Full wwPDB X-ray Structure Validation Report

Sep 2, 2026 – 10:39 PM EDT

PDB ID	:	9Q6Q / pdb_00009q6q
Title	:	Crystal structure of the wild-type Thermus thermophilus 70S ribosome in complex with pleuromutilin-18 triazole derivative and protein Y at 2.90A resolution
Authors	:	Killam, B.Y.; Kopec, I.; Breiner, L.M.; Hoernig, M.; LoPresti, M.; Abdelsattar, A.S.; Abouelkhair, A.A.; Briganti, A.J.; Slowinski, R.P.; Vogelaar, N.J.; Seleem, M.N.; Brown, A.M.; Lowell, A.N.; Polikanov, Y.S.
Deposited on	:	2025-08-22
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

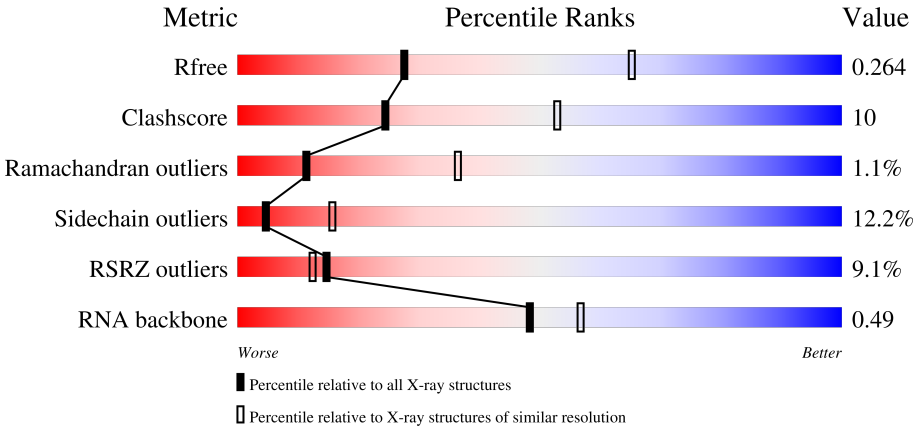
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2915	5% 60% 33% 6%
1	2A	2915	6% 56% 35% 8%
2	1B	121	% 64% 32%
2	2B	121	9% 57% 37% 5%

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Mol	Chain	Length	Quality of chain
3	1D	276	2% 75% 22%
3	2D	276	3% 76% 20%
4	1E	206	67% 26% 6%
4	2E	206	2% 62% 31% 6%
5	1F	210	68% 24% 5%
5	2F	210	3% 59% 30% 8%
6	1G	182	8% 59% 35% 5%
6	2G	182	30% 53% 43%
7	1H	180	2% 71% 23%
7	2H	180	14% 47% 43% 6%
8	1I	148	9% 64% 26% 9%
8	2I	148	9% 70% 25%
9	1N	140	% 74% 22%
9	2N	140	3% 69% 27%
10	1O	122	% 70% 25% 5%
10	2O	122	6% 72% 26%
11	1P	150	3% 71% 27%
11	2P	150	2% 66% 30%
12	1Q	141	2% 75% 21%
12	2Q	141	6% 70% 26%
13	1R	118	65% 30% 5%
13	2R	118	% 57% 40%
14	1S	112	% 70% 24%
14	2S	112	13% 53% 40% 5%
15	1T	146	3% 64% 23% 10%

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Mol	Chain	Length	Quality of chain
15	2T	146	3% 61% 25% 10%
16	1U	118	2% 78% 19%
16	2U	118	4% 73% 22%
17	1V	101	% 75% 20%
17	2V	101	4% 66% 28%
18	1W	113	% 74% 19% 5%
18	2W	113	% 72% 20% 6%
19	1X	96	% 73% 22%
19	2X	96	3% 70% 27%
20	1Y	110	2% 66% 28%
20	2Y	110	20% 58% 35%
21	1Z	206	5% 67% 28%
21	2Z	206	17% 62% 31% 5%
22	10	85	2% 66% 21% 9%
22	20	85	6% 64% 26% 9%
23	11	98	4% 80% 16%
23	21	98	4% 62% 31% 6%
24	12	72	% 71% 24%
24	22	72	15% 64% 28% 6%
25	13	60	2% 73% 20% 5%
25	23	60	2% 60% 32% 7%
26	14	71	15% 51% 37% 8%
26	24	71	51% 54% 31% 11%
27	15	60	3% 72% 23%
27	25	60	2% 72% 25%

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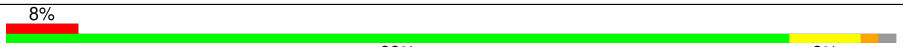
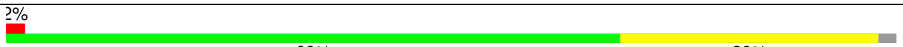
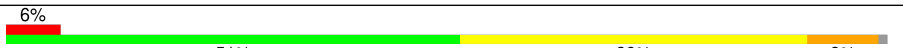
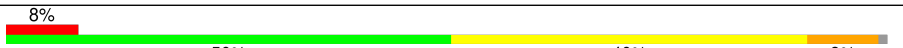
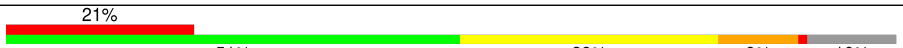
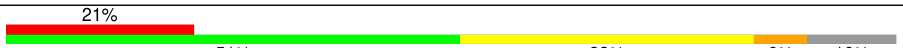
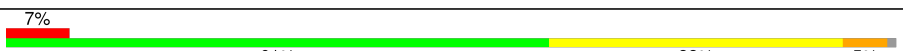
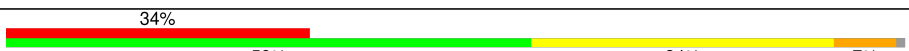
Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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Mol	Chain	Length	Quality of chain
40	2i	128	53% 41% 48% 10%
41	1j	105	39% 50% 32% 10% 8%
41	2j	105	49% 52% 34% 5% 9%
42	1k	129	9% 56% 27% 5% 12%
42	2k	129	7% 59% 25% 5% 12%
43	1l	132	2% 63% 26% 8%
43	2l	132	6% 61% 27% 5% 8%
44	1m	126	17% 54% 33% 6% 8%
44	2m	126	30% 51% 33% 6% 10%
45	1n	61	36% 41% 49% 8%
45	2n	61	49% 62% 33%
46	1o	89	9% 67% 28%
46	2o	89	3% 64% 31%
47	1p	88	14% 49% 38% 7% 7%
47	2p	88	11% 56% 35% 7%
48	1q	105	5% 62% 30% 6%
48	2q	105	5% 69% 22% 6%
49	1r	88	9% 56% 19% 23%
49	2r	88	6% 52% 22% 23%
50	1s	93	29% 55% 31% 11%
50	2s	93	40% 48% 37% 11%
51	1t	106	21% 61% 25% 9%
51	2t	106	8% 64% 26% 8%
52	1u	27	33% 56% 26% 15%
52	2u	27	48% 63% 22% 15%

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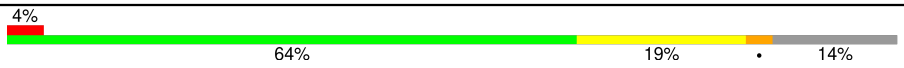
Mol	Chain	Length	Quality of chain
53	1y	113	
53	2y	113	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	1A	3856	-	-	-	X
54	MG	1A	3996	-	-	-	X
54	MG	2A	3706	-	-	-	X

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 297540 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2872	Total	C	N	O	P	0	0	0
			61869	27540	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	2E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
11	2P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	1Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	2Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	2R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			877	553	175	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
15	2T	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	2U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	1W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	2W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	1X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	2X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	13	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	23	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	16	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	26	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	17	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	27	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	18	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	28	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	19	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	29	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	131			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			834	520	156	155	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	1l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
43	2l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	2			

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
46	2o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
47	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	1r	68	Total	C	N	O	0	0	0
			555	355	108	92			
49	2r	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1y	97	Total 764	C 478	N 144	O 139	S 3	0	0	0
53	2y	96	Total 749	C 468	N 141	O 137	S 3	0	0	0

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1A	1011	Total 1011	Mg 1011	0	0
54	1B	30	Total 30	Mg 30	0	0
54	1D	18	Total 18	Mg 18	0	0
54	1E	9	Total 9	Mg 9	0	0
54	1F	16	Total 16	Mg 16	0	0
54	1G	4	Total 4	Mg 4	0	0
54	1H	3	Total 3	Mg 3	0	0
54	1N	2	Total 2	Mg 2	0	0
54	1O	2	Total 2	Mg 2	0	0
54	1P	6	Total 6	Mg 6	0	0
54	1Q	7	Total 7	Mg 7	0	0
54	1R	8	Total 8	Mg 8	0	0
54	1S	1	Total 1	Mg 1	0	0
54	1T	5	Total 5	Mg 5	0	0
54	1U	5	Total 5	Mg 5	0	0
54	1V	6	Total 6	Mg 6	0	0
54	1W	3	Total 3	Mg 3	0	0
54	1Y	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	1Z	1	Total Mg 1 1	0	0
54	10	7	Total Mg 7 7	0	0
54	11	4	Total Mg 4 4	0	0
54	13	3	Total Mg 3 3	0	0
54	15	6	Total Mg 6 6	0	0
54	17	4	Total Mg 4 4	0	0
54	18	4	Total Mg 4 4	0	0
54	19	2	Total Mg 2 2	0	0
54	1a	270	Total Mg 270 270	0	0
54	1b	1	Total Mg 1 1	0	0
54	1d	5	Total Mg 5 5	0	0
54	1e	4	Total Mg 4 4	0	0
54	1f	2	Total Mg 2 2	0	0
54	1g	3	Total Mg 3 3	0	0
54	1h	2	Total Mg 2 2	0	0
54	1i	1	Total Mg 1 1	0	0
54	1l	2	Total Mg 2 2	0	0
54	1m	1	Total Mg 1 1	0	0
54	1n	2	Total Mg 2 2	0	0
54	1o	2	Total Mg 2 2	0	0
54	1p	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	1t	2	Total Mg 2 2	0	0
54	1y	5	Total Mg 5 5	0	0
54	2A	732	Total Mg 732 732	0	0
54	2B	20	Total Mg 20 20	0	0
54	2D	7	Total Mg 7 7	0	0
54	2E	8	Total Mg 8 8	0	0
54	2F	4	Total Mg 4 4	0	0
54	2G	3	Total Mg 3 3	0	0
54	2I	1	Total Mg 1 1	0	0
54	2N	1	Total Mg 1 1	0	0
54	2O	1	Total Mg 1 1	0	0
54	2P	3	Total Mg 3 3	0	0
54	2Q	4	Total Mg 4 4	0	0
54	2R	2	Total Mg 2 2	0	0
54	2T	3	Total Mg 3 3	0	0
54	2U	1	Total Mg 1 1	0	0
54	2V	1	Total Mg 1 1	0	0
54	2W	3	Total Mg 3 3	0	0
54	2X	1	Total Mg 1 1	0	0
54	2Y	1	Total Mg 1 1	0	0
54	20	2	Total Mg 2 2	0	0

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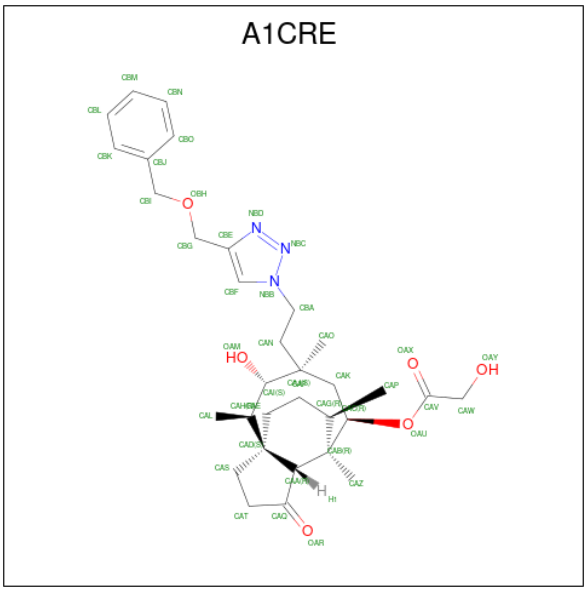
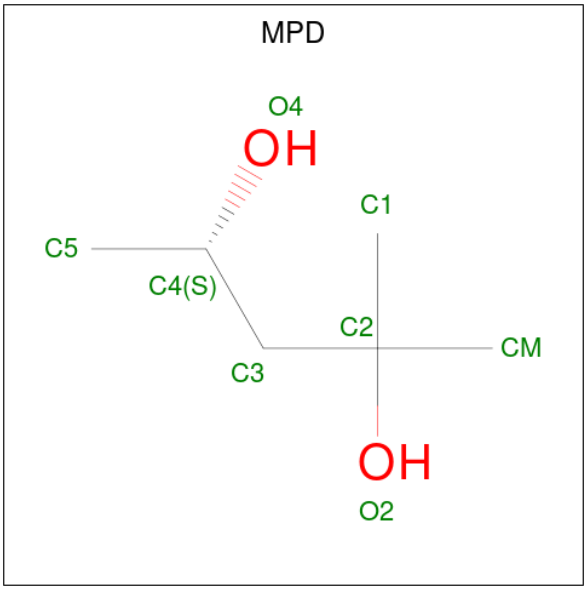
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	21	1	Total Mg 1 1	0	0
54	23	1	Total Mg 1 1	0	0
54	25	3	Total Mg 3 3	0	0
54	27	1	Total Mg 1 1	0	0
54	28	2	Total Mg 2 2	0	0
54	2a	192	Total Mg 192 192	0	0
54	2e	2	Total Mg 2 2	0	0
54	2f	1	Total Mg 1 1	0	0
54	2j	1	Total Mg 1 1	0	0
54	2k	1	Total Mg 1 1	0	0
54	2l	1	Total Mg 1 1	0	0
54	2o	1	Total Mg 1 1	0	0
54	2q	1	Total Mg 1 1	0	0
54	2r	1	Total Mg 1 1	0	0
54	2t	1	Total Mg 1 1	0	0
54	2y	1	Total Mg 1 1	0	0

- Molecule 55 is (3aS,4R,5S,6S,8R,9R,9aR,10R)-6-(2-{4-[(benzyloxy)methyl]-1H-1,2,3-triazol-1-yl}ethyl)-5-hydroxy-4,6,9,10-tetramethyl-1-oxodecahydro-3a,9-propanocyclopenta[8]annulen-8-yl hydroxyacetate (CCD ID: A1CRE) (formula: $C_{32}H_{45}N_3O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1A	1	Total C N O 41 32 3 6	0	0
55	2A	1	Total C N O 41 32 3 6	0	0

- Molecule 56 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1A	1	Total C O 8 6 2	0	0
56	18	1	Total C O 8 6 2	0	0

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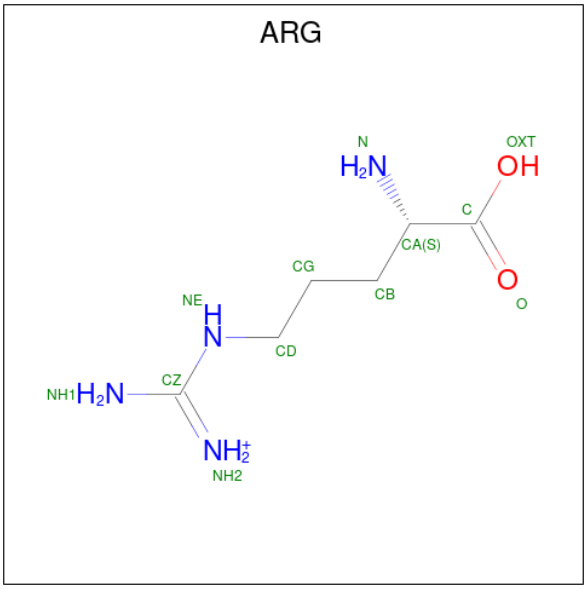
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1a	1	Total C O 8 6 2	0	0
56	1a	1	Total C O 8 6 2	0	0
56	2A	1	Total C O 8 6 2	0	0
56	2A	1	Total C O 8 6 2	0	0
56	2B	1	Total C O 8 6 2	0	0

- Molecule 57 is ARGININE (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1B	1	Total C N O 12 6 4 2	0	0
57	1F	1	Total C N O 12 6 4 2	0	0

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1Y	1	Total Zn 1 1	0	0
58	14	1	Total Zn 1 1	0	0

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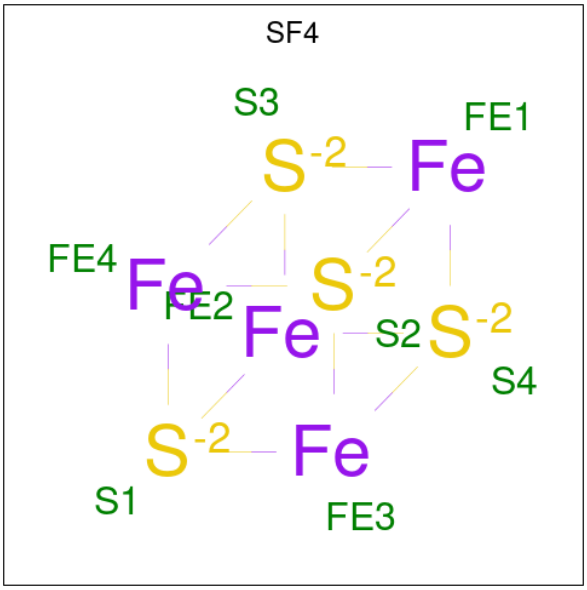
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	15	1	Total Zn 1 1	0	0
58	16	1	Total Zn 1 1	0	0
58	19	1	Total Zn 1 1	0	0
58	1n	1	Total Zn 1 1	0	0
58	2Y	1	Total Zn 1 1	0	0
58	24	1	Total Zn 1 1	0	0
58	25	1	Total Zn 1 1	0	0
58	26	1	Total Zn 1 1	0	0
58	29	1	Total Zn 1 1	0	0
58	2n	1	Total Zn 1 1	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1d	1	Total Fe S 8 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	2d	1	Total Fe S 8 4 4	0	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1A	3794	Total O 3794 3794	0	0
60	1B	98	Total O 98 98	0	0
60	1D	112	Total O 112 112	0	0
60	1E	73	Total O 73 73	0	0
60	1F	61	Total O 61 61	0	0
60	1G	20	Total O 20 20	0	0
60	1H	14	Total O 14 14	0	0
60	1I	8	Total O 8 8	0	0
60	1N	51	Total O 51 51	0	0
60	1O	20	Total O 20 20	0	0
60	1P	64	Total O 64 64	0	0
60	1Q	39	Total O 39 39	0	0
60	1R	30	Total O 30 30	0	0
60	1S	8	Total O 8 8	0	0
60	1T	39	Total O 39 39	0	0
60	1U	39	Total O 39 39	0	0
60	1V	38	Total O 38 38	0	0
60	1W	28	Total O 28 28	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1X	26	Total O 26 26	0	0
60	1Y	15	Total O 15 15	0	0
60	1Z	11	Total O 11 11	0	0
60	10	26	Total O 26 26	0	0
60	11	25	Total O 25 25	0	0
60	12	15	Total O 15 15	0	0
60	13	23	Total O 23 23	0	0
60	14	1	Total O 1 1	0	0
60	15	29	Total O 29 29	0	0
60	16	14	Total O 14 14	0	0
60	17	13	Total O 13 13	0	0
60	18	28	Total O 28 28	0	0
60	19	11	Total O 11 11	0	0
60	1a	532	Total O 532 532	0	0
60	1b	1	Total O 1 1	0	0
60	1d	9	Total O 9 9	0	0
60	1e	6	Total O 6 6	0	0
60	1f	2	Total O 2 2	0	0
60	1g	1	Total O 1 1	0	0
60	1h	2	Total O 2 2	0	0
60	1i	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1j	1	Total O 1 1	0	0
60	1l	5	Total O 5 5	0	0
60	1m	2	Total O 2 2	0	0
60	1o	2	Total O 2 2	0	0
60	1p	3	Total O 3 3	0	0
60	1q	1	Total O 1 1	0	0
60	1r	1	Total O 1 1	0	0
60	1t	1	Total O 1 1	0	0
60	1u	1	Total O 1 1	0	0
60	1y	6	Total O 6 6	0	0
60	2A	2275	Total O 2275 2275	0	0
60	2B	60	Total O 60 60	0	0
60	2D	50	Total O 50 50	0	0
60	2E	29	Total O 29 29	0	0
60	2F	20	Total O 20 20	0	0
60	2G	6	Total O 6 6	0	0
60	2H	3	Total O 3 3	0	0
60	2I	3	Total O 3 3	0	0
60	2N	5	Total O 5 5	0	0
60	2O	15	Total O 15 15	0	0
60	2P	26	Total O 26 26	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	2Q	20	Total O 20 20	0	0
60	2R	17	Total O 17 17	0	0
60	2S	5	Total O 5 5	0	0
60	2T	13	Total O 13 13	0	0
60	2U	8	Total O 8 8	0	0
60	2V	7	Total O 7 7	0	0
60	2W	21	Total O 21 21	0	0
60	2X	7	Total O 7 7	0	0
60	2Y	3	Total O 3 3	0	0
60	2Z	13	Total O 13 13	0	0
60	20	12	Total O 12 12	0	0
60	21	19	Total O 19 19	0	0
60	23	3	Total O 3 3	0	0
60	24	1	Total O 1 1	0	0
60	25	11	Total O 11 11	0	0
60	26	5	Total O 5 5	0	0
60	27	11	Total O 11 11	0	0
60	28	14	Total O 14 14	0	0
60	29	1	Total O 1 1	0	0
60	2a	436	Total O 436 436	0	0
60	2d	5	Total O 5 5	0	0

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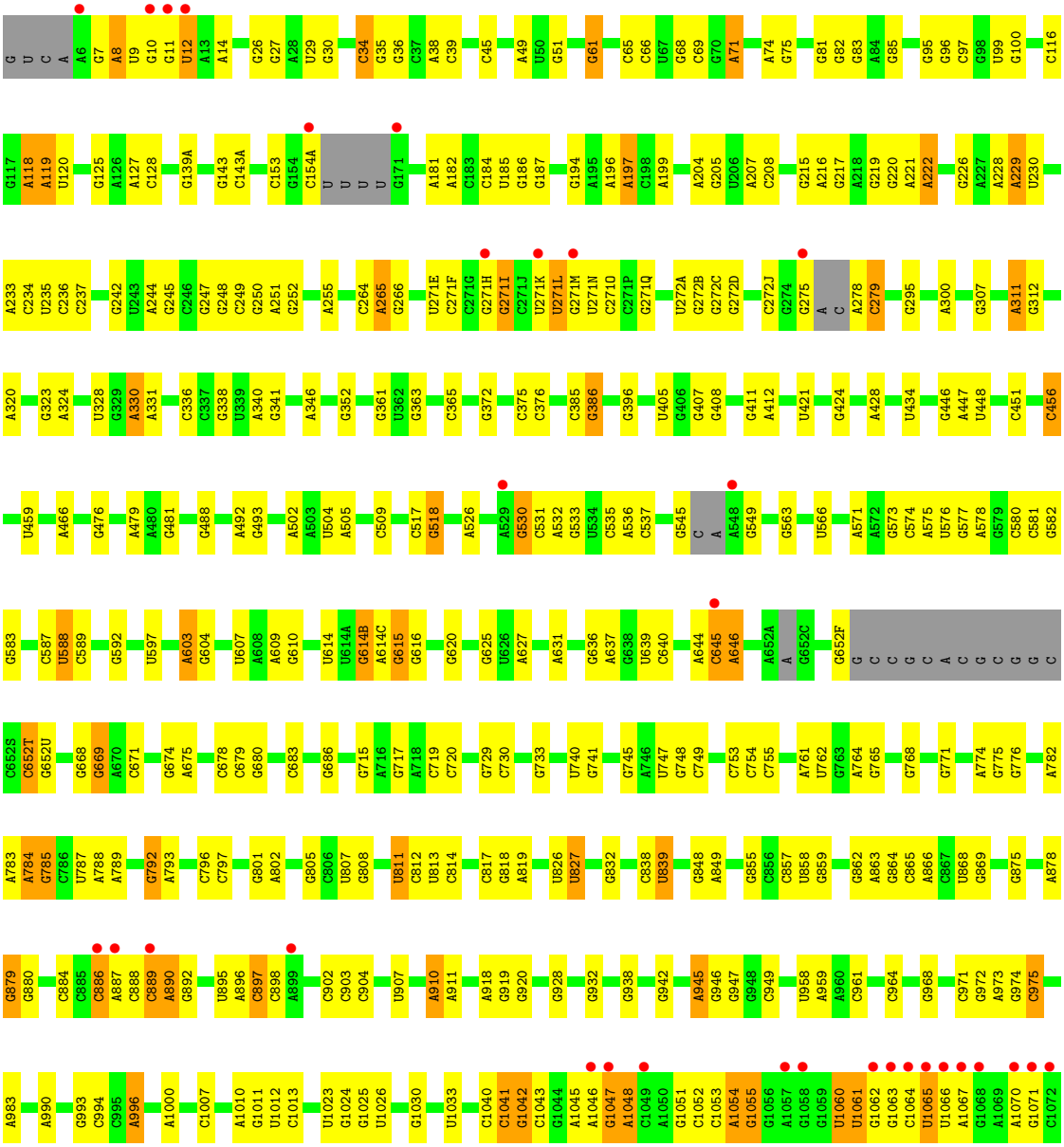
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	2e	3	Total O 3 3	0	0
60	2f	2	Total O 2 2	0	0
60	2j	2	Total O 2 2	0	0
60	2l	4	Total O 4 4	0	0
60	2m	1	Total O 1 1	0	0
60	2n	1	Total O 1 1	0	0
60	2o	4	Total O 4 4	0	0
60	2p	4	Total O 4 4	0	0
60	2q	1	Total O 1 1	0	0
60	2r	3	Total O 3 3	0	0
60	2t	1	Total O 1 1	0	0
60	2u	1	Total O 1 1	0	0
60	2y	8	Total O 8 8	0	0

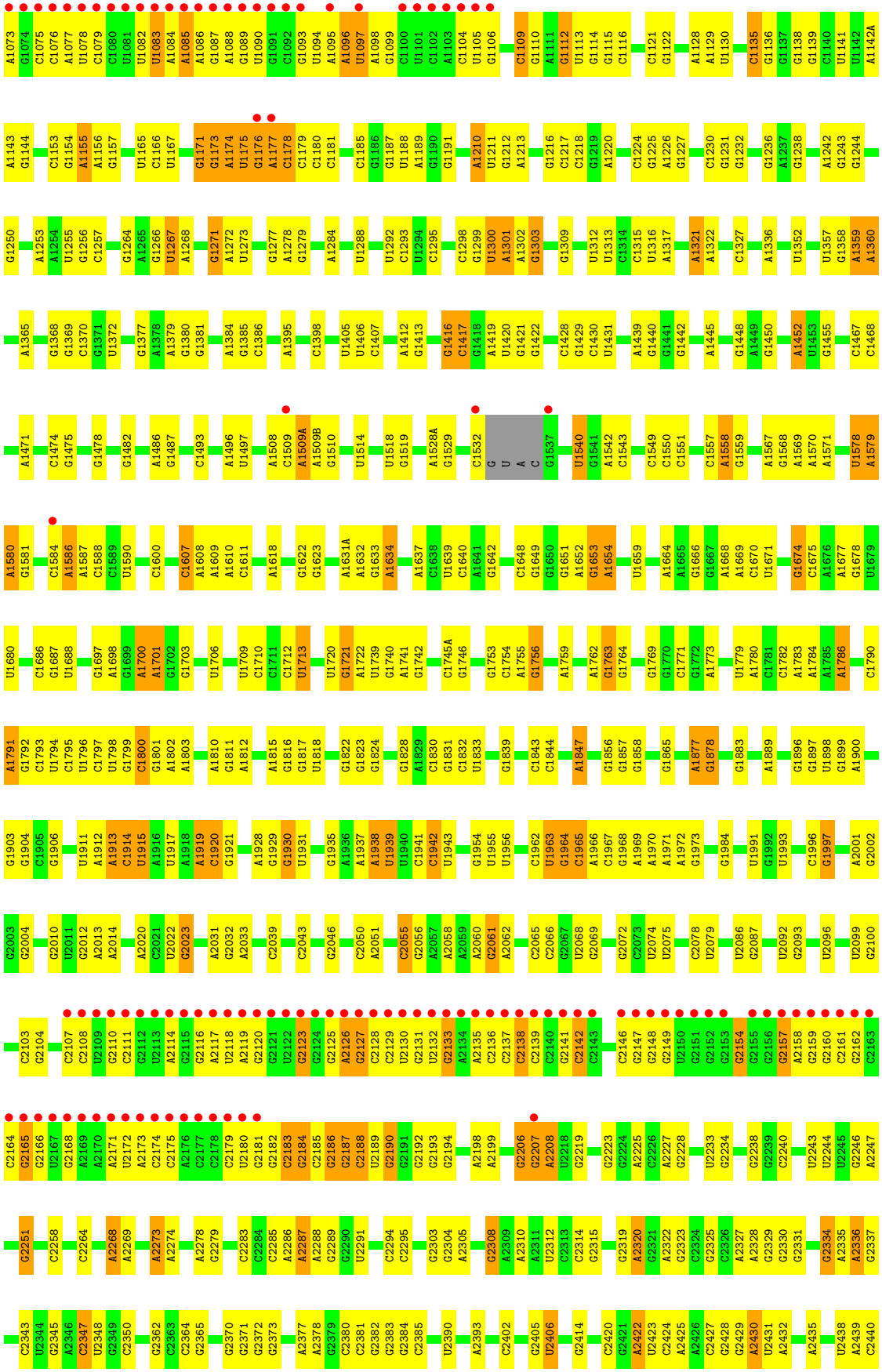
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S Ribosomal RNA

Chain 1A:




A1073 G1074 C1075 C1076 A1077 U1078 C1079 C1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 C1109 G1110 A1111 G1112 U1113 G1114 G1115 C1116 C1121 G1122 A1128 A1129 U1130 C1135 G1136 G1137 G1138 G1139 C1140 U1141 U1142 A1142A
A1143 G1144 C1153 G1154 A1155 A1156 G1157 U1165 C1166 U1167 G1171 C1173 A1174 U1175 C1176 A1177 C1178 C1179 C1180 C1181 C1185 G1186 G1187 U1188 A1189 G1190 G1191 A1210 U1211 G1212 A1213 G1216 C1217 C1218 G1219 A1220 C1224 G1225 A1226 G1227 C1230 G1231 G1232 G1236 A1237 G1238 A1242 G1243 G1244
G1250 A1253 A1254 U1255 G1256 C1257 G1264 A1265 G1266 U1267 A1268 G1271 A1272 U1273 G1277 A1278 G1279 A1284 U1288 U1292 C1293 U1294 C1295 C1298 G1299 U1300 A1301 A1302 G1303 G1309 U1312 U1313 C1314 C1315 U1316 A1317 A1321 A1322 C1327 A1336 U1352 U1357 G1358 A1359 A1360
A1365 G1368 G1369 C1370 G1371 U1372 G1377 A1378 A1379 G1380 G1381 A1384 G1385 C1386 A1395 C1398 U1405 U1406 C1407 A1412 G1413 G1416 C1417 G1418 A1419 U1420 G1421 G1422 C1428 G1429 C1430 U1431 A1439 G1440 G1441 G1442 A1445 G1448 A1449 G1450 A1452 U1453 G1455 C1467 C1468
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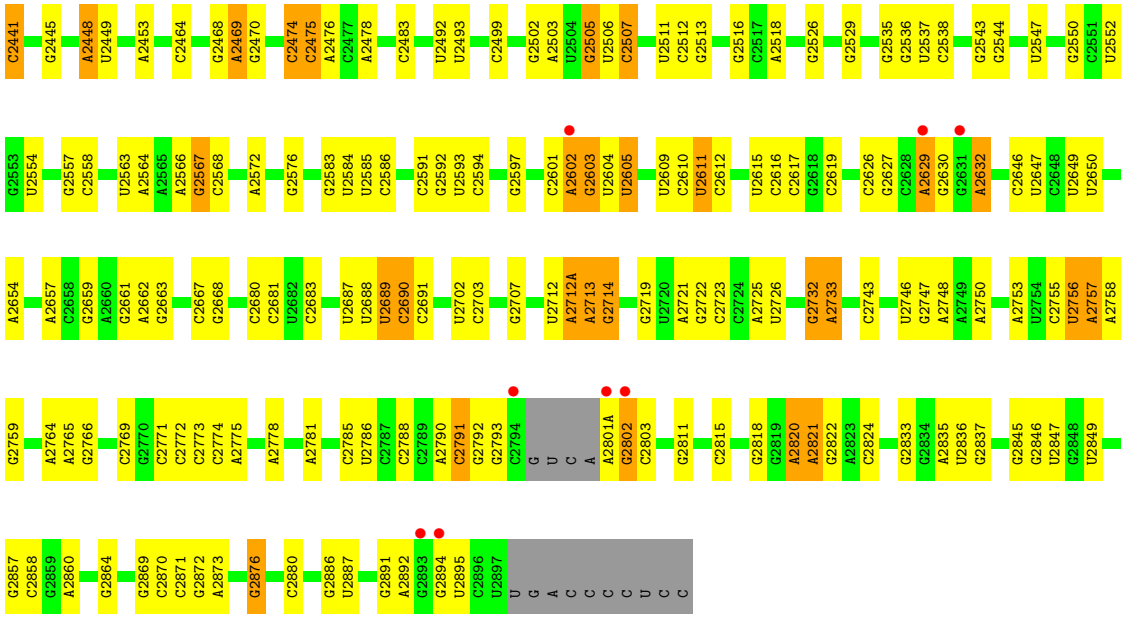

• Molecule 1: 23S Ribosomal RNA

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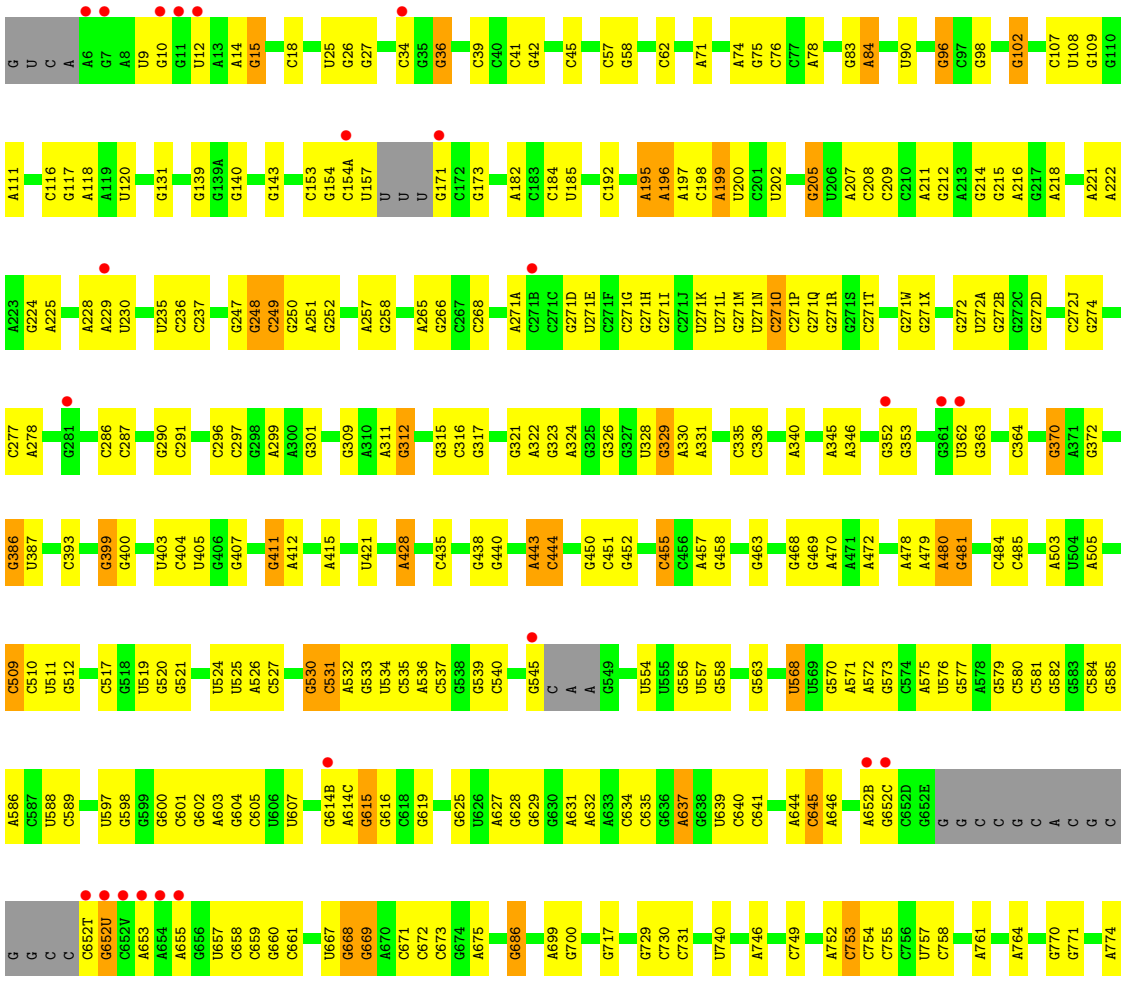

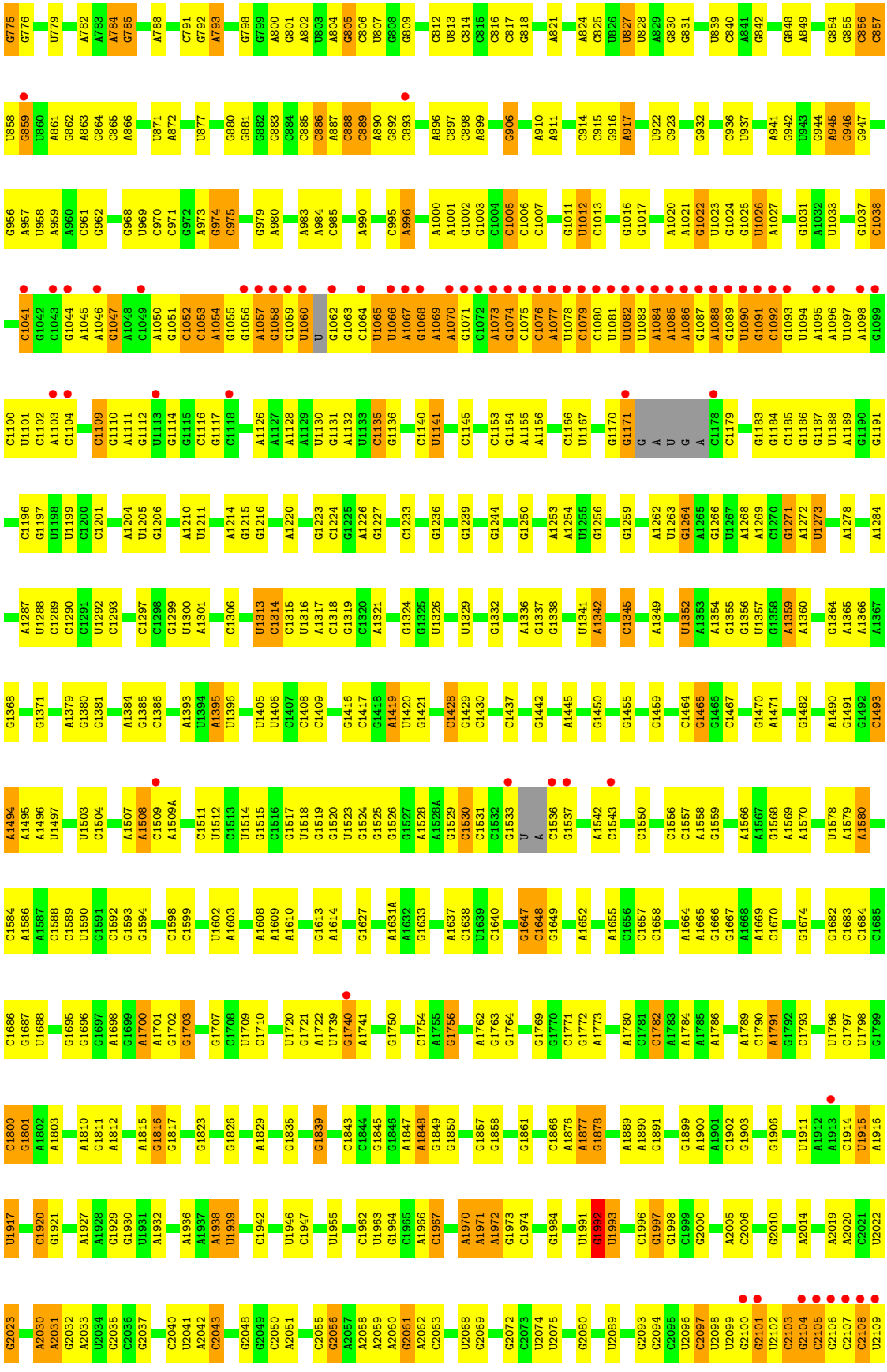
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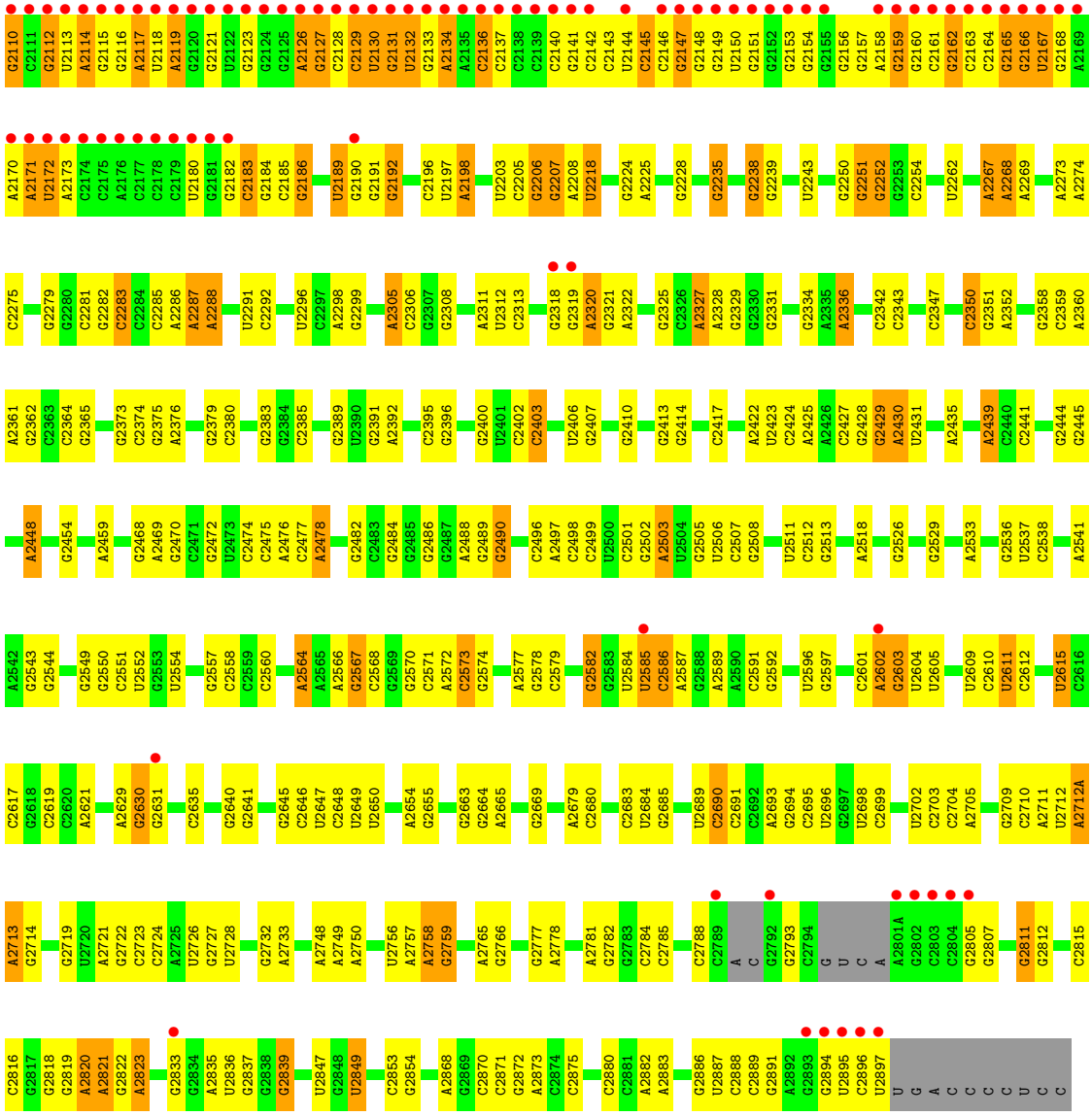
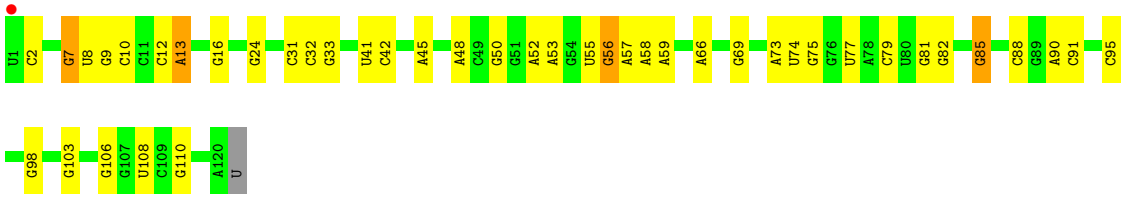


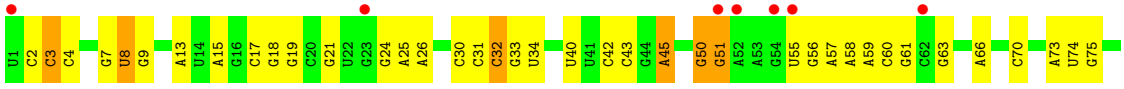
• Molecule 2: 5S Ribosomal RNA

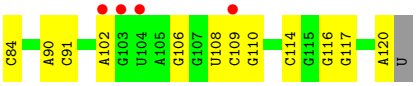
Chain 1B:



• Molecule 2: 5S Ribosomal RNA

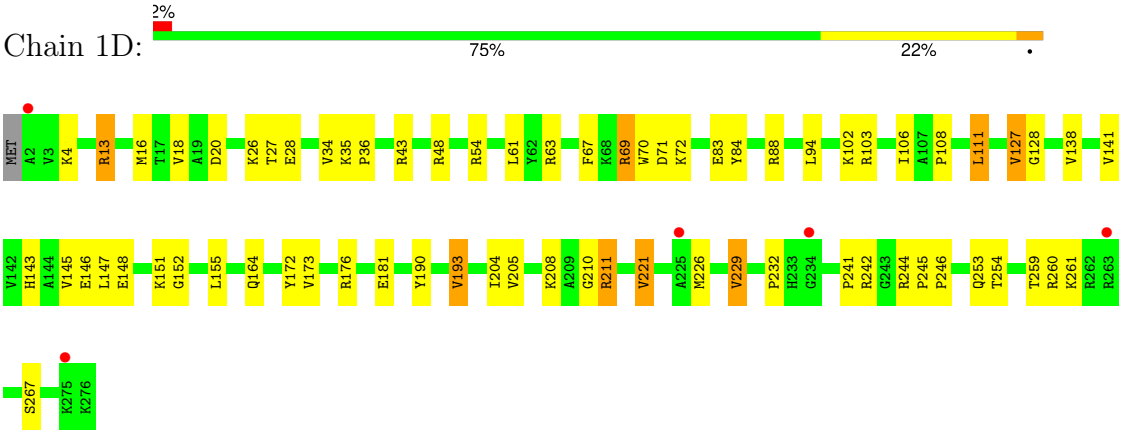
Chain 2B:





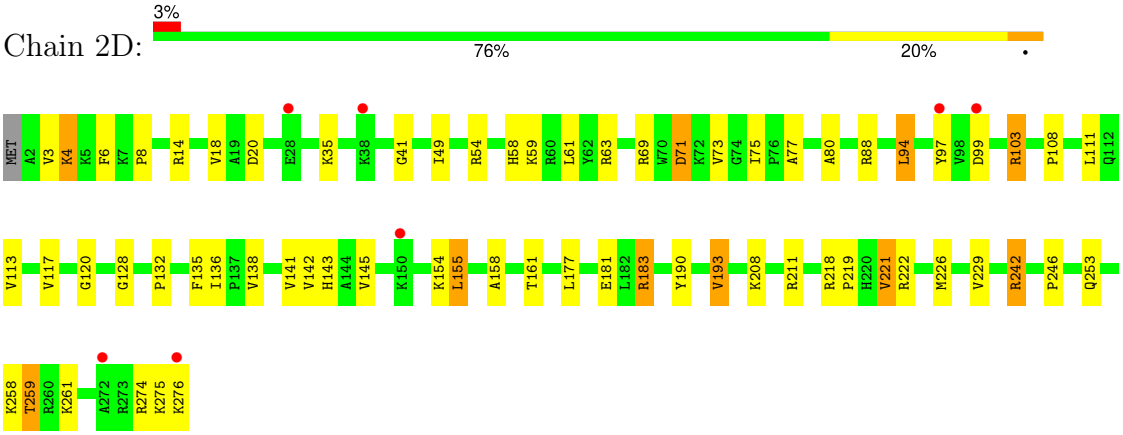
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



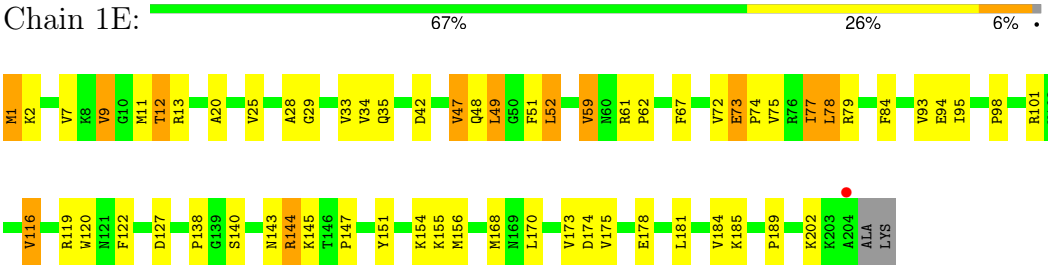
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



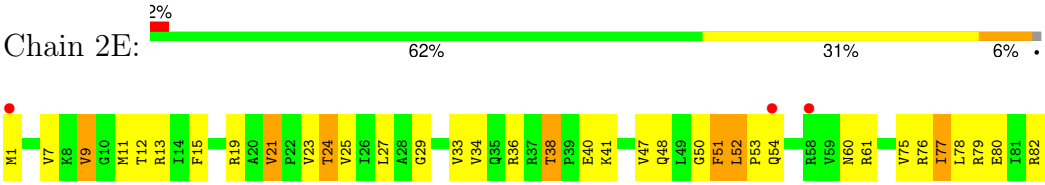
• Molecule 4: 50S ribosomal protein L3

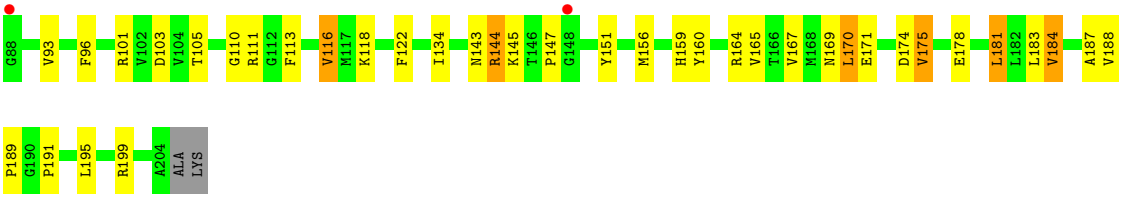
Chain 1E:



• Molecule 4: 50S ribosomal protein L3

Chain 2E:





• Molecule 5: 50S ribosomal protein L4

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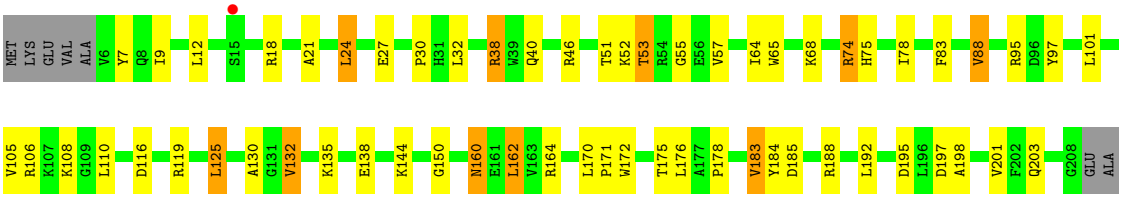
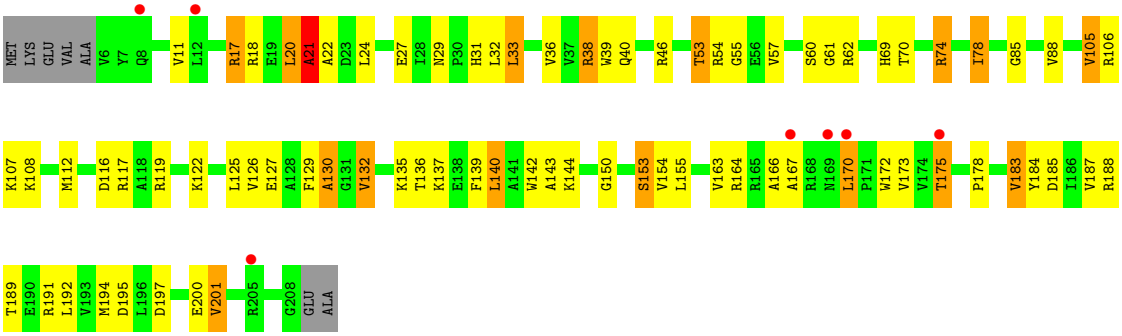


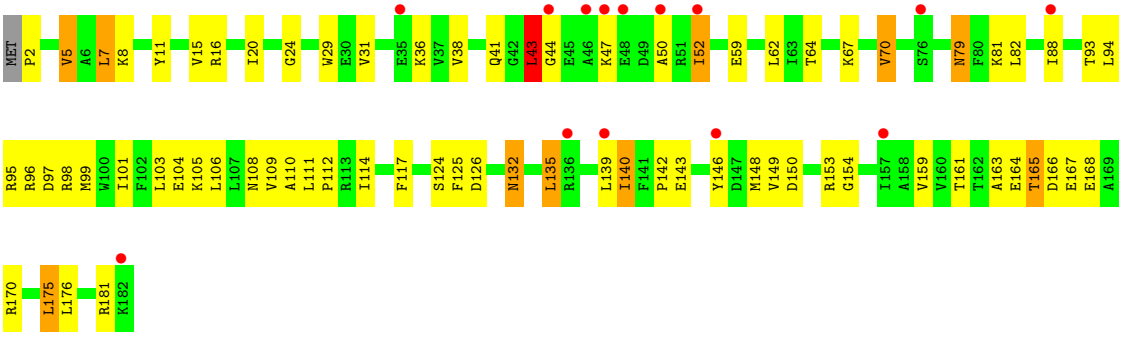
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



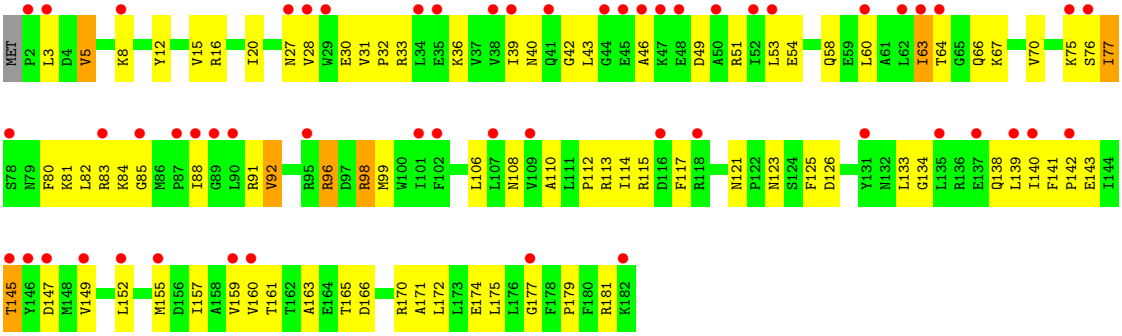
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



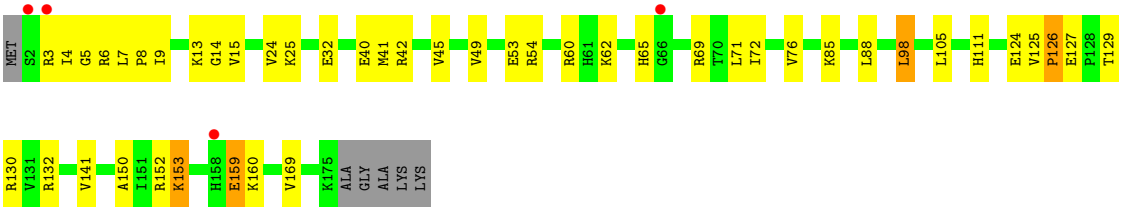
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



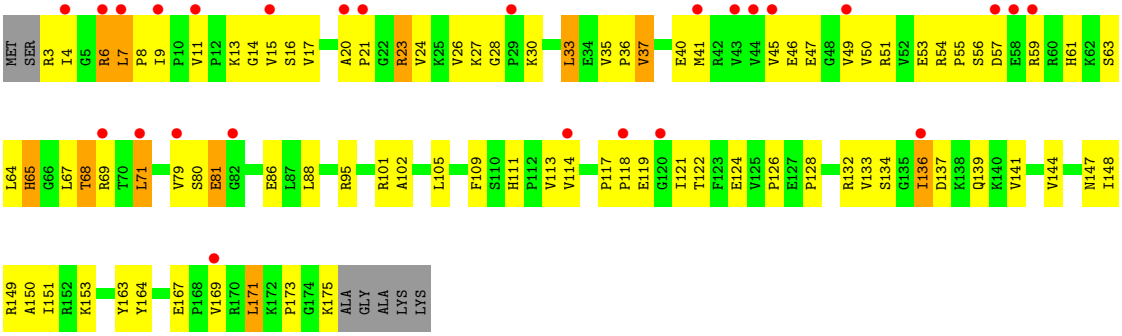
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



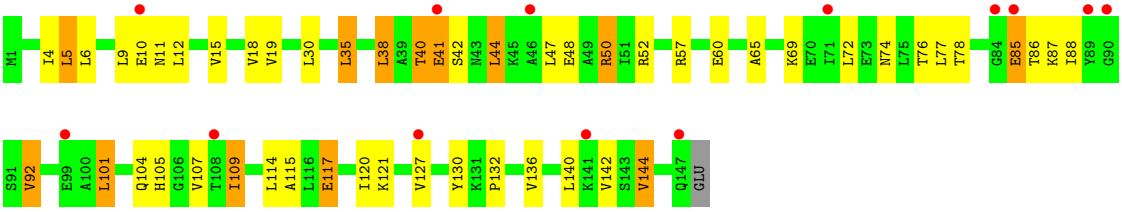
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



• Molecule 8: 50S ribosomal protein L9

Chain 1I:



• Molecule 8: 50S ribosomal protein L9

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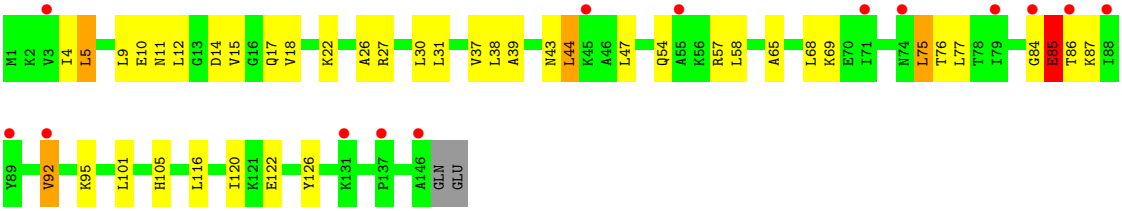
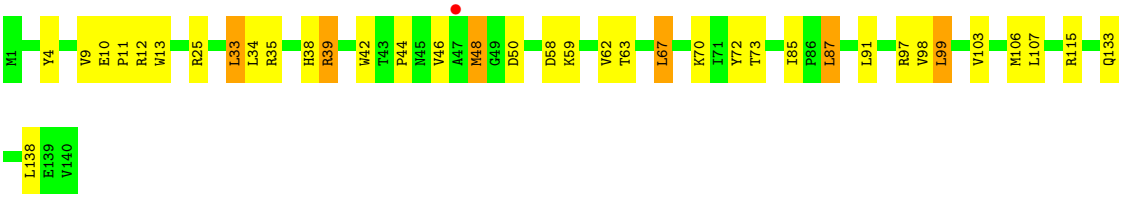


• Molecule 9: 50S ribosomal protein L13

Chain 1N:



• Molecule 9: 50S ribosomal protein L13

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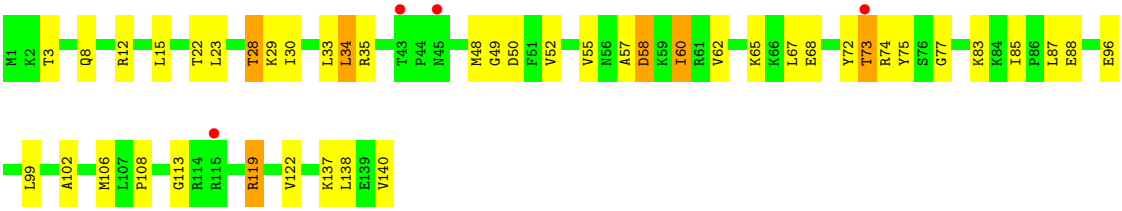

• Molecule 10: 50S ribosomal protein L14

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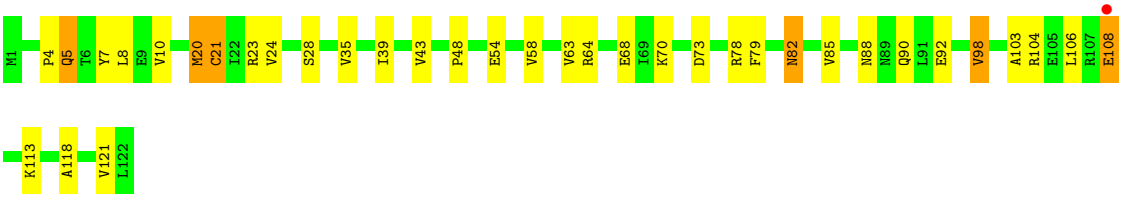
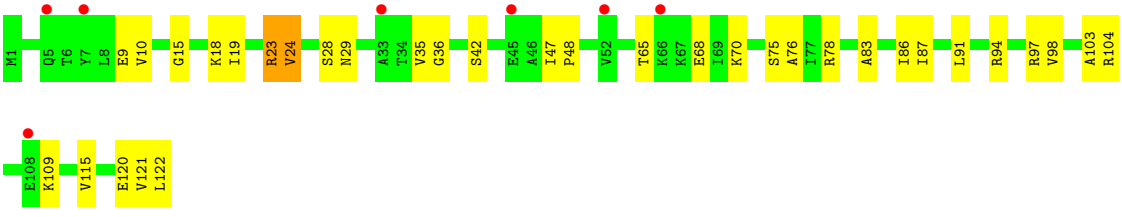


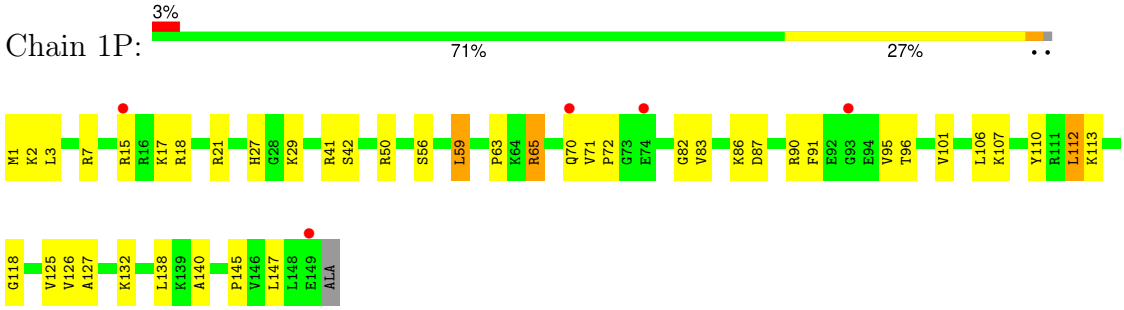
• Molecule 10: 50S ribosomal protein L14

Chain 2O:



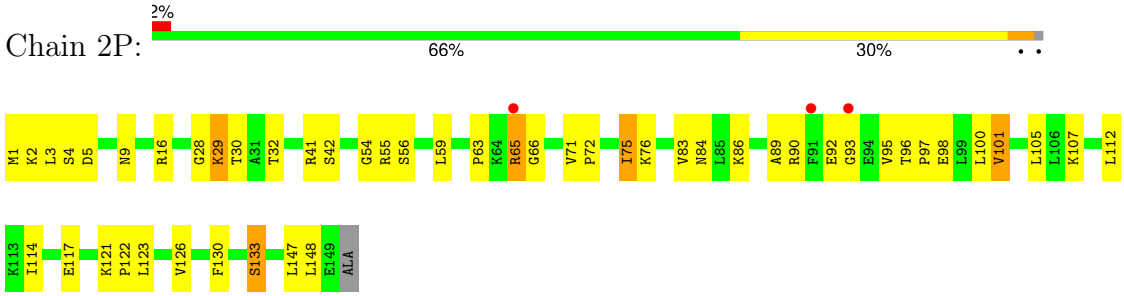
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



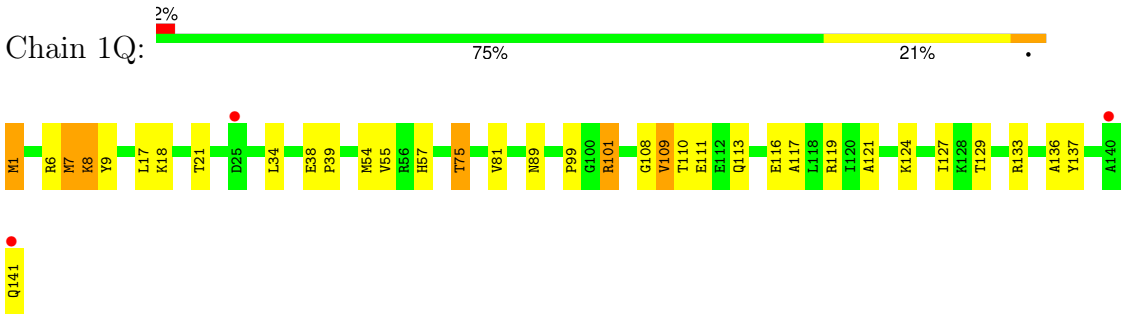
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



• Molecule 12: 50S ribosomal protein L16

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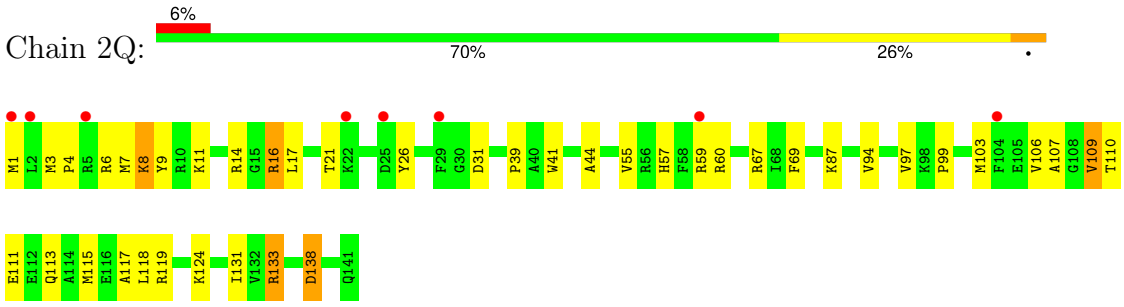
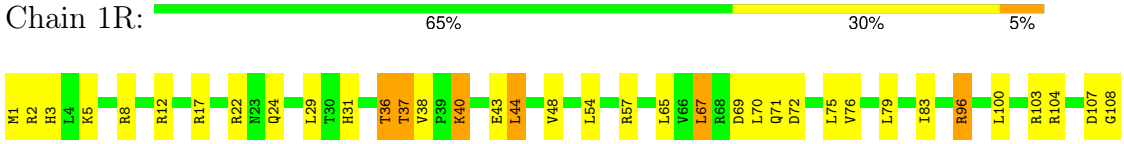
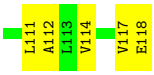


• Molecule 13: 50S ribosomal protein L17

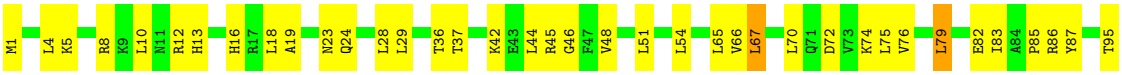
Chain 1R:

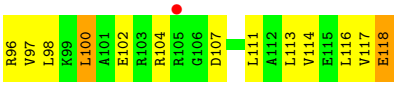




• Molecule 13: 50S ribosomal protein L17

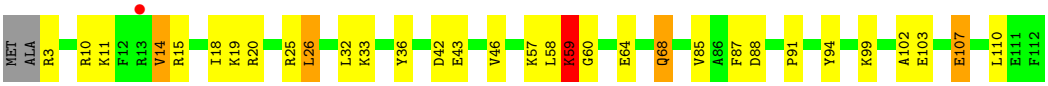
Chain 2R:





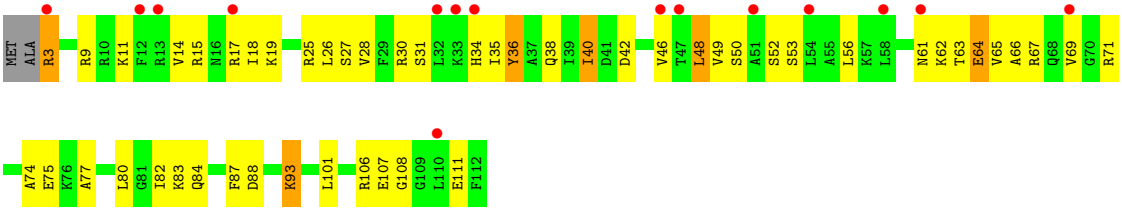
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



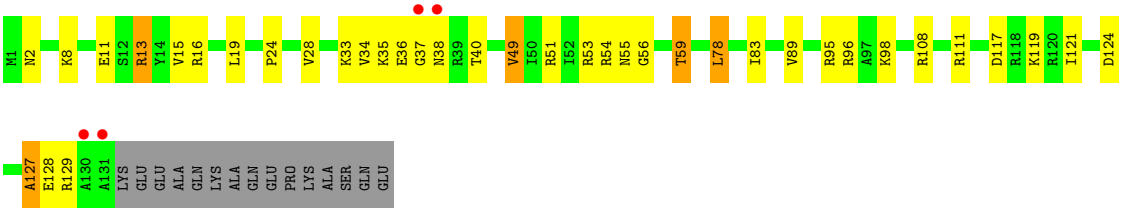
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



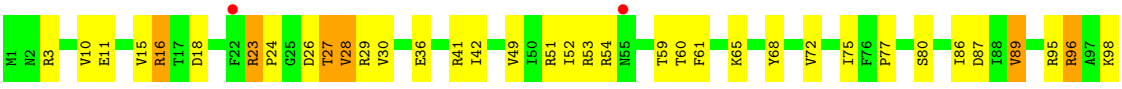
• Molecule 15: 50S ribosomal protein L19

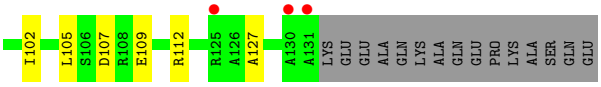
Chain 1T:



• Molecule 15: 50S ribosomal protein L19

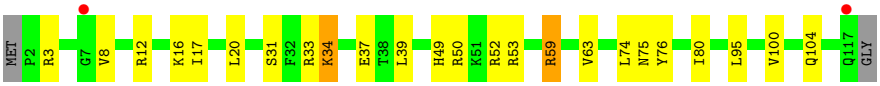
Chain 2T:





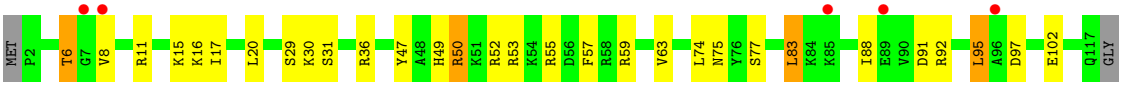
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



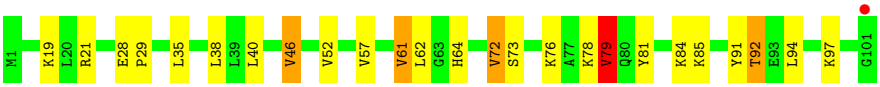
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



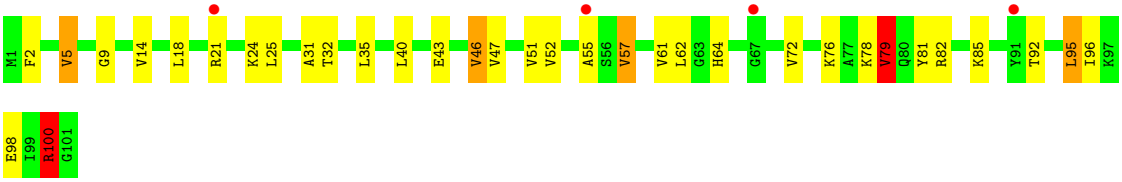
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



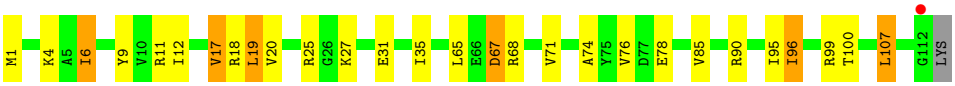
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



• Molecule 18: 50S ribosomal protein L22

Chain 1W:

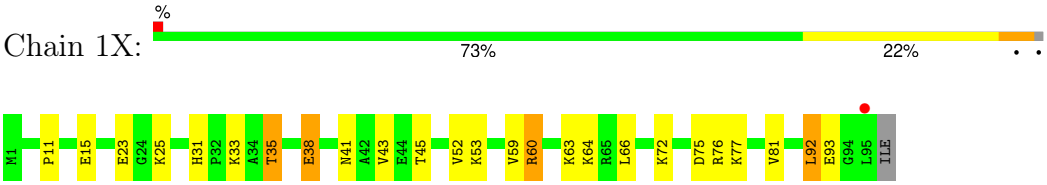


• Molecule 18: 50S ribosomal protein L22

Chain 2W:

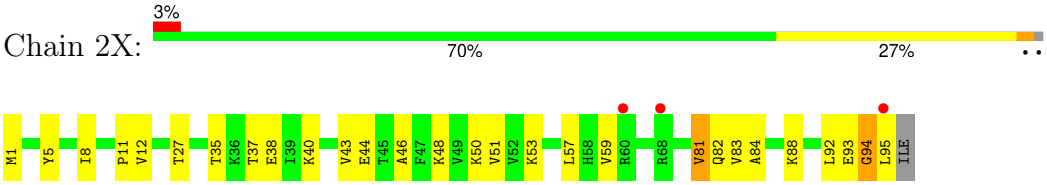
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



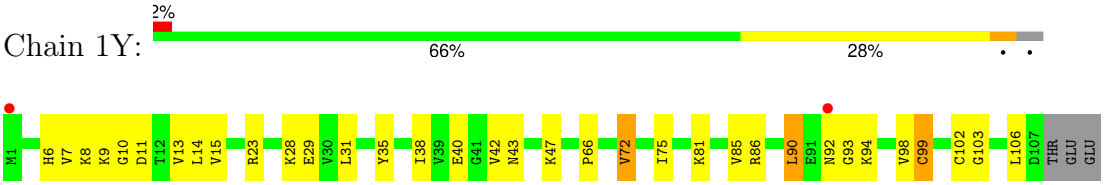
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



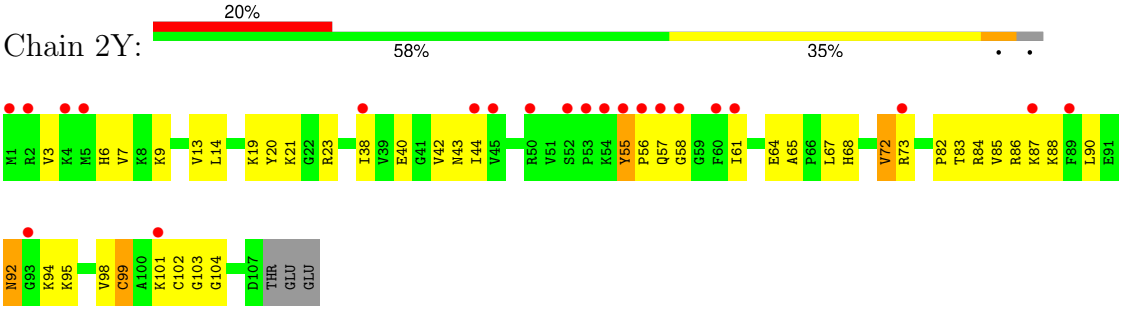
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



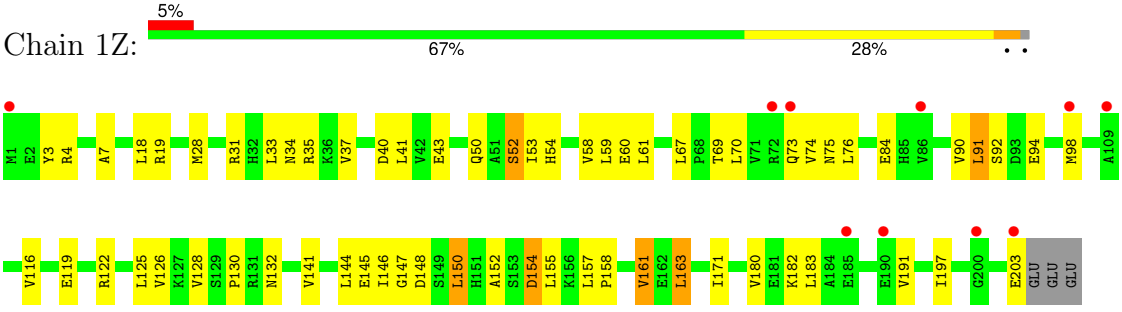
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



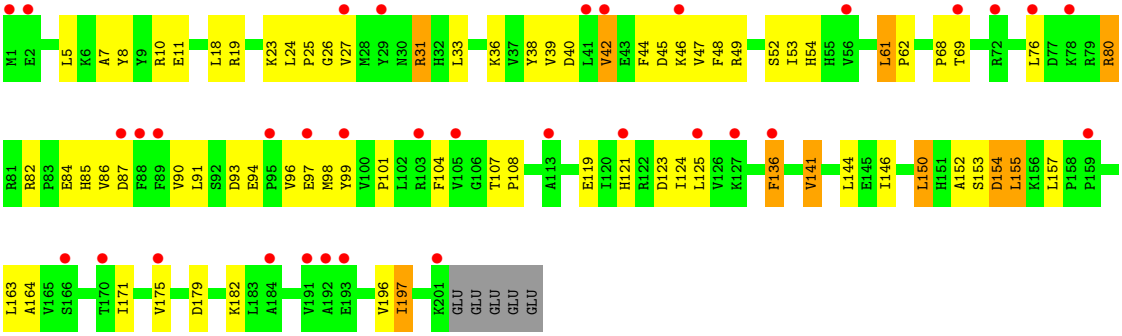
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:

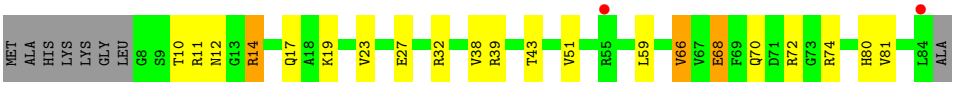


• Molecule 21: 50S ribosomal protein L25

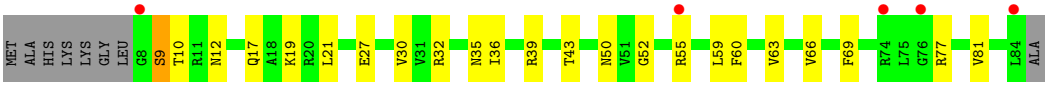
Chain 2Z:



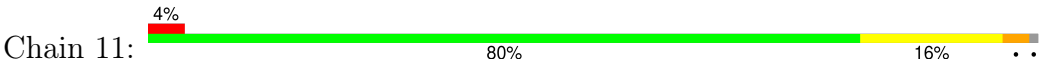
• Molecule 22: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L27

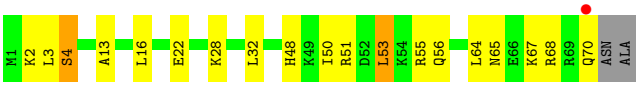


• Molecule 23: 50S ribosomal protein L28



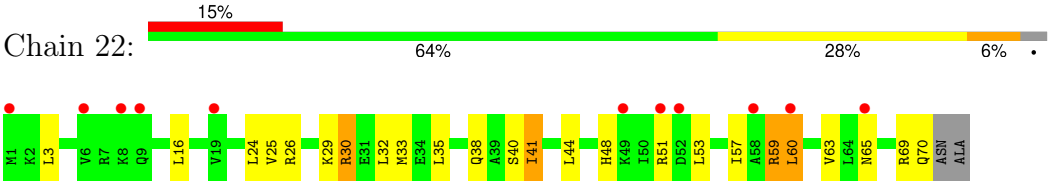
• Molecule 23: 50S ribosomal protein L28

• Molecule 24: 50S ribosomal protein L29



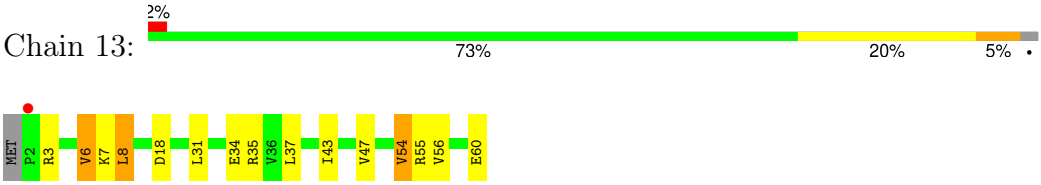
• Molecule 24: 50S ribosomal protein L29

Chain 22:



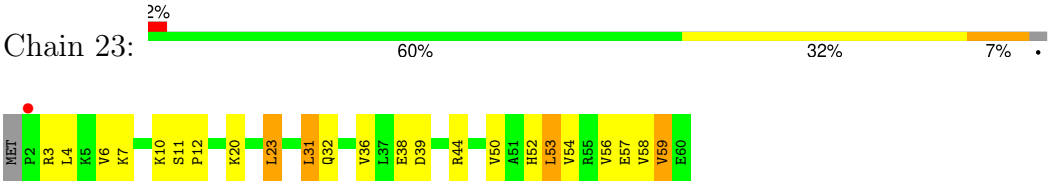
• Molecule 25: 50S ribosomal protein L30

Chain 13:



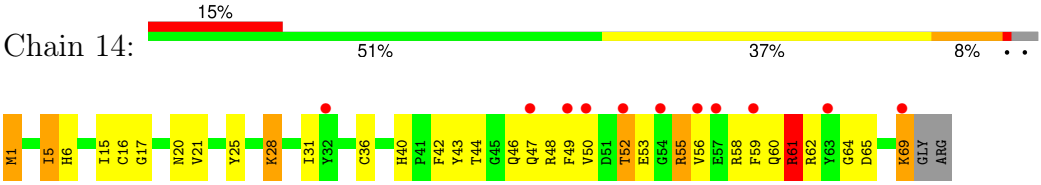
• Molecule 25: 50S ribosomal protein L30

Chain 23:



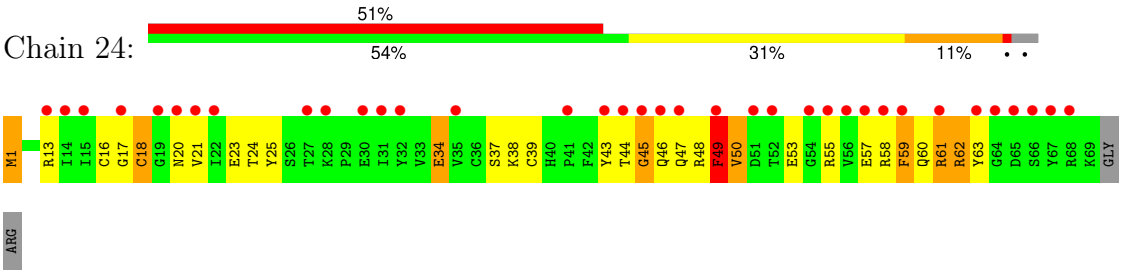
• Molecule 26: 50S ribosomal protein L31

Chain 14:



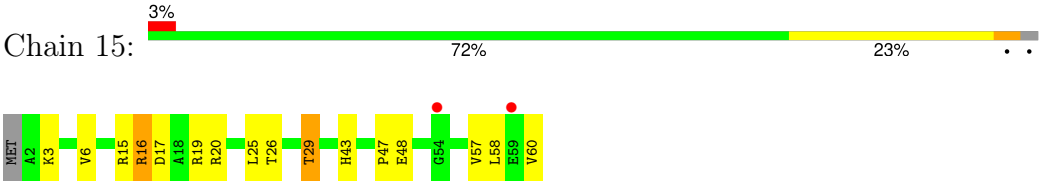
• Molecule 26: 50S ribosomal protein L31

Chain 24:



• Molecule 27: 50S ribosomal protein L32

Chain 15:

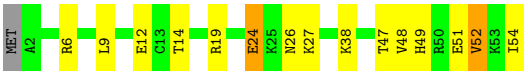


• Molecule 27: 50S ribosomal protein L32

Chain 25:

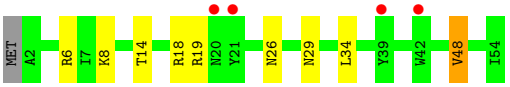
• Molecule 28: 50S ribosomal protein L33

Chain 16:



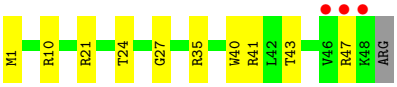
• Molecule 28: 50S ribosomal protein L33

Chain 26:



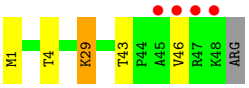
• Molecule 29: 50S ribosomal protein L34

Chain 17:



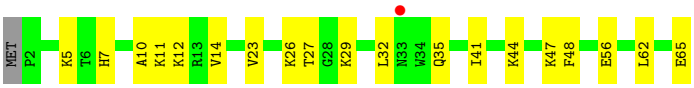
• Molecule 29: 50S ribosomal protein L34

Chain 27:



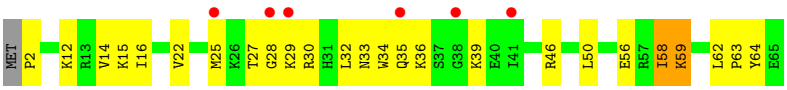
• Molecule 30: 50S ribosomal protein L35

Chain 18:



• Molecule 30: 50S ribosomal protein L35

Chain 28:



• Molecule 31: 50S ribosomal protein L36

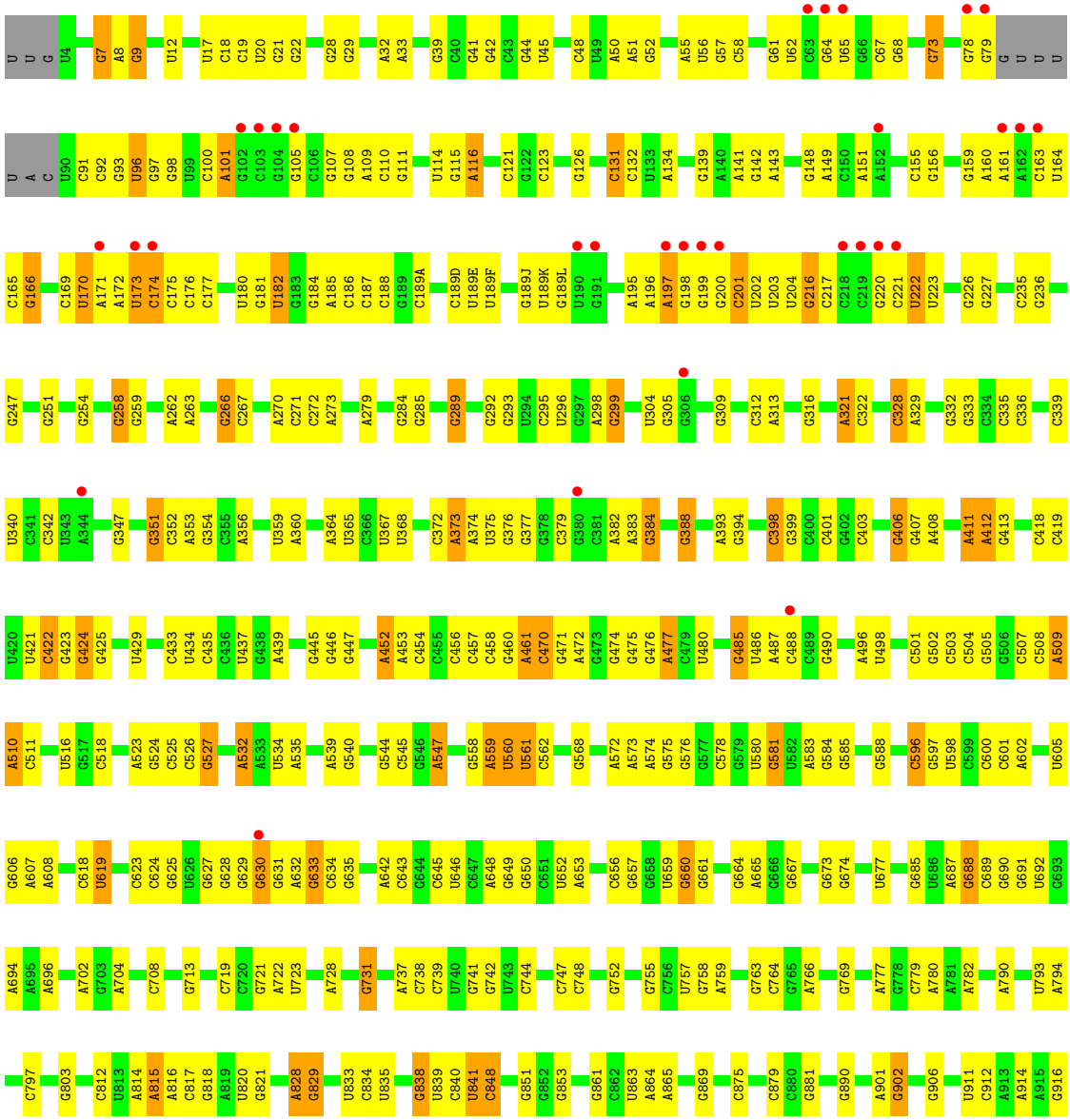
Chain 19:

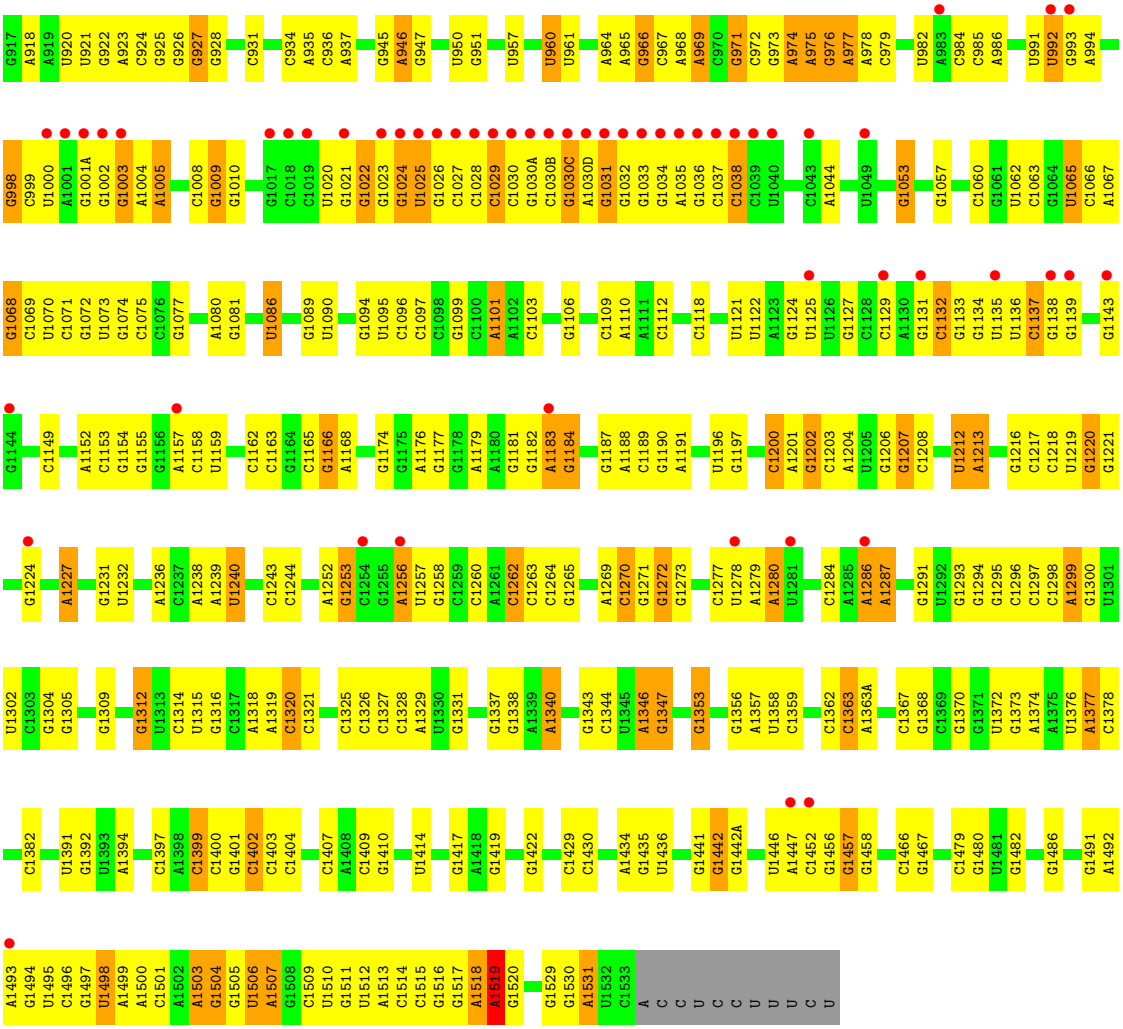
• Molecule 31: 50S ribosomal protein L36

Chain 29:

• Molecule 32: 16S Ribosomal RNA

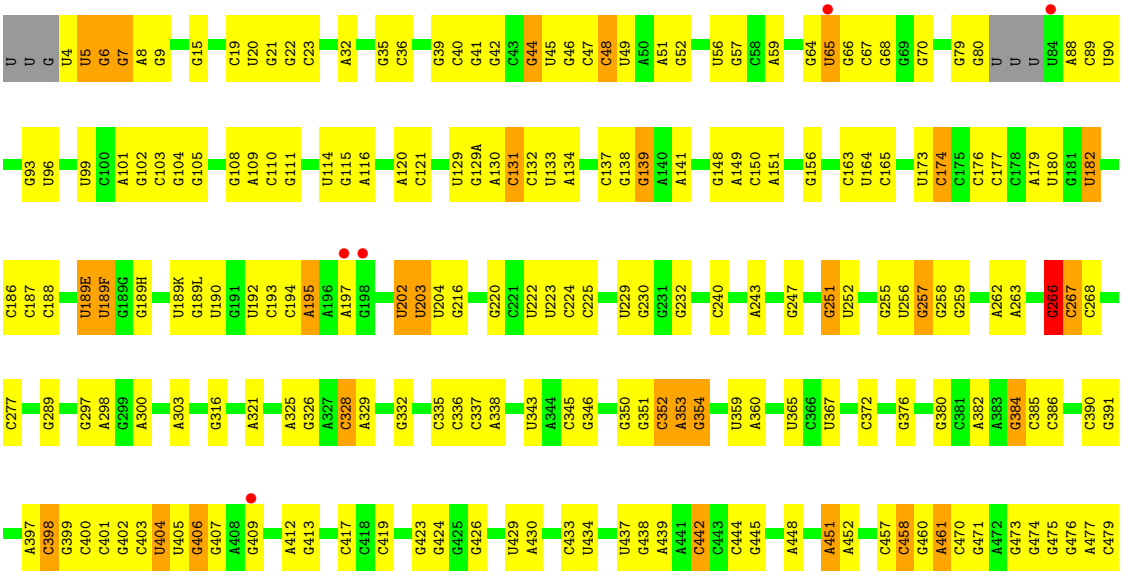
Chain 1a:

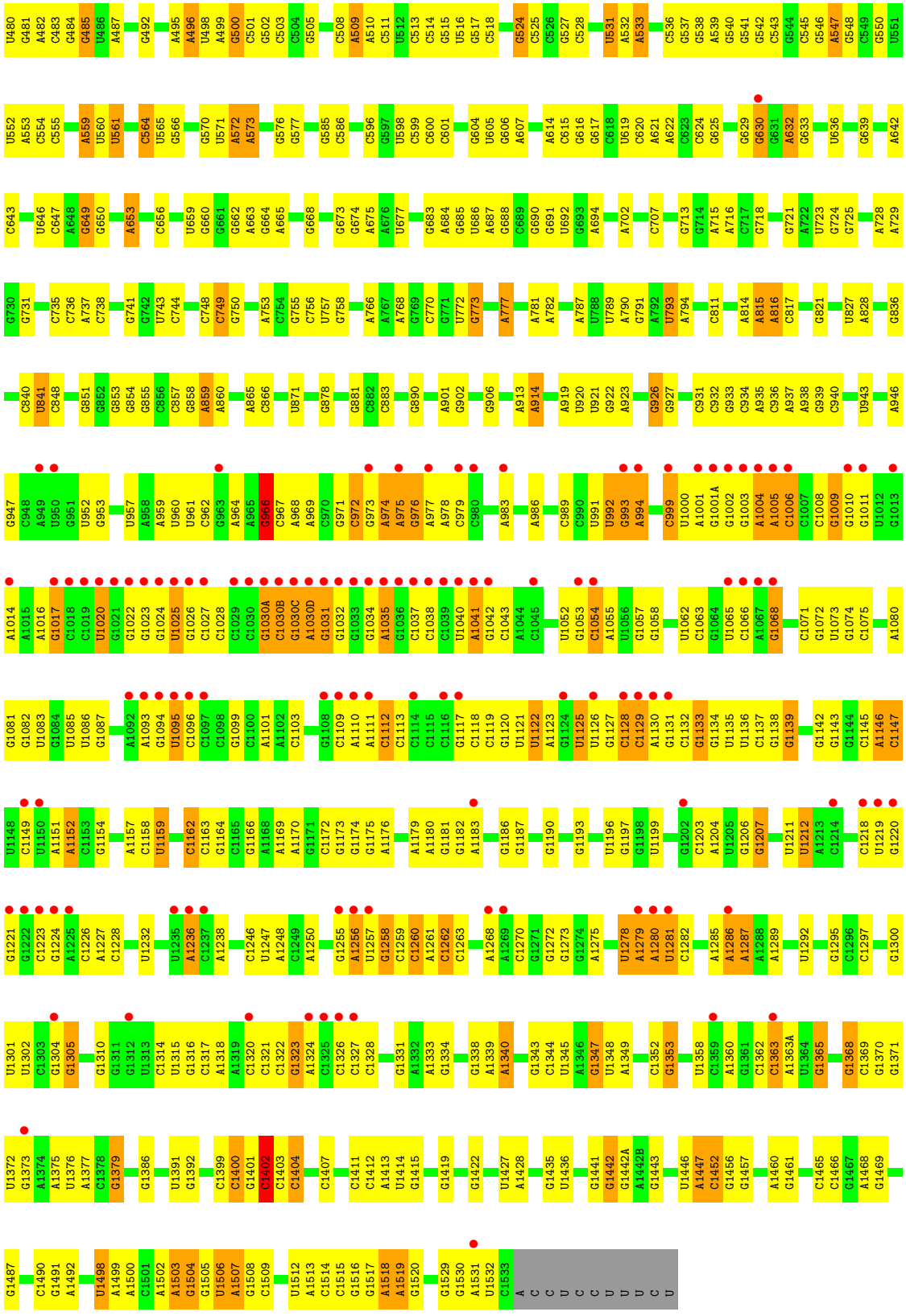




• Molecule 32: 16S Ribosomal RNA

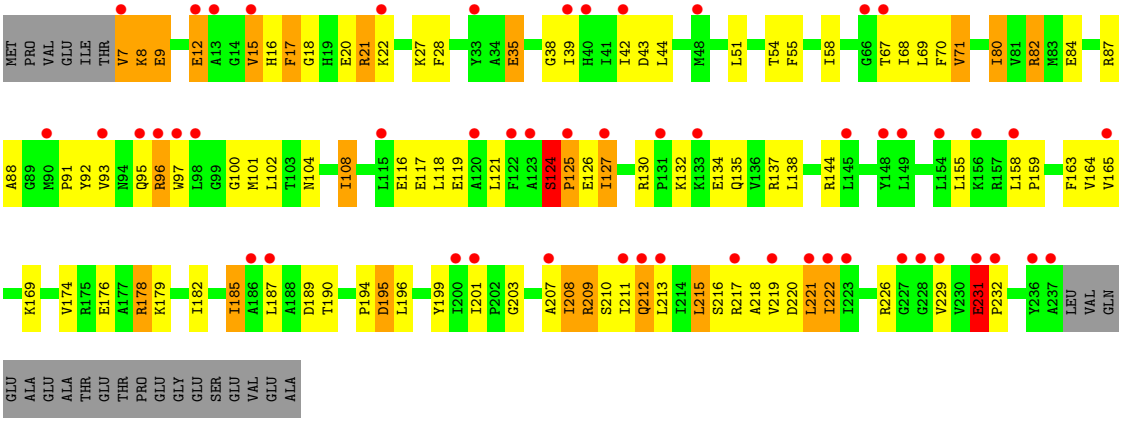
Chain 2a:





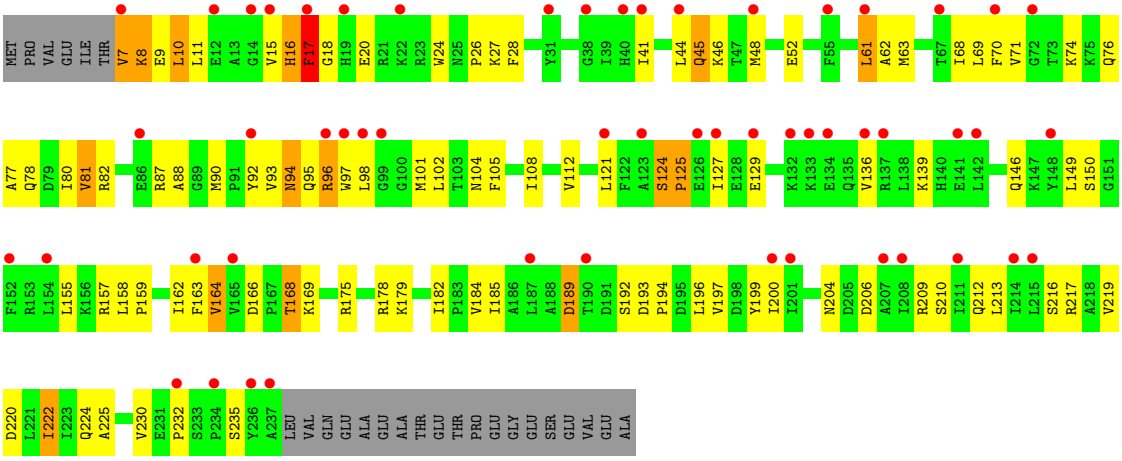
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



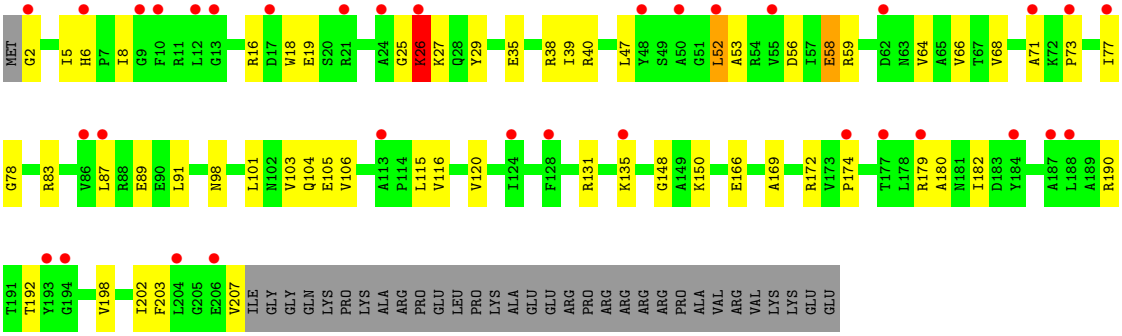
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



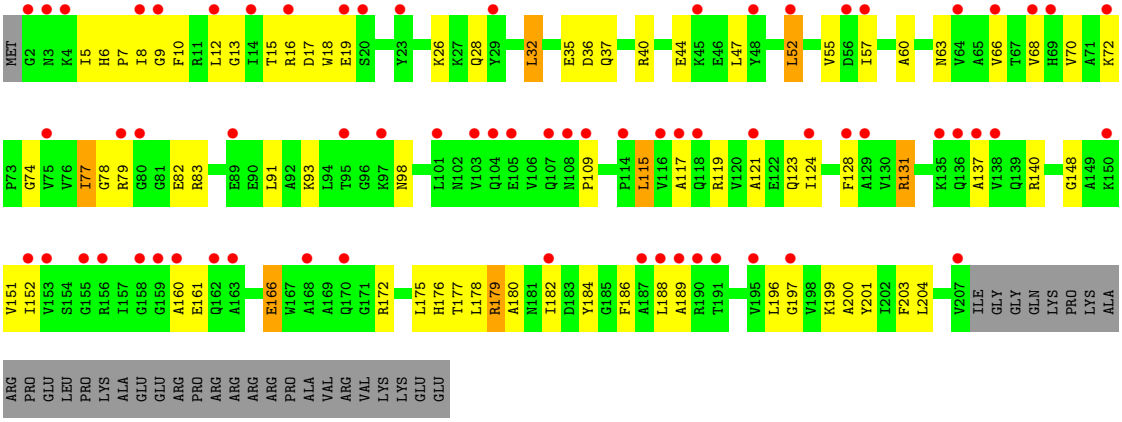
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



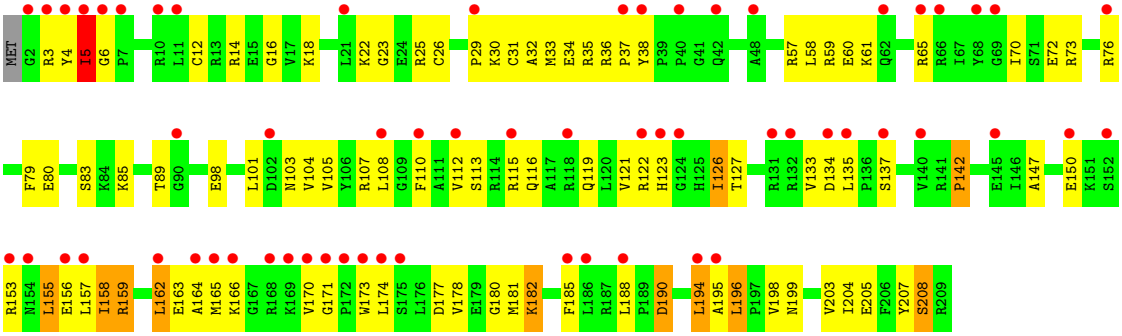
• Molecule 34: 30S ribosomal protein S3

Chain 2c:



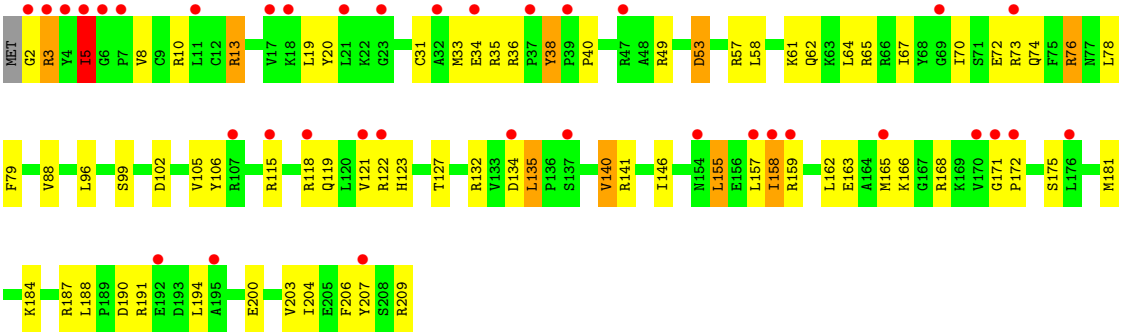
• Molecule 35: 30S ribosomal protein S4

Chain 1d:



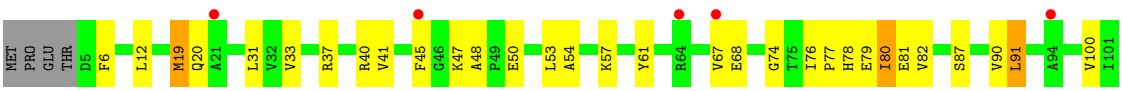
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



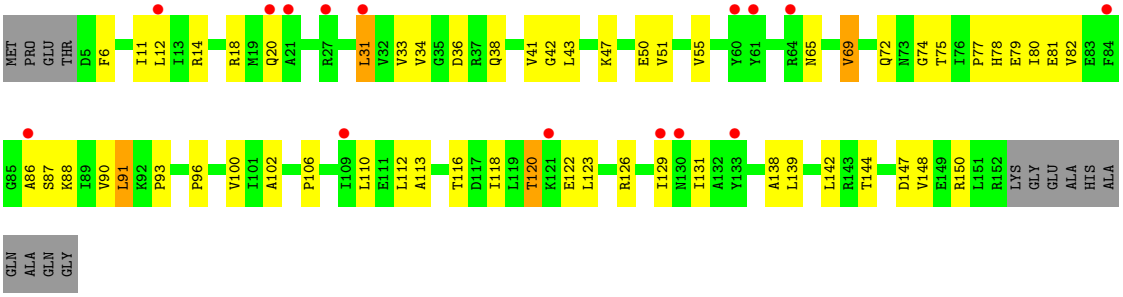
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



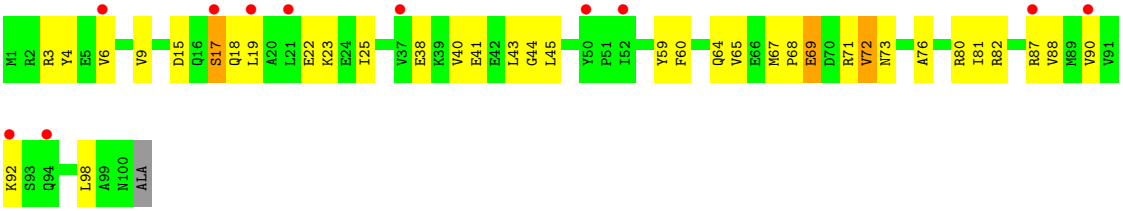
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



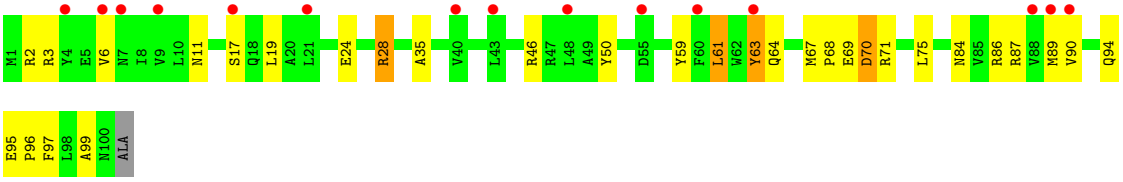
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



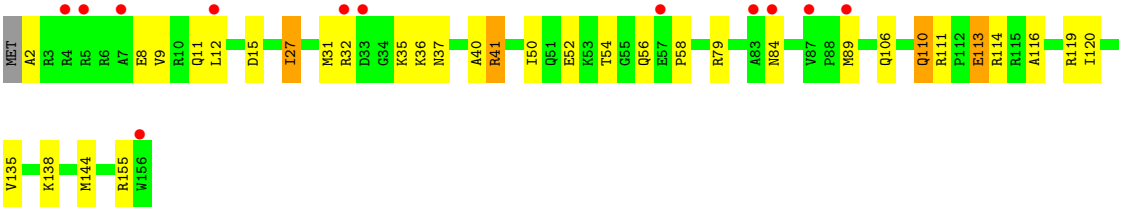
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



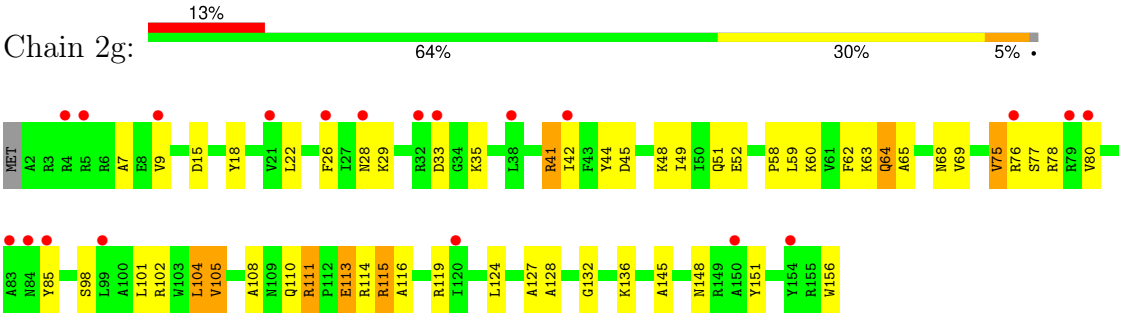
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



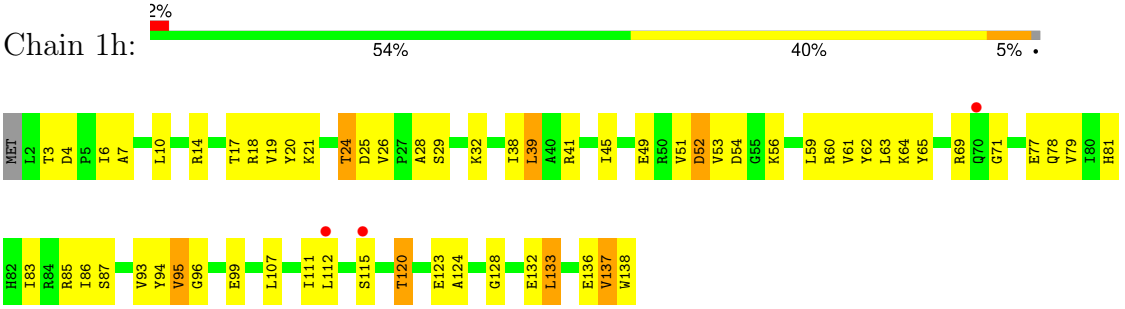
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



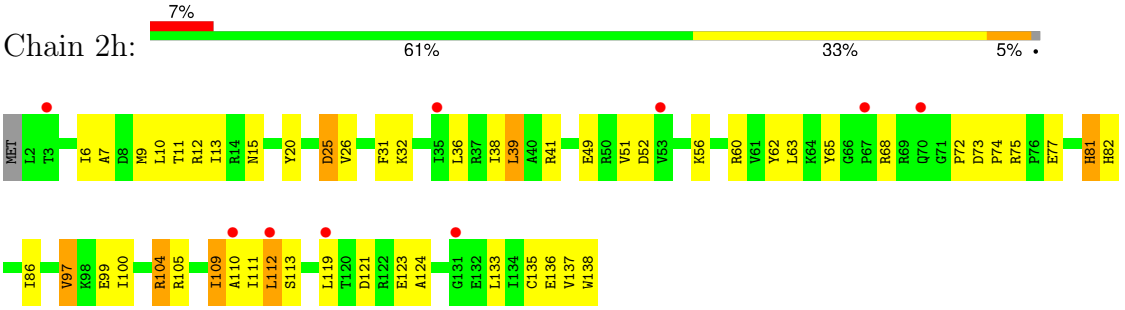
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



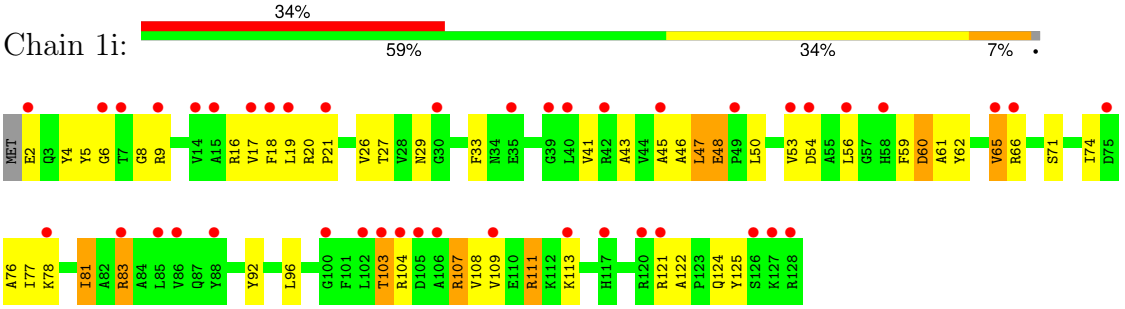
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



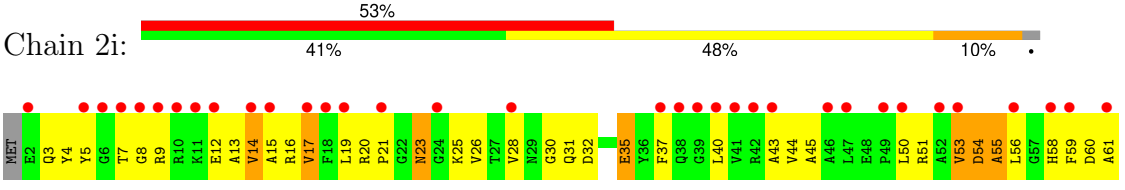
• Molecule 40: 30S ribosomal protein S9

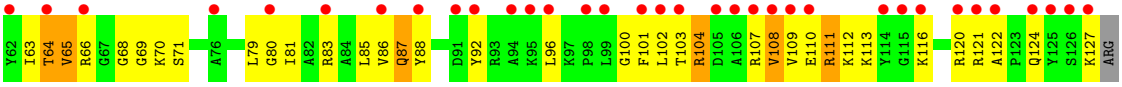
Chain 1i:



• Molecule 40: 30S ribosomal protein S9

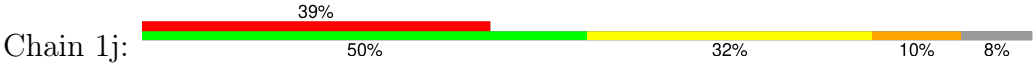
Chain 2i:

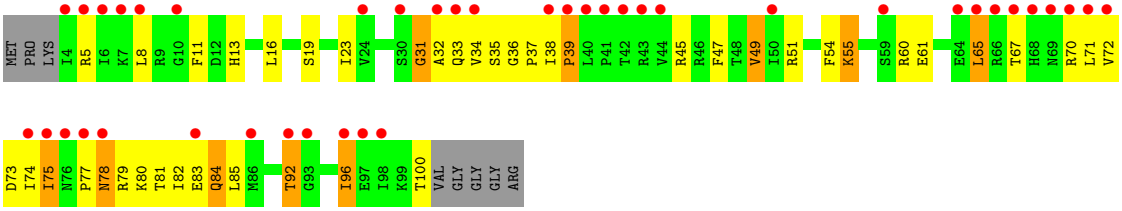




• Molecule 41: 30S ribosomal protein S10

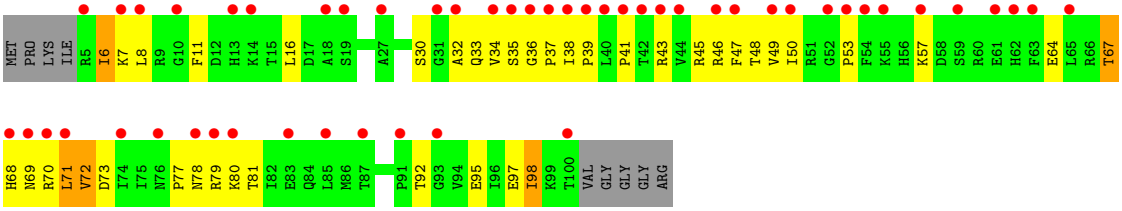
Chain 1j:





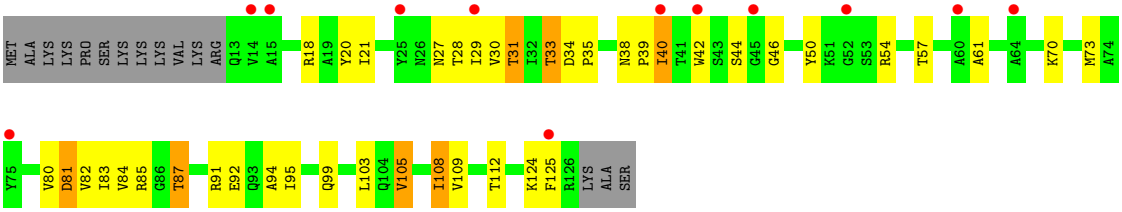
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



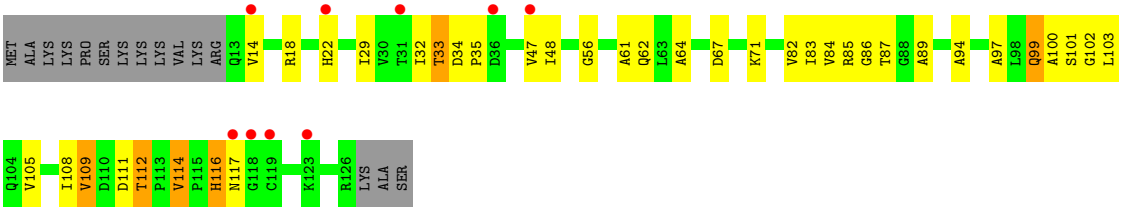
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



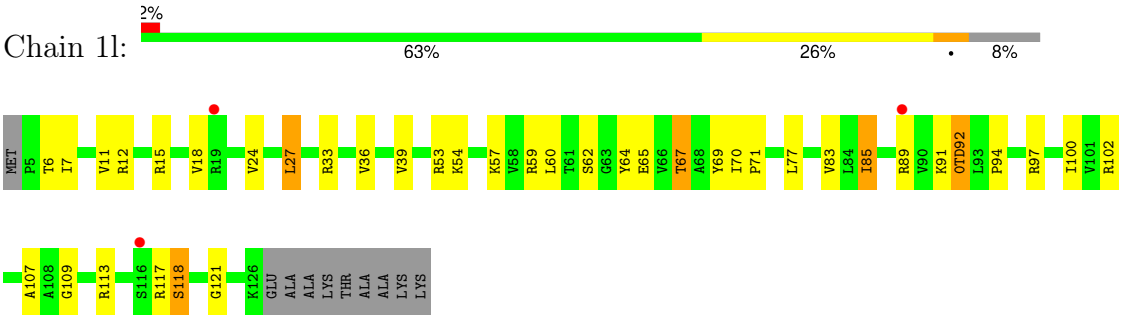
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



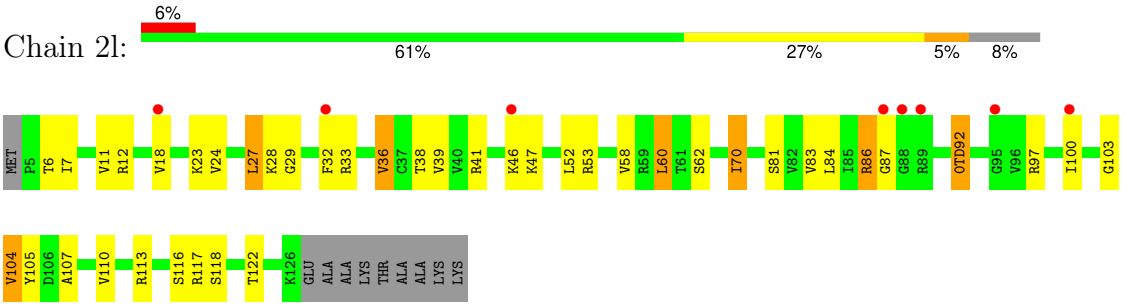
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



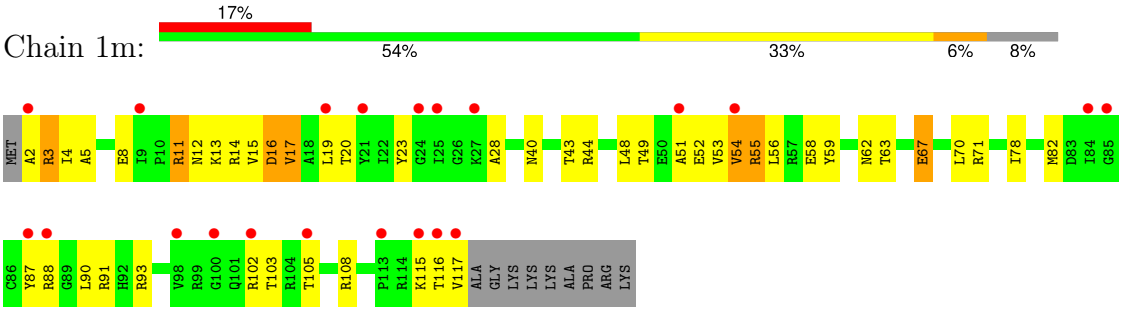
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



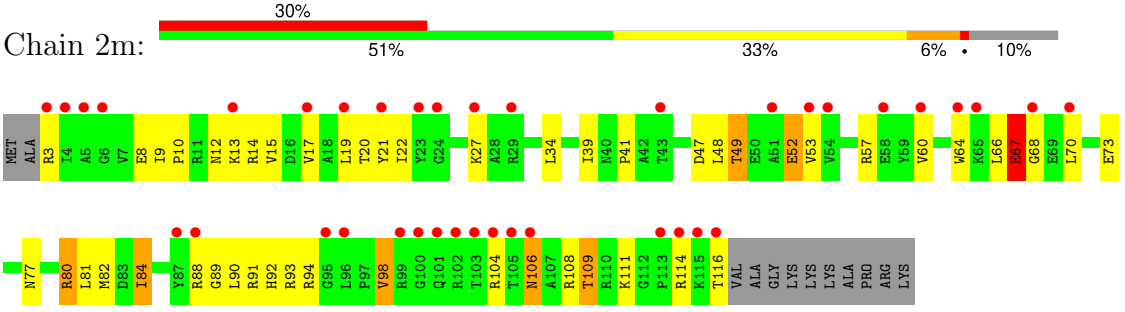
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



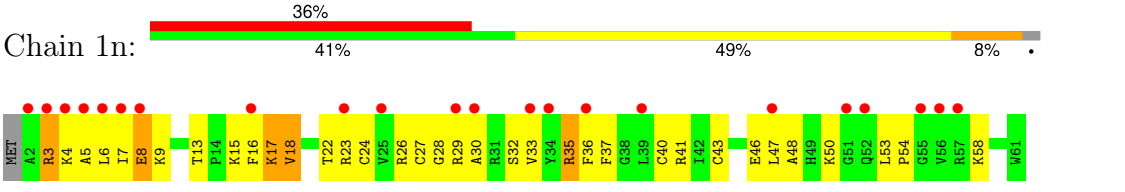
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



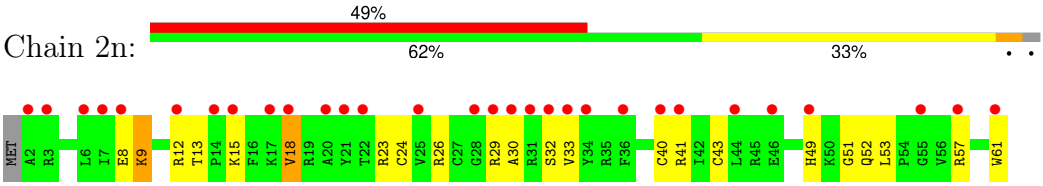
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



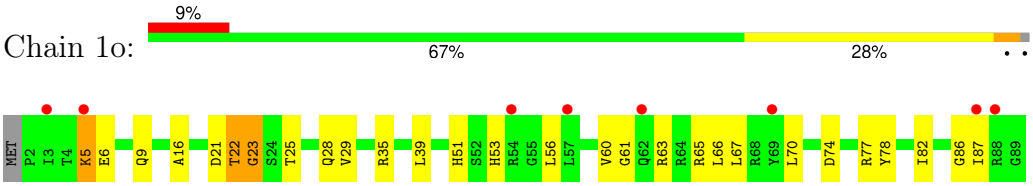
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



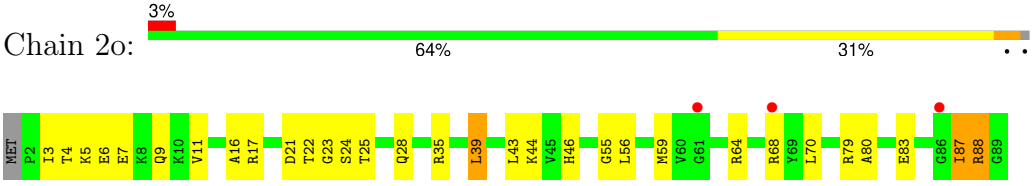
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



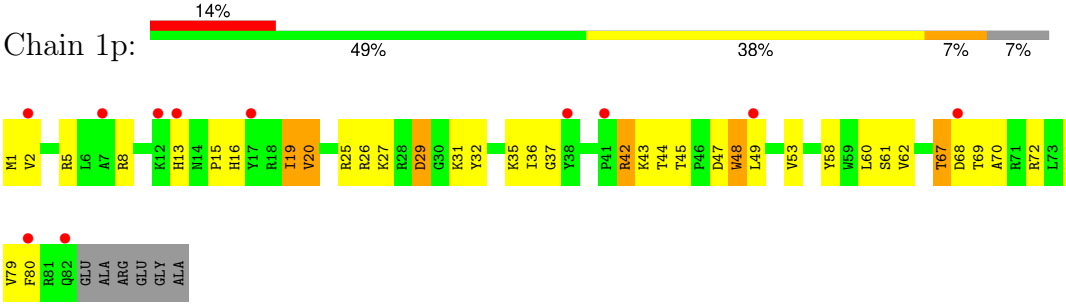
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



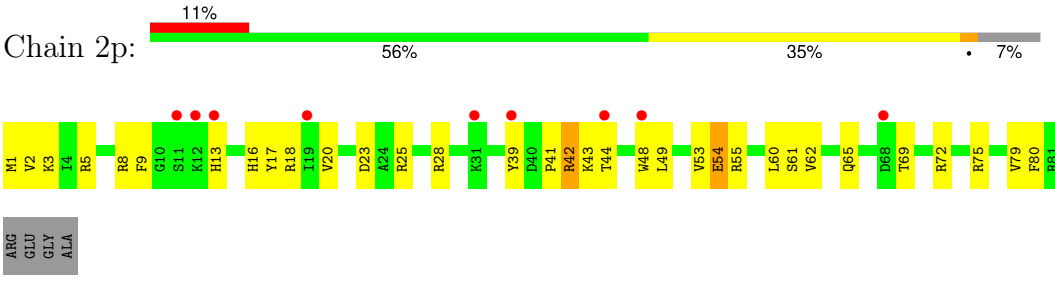
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



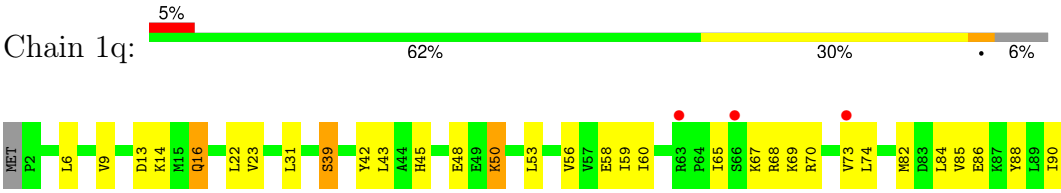
• Molecule 47: 30S ribosomal protein S16

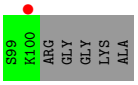
Chain 2p:



• Molecule 48: 30S ribosomal protein S17

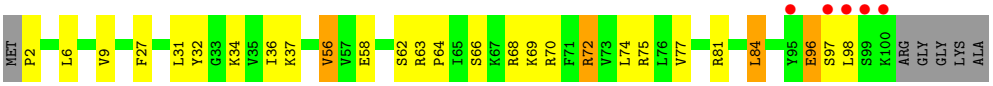
Chain 1q:





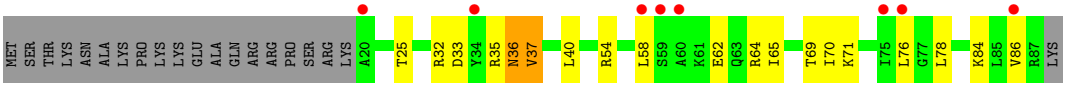
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



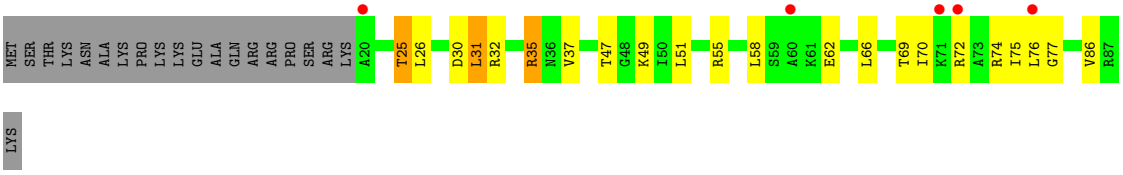
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



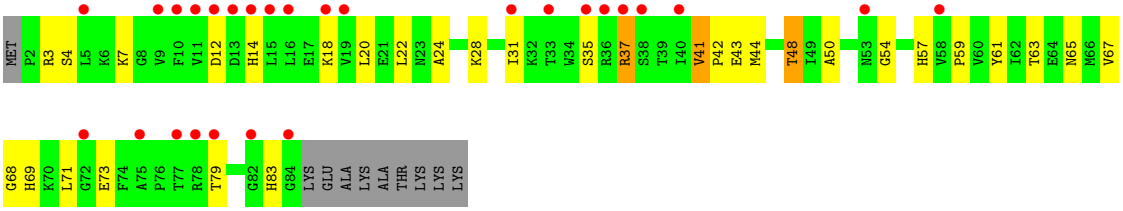
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



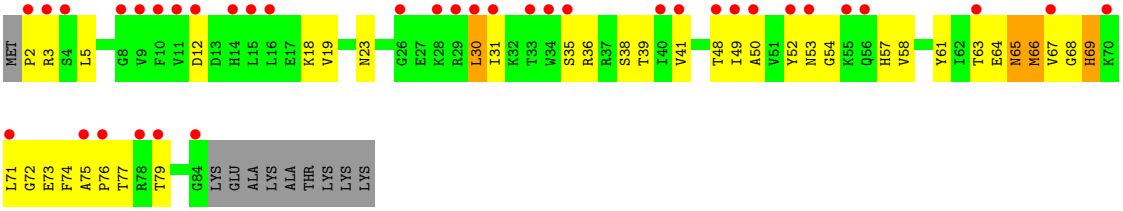
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



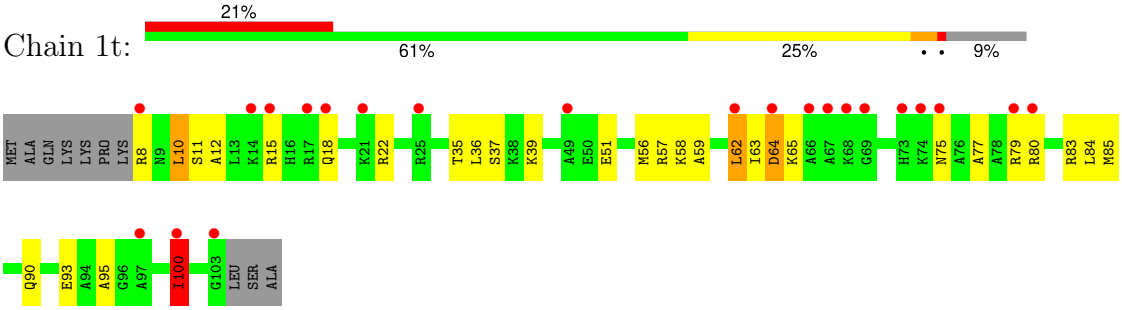
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



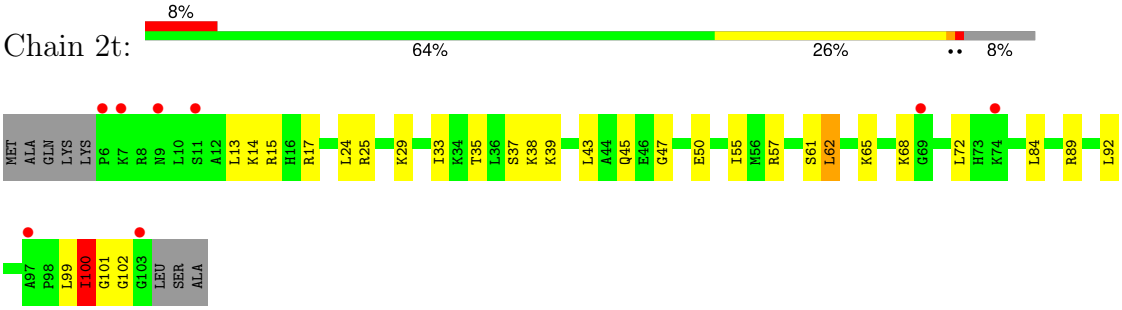
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



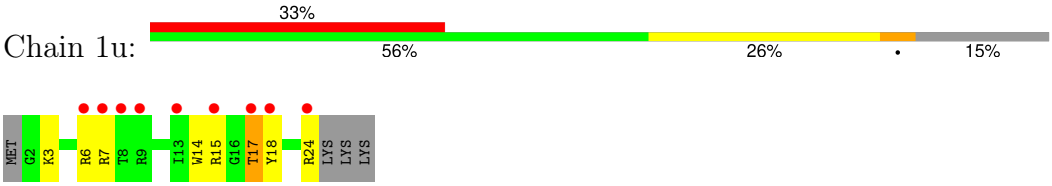
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



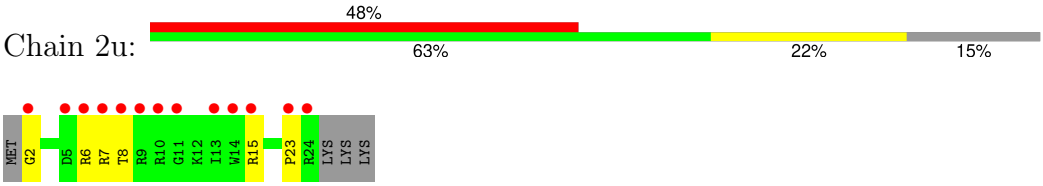
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



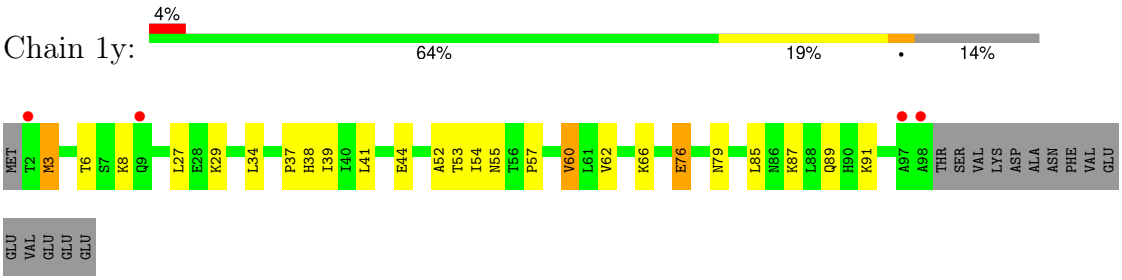
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



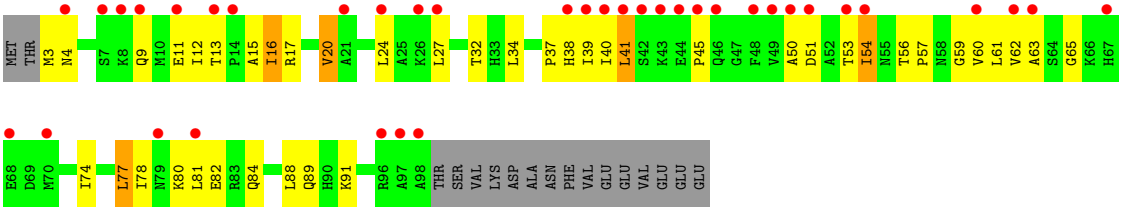
• Molecule 53: Ribosome-associated inhibitor A

Chain 1y:



• Molecule 53: Ribosome-associated inhibitor A

Chain 2y:


MET THR M3 N4 S7 K8 Q9 M10 E11 I12 T13 P14 A15 I16 R17 V20 A21 L24 A25 K26 L27 T32 H33 L34 P37 H38 I39 I40 L41 S42 K43 E44 P45 Q46 G47 F48 V49 A50 D51 A52 T53 I54 N55 T56 P57 N58 G59 V60 L61 V62 A63 S64 G65 K66 H67
E68 D69 M70 I74 L77 I78 N79 K80 L81 E82 R83 Q84 L88 Q89 H90 K91 R96 A97 A98 THR SER VAL LYS ASP ALA ASN PHE VAL GLU GLU VAL GLU GLU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.38Å 452.11Å 624.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	366.21 – 2.90 366.21 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (366.21-2.90) 99.5 (366.21-2.90)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.213 , 0.267 0.212 , 0.264	Depositor DCC
R_{free} test set	64774 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	50.6	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 337.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	297540	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, OMC, 2MA, 4OC, M2G, 5MC, ZN, 0TD, UR3, A1CRE, 5MU, MPD, SF4, MA6, OMU, PSU, 2MG, G7M, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1A	0.29	1/69031 (0.0%)	0.45	0/107754
1	2A	0.23	0/68903	0.40	1/107552 (0.0%)
2	1B	0.22	0/2876	0.40	0/4486
2	2B	0.20	0/2878	0.38	0/4490
3	1D	0.30	0/2181	0.51	0/2940
3	2D	0.24	0/2186	0.50	1/2944 (0.0%)
4	1E	0.28	0/1592	0.51	0/2149
4	2E	0.24	0/1592	0.49	0/2149
5	1F	0.28	0/1619	0.50	0/2193
5	2F	0.23	0/1615	0.47	2/2188 (0.1%)
6	1G	0.27	0/1451	0.45	0/1961
6	2G	0.21	0/1449	0.44	0/1957
7	1H	0.22	0/1356	0.47	0/1834
7	2H	0.21	0/1350	0.42	0/1826
8	1I	0.25	0/1109	0.48	0/1512
8	2I	0.20	0/1091	0.45	0/1490
9	1N	0.25	0/1148	0.45	0/1547
9	2N	0.22	0/1144	0.43	0/1543
10	1O	0.29	0/943	0.50	0/1269
10	2O	0.23	0/943	0.47	0/1269
11	1P	0.27	0/1152	0.50	0/1533
11	2P	0.22	0/1152	0.49	0/1533
12	1Q	0.26	0/1143	0.46	0/1527
12	2Q	0.25	0/1143	0.44	0/1527
13	1R	0.28	0/982	0.55	0/1312
13	2R	0.24	0/982	0.51	0/1312
14	1S	0.22	0/887	0.48	0/1180
14	2S	0.21	0/880	0.45	0/1172
15	1T	0.27	0/1105	0.48	0/1477
15	2T	0.23	0/1097	0.46	0/1468
16	1U	0.30	0/977	0.49	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.21	0/977	0.41	0/1301
17	1V	0.25	0/786	0.46	0/1053
17	2V	0.22	0/782	0.46	0/1049
18	1W	0.27	0/897	0.48	0/1205
18	2W	0.24	0/897	0.43	0/1205
19	1X	0.27	0/764	0.46	0/1025
19	2X	0.22	0/764	0.51	0/1025
20	1Y	0.26	0/823	0.52	0/1099
20	2Y	0.24	0/823	0.50	0/1100
21	1Z	0.22	0/1620	0.44	0/2200
21	2Z	0.24	0/1590	0.45	0/2162
22	10	0.29	0/616	0.56	0/821
22	20	0.22	0/616	0.45	0/821
23	11	0.26	0/761	0.47	0/1013
23	21	0.23	0/766	0.41	0/1018
24	12	0.24	0/590	0.45	0/781
24	22	0.21	0/594	0.39	0/785
25	13	0.26	0/474	0.49	0/635
25	23	0.20	0/469	0.42	0/630
26	14	0.28	0/559	0.58	0/754
26	24	0.29	0/549	0.68	2/741 (0.3%)
27	15	0.29	0/473	0.51	0/639
27	25	0.23	0/469	0.47	0/635
28	16	0.27	0/460	0.50	0/613
28	26	0.22	0/456	0.43	0/608
29	17	0.31	0/426	0.55	0/561
29	27	0.27	0/426	0.50	0/561
30	18	0.27	0/525	0.53	0/691
30	28	0.24	0/525	0.44	0/691
31	19	0.26	0/310	0.44	0/407
31	29	0.22	0/310	0.45	0/407
32	1a	0.21	0/35795	0.39	0/55864
32	2a	0.20	0/35890	0.38	1/56012 (0.0%)
33	1b	0.25	0/1876	0.56	1/2533 (0.0%)
33	2b	0.25	0/1860	0.50	0/2518
34	1c	0.21	0/1582	0.43	0/2137
34	2c	0.27	0/1566	0.48	0/2119
35	1d	0.21	0/1695	0.44	0/2274
35	2d	0.22	0/1698	0.45	0/2277
36	1e	0.23	0/1149	0.48	0/1548
36	2e	0.21	0/1149	0.46	0/1548
37	1f	0.20	0/827	0.42	0/1120
37	2f	0.23	0/829	0.46	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.21	0/1254	0.39	0/1683
38	2g	0.19	0/1248	0.40	0/1676
39	1h	0.20	0/1118	0.43	0/1506
39	2h	0.20	0/1108	0.44	0/1494
40	1i	0.21	0/1005	0.46	0/1351
40	2i	0.22	0/985	0.49	0/1329
41	1j	0.23	0/732	0.48	0/993
41	2j	0.22	0/723	0.50	0/984
42	1k	0.25	0/849	0.54	1/1150 (0.1%)
42	2k	0.21	0/848	0.49	1/1149 (0.1%)
43	1l	0.23	0/937	0.49	0/1260
43	2l	0.21	0/937	0.50	0/1260
44	1m	0.21	0/924	0.46	0/1242
44	2m	0.21	0/905	0.44	0/1217
45	1n	0.24	0/501	0.45	0/664
45	2n	0.25	0/501	0.47	0/664
46	1o	0.21	0/739	0.41	0/985
46	2o	0.21	0/739	0.48	1/985 (0.1%)
47	1p	0.23	0/697	0.51	0/939
47	2p	0.20	0/693	0.47	0/935
48	1q	0.21	0/836	0.45	0/1117
48	2q	0.24	0/836	0.45	0/1117
49	1r	0.37	0/560	0.48	0/746
49	2r	0.27	0/560	0.40	0/746
50	1s	0.19	0/663	0.43	0/895
50	2s	0.21	0/660	0.46	0/893
51	1t	0.21	0/734	0.47	0/969
51	2t	0.20	0/736	0.43	0/976
52	1u	0.28	0/203	0.48	0/266
52	2u	0.22	0/203	0.52	0/266
53	1y	0.20	0/776	0.34	0/1048
53	2y	0.25	0/761	0.45	0/1030
All	All	0.24	1/309941 (0.0%)	0.43	11/463239 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	2I	0	1
14	1S	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
19	1X	0	1
21	2Z	0	1
26	14	0	1
26	24	0	1
33	1b	0	2
43	2l	0	1
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2552	OMU	O3'-P	5.01	1.61	1.56

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	1b	222	ILE	N-CA-C	-10.39	102.53	112.29
42	1k	40	ILE	N-CA-C	-10.19	103.56	112.12
3	2D	41	GLY	N-CA-C	-7.33	105.12	115.30
32	2a	266	G	C2'-C3'-O3'	5.47	117.71	109.50
5	2F	21	ALA	CA-C-N	5.44	131.49	121.70
5	2F	21	ALA	C-N-CA	5.44	131.49	121.70
46	2o	44	LYS	N-CA-C	-5.43	106.63	113.20
26	24	59	PHE	CA-C-N	5.41	131.44	121.70
26	24	59	PHE	C-N-CA	5.41	131.44	121.70
1	2A	1992	G	C2'-C3'-O3'	5.40	117.60	109.50
42	2k	100	ALA	N-CA-C	-5.22	106.94	113.15

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	52	THR	Peptide
14	1S	58	LEU	Peptide
19	1X	93	GLU	Peptide
33	1b	220	ASP	Peptide
33	1b	231	GLU	Peptide
26	24	18	CYS	Peptide
8	2I	85	GLU	Peptide
21	2Z	136	PHE	Peptide
43	2l	86	ARG	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61869	0	31203	704	0
1	2A	61758	0	31153	830	0
2	1B	2572	0	1305	31	0
2	2B	2573	0	1306	32	0
3	1D	2131	0	2207	47	0
3	2D	2136	0	2218	47	0
4	1E	1559	0	1618	42	0
4	2E	1559	0	1618	54	0
5	1F	1584	0	1625	36	0
5	2F	1580	0	1619	54	0
6	1G	1426	0	1445	48	0
6	2G	1424	0	1441	50	0
7	1H	1330	0	1407	31	0
7	2H	1324	0	1402	52	0
8	1I	1094	0	1127	26	0
8	2I	1076	0	1094	21	0
9	1N	1121	0	1195	27	0
9	2N	1117	0	1184	28	0
10	1O	933	0	996	23	0
10	2O	933	0	996	27	0
11	1P	1135	0	1212	30	0
11	2P	1135	0	1212	32	0
12	1Q	1122	0	1179	23	0
12	2Q	1122	0	1179	27	0
13	1R	968	0	1033	25	0
13	2R	968	0	1033	32	0
14	1S	877	0	938	19	0
14	2S	870	0	923	32	0
15	1T	1091	0	1151	26	0
15	2T	1083	0	1136	26	0
16	1U	959	0	1019	15	0
16	2U	959	0	1019	17	0
17	1V	775	0	841	14	0
17	2V	771	0	830	21	0
18	1W	886	0	940	14	0
18	2W	886	0	940	24	0
19	1X	750	0	814	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2X	750	0	814	15	0
20	1Y	810	0	892	25	0
20	2Y	810	0	887	26	0
21	1Z	1587	0	1598	35	0
21	2Z	1557	0	1564	48	0
22	10	608	0	622	16	0
22	20	608	0	622	17	0
23	11	754	0	823	11	0
23	21	759	0	837	24	0
24	12	588	0	643	12	0
24	22	592	0	654	12	0
25	13	469	0	518	10	0
25	23	464	0	514	12	0
26	14	546	0	522	24	0
26	24	536	0	514	30	0
27	15	459	0	476	12	0
27	25	455	0	465	11	0
28	16	453	0	473	9	0
28	26	449	0	469	5	0
29	17	418	0	467	7	0
29	27	418	0	467	1	0
30	18	517	0	582	12	0
30	28	517	0	582	17	0
31	19	307	0	335	6	0
31	29	307	0	335	5	0
32	1a	32246	0	16294	512	0
32	2a	32331	0	16338	517	0
33	1b	1842	0	1862	66	0
33	2b	1825	0	1828	73	0
34	1c	1558	0	1557	37	0
34	2c	1542	0	1517	51	0
35	1d	1665	0	1687	68	0
35	2d	1668	0	1703	51	0
36	1e	1133	0	1190	33	0
36	2e	1133	0	1191	35	0
37	1f	814	0	808	22	0
37	2f	816	0	808	19	0
38	1g	1235	0	1249	19	0
38	2g	1229	0	1238	37	0
39	1h	1098	0	1143	35	0
39	2h	1088	0	1126	41	0
40	1i	986	0	990	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	2i	966	0	953	61	0
41	1j	719	0	672	30	0
41	2j	710	0	661	26	0
42	1k	834	0	838	22	0
42	2k	833	0	836	21	0
43	1l	932	0	981	23	0
43	2l	932	0	981	23	0
44	1m	914	0	954	29	0
44	2m	895	0	920	36	0
45	1n	492	0	529	27	0
45	2n	492	0	529	21	0
46	1o	728	0	760	20	0
46	2o	728	0	760	20	0
47	1p	681	0	697	28	0
47	2p	677	0	686	21	0
48	1q	823	0	891	20	0
48	2q	823	0	891	15	0
49	1r	555	0	618	9	0
49	2r	555	0	618	13	0
50	1s	648	0	658	23	0
50	2s	645	0	635	31	0
51	1t	732	0	809	23	0
51	2t	733	0	795	23	0
52	1u	199	0	208	6	0
52	2u	199	0	208	3	0
53	1y	764	0	786	19	0
53	2y	749	0	757	23	0
54	10	7	0	0	0	0
54	11	4	0	0	0	0
54	13	3	0	0	0	0
54	15	6	0	0	0	0
54	17	4	0	0	0	0
54	18	4	0	0	0	0
54	19	2	0	0	0	0
54	1A	1011	0	0	0	0
54	1B	30	0	0	0	0
54	1D	18	0	0	0	0
54	1E	9	0	0	0	0
54	1F	16	0	0	0	0
54	1G	4	0	0	0	0
54	1H	3	0	0	0	0
54	1N	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1O	2	0	0	0	0
54	1P	6	0	0	0	0
54	1Q	7	0	0	0	0
54	1R	8	0	0	0	0
54	1S	1	0	0	0	0
54	1T	5	0	0	0	0
54	1U	5	0	0	0	0
54	1V	6	0	0	0	0
54	1W	3	0	0	0	0
54	1Y	1	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	270	0	0	0	0
54	1b	1	0	0	0	0
54	1d	5	0	0	0	0
54	1e	4	0	0	0	0
54	1f	2	0	0	0	0
54	1g	3	0	0	0	0
54	1h	2	0	0	0	0
54	1i	1	0	0	0	0
54	1l	2	0	0	0	0
54	1m	1	0	0	0	0
54	1n	2	0	0	0	0
54	1o	2	0	0	0	0
54	1p	1	0	0	0	0
54	1t	2	0	0	0	0
54	1y	5	0	0	0	0
54	20	2	0	0	0	0
54	21	1	0	0	0	0
54	23	1	0	0	0	0
54	25	3	0	0	0	0
54	27	1	0	0	0	0
54	28	2	0	0	0	0
54	2A	732	0	0	0	0
54	2B	20	0	0	0	0
54	2D	7	0	0	0	0
54	2E	8	0	0	0	0
54	2F	4	0	0	0	0
54	2G	3	0	0	0	0
54	2I	1	0	0	0	0
54	2N	1	0	0	0	0
54	2O	1	0	0	0	0
54	2P	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	2Q	4	0	0	0	0
54	2R	2	0	0	0	0
54	2T	3	0	0	0	0
54	2U	1	0	0	0	0
54	2V	1	0	0	0	0
54	2W	3	0	0	0	0
54	2X	1	0	0	0	0
54	2Y	1	0	0	0	0
54	2a	192	0	0	0	0
54	2e	2	0	0	0	0
54	2f	1	0	0	0	0
54	2j	1	0	0	0	0
54	2k	1	0	0	0	0
54	2l	1	0	0	0	0
54	2o	1	0	0	0	0
54	2q	1	0	0	0	0
54	2r	1	0	0	0	0
54	2t	1	0	0	0	0
54	2y	1	0	0	0	0
55	1A	41	0	0	0	0
55	2A	41	0	0	0	0
56	18	8	0	12	1	0
56	1A	8	0	14	1	0
56	1a	16	0	27	2	0
56	2A	16	0	28	0	0
56	2B	8	0	14	1	0
57	1B	12	0	12	2	0
57	1F	12	0	12	2	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	1	0
59	2d	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	10	26	0	0	1	0
60	11	25	0	0	0	0
60	12	15	0	0	1	0
60	13	23	0	0	3	0
60	14	1	0	0	0	0
60	15	29	0	0	1	0
60	16	14	0	0	0	0
60	17	13	0	0	2	0
60	18	28	0	0	2	0
60	19	11	0	0	1	0
60	1A	3794	0	0	183	0
60	1B	98	0	0	11	0
60	1D	112	0	0	2	0
60	1E	73	0	0	4	0
60	1F	61	0	0	3	0
60	1G	20	0	0	1	0
60	1H	14	0	0	0	0
60	1I	8	0	0	0	0
60	1N	51	0	0	3	0
60	1O	20	0	0	3	0
60	1P	64	0	0	2	0
60	1Q	39	0	0	1	0
60	1R	30	0	0	3	0
60	1S	8	0	0	0	0
60	1T	39	0	0	2	0
60	1U	39	0	0	1	0
60	1V	38	0	0	0	0
60	1W	28	0	0	0	0
60	1X	26	0	0	2	0
60	1Y	15	0	0	2	0
60	1Z	11	0	0	2	0
60	1a	532	0	0	42	0
60	1b	1	0	0	0	0
60	1d	9	0	0	3	0
60	1e	6	0	0	0	0
60	1f	2	0	0	0	0
60	1g	1	0	0	0	0
60	1h	2	0	0	0	0
60	1i	1	0	0	0	0
60	1j	1	0	0	0	0
60	1l	5	0	0	0	0
60	1m	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	1o	2	0	0	0	0
60	1p	3	0	0	0	0
60	1q	1	0	0	0	0
60	1r	1	0	0	0	0
60	1t	1	0	0	0	0
60	1u	1	0	0	0	0
60	1y	6	0	0	0	0
60	20	12	0	0	1	0
60	21	19	0	0	3	0
60	23	3	0	0	0	0
60	24	1	0	0	0	0
60	25	11	0	0	0	0
60	26	5	0	0	1	0
60	27	11	0	0	1	0
60	28	14	0	0	4	0
60	29	1	0	0	0	0
60	2A	2275	0	0	194	0
60	2B	60	0	0	7	0
60	2D	50	0	0	2	0
60	2E	29	0	0	2	0
60	2F	20	0	0	1	0
60	2G	6	0	0	1	0
60	2H	3	0	0	1	0
60	2I	3	0	0	1	0
60	2N	5	0	0	0	0
60	2O	15	0	0	1	0
60	2P	26	0	0	3	0
60	2Q	20	0	0	2	0
60	2R	17	0	0	2	0
60	2S	5	0	0	0	0
60	2T	13	0	0	0	0
60	2U	8	0	0	1	0
60	2V	7	0	0	0	0
60	2W	21	0	0	2	0
60	2X	7	0	0	0	0
60	2Y	3	0	0	0	0
60	2Z	13	0	0	2	0
60	2a	436	0	0	29	0
60	2d	5	0	0	0	0
60	2e	3	0	0	0	0
60	2f	2	0	0	0	0
60	2j	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	2l	4	0	0	1	0
60	2m	1	0	0	0	0
60	2n	1	0	0	0	0
60	2o	4	0	0	1	0
60	2p	4	0	0	0	0
60	2q	1	0	0	0	0
60	2r	3	0	0	0	0
60	2t	1	0	0	0	0
60	2u	1	0	0	0	0
60	2y	8	0	0	1	0
All	All	297540	0	194512	4638	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (4638) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.34	1.25
32:2a:1003:G:H2'	32:2a:1004:A:H4'	1.40	1.02
20:1Y:92:ASN:HB2	20:1Y:94:LYS:H	1.26	0.97
32:2a:1256:A:H61	32:2a:1278:U:H1'	1.27	0.96
1:1A:1082:U:O4	1:1A:1086:A:N1	1.99	0.95
32:1a:201:C:H42	32:1a:216:G:H1	1.14	0.94
15:1T:55:ASN:H	15:1T:59:THR:HG22	1.31	0.94
1:1A:2127:G:H21	1:1A:2173:A:H1'	1.32	0.92
32:2a:1278:U:H5"	32:2a:1279:A:H5'	1.54	0.90
32:2a:1286:A:H8	32:2a:1287:A:H4'	1.35	0.88
1:1A:194:G:OP2	60:1A:4117:HOH:O	1.93	0.86
1:1A:1060:U:H4'	1:1A:1061:U:H5'	1.58	0.86
32:2a:1441:G:H5"	32:2a:1442:G:H5'	1.58	0.86
1:1A:2319:G:H22	14:1S:3:ARG:HD2	1.41	0.85
1:1A:517:C:OP1	27:15:16:ARG:NH2	2.09	0.85
26:24:20:ASN:HD21	26:24:38:LYS:HE2	1.41	0.85
1:1A:1315:C:OP2	60:1A:4118:HOH:O	1.93	0.85
1:2A:1047:G:H2'	1:2A:1110:G:H22	1.41	0.85
1:2A:2499:C:OP1	60:2A:3814:HOH:O	1.95	0.84
46:2o:16:ALA:HB1	46:2o:21:ASP:HB3	1.58	0.84
1:1A:1082:U:N3	1:1A:1086:A:N6	2.09	0.83
1:1A:1085:A:O2'	1:1A:1104:C:O2'	1.95	0.83
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2k:86:GLY:H	42:2k:112:THR:HG23	1.43	0.83
1:1A:2304:G:H22	1:1A:2312:U:H3	1.23	0.83
1:2A:1063:G:H22	1:2A:1075:C:H42	1.27	0.83
1:1A:1701:A:OP2	60:1A:4119:HOH:O	1.97	0.82
1:2A:1041:C:H42	1:2A:1114:G:H1	1.24	0.82
3:2D:221:VAL:HG22	3:2D:226:MET:HE2	1.59	0.82
32:2a:79:G:H1	32:2a:90:U:H3	1.25	0.82
12:1Q:34:LEU:HD11	12:1Q:129:THR:HB	1.62	0.82
10:2O:48:PRO:HB3	32:2a:1422:G:H5"	1.59	0.82
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.62	0.82
32:2a:1500:A:OP1	60:2a:3205:HOH:O	1.96	0.82
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.13	0.81
32:2a:975:A:H4'	32:2a:976:G:H5"	1.60	0.81
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	1.63	0.81
1:2A:1090:U:H2'	1:2A:1091:G:H8	1.42	0.81
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.13	0.80
33:2b:8:LYS:HD2	33:2b:48:MET:HG2	1.61	0.80
1:1A:1175:U:OP1	1:1A:1177:A:N6	2.15	0.80
32:1a:1500:A:OP1	60:1a:3304:HOH:O	1.99	0.80
1:1A:971:C:OP2	60:1A:4120:HOH:O	1.99	0.80
1:2A:364:C:OP2	60:2A:3815:HOH:O	1.99	0.80
40:2i:5:TYR:H	40:2i:87:GLN:HE22	1.29	0.79
32:2a:1518:MA6:H93	32:2a:1519:MA6:H102	1.65	0.79
32:2a:70:G:H1	32:2a:99:U:H3	1.31	0.79
8:2I:26:ALA:HA	8:2I:30:LEU:HB2	1.64	0.79
32:1a:411:A:OP1	35:1d:30:LYS:NZ	2.16	0.79
30:28:56:GLU:HA	30:28:59:LYS:HG3	1.64	0.79
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.64	0.78
32:2a:1285:A:H4'	32:2a:1286:A:H5'	1.63	0.78
32:1a:472:A:H5"	47:1p:80:PHE:HB3	1.64	0.78
48:2q:62:SER:OG	48:2q:72:ARG:NH1	2.16	0.78
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.65	0.78
34:2c:109:PRO:HB3	34:2c:115:LEU:HD23	1.64	0.78
1:1A:11:G:H2'	1:1A:12:U:H5"	1.66	0.78
1:2A:2526:G:O6	60:2A:3816:HOH:O	2.00	0.78
1:2A:2640:G:O3'	9:2N:74:ARG:NH2	2.16	0.78
40:2i:53:VAL:O	40:2i:55:ALA:N	2.16	0.78
7:1H:98:LEU:HD22	7:1H:125:VAL:HG23	1.65	0.77
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.17	0.77
1:1A:942:G:O6	60:1A:4124:HOH:O	2.02	0.77
1:1A:975:C:O2	60:1A:4121:HOH:O	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:217:G:OP2	60:1A:4122:HOH:O	2.02	0.77
32:1a:964:A:OP1	60:1a:3305:HOH:O	2.01	0.77
1:2A:947:G:OP2	60:2A:3821:HOH:O	2.03	0.77
1:1A:1064:C:H3'	1:1A:1065:U:H5"	1.67	0.77
3:1D:69:ARG:NH2	3:1D:128:GLY:O	2.17	0.77
1:2A:1903:G:O2'	60:2A:3820:HOH:O	2.03	0.77
1:2A:1332:G:OP1	60:2A:3817:HOH:O	2.01	0.77
1:2A:740:U:OP2	60:2A:3818:HOH:O	2.02	0.77
32:1a:1003:G:N2	32:1a:1004:A:N3	2.34	0.76
1:1A:1753:G:N7	60:1A:4209:HOH:O	2.17	0.76
45:1n:24:CYS:HB3	45:1n:28:GLY:H	1.50	0.76
1:1A:320:A:OP1	5:1F:135:LYS:NZ	2.18	0.76
1:1A:827:U:OP1	60:1A:4123:HOH:O	2.02	0.76
1:2A:1315:C:OP2	60:2A:3817:HOH:O	2.03	0.76
6:2G:5:VAL:HG22	6:2G:8:LYS:HB2	1.66	0.76
1:1A:2615:U:OP2	60:1A:4125:HOH:O	2.03	0.76
16:1U:34:LYS:NZ	16:1U:37:GLU:OE1	2.19	0.76
1:2A:1023:U:OP2	60:2A:3819:HOH:O	2.03	0.76
21:2Z:157:LEU:HD11	21:2Z:163:LEU:HB2	1.68	0.76
5:1F:38:ARG:NH2	60:1F:402:HOH:O	2.18	0.76
1:1A:1242:A:N1	60:1A:4222:HOH:O	2.19	0.76
12:2Q:26:TYR:O	60:2Q:301:HOH:O	2.04	0.76
23:21:50:ARG:HG2	23:21:59:THR:HG22	1.68	0.76
1:1A:197:A:OP1	60:1A:4128:HOH:O	2.04	0.75
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.05	0.75
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.68	0.75
1:2A:2551:C:OP2	60:2A:3822:HOH:O	2.03	0.75
34:2c:9:GLY:HA3	45:2n:49:HIS:HA	1.68	0.75
21:1Z:19:ARG:NH1	21:1Z:84:GLU:O	2.19	0.75
39:1h:14:ARG:NH1	39:1h:83:ILE:O	2.19	0.75
1:2A:323:G:HO2'	1:2A:1205:U:H3	1.34	0.75
4:2E:110:GLY:O	60:2R:301:HOH:O	2.04	0.75
6:2G:112:PRO:HG3	26:24:43:TYR:HE2	1.49	0.75
11:2P:89:ALA:O	11:2P:121:LYS:NZ	2.19	0.75
1:1A:219:G:O6	60:1A:4129:HOH:O	2.04	0.75
1:1A:1271:G:OP2	60:1A:4126:HOH:O	2.03	0.75
35:1d:153:ARG:O	35:1d:159:ARG:NH2	2.19	0.75
32:1a:116:A:OP1	60:1a:3306:HOH:O	2.04	0.75
1:2A:585:G:OP2	60:2A:3823:HOH:O	2.04	0.75
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.20	0.75
1:2A:1002:G:N7	60:2A:3938:HOH:O	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1505:G:OP1	60:2a:3205:HOH:O	2.03	0.75
35:2d:163:GLU:HA	35:2d:166:LYS:HD3	1.67	0.75
1:2A:1670:C:OP1	60:2A:3825:HOH:O	2.05	0.75
1:1A:2243:U:OP2	60:1A:4132:HOH:O	2.05	0.74
30:28:34:TRP:O	60:28:201:HOH:O	2.05	0.74
32:2a:1009:G:H1	32:2a:1020:U:H3	1.35	0.74
33:2b:101:MET:HA	33:2b:108:ILE:HG13	1.68	0.74
44:2m:82:MET:HE2	44:2m:92:HIS:HB3	1.68	0.74
1:1A:2746:U:OP2	60:1A:4134:HOH:O	2.05	0.74
32:1a:803:G:OP1	60:1a:3308:HOH:O	2.05	0.74
1:2A:399:G:OP2	60:2A:3824:HOH:O	2.04	0.74
1:2A:1216:G:OP1	60:2A:3829:HOH:O	2.05	0.74
5:1F:53:THR:HG22	5:1F:55:GLY:H	1.52	0.74
1:2A:1602:U:O4	60:2A:3828:HOH:O	2.05	0.74
1:1A:1024:G:OP2	60:1A:4130:HOH:O	2.04	0.74
1:2A:1065:U:H3	1:2A:1073:A:H61	1.33	0.74
32:2a:624:C:H2'	32:2a:625:G:H8	1.52	0.74
39:2h:25:ASP:N	39:2h:25:ASP:OD1	2.20	0.74
1:1A:187:G:OP2	60:1A:4133:HOH:O	2.05	0.74
26:14:40:HIS:HB3	26:14:43:TYR:HD2	1.52	0.74
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.23	0.74
39:1h:86:ILE:HG21	39:1h:133:LEU:HD13	1.69	0.74
40:1i:4:TYR:HB2	40:1i:19:LEU:HB2	1.70	0.74
1:2A:805:G:OP1	60:2A:3832:HOH:O	2.06	0.74
1:1A:2258:C:OP1	60:1A:4135:HOH:O	2.06	0.74
47:1p:20:VAL:HG23	47:1p:35:LYS:HA	1.70	0.74
1:2A:2267:A:H5"	1:2A:2268:A:H5'	1.70	0.74
32:2a:766:A:OP2	60:2a:3206:HOH:O	2.05	0.74
1:1A:1823:G:N3	60:1A:4231:HOH:O	2.20	0.73
23:21:76:ARG:NH1	23:21:97:LEU:O	2.21	0.73
1:2A:2589:A:OP1	60:2A:3827:HOH:O	2.05	0.73
1:2A:2685:G:O6	60:2A:3831:HOH:O	2.06	0.73
33:2b:178:ARG:HB3	39:2h:72:PRO:HA	1.69	0.73
1:1A:1631(A):A:OP1	60:1A:4127:HOH:O	2.04	0.73
32:1a:1069:C:OP2	60:1a:3307:HOH:O	2.05	0.73
6:1G:161:THR:HG22	6:1G:163:ALA:H	1.52	0.73
1:2A:572:A:OP2	17:2V:78:LYS:NZ	2.22	0.73
1:1A:2072:G:N2	60:1A:4248:HOH:O	2.22	0.73
32:1a:812:C:O2	60:1a:3309:HOH:O	2.06	0.73
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.70	0.73
17:2V:40:LEU:HB2	17:2V:46:VAL:HG13	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1310:G:H5'	44:2m:77:ASN:HD22	1.54	0.73
1:1A:1295:C:OP2	60:1A:4136:HOH:O	2.06	0.73
1:2A:1314:C:OP1	60:2A:3817:HOH:O	2.06	0.73
35:2d:13:ARG:HB2	35:2d:40:PRO:HD3	1.68	0.73
32:1a:664:G:H22	32:1a:741:G:H1	1.37	0.73
32:1a:951:G:OP1	60:1a:3310:HOH:O	2.06	0.73
1:2A:1288:U:OP1	60:2A:3836:HOH:O	2.07	0.73
39:1h:120:THR:H	39:1h:123:GLU:HB2	1.53	0.72
1:2A:2051:A:OP2	60:2A:3830:HOH:O	2.06	0.72
32:2a:1402:4OC:HM22	32:2a:1403:C:H5'	1.70	0.72
1:2A:1345:C:OP2	60:2A:3838:HOH:O	2.07	0.72
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.24	0.72
1:2A:2427:C:OP1	60:2A:3826:HOH:O	2.05	0.72
1:2A:2712(A):A:OP2	60:2A:3835:HOH:O	2.07	0.72
32:2a:768:A:OP2	60:2a:3208:HOH:O	2.08	0.72
1:1A:365:C:OP2	60:1A:4131:HOH:O	2.05	0.72
8:2I:85:GLU:HB3	8:2I:87:LYS:H	1.53	0.72
33:2b:87:ARG:NH2	33:2b:220:ASP:OD1	2.22	0.72
32:1a:394:G:O6	60:1a:3312:HOH:O	2.08	0.72
33:1b:231:GLU:HB3	33:1b:232:PRO:HD2	1.70	0.72
40:1i:6:GLY:HA3	40:1i:83:ARG:HB2	1.71	0.72
1:1A:85:G:O6	60:1A:4138:HOH:O	2.06	0.72
1:1A:2507:C:OP2	60:1A:4137:HOH:O	2.06	0.72
4:1E:110:GLY:O	60:1R:301:HOH:O	2.07	0.72
1:2A:958:U:OP2	12:2Q:14:ARG:NH1	2.22	0.72
1:2A:1199:U:OP1	60:2A:3833:HOH:O	2.06	0.72
40:2i:9:ARG:HG2	40:2i:14:VAL:HG12	1.71	0.72
1:2A:1155:A:H5"	16:2U:55:ARG:HD3	1.72	0.72
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.72	0.72
41:1j:54:PHE:HD2	41:1j:55:LYS:HG2	1.54	0.72
1:1A:1398:C:OP1	19:1X:53:LYS:NZ	2.23	0.72
15:1T:127:ALA:O	15:1T:129:ARG:N	2.22	0.72
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.70	0.72
17:1V:40:LEU:HB2	17:1V:46:VAL:HG13	1.70	0.72
1:2A:450:G:N7	60:2A:3962:HOH:O	2.22	0.72
1:1A:1818:U:OP1	60:1A:4139:HOH:O	2.07	0.71
32:1a:803:G:OP1	60:1a:3311:HOH:O	2.07	0.71
1:2A:1084:A:N6	1:2A:1086:A:N7	2.38	0.71
32:2a:572:A:OP1	60:2a:3207:HOH:O	2.07	0.71
32:1a:1409:C:H2'	32:1a:1410:G:H8	1.56	0.71
32:1a:1414:U:H3	32:1a:1486:G:H1	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:78:GLY:HA3	34:1c:83:ARG:H	1.54	0.71
39:1h:95:VAL:HG12	39:1h:99:GLU:HG3	1.72	0.71
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.70	0.71
1:1A:1973:G:OP1	60:1A:4142:HOH:O	2.08	0.71
47:1p:43:LYS:HG2	47:1p:48:TRP:CD2	2.24	0.71
1:2A:1297:C:OP2	60:2A:3843:HOH:O	2.09	0.71
1:2A:2448:A:OP1	60:2A:3814:HOH:O	2.07	0.71
32:1a:73:G:H1	32:1a:96:U:H3	1.39	0.71
32:2a:401:C:OP2	35:2d:73:ARG:NH2	2.22	0.71
1:2A:946:G:OP1	60:2A:3840:HOH:O	2.08	0.71
1:2A:1356:G:OP2	60:2A:3834:HOH:O	2.07	0.71
1:2A:2849:U:O4	15:2T:23:ARG:NH2	2.23	0.71
32:2a:1005:A:H5"	32:2a:1006:C:C5	2.25	0.71
34:2c:121:ALA:HB1	34:2c:189:ALA:HB2	1.71	0.71
40:2i:4:TYR:O	40:2i:19:LEU:N	2.22	0.71
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.07	0.71
26:14:16:CYS:SG	26:14:17:GLY:N	2.64	0.71
32:1a:1402:4OC:HM22	32:1a:1403:C:H5'	1.72	0.71
45:1n:23:ARG:HH12	45:1n:30:ALA:HB2	1.55	0.71
26:24:16:CYS:SG	26:24:17:GLY:N	2.64	0.71
32:2a:664:G:H22	32:2a:741:G:H1	1.37	0.71
1:1A:2384:G:O6	60:1A:4144:HOH:O	2.08	0.71
2:1B:58:A:OP2	60:1B:301:HOH:O	2.07	0.71
1:2A:2822:G:OP2	60:2A:3839:HOH:O	2.08	0.71
28:26:8:LYS:NZ	60:26:601:HOH:O	2.22	0.71
1:1A:2602:A:N7	60:1A:4283:HOH:O	2.24	0.71
19:1X:60:ARG:HH12	29:17:47:ARG:HH22	1.36	0.71
1:2A:1239:G:OP1	60:2A:3844:HOH:O	2.09	0.71
1:1A:855:G:N2	60:1A:4252:HOH:O	2.22	0.71
1:1A:2227:A:N7	60:1A:4277:HOH:O	2.24	0.71
1:2A:615:G:OP1	5:2F:40:GLN:NE2	2.24	0.71
13:2R:97:VAL:HG22	13:2R:114:VAL:HG12	1.72	0.71
1:1A:1267:U:OP1	60:1A:4143:HOH:O	2.08	0.71
5:1F:185:ASP:OD1	5:1F:188:ARG:NH1	2.24	0.71
22:10:10:THR:HG22	22:10:12:ASN:H	1.55	0.71
51:1t:36:LEU:HD13	51:1t:58:LYS:HG3	1.73	0.71
1:1A:1185:C:OP2	60:1A:4141:HOH:O	2.08	0.70
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.23	0.70
17:2V:98:GLU:OE2	17:2V:100:ARG:NH1	2.23	0.70
1:1A:1784:A:OP2	60:1A:4145:HOH:O	2.09	0.70
32:1a:1086:U:H3	32:1a:1099:G:H22	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.73	0.70
1:1A:1023:U:OP2	60:1A:4130:HOH:O	2.08	0.70
1:1A:1670:C:OP1	60:1A:4140:HOH:O	2.08	0.70
32:1a:975:A:H4'	32:1a:976:G:H5"	1.74	0.70
1:2A:154(A):C:H42	1:2A:171:G:H1	1.39	0.70
40:2i:3:GLN:HG2	40:2i:20:ARG:HE	1.55	0.70
17:1V:72:VAL:HG13	17:1V:85:LYS:HB3	1.73	0.70
32:1a:966:M2G:H1'	53:1y:53:THR:HG21	1.73	0.70
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.25	0.70
1:1A:671:C:N4	60:1A:4292:HOH:O	2.24	0.70
57:1B:231:ARG:N	60:1B:311:HOH:O	2.25	0.70
1:2A:731:C:OP1	60:2A:3848:HOH:O	2.10	0.70
11:2P:54:GLY:O	60:2P:301:HOH:O	2.09	0.70
30:28:33:ASN:HA	30:28:36:LYS:HD2	1.72	0.70
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.74	0.70
36:2e:88:LYS:HB3	36:2e:123:LEU:HB2	1.72	0.70
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.26	0.70
32:1a:673:G:H2'	32:1a:674:G:C8	2.27	0.70
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.25	0.70
1:2A:1371:G:O6	60:2A:3841:HOH:O	2.08	0.70
23:21:21:ARG:NH2	60:21:202:HOH:O	2.22	0.70
1:1A:139(A):G:N3	60:1A:4263:HOH:O	2.22	0.70
1:1A:1509(A):A:H2'	1:1A:1509(B):A:O4'	1.92	0.70
1:1A:1793:C:OP1	60:1A:4147:HOH:O	2.09	0.70
1:1A:2610:C:O2	60:1A:4148:HOH:O	2.09	0.70
1:2A:2445:G:OP1	5:2F:74:ARG:NH2	2.24	0.70
32:2a:617:G:OP2	60:2a:3213:HOH:O	2.10	0.70
32:2a:1500:A:OP2	60:2a:3209:HOH:O	2.09	0.70
1:1A:2199:A:OP2	60:1A:4150:HOH:O	2.10	0.70
2:1B:48:A:OP1	60:1B:302:HOH:O	2.10	0.70
32:1a:393:A:OP1	60:1a:3314:HOH:O	2.09	0.70
56:1a:3271:MPD:O2	60:1a:3313:HOH:O	2.09	0.70
1:2A:1199:U:O2'	60:2A:3851:HOH:O	2.10	0.70
21:2Z:144:LEU:HD21	21:2Z:150:LEU:HD13	1.74	0.70
47:2p:13:HIS:O	47:2p:42:ARG:NH1	2.24	0.70
20:1Y:23:ARG:NH2	60:1Y:302:HOH:O	2.25	0.69
1:2A:675:A:OP2	60:2A:3846:HOH:O	2.09	0.69
1:2A:864:G:H1'	1:2A:914:C:H42	1.57	0.69
32:1a:263:A:P	51:1t:79:ARG:HH12	2.15	0.69
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.74	0.69
32:2a:376:G:N7	60:2a:3242:HOH:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2499:C:OP1	60:1A:4146:HOH:O	2.09	0.69
40:2i:9:ARG:HB2	40:2i:104:ARG:HE	1.57	0.69
29:27:29:LYS:NZ	60:27:201:HOH:O	2.24	0.69
32:2a:547:A:OP1	60:2a:3211:HOH:O	2.10	0.69
32:2a:1503:A:OP1	32:2a:1531:A:O2'	2.10	0.69
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.24	0.69
32:1a:1030(C):G:H2'	32:1a:1030(D):A:H8	1.57	0.69
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.57	0.69
32:2a:1345:U:OP1	60:2a:3212:HOH:O	2.10	0.69
1:1A:65:C:OP2	60:1A:4151:HOH:O	2.10	0.69
1:2A:791:C:OP2	60:2A:3847:HOH:O	2.09	0.69
1:2A:2596:U:OP2	60:2A:3845:HOH:O	2.09	0.69
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.73	0.69
32:2a:437:U:H5"	35:2d:155:LEU:HD11	1.73	0.69
32:2a:1199:U:OP1	60:2a:3210:HOH:O	2.09	0.69
39:1h:29:SER:HB3	39:1h:32:LYS:HG3	1.74	0.69
1:2A:2587:A:OP2	60:2A:3854:HOH:O	2.11	0.69
1:1A:81:G:OP2	60:1A:4159:HOH:O	2.11	0.69
1:1A:578:A:OP2	60:1A:4158:HOH:O	2.11	0.69
32:1a:1158:C:H5	32:1a:1181:G:H1	1.41	0.69
1:2A:511:U:OP2	60:2A:3856:HOH:O	2.11	0.69
1:2A:827:U:OP1	60:2A:3842:HOH:O	2.09	0.69
1:2A:1084:A:H3'	1:2A:1085:A:H4'	1.74	0.69
1:2A:1170:G:H1	1:2A:1179:C:H42	1.40	0.69
1:2A:2104:G:O6	1:2A:2185:C:N3	2.26	0.69
1:2A:2362:G:N3	60:2A:3996:HOH:O	2.25	0.69
21:2Z:85:HIS:ND1	60:2Z:301:HOH:O	2.26	0.69
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.26	0.69
32:2a:7:G:O2'	36:2e:120:THR:O	2.11	0.69
34:2c:70:VAL:HG22	34:2c:72:LYS:H	1.57	0.69
35:2d:162:LEU:HD13	35:2d:181:MET:HG2	1.75	0.69
49:2r:25:THR:O	49:2r:25:THR:OG1	2.11	0.69
32:1a:1291:G:OP1	38:1g:37:ASN:ND2	2.25	0.69
1:2A:1153:C:OP2	60:2A:3859:HOH:O	2.11	0.69
1:2A:1769:G:N7	60:2A:4006:HOH:O	2.26	0.69
10:2O:35:VAL:HG23	10:2O:65:THR:HG23	1.74	0.69
35:2d:140:VAL:HG11	35:2d:146:ILE:HD11	1.75	0.69
1:1A:2319:G:N2	14:1S:3:ARG:HD2	2.08	0.69
1:2A:570:G:O6	60:2A:3814:HOH:O	2.09	0.69
1:2A:793:A:OP1	60:2A:3857:HOH:O	2.11	0.69
1:2A:945:A:OP2	60:2A:3850:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1603:A:OP1	60:2A:3849:HOH:O	2.10	0.69
1:2A:2048:G:OP1	60:2A:3855:HOH:O	2.11	0.69
32:2a:40:C:H42	32:2a:402:G:H1	1.39	0.69
32:2a:677:U:H3	32:2a:713:G:H22	1.41	0.69
13:2R:29:LEU:HB3	13:2R:75:LEU:HD21	1.75	0.68
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.25	0.68
21:1Z:144:LEU:HD21	21:1Z:150:LEU:HD13	1.74	0.68
22:10:11:ARG:O	22:10:14:ARG:NH2	2.17	0.68
33:1b:7:VAL:O	33:1b:217:ARG:NH2	2.25	0.68
1:2A:387:U:OP1	60:2A:3852:HOH:O	2.10	0.68
1:1A:2427:C:OP1	60:1A:4156:HOH:O	2.11	0.68
32:1a:1021:G:C2	32:1a:1022:G:H1'	2.29	0.68
32:1a:1189:C:O2	60:1a:3315:HOH:O	2.11	0.68
1:2A:326:G:N7	60:2A:4009:HOH:O	2.26	0.68
1:2A:1214:A:OP2	60:2A:3862:HOH:O	2.11	0.68
6:2G:114:ILE:HA	6:2G:140:ILE:HD12	1.75	0.68
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.24	0.68
35:2d:61:LYS:NZ	35:2d:72:GLU:OE1	2.26	0.68
1:1A:220:G:O6	60:1A:4149:HOH:O	2.10	0.68
1:1A:2602:A:H1'	1:1A:2603:G:H5"	1.75	0.68
1:2A:1970:A:OP1	60:2A:3860:HOH:O	2.11	0.68
4:2E:77:ILE:HD13	4:2E:195:LEU:HD13	1.74	0.68
1:1A:614(C):A:N7	60:1A:4318:HOH:O	2.27	0.68
35:1d:25:ARG:NH1	35:1d:30:LYS:O	2.26	0.68
47:1p:45:THR:HG23	47:1p:47:ASP:H	1.58	0.68
1:2A:1024:G:OP2	60:2A:3819:HOH:O	2.10	0.68
19:2X:35:THR:HG22	19:2X:37:THR:H	1.57	0.68
1:1A:1452:A:OP2	60:1A:4163:HOH:O	2.11	0.68
20:1Y:15:VAL:HG21	20:1Y:42:VAL:HG11	1.75	0.68
1:2A:1652:A:OP2	60:2A:3853:HOH:O	2.11	0.68
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.29	0.68
1:2A:2685:G:N7	60:2A:4019:HOH:O	2.26	0.68
5:2F:20:LEU:HD23	5:2F:21:ALA:H	1.59	0.68
32:2a:1226:C:N4	44:2m:104:ARG:HD2	2.08	0.68
1:1A:2303:G:O2'	6:1G:132:ASN:ND2	2.26	0.68
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.26	0.68
1:2A:2014:A:H4'	18:2W:92:ARG:HH22	1.57	0.68
1:2A:2430:A:OP2	60:2A:3842:HOH:O	2.12	0.68
5:2F:116:ASP:OD1	5:2F:119:ARG:NH2	2.26	0.68
1:2A:192:C:N3	60:2A:4018:HOH:O	2.26	0.68
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:162:LEU:HD13	35:1d:181:MET:HE2	1.75	0.68
1:2A:2218:U:O2	23:21:52:ARG:NH1	2.27	0.68
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.26	0.68
1:1A:1030:G:OP1	60:1A:4152:HOH:O	2.10	0.68
1:2A:517:C:OP1	27:25:16:ARG:NH2	2.26	0.68
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.74	0.68
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.76	0.67
1:1A:1856:G:OP2	60:1A:4162:HOH:O	2.11	0.67
1:2A:1631(A):A:N6	60:2A:3872:HOH:O	2.18	0.67
1:1A:1224:C:O2	60:1A:4166:HOH:O	2.12	0.67
10:1O:73:ASP:O	60:1O:301:HOH:O	2.12	0.67
35:1d:89:THR:OG1	60:1d:401:HOH:O	2.11	0.67
1:2A:1920:OMC:HM22	1:2A:1921:G:H5'	1.75	0.67
32:2a:1457:G:OP1	51:2t:39:LYS:NZ	2.27	0.67
1:1A:733:G:OP1	60:1A:4157:HOH:O	2.11	0.67
1:1A:1138:G:OP1	60:1A:4161:HOH:O	2.11	0.67
1:1A:1143:A:OP2	60:1A:4168:HOH:O	2.12	0.67
1:1A:1669:A:OP2	60:1A:4154:HOH:O	2.11	0.67
8:1I:38:LEU:HB3	8:1I:40:THR:HG22	1.76	0.67
21:1Z:69:THR:HG22	21:1Z:90:VAL:HA	1.76	0.67
1:2A:527:C:OP1	60:2A:3864:HOH:O	2.12	0.67
25:23:39:ASP:OD1	25:23:44:ARG:NH1	2.28	0.67
32:2a:1295:G:O2'	44:2m:14:ARG:NH1	2.28	0.67
13:1R:96:ARG:NH2	13:1R:118:GLU:OE2	2.27	0.67
32:1a:1505:G:OP1	60:1a:3304:HOH:O	2.12	0.67
1:1A:1670:C:OP2	60:1A:4154:HOH:O	2.12	0.67
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.27	0.67
32:1a:608:A:OP2	60:1a:3317:HOH:O	2.13	0.67
32:1a:1231:G:N3	60:1a:3328:HOH:O	2.28	0.67
1:1A:1677:A:OP1	60:1A:4155:HOH:O	2.11	0.67
1:1A:2721:A:N3	60:1A:4339:HOH:O	2.28	0.67
1:2A:1528:A:OP2	60:2A:3858:HOH:O	2.11	0.67
21:2Z:87:ASP:OD1	60:2Z:301:HOH:O	2.13	0.67
32:1a:945:G:OP2	60:1a:3318:HOH:O	2.13	0.67
36:1e:100:VAL:O	36:1e:107:ARG:NH2	2.28	0.67
1:2A:818:G:OP2	60:2A:3865:HOH:O	2.12	0.67
1:2A:1026:U:OP1	60:2A:3819:HOH:O	2.13	0.67
22:20:36:ILE:O	60:20:201:HOH:O	2.13	0.67
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.27	0.67
15:2T:30:VAL:HG22	15:2T:86:ILE:HG12	1.77	0.67
17:2V:35:LEU:HB2	17:2V:57:VAL:HG23	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:23:6:VAL:HG13	25:23:56:VAL:HG22	1.77	0.67
32:2a:656:C:O2'	46:2o:28:GLN:NE2	2.27	0.67
1:1A:1143:A:OP1	9:1N:25:ARG:NH2	2.28	0.67
10:1O:48:PRO:HB3	32:1a:1422:G:H5"	1.75	0.67
32:1a:1374:A:OP1	38:1g:36:LYS:NZ	2.28	0.67
1:2A:1090:U:H2'	1:2A:1091:G:C8	2.28	0.67
1:2A:1890:A:N7	60:2A:4038:HOH:O	2.28	0.67
15:2T:29:ARG:HB3	15:2T:87:ASP:HB2	1.77	0.67
43:2l:86:ARG:HH11	43:2l:87:GLY:HA3	1.60	0.67
1:1A:251:A:OP2	60:1A:4173:HOH:O	2.13	0.66
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.75	0.66
21:1Z:144:LEU:HD11	21:1Z:150:LEU:HD22	1.78	0.66
36:1e:37:ARG:HH12	36:1e:112:LEU:HD23	1.60	0.66
1:2A:1932:A:OP2	60:2A:3863:HOH:O	2.12	0.66
1:1A:1963:U:OP1	60:1A:4164:HOH:O	2.11	0.66
2:1B:55:U:OP2	60:1B:304:HOH:O	2.13	0.66
1:2A:393:C:OP2	60:2A:3866:HOH:O	2.13	0.66
1:2A:731:C:OP2	60:2A:3861:HOH:O	2.11	0.66
1:2A:770:G:OP2	60:2A:3868:HOH:O	2.13	0.66
1:2A:804:A:OP1	60:2A:3874:HOH:O	2.14	0.66
35:2d:165:MET:SD	35:2d:168:ARG:NH1	2.69	0.66
1:2A:2130:U:H2'	1:2A:2158:A:H61	1.61	0.66
1:1A:2058:A:OP1	60:1A:4169:HOH:O	2.12	0.66
1:2A:1031:G:H5"	31:29:8:LYS:HE3	1.76	0.66
11:2P:32:THR:O	60:2P:302:HOH:O	2.14	0.66
32:2a:1187:G:H5'	40:2i:113:LYS:HE2	1.77	0.66
1:1A:597:U:O4	60:1A:4153:HOH:O	2.11	0.66
3:2D:75:ILE:HG21	3:2D:99:ASP:HB2	1.75	0.66
7:2H:150:ALA:HA	7:2H:153:LYS:HG3	1.77	0.66
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.29	0.66
1:1A:1913:A:N6	32:1a:1409:C:O2	2.28	0.66
24:12:22:GLU:OE2	24:12:68:ARG:NH2	2.29	0.66
34:1c:52:LEU:HD13	34:1c:68:VAL:HG13	1.75	0.66
1:2A:520:G:OP2	60:2A:3871:HOH:O	2.13	0.66
1:2A:1682:G:O3'	60:2A:3872:HOH:O	2.13	0.66
4:2E:183:LEU:HD21	15:2T:10:VAL:HG11	1.77	0.66
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.29	0.66
32:2a:1110:A:OP2	60:2a:3214:HOH:O	2.13	0.66
1:1A:975:C:OP1	60:1A:4171:HOH:O	2.13	0.66
1:1A:2543:G:OP2	60:1A:4175:HOH:O	2.14	0.66
2:1B:91:C:OP2	60:1B:303:HOH:O	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:152:ALA:HA	21:1Z:155:LEU:HD13	1.77	0.66
1:2A:2292:C:OP1	14:2S:17:ARG:NH2	2.27	0.66
35:1d:18:LYS:NZ	35:1d:31:CYS:SG	2.68	0.66
45:1n:48:ALA:HB2	45:1n:53:LEU:HD12	1.77	0.66
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.31	0.66
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.29	0.66
44:2m:15:VAL:HG11	44:2m:48:LEU:HD21	1.77	0.66
1:2A:1342:A:OP2	60:2A:3828:HOH:O	2.13	0.66
35:2d:158:ILE:HG22	35:2d:162:LEU:HD12	1.77	0.66
40:1i:17:VAL:HG21	40:1i:81:ILE:HG22	1.76	0.66
43:1l:57:LYS:HE2	43:1l:67:THR:HG22	1.78	0.66
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.77	0.66
1:2A:1273:U:OP2	60:2A:3876:HOH:O	2.14	0.66
1:2A:2431:U:OP1	60:2A:3882:HOH:O	2.14	0.66
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.60	0.66
51:2t:57:ARG:HH22	51:2t:100:ILE:HD12	1.60	0.66
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.28	0.65
32:1a:1057:G:OP2	60:1a:3319:HOH:O	2.14	0.65
43:1l:89:ARG:HB2	43:1l:97:ARG:HA	1.78	0.65
1:2A:198:C:OP2	60:2A:3808:HOH:O	2.15	0.65
22:20:50:ASN:ND2	22:20:81:VAL:O	2.29	0.65
18:1W:18:ARG:NH1	18:1W:76:VAL:O	2.30	0.65
6:2G:66:GLN:HE21	6:2G:92:VAL:HG23	1.60	0.65
32:2a:890:G:O2'	32:2a:906:G:O6	2.14	0.65
32:2a:1256:A:N6	32:2a:1278:U:H1'	2.05	0.65
1:2A:1299:G:O6	60:2A:3867:HOH:O	2.13	0.65
1:2A:1972:A:OP1	60:2A:3870:HOH:O	2.13	0.65
1:2A:2602:A:H1'	1:2A:2603:G:H5"	1.78	0.65
38:2g:78:ARG:HE	38:2g:80:VAL:HG21	1.60	0.65
1:1A:1284:A:N3	60:1A:4342:HOH:O	2.28	0.65
1:1A:2377:A:N3	60:1A:4357:HOH:O	2.29	0.65
2:1B:82:G:N7	60:1B:315:HOH:O	2.30	0.65
18:1W:65:LEU:HB2	18:1W:68:ARG:HD2	1.78	0.65
21:1Z:52:SER:OG	21:1Z:53:ILE:N	2.29	0.65
32:1a:309:G:O2'	32:1a:607:A:N1	2.30	0.65
32:1a:588:G:OP2	60:1a:3321:HOH:O	2.14	0.65
32:1a:780:A:OP2	60:1a:3325:HOH:O	2.15	0.65
32:1a:921:U:O2	36:1e:19:MET:HB2	1.96	0.65
1:1A:1756:G:O6	60:1A:4170:HOH:O	2.12	0.65
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.76	0.65
32:1a:600:C:H2'	32:1a:601:C:C6	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1500:A:OP2	60:1a:3324:HOH:O	2.14	0.65
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.79	0.65
32:2a:258:G:H1	32:2a:268:C:H42	1.43	0.65
41:2j:6:ILE:HB	41:2j:72:VAL:HG23	1.78	0.65
1:1A:312:G:OP2	60:1A:4178:HOH:O	2.14	0.65
1:1A:1175:U:O2'	1:1A:1176:G:O5'	2.14	0.65
4:1E:127:ASP:OD2	60:1E:402:HOH:O	2.14	0.65
6:1G:164:GLU:OE1	60:1G:301:HOH:O	2.13	0.65
10:1O:68:GLU:OE1	60:1O:302:HOH:O	2.14	0.65
32:1a:1409:C:H2'	32:1a:1410:G:C8	2.31	0.65
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.30	0.65
32:2a:49:U:OP2	60:2a:3215:HOH:O	2.14	0.65
1:1A:2516:G:OP2	60:1A:4176:HOH:O	2.14	0.65
1:1A:2550:G:OP1	60:1A:4154:HOH:O	2.14	0.65
2:1B:81:G:N7	57:1B:231:ARG:NH2	2.44	0.65
38:1g:111:ARG:NH1	38:1g:113:GLU:OE2	2.26	0.65
45:1n:4:LYS:HA	45:1n:7:ILE:HG12	1.78	0.65
1:2A:468:G:O2'	5:2F:62:ARG:NH2	2.30	0.65
1:2A:2089:U:O4	60:2A:3873:HOH:O	2.13	0.65
32:2a:48:C:OP2	60:2a:3215:HOH:O	2.14	0.65
32:2a:1073:U:H2'	32:2a:1074:G:H8	1.61	0.65
1:1A:249:C:O2	30:18:12:LYS:NZ	2.28	0.65
1:1A:2499:C:OP2	60:1A:4182:HOH:O	2.14	0.65
32:1a:971:G:OP2	60:1a:3328:HOH:O	2.15	0.65
3:2D:158:ALA:O	3:2D:161:THR:OG1	2.15	0.65
40:2i:28:VAL:HG22	40:2i:63:ILE:HB	1.78	0.65
41:2j:8:LEU:HB2	41:2j:70:ARG:HB2	1.78	0.65
51:2t:33:ILE:HD13	51:2t:62:LEU:HB3	1.78	0.65
1:1A:9:U:H3	1:1A:2629:A:H2	1.45	0.65
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.79	0.65
44:1m:58:GLU:O	44:1m:62:ASN:ND2	2.24	0.65
1:2A:62:C:OP1	60:2A:3880:HOH:O	2.14	0.65
1:2A:1669:A:OP2	60:2A:3869:HOH:O	2.13	0.65
42:2k:67:ASP:OD2	42:2k:71:LYS:NZ	2.21	0.65
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.79	0.65
30:18:41:ILE:O	60:18:201:HOH:O	2.15	0.65
2:2B:15:A:OP1	60:2B:304:HOH:O	2.14	0.65
2:2B:61:G:O6	60:2B:303:HOH:O	2.09	0.65
1:1A:668:G:H5'	1:1A:669:G:OP2	1.97	0.64
32:1a:584:G:H5'	48:1q:91:ARG:HH22	1.62	0.64
32:1a:1031:G:H2'	32:1a:1032:G:H8	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:83:SER:O	60:1d:402:HOH:O	2.13	0.64
1:2A:597:U:H2'	1:2A:598:G:C8	2.31	0.64
1:2A:1971:A:OP1	60:2A:3875:HOH:O	2.14	0.64
32:2a:1126:U:O4'	32:2a:1281:U:H1'	1.98	0.64
1:1A:1309:G:OP2	60:1A:4188:HOH:O	2.15	0.64
1:1A:1783:A:N7	60:1A:4369:HOH:O	2.30	0.64
1:1A:1954:G:N2	60:1A:4350:HOH:O	2.29	0.64
1:1A:2126:A:H4'	1:1A:2127:G:O5'	1.96	0.64
1:1A:2507:C:OP1	60:1A:4185:HOH:O	2.15	0.64
4:1E:35:GLN:HB3	4:1E:48:GLN:HE21	1.62	0.64
32:1a:200:G:H1	32:1a:217:C:H42	1.45	0.64
32:1a:1067:A:O3'	60:1a:3326:HOH:O	2.15	0.64
39:1h:49:GLU:HG2	39:1h:62:TYR:HE2	1.62	0.64
1:2A:2597:G:OP1	60:2A:3878:HOH:O	2.14	0.64
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.79	0.64
34:2c:182:ILE:HG12	34:2c:203:PHE:HD1	1.62	0.64
1:1A:740:U:OP2	60:1A:4145:HOH:O	2.14	0.64
1:1A:1865:G:OP1	60:1A:4187:HOH:O	2.15	0.64
1:1A:2847:U:OP1	15:1T:98:LYS:NZ	2.30	0.64
32:1a:535:A:OP1	60:1a:3323:HOH:O	2.14	0.64
1:2A:1993:U:OP2	60:2A:3885:HOH:O	2.15	0.64
15:2T:109:GLU:HG2	15:2T:112:ARG:HH22	1.60	0.64
33:2b:78:GLN:HE22	33:2b:95:GLN:HA	1.62	0.64
33:2b:212:GLN:NE2	33:2b:235:SER:OG	2.30	0.64
6:1G:104:GLU:O	6:1G:108:ASN:ND2	2.27	0.64
35:1d:163:GLU:O	35:1d:165:MET:N	2.31	0.64
1:2A:1352:U:OP1	60:2A:3877:HOH:O	2.14	0.64
1:2A:1754:C:OP1	15:2T:96:ARG:NH1	2.30	0.64
1:2A:1793:C:OP1	60:2A:3883:HOH:O	2.15	0.64
32:2a:1259:C:C4	32:2a:1260:C:H1'	2.32	0.64
36:2e:144:THR:H	36:2e:147:ASP:HB2	1.62	0.64
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.79	0.64
32:1a:976:G:H5'	32:1a:1358:U:O2'	1.98	0.64
1:2A:197:A:OP1	60:2A:3808:HOH:O	2.14	0.64
1:2A:971:C:OP2	60:2A:3889:HOH:O	2.15	0.64
1:2A:979:G:N7	60:2A:4061:HOH:O	2.30	0.64
1:2A:1012:U:H5	9:2N:28:THR:HG21	1.62	0.64
1:2A:1655:A:OP1	60:2A:3886:HOH:O	2.15	0.64
32:2a:673:G:H2'	32:2a:674:G:C8	2.32	0.64
1:1A:488:G:OP1	60:1A:4191:HOH:O	2.15	0.64
1:1A:2605:PSU:OP1	60:1A:4180:HOH:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:51:ARG:NH1	60:1T:301:HOH:O	2.29	0.64
33:1b:163:PHE:HD1	33:1b:185:ILE:HG13	1.62	0.64
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.45	0.64
36:1e:147:ASP:OD1	36:1e:147:ASP:N	2.31	0.64
32:2a:45:U:H2'	32:2a:46:G:C8	2.33	0.64
32:1a:1202:G:O4'	45:1n:29:ARG:NH1	2.30	0.64
3:2D:69:ARG:NH2	3:2D:128:GLY:O	2.28	0.64
15:2T:54:ARG:HA	15:2T:59:THR:HG23	1.80	0.64
32:2a:1258:G:H2'	32:2a:1259:C:H6	1.62	0.64
12:1Q:136:ALA:HB1	21:1Z:52:SER:HB2	1.80	0.64
21:1Z:145:GLU:O	21:1Z:148:ASP:N	2.27	0.64
32:1a:107:G:N7	51:1t:15:ARG:NH2	2.45	0.64
1:1A:2707:G:OP1	60:1A:4189:HOH:O	2.15	0.64
60:1A:4222:HOH:O	11:1P:2:LYS:NZ	2.30	0.64
32:2a:1376:U:OP1	38:2g:98:SER:OG	2.13	0.64
53:2y:3:MET:HE2	53:2y:37:PRO:HB2	1.78	0.64
32:1a:600:C:H2'	32:1a:601:C:H6	1.63	0.64
1:2A:749:C:OP2	60:2A:3879:HOH:O	2.14	0.64
1:2A:2572:A:OP1	1:2A:2574:G:O2'	2.15	0.64
32:2a:952:U:H2'	32:2a:953:G:H8	1.63	0.64
2:1B:8:U:O3'	14:1S:25:ARG:NH2	2.31	0.63
32:1a:547:A:OP1	60:1a:3327:HOH:O	2.15	0.63
33:1b:70:PHE:HD1	33:1b:163:PHE:HB3	1.64	0.63
1:2A:1075:C:H2'	1:2A:1076:C:H5'	1.79	0.63
32:2a:1008:C:H2'	32:2a:1009:G:C8	2.33	0.63
38:2g:22:LEU:HD23	38:2g:63:LYS:HG2	1.79	0.63
1:1A:1264:G:OP1	27:15:19:ARG:NH2	2.20	0.63
39:1h:83:ILE:HB	39:1h:137:VAL:HG13	1.80	0.63
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.79	0.63
32:1a:1456:G:N1	51:1t:51:GLU:OE2	2.29	0.63
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.62	0.63
1:2A:39:C:O2	5:2F:46:ARG:NH2	2.31	0.63
32:2a:1314:C:N4	50:2s:2:PRO:O	2.32	0.63
34:2c:9:GLY:HA2	34:2c:12:LEU:HG	1.80	0.63
38:2g:132:GLY:O	38:2g:136:LYS:HG2	1.98	0.63
47:2p:17:TYR:HE2	47:2p:41:PRO:HG3	1.61	0.63
1:1A:792:G:OP2	60:1A:4192:HOH:O	2.16	0.63
1:2A:1890:A:OP2	60:2A:3881:HOH:O	2.14	0.63
1:2A:2072:G:N2	60:2A:4075:HOH:O	2.31	0.63
1:2A:2112:G:H2'	1:2A:2113:U:C6	2.34	0.63
5:2F:33:LEU:HD22	5:2F:112:MET:HE3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:134:A:N1	47:2p:25:ARG:NH2	2.45	0.63
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.33	0.63
15:1T:19:LEU:HD12	15:1T:78:LEU:HD23	1.80	0.63
32:1a:96:U:H2'	32:1a:97:G:H8	1.63	0.63
6:2G:12:TYR:HA	6:2G:16:ARG:HG3	1.80	0.63
17:2V:24:LYS:HG3	17:2V:64:HIS:HD2	1.64	0.63
18:2W:53:SER:OG	60:2W:301:HOH:O	2.16	0.63
26:24:44:THR:O	26:24:46:GLN:N	2.31	0.63
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.30	0.63
1:1A:346:A:OP1	60:1A:4190:HOH:O	2.15	0.63
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.81	0.63
1:1A:1815:A:OP2	3:1D:54:ARG:NH2	2.32	0.63
20:1Y:92:ASN:N	20:1Y:93:GLY:HA2	2.14	0.63
35:1d:122:ARG:NH1	35:1d:134:ASP:OD2	2.32	0.63
32:2a:999:C:H42	32:2a:1042:G:H1	1.46	0.63
32:1a:881:G:P	43:1l:12:ARG:HH22	2.22	0.63
1:2A:652(T):C:H2'	1:2A:652(U):G:C8	2.34	0.63
3:2D:61:LEU:O	3:2D:63:ARG:NH1	2.32	0.63
32:2a:56:U:H2'	32:2a:57:G:C8	2.34	0.63
36:2e:12:LEU:HD21	36:2e:14:ARG:HG2	1.80	0.63
43:2l:84:LEU:HB3	43:2l:104:VAL:HG11	1.81	0.63
1:1A:153:C:OP2	23:11:92:LYS:NZ	2.29	0.63
22:10:27:GLU:HG3	22:10:68:GLU:HA	1.80	0.63
1:2A:2511:U:OP1	60:2A:3892:HOH:O	2.15	0.63
26:24:59:PHE:HA	26:24:60:GLN:C	2.23	0.63
44:2m:80:ARG:NH2	50:2s:65:ASN:O	2.31	0.63
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.17	0.63
5:2F:18:ARG:NH2	5:2F:127:GLU:OE1	2.32	0.63
6:2G:46:ALA:HB1	6:2G:51:ARG:HA	1.81	0.63
40:2i:13:ALA:HB2	40:2i:68:GLY:HA3	1.79	0.63
32:1a:401:C:OP2	35:1d:73:ARG:NH2	2.32	0.62
32:1a:971:G:N2	32:1a:1363(A):A:OP2	2.29	0.62
32:2a:419:C:OP1	32:2a:513:C:O2'	2.16	0.62
32:2a:1134:G:C2	32:2a:1135:U:H1'	2.34	0.62
1:2A:1091:G:N2	1:2A:1100:C:O2	2.32	0.62
32:1a:1240:U:OP2	38:1g:116:ALA:N	2.32	0.62
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.31	0.62
14:2S:48:LEU:HD23	14:2S:82:ILE:HD11	1.81	0.62
17:1V:64:HIS:HD1	17:1V:92:THR:HG1	1.47	0.62
32:1a:1103:C:OP1	33:1b:96:ARG:NH2	2.32	0.62
32:2a:624:C:H2'	32:2a:625:G:C8	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1Y:92:ASN:HB2	20:1Y:94:LYS:N	2.08	0.62
37:1f:4:TYR:HD1	37:1f:92:LYS:HA	1.63	0.62
1:2A:1550:C:OP1	1:2A:1720:U:O2'	2.18	0.62
44:2m:91:ARG:HB2	44:2m:98:VAL:HG13	1.82	0.62
14:1S:15:ARG:O	14:1S:19:LYS:HG2	2.00	0.62
32:1a:692:U:OP1	42:1k:124:LYS:NZ	2.25	0.62
32:1a:742:G:OP2	46:1o:35:ARG:NH2	2.29	0.62
31:29:29:ASN:HD22	31:29:32:HIS:CE1	2.18	0.62
32:2a:343:U:H2'	32:2a:345:C:H5	1.63	0.62
25:13:37:LEU:HB3	25:13:43:ILE:HD13	1.81	0.62
42:1k:29:ILE:HG23	42:1k:44:SER:HB3	1.82	0.62
35:2d:10:ARG:HA	35:2d:13:ARG:HG3	1.81	0.62
35:2d:62:GLN:OE1	35:2d:65:ARG:NH1	2.33	0.62
9:1N:12:ARG:NH1	9:1N:50:ASP:OD2	2.33	0.62
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.46	0.62
25:13:3:ARG:NH1	25:13:60:GLU:OE2	2.30	0.62
15:2T:27:THR:HB	15:2T:89:VAL:HG22	1.82	0.62
21:2Z:152:ALA:HB1	21:2Z:163:LEU:HD21	1.82	0.62
1:1A:592:G:O6	60:1A:4160:HOH:O	2.11	0.62
1:1A:2165:G:H2'	1:1A:2166:G:C8	2.35	0.62
18:1W:71:VAL:HA	18:1W:107:LEU:HD12	1.82	0.62
34:1c:150:LYS:HG3	34:1c:169:ALA:HB2	1.81	0.62
38:1g:50:ILE:HD11	38:1g:58:PRO:HA	1.82	0.62
44:1m:2:ALA:HA	44:1m:8:GLU:HB2	1.81	0.62
1:2A:1493:C:N4	1:2A:2206:G:O2'	2.33	0.62
5:2F:132:VAL:HG21	5:2F:163:VAL:HG22	1.82	0.62
32:2a:64:G:H4'	32:2a:65:U:H3'	1.81	0.62
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.82	0.62
34:1c:35:GLU:OE2	34:1c:59:ARG:NH2	2.28	0.62
41:1j:38:ILE:HD11	41:1j:71:LEU:HB3	1.81	0.62
42:1k:34:ASP:OD1	42:1k:38:ASN:N	2.26	0.62
1:2A:2112:G:H2'	1:2A:2113:U:H6	1.65	0.62
37:1f:4:TYR:HD2	37:1f:67:MET:HE3	1.65	0.61
45:1n:47:LEU:HD23	45:1n:50:LYS:HD3	1.82	0.61
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.47	0.61
28:16:6:ARG:NE	28:16:24:GLU:OE2	2.32	0.61
32:1a:376:G:H5"	47:1p:5:ARG:HD2	1.81	0.61
42:1k:21:ILE:HG12	42:1k:30:VAL:HG22	1.82	0.61
1:2A:1782:C:OP1	60:2A:3894:HOH:O	2.16	0.61
7:2H:86:GLU:OE2	7:2H:132:ARG:NH2	2.33	0.61
23:21:3:LYS:HB2	23:21:61:ARG:HH12	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:811:C:O2'	32:2a:901:A:N1	2.33	0.61
32:2a:1132:C:H2'	32:2a:1133:G:H8	1.65	0.61
38:2g:108:ALA:HA	38:2g:111:ARG:HD2	1.81	0.61
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.35	0.61
48:1q:48:GLU:HB2	48:1q:50:LYS:HG2	1.81	0.61
32:2a:1030(C):G:N7	32:2a:1031:G:N2	2.48	0.61
39:2h:41:ARG:NH2	39:2h:123:GLU:OE2	2.33	0.61
41:2j:50:ILE:HD11	41:2j:57:LYS:HD2	1.83	0.61
42:2k:33:THR:OG1	42:2k:34:ASP:N	2.31	0.61
1:1A:858:U:OP1	60:1A:4197:HOH:O	2.16	0.61
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.65	0.61
12:1Q:57:HIS:CD2	12:1Q:117:ALA:HB2	2.35	0.61
32:1a:342:C:O2'	60:1a:3330:HOH:O	2.16	0.61
32:2a:1129:C:H2'	32:2a:1139:G:N7	2.16	0.61
47:2p:5:ARG:HH21	47:2p:28:ARG:HA	1.64	0.61
47:2p:42:ARG:HB3	47:2p:44:THR:HG23	1.82	0.61
50:2s:19:VAL:O	50:2s:23:ASN:ND2	2.33	0.61
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.64	0.61
32:1a:1003:G:H2'	32:1a:1004:A:H4'	1.82	0.61
33:1b:195:ASP:OD1	33:1b:195:ASP:N	2.23	0.61
36:1e:144:THR:OG1	36:1e:147:ASP:OD1	2.18	0.61
1:2A:1041:C:N4	1:2A:1114:G:H1	1.97	0.61
1:2A:1316:U:H2'	1:2A:1317:A:H8	1.65	0.61
5:2F:78:ILE:HD13	5:2F:78:ILE:H	1.65	0.61
20:2Y:92:ASN:HD21	20:2Y:94:LYS:HG2	1.65	0.61
32:2a:258:G:H2'	32:2a:259:G:H8	1.65	0.61
14:1S:11:LYS:HG3	14:1S:91:PRO:HD3	1.81	0.61
33:1b:17:PHE:HA	33:1b:44:LEU:HD11	1.83	0.61
34:1c:6:HIS:CD2	34:1c:8:ILE:H	2.18	0.61
47:1p:20:VAL:HG21	47:1p:32:TYR:CD2	2.35	0.61
50:1s:41:VAL:HG12	50:1s:44:MET:HG3	1.83	0.61
1:2A:671:C:OP1	60:2A:3891:HOH:O	2.15	0.61
1:2A:2037:G:OP2	60:2A:3890:HOH:O	2.15	0.61
1:2A:2042:A:OP1	60:2A:3896:HOH:O	2.16	0.61
1:2A:2602:A:H4'	1:2A:2603:G:OP1	1.99	0.61
32:2a:1035:A:H2'	32:2a:1037:C:H41	1.65	0.61
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.24	0.61
8:1I:77:LEU:HB3	8:1I:142:VAL:HG22	1.81	0.61
32:1a:974:A:H8	32:1a:974:A:OP1	1.84	0.61
32:1a:1220:G:N2	50:1s:54:GLY:O	2.31	0.61
39:1h:112:LEU:HD22	39:1h:133:LEU:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:1q:13:ASP:OD1	48:1q:14:LYS:NZ	2.27	0.61
1:2A:906:G:O2'	12:2Q:67:ARG:NH2	2.33	0.61
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.36	0.61
8:1I:4:ILE:HG12	8:1I:18:VAL:HG22	1.82	0.61
1:2A:1087:G:H22	1:2A:1102:C:H42	1.49	0.61
5:2F:154:VAL:HG22	5:2F:191:ARG:HB2	1.81	0.61
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.82	0.61
8:2I:122:GLU:O	8:2I:126:TYR:OH	2.16	0.61
34:2c:117:ALA:HB2	34:2c:200:ALA:HB2	1.83	0.61
32:1a:501:C:OP1	43:1l:117:ARG:NH2	2.34	0.61
32:1a:544:G:OP1	35:1d:59:ARG:NH2	2.34	0.61
32:1a:1212:U:H5'	32:1a:1213:A:H5'	1.81	0.61
1:2A:2376:A:N3	14:2S:106:ARG:NH2	2.48	0.61
36:2e:77:PRO:HD2	36:2e:142:LEU:HD22	1.81	0.61
50:2s:30:LEU:HD11	50:2s:50:ALA:HB2	1.83	0.61
19:1X:76:ARG:NH1	60:1X:103:HOH:O	2.33	0.60
25:13:35:ARG:NH2	60:13:201:HOH:O	2.34	0.60
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.36	0.60
32:1a:532:A:N6	32:1a:1206:G:O2'	2.32	0.60
3:2D:275:LYS:HE3	3:2D:276:LYS:HA	1.82	0.60
32:2a:962:C:O2'	60:2a:3216:HOH:O	2.16	0.60
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	1.82	0.60
6:1G:7:LEU:HD22	6:1G:176:LEU:HD22	1.83	0.60
35:1d:163:GLU:C	35:1d:165:MET:H	2.09	0.60
40:1i:6:GLY:H	40:1i:17:VAL:HG12	1.66	0.60
1:2A:1215:G:O6	60:2A:3901:HOH:O	2.16	0.60
32:2a:619:U:N3	35:2d:134:ASP:OD1	2.26	0.60
32:2a:1071:C:H2'	32:2a:1072:G:H8	1.66	0.60
1:1A:2055:C:O2	60:1A:4183:HOH:O	2.15	0.60
1:1A:2240:C:OP2	60:1A:4198:HOH:O	2.16	0.60
6:1G:79:ASN:OD1	6:1G:79:ASN:N	2.31	0.60
7:1H:3:ARG:HH11	7:1H:4:ILE:H	1.48	0.60
31:19:27:CYS:O	60:19:201:HOH:O	2.16	0.60
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.82	0.60
1:2A:2105:C:H42	1:2A:2184:G:H1	1.49	0.60
1:2A:2115:G:H22	1:2A:2119:A:H5'	1.67	0.60
32:2a:881:G:P	43:2l:12:ARG:HH22	2.24	0.60
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.37	0.60
32:2a:1203:C:H2'	32:2a:1204:A:H8	1.66	0.60
32:1a:539:A:H2'	32:1a:540:G:C8	2.36	0.60
1:2A:192:C:O2	60:2A:3893:HOH:O	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1652:A:OP1	13:2R:8:ARG:NH1	2.35	0.60
13:2R:36:THR:HG22	13:2R:37:THR:H	1.66	0.60
39:2h:119:LEU:HB3	39:2h:123:GLU:HB2	1.84	0.60
40:2i:85:LEU:HB3	40:2i:92:TYR:HD2	1.65	0.60
44:2m:22:ILE:HG21	44:2m:66:LEU:HD13	1.81	0.60
53:2y:12:ILE:O	53:2y:17:ARG:NH2	2.34	0.60
5:1F:164:ARG:HE	57:1F:317:ARG:HH12	1.50	0.60
11:1P:87:ASP:O	11:1P:90:ARG:NH1	2.34	0.60
32:2a:417:C:H42	32:2a:426:G:H1	1.47	0.60
32:2a:1226:C:OP2	44:2m:91:ARG:NH1	2.33	0.60
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.36	0.60
35:2d:159:ARG:O	35:2d:163:GLU:N	2.34	0.60
1:1A:184:C:H2'	1:1A:185:U:C6	2.36	0.60
1:1A:588:U:H2'	1:1A:589:C:C6	2.37	0.60
1:1A:1336:A:OP2	19:1X:64:LYS:NZ	2.34	0.60
26:14:56:VAL:HB	26:14:60:GLN:HG2	1.83	0.60
32:1a:1504:G:OP1	32:1a:1507:A:H4'	2.01	0.60
32:2a:1310:G:H5'	44:2m:77:ASN:ND2	2.15	0.60
34:2c:137:ALA:HA	34:2c:140:ARG:HE	1.65	0.60
1:1A:447:A:OP2	60:1A:4193:HOH:O	2.16	0.60
26:14:59:PHE:HE1	50:1s:67:VAL:HG21	1.67	0.60
1:2A:1062:G:H2'	1:2A:1063:G:H8	1.65	0.60
21:2Z:45:ASP:OD1	21:2Z:49:ARG:NH2	2.31	0.60
32:2a:1002:G:C4	32:2a:1003:G:H8	2.19	0.60
3:1D:34:VAL:HG12	3:1D:63:ARG:HG3	1.84	0.60
32:1a:486:U:H2'	32:1a:487:A:H8	1.67	0.60
1:2A:2781:A:H5"	1:2A:2782:G:H5'	1.82	0.60
7:2H:45:VAL:HG13	7:2H:50:VAL:HG22	1.84	0.60
9:2N:15:LEU:HD23	9:2N:137:LYS:HD2	1.83	0.60
25:23:12:PRO:HB2	25:23:20:LYS:HG2	1.82	0.60
32:2a:620:C:C2	35:2d:135:LEU:HG	2.37	0.60
32:2a:1256:A:OP1	34:2c:26:LYS:NZ	2.29	0.60
34:2c:63:ASN:HB2	34:2c:98:ASN:HB2	1.83	0.60
46:2o:39:LEU:HD13	46:2o:56:LEU:HB2	1.82	0.60
1:1A:1011:G:OP1	16:1U:75:ASN:ND2	2.35	0.60
1:1A:1474:C:H2'	1:1A:1475:G:H8	1.65	0.60
11:1P:18:ARG:NH2	60:1P:305:HOH:O	2.29	0.60
21:1Z:154:ASP:OD1	21:1Z:154:ASP:N	2.35	0.60
35:1d:155:LEU:HB3	35:1d:158:ILE:HG23	1.83	0.60
48:1q:6:LEU:HD23	48:1q:23:VAL:HG21	1.84	0.60
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1064:C:N4	1:2A:1074:G:O6	2.35	0.60
1:2A:1352:U:OP2	60:2A:3895:HOH:O	2.16	0.60
26:24:24:THR:OG1	26:24:25:TYR:N	2.35	0.60
33:2b:104:ASN:O	33:2b:108:ILE:HG12	2.02	0.60
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.36	0.60
1:1A:1312:U:OP2	19:1X:63:LYS:NZ	2.29	0.60
32:1a:171:A:H2'	32:1a:172:A:C8	2.37	0.60
32:1a:1003:G:C2'	32:1a:1004:A:H4'	2.32	0.60
34:1c:29:TYR:OH	45:1n:54:PRO:O	2.20	0.60
37:1f:19:LEU:HD11	37:1f:59:TYR:CE1	2.37	0.60
40:1i:92:TYR:HB3	40:1i:96:LEU:HD12	1.84	0.60
1:2A:2570:G:O6	60:2A:3887:HOH:O	2.15	0.60
7:2H:95:ARG:HB2	7:2H:128:PRO:HB3	1.84	0.60
32:2a:501:C:H2'	32:2a:502:G:H8	1.67	0.60
32:2a:815:A:N7	32:2a:1509:C:O2'	2.35	0.60
32:2a:1030(B):C:H41	32:2a:1030(C):G:H21	1.49	0.60
1:1A:1419:A:OP2	60:1A:4196:HOH:O	2.16	0.59
32:1a:92:C:H2'	32:1a:93:G:C8	2.37	0.59
33:1b:102:LEU:HD23	33:1b:182:ILE:HD12	1.84	0.59
1:2A:2837:G:N7	60:2A:4076:HOH:O	2.32	0.59
17:2V:14:VAL:HB	17:2V:96:ILE:HG13	1.83	0.59
20:2Y:7:VAL:HG21	20:2Y:72:VAL:HG12	1.84	0.59
32:1a:356:A:N3	32:1a:368:U:O2'	2.34	0.59
32:1a:523:A:H61	43:1l:92:0TD:CG	2.15	0.59
32:1a:1295:G:O2'	44:1m:14:ARG:NH1	2.35	0.59
34:1c:52:LEU:HD12	34:1c:53:ALA:H	1.67	0.59
42:1k:18:ARG:NH2	42:1k:35:PRO:O	2.34	0.59
1:2A:2560:C:OP2	60:2A:3897:HOH:O	2.16	0.59
34:2c:78:GLY:HA3	34:2c:83:ARG:H	1.65	0.59
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.35	0.59
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.38	0.59
1:2A:1849:G:H2'	1:2A:1850:G:H8	1.65	0.59
1:2A:2252:G:N3	60:2A:4060:HOH:O	2.30	0.59
32:2a:539:A:H2'	32:2a:540:G:C8	2.38	0.59
32:2a:1368:G:OP1	40:2i:111:ARG:NH2	2.34	0.59
40:2i:9:ARG:H	40:2i:79:LEU:HD23	1.68	0.59
1:1A:945:A:N7	60:1A:4389:HOH:O	2.32	0.59
32:1a:790:A:C2	53:1y:29:LYS:HD3	2.38	0.59
32:1a:1158:C:H5	32:1a:1181:G:N1	2.01	0.59
32:1a:1377:A:HO2'	38:1g:2:ALA:N	1.99	0.59
1:2A:1324:G:O2'	1:2A:1326:U:OP2	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2022:U:OP1	60:2A:3903:HOH:O	2.17	0.59
1:1A:1771:C:OP1	60:1A:4204:HOH:O	2.17	0.59
13:1R:36:THR:HG22	13:1R:37:THR:H	1.65	0.59
26:14:61:ARG:HG3	26:14:62:ARG:H	1.67	0.59
47:1p:53:VAL:HG13	47:1p:79:VAL:HG12	1.84	0.59
1:2A:922:U:H2'	1:2A:923:C:C6	2.36	0.59
1:2A:975:C:OP1	60:2A:3899:HOH:O	2.16	0.59
32:2a:187:C:O2'	51:2t:89:ARG:HD3	2.02	0.59
33:2b:15:VAL:O	33:2b:17:PHE:N	2.33	0.59
33:2b:212:GLN:O	33:2b:216:SER:OG	2.18	0.59
40:2i:21:PRO:HA	40:2i:59:PHE:HD1	1.67	0.59
1:1A:1377:G:O6	60:1A:4201:HOH:O	2.17	0.59
1:1A:1762:A:H2'	60:1A:7327:HOH:O	2.00	0.59
1:1A:2611:U:C4	27:15:3:LYS:HG2	2.37	0.59
32:1a:812:C:N3	60:1a:3369:HOH:O	2.32	0.59
1:2A:236:C:H2'	1:2A:237:C:C6	2.37	0.59
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.17	0.59
3:2D:142:VAL:HG23	3:2D:193:VAL:HA	1.84	0.59
21:2Z:97:GLU:HB3	21:2Z:125:LEU:HD11	1.84	0.59
25:23:10:LYS:HB3	25:23:53:LEU:HA	1.85	0.59
32:2a:316:G:OP2	32:2a:351:G:O2'	2.20	0.59
1:1A:97:C:OP1	24:12:2:LYS:NZ	2.32	0.59
2:1B:59:A:N6	60:1B:314:HOH:O	2.27	0.59
32:1a:708:C:OP1	42:1k:85:ARG:NH2	2.34	0.59
37:1f:38:GLU:OE1	37:1f:64:GLN:NE2	2.34	0.59
1:2A:1109:C:H3'	1:2A:1110:G:C8	2.38	0.59
1:2A:1186:G:OP2	60:2A:3905:HOH:O	2.17	0.59
12:2Q:1:MET:HG3	12:2Q:44:ALA:HB1	1.85	0.59
32:2a:328:C:H4'	32:2a:329:A:H5'	1.85	0.59
32:2a:448:A:OP2	32:2a:485:G:N2	2.24	0.59
32:2a:1030(A):G:N2	32:2a:1030(D):A:OP2	2.36	0.59
1:1A:1607:C:N4	1:1A:1622:G:OP2	2.34	0.59
8:1I:101:LEU:HD22	8:1I:107:VAL:HB	1.85	0.59
46:1o:29:VAL:HG11	46:1o:67:LEU:HD21	1.83	0.59
1:2A:251:A:C5	1:2A:252:G:H1'	2.38	0.59
12:2Q:97:VAL:HG21	12:2Q:103:MET:HE3	1.84	0.59
32:2a:538:G:O6	60:2a:3217:HOH:O	2.17	0.59
41:2j:78:ASN:O	41:2j:80:LYS:N	2.36	0.59
1:1A:336:C:HO2'	20:1Y:35:TYR:HH	1.49	0.59
1:1A:947:G:O6	60:1A:4177:HOH:O	2.14	0.59
18:1W:4:LYS:HE3	18:1W:6:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:8:A:N7	35:1d:208:SER:OG	2.36	0.59
32:1a:597:G:OP2	60:1a:3329:HOH:O	2.15	0.59
1:2A:2184:G:N1	1:2A:2185:C:O2	2.36	0.59
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.68	0.59
32:2a:1132:C:H2'	32:2a:1133:G:C8	2.38	0.59
1:1A:949:C:OP2	60:1A:4200:HOH:O	2.17	0.59
1:1A:2183:C:H2'	1:1A:2184:G:C8	2.37	0.59
1:1A:2759:G:N7	60:1A:4382:HOH:O	2.31	0.59
32:1a:406:G:H5'	35:1d:5:ILE:HD11	1.85	0.59
1:2A:1076:C:H4'	1:2A:1077:A:OP1	2.02	0.59
1:2A:2022:U:OP2	27:25:15:ARG:NH2	2.35	0.59
1:2A:2318:G:H21	14:2S:3:ARG:HD3	1.68	0.59
1:2A:2468:G:OP1	12:2Q:119:ARG:NH2	2.35	0.59
4:2E:9:VAL:HB	15:2T:3:ARG:HG2	1.84	0.59
26:24:18:CYS:HB2	26:24:20:ASN:HB2	1.84	0.59
38:2g:116:ALA:HA	38:2g:119:ARG:HG3	1.85	0.59
40:2i:116:LYS:HD2	40:2i:122:ALA:HA	1.85	0.59
1:1A:968:G:O6	60:1A:4165:HOH:O	2.11	0.58
4:1E:78:LEU:O	4:1E:79:ARG:NH1	2.33	0.58
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.84	0.58
18:1W:12:ILE:HD13	18:1W:17:VAL:HG13	1.85	0.58
29:17:35:ARG:NH1	60:17:202:HOH:O	2.35	0.58
32:1a:757:U:H2'	32:1a:758:G:O4'	2.03	0.58
32:1a:757:U:O2'	32:1a:879:C:O2	2.21	0.58
42:1k:81:ASP:N	42:1k:81:ASP:OD1	2.36	0.58
1:2A:526:A:OP1	60:2A:3864:HOH:O	2.16	0.58
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.03	0.58
5:2F:135:LYS:HG2	5:2F:137:LYS:HG2	1.83	0.58
36:2e:93:PRO:HG2	39:2h:105:ARG:HG3	1.85	0.58
36:2e:139:LEU:HA	36:2e:142:LEU:HD12	1.84	0.58
40:2i:14:VAL:HG23	40:2i:66:ARG:HB2	1.85	0.58
1:1A:236:C:H2'	1:1A:237:C:C6	2.37	0.58
10:1O:68:GLU:HB3	10:1O:78:ARG:HB2	1.85	0.58
1:2A:268:C:O2'	60:2A:3907:HOH:O	2.17	0.58
1:2A:2313:C:H5"	6:2G:91:ARG:HD3	1.85	0.58
26:24:46:GLN:O	26:24:48:ARG:NH1	2.35	0.58
1:1A:83:G:OP1	60:1A:4195:HOH:O	2.16	0.58
32:1a:424:G:H2'	32:1a:425:G:H8	1.67	0.58
32:1a:985:C:H2'	32:1a:986:A:C8	2.38	0.58
36:1e:137:GLU:OE2	36:1e:141:GLN:NE2	2.31	0.58
42:1k:87:THR:O	42:1k:87:THR:OG1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1m:78:ILE:HG22	44:1m:82:MET:HE2	1.85	0.58
1:2A:855:G:O2'	22:20:27:GLU:OE2	2.19	0.58
32:1a:96:U:H2'	32:1a:97:G:C8	2.38	0.58
32:1a:815:A:N7	32:1a:1509:C:O2'	2.37	0.58
34:1c:19:GLU:O	34:1c:40:ARG:NH2	2.36	0.58
1:2A:2417:C:O3'	60:2A:3911:HOH:O	2.17	0.58
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.67	0.58
35:1d:85:LYS:O	60:1d:402:HOH:O	2.17	0.58
50:1s:41:VAL:HG13	50:1s:43:GLU:H	1.69	0.58
8:2I:65:ALA:O	8:2I:69:LYS:N	2.36	0.58
13:2R:98:LEU:HD12	13:2R:113:LEU:HD11	1.85	0.58
36:1e:148:VAL:HG21	39:1h:107:LEU:HB3	1.86	0.58
1:2A:271(R):G:H5"	23:21:97:LEU:HD21	1.85	0.58
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.04	0.58
14:2S:77:ALA:HB1	14:2S:82:ILE:HB	1.86	0.58
33:2b:16:HIS:O	33:2b:18:GLY:N	2.37	0.58
1:1A:1173:G:O2'	1:1A:1174:A:O4'	2.21	0.58
1:1A:1174:A:H1'	1:1A:1175:U:O4'	2.04	0.58
1:1A:1430:C:H2'	1:1A:1431:U:C6	2.38	0.58
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.18	0.58
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.77	0.58
32:1a:373:A:H2'	32:1a:374:A:H8	1.67	0.58
32:1a:1129:C:H4'	40:1i:16:ARG:HH22	1.68	0.58
1:2A:775:G:OP1	60:2A:3906:HOH:O	2.17	0.58
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.85	0.58
1:1A:1010:A:OP2	60:1A:4202:HOH:O	2.17	0.58
32:1a:263:A:OP1	51:1t:79:ARG:NH1	2.37	0.58
41:1j:11:PHE:HE1	41:1j:67:THR:HG22	1.69	0.58
1:2A:387:U:OP1	60:2A:3904:HOH:O	2.17	0.58
42:2k:82:VAL:HB	42:2k:108:ILE:HG12	1.86	0.58
1:1A:1653:G:H3'	13:1R:2:ARG:HD3	1.86	0.58
1:1A:1973:G:O6	60:1A:4174:HOH:O	2.14	0.58
1:1A:2583:G:OP2	60:1A:4207:HOH:O	2.17	0.58
21:1Z:141:VAL:HB	21:1Z:144:LEU:HD12	1.85	0.58
35:1d:23:GLY:HA3	35:1d:112:VAL:HB	1.86	0.58
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.85	0.58
1:1A:1474:C:H2'	1:1A:1475:G:C8	2.39	0.58
1:1A:1844:C:OP1	60:1A:4206:HOH:O	2.17	0.58
1:1A:2390:U:P	30:18:35:GLN:HE22	2.27	0.58
3:1D:70:TRP:HB3	3:1D:190:TYR:CE2	2.39	0.58
6:1G:50:ALA:HB1	6:1G:52:ILE:HG12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:150:ASP:OD1	6:1G:153:ARG:NH1	2.36	0.58
32:1a:976:G:OP2	32:1a:1358:U:O2'	2.19	0.58
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.39	0.58
1:2A:2823:A:OP1	4:2E:159:HIS:NE2	2.37	0.58
32:2a:642:A:N3	39:2h:113:SER:OG	2.37	0.58
1:1A:745:G:O6	60:1A:4194:HOH:O	2.16	0.57
1:1A:1486:A:H2'	1:1A:1487:G:H8	1.69	0.57
2:1B:85:G:O6	60:1B:305:HOH:O	2.13	0.57
34:1c:47:LEU:HD13	34:1c:68:VAL:HG11	1.86	0.57
1:2A:962:G:OP1	60:2A:3912:HOH:O	2.17	0.57
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.85	0.57
3:2D:132:PRO:HG2	3:2D:135:PHE:HD2	1.69	0.57
32:2a:975:A:N1	41:2j:48:THR:HB	2.19	0.57
32:2a:1186:G:N2	45:2n:61:TRP:OXT	2.36	0.57
36:2e:33:VAL:HG13	36:2e:112:LEU:HD12	1.85	0.57
37:2f:6:VAL:HG22	37:2f:90:VAL:HG22	1.83	0.57
1:1A:1243:G:O2'	11:1P:7:ARG:NH2	2.37	0.57
8:1I:85:GLU:HG3	8:1I:86:THR:N	2.18	0.57
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.39	0.57
37:1f:80:ARG:NH1	37:1f:88:VAL:O	2.37	0.57
32:2a:1073:U:H2'	32:2a:1074:G:C8	2.39	0.57
32:2a:1258:G:H2'	32:2a:1259:C:C6	2.39	0.57
9:1N:70:LYS:HB3	9:1N:87:LEU:HB2	1.85	0.57
45:1n:23:ARG:NH1	45:1n:30:ALA:HB2	2.18	0.57
1:2A:2847:U:OP1	15:2T:98:LYS:NZ	2.37	0.57
9:2N:12:ARG:NH1	9:2N:50:ASP:OD2	2.37	0.57
16:2U:49:HIS:HA	16:2U:52:ARG:HB3	1.85	0.57
18:2W:68:ARG:HB2	18:2W:109:GLU:HG2	1.86	0.57
33:2b:185:ILE:HG13	33:2b:199:TYR:HB2	1.86	0.57
23:11:77:ALA:HA	23:11:80:LEU:HD13	1.86	0.57
32:1a:1417:G:O6	60:1a:3316:HOH:O	2.12	0.57
39:1h:6:ILE:HB	39:1h:85:ARG:NH1	2.19	0.57
32:2a:4:U:H3	39:2h:105:ARG:HD3	1.68	0.57
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.40	0.57
1:1A:1642:G:N7	60:1A:4276:HOH:O	2.33	0.57
1:1A:2181:G:H2'	1:1A:2182:G:H8	1.70	0.57
32:1a:407:G:OP1	35:1d:115:ARG:NH2	2.38	0.57
32:1a:560:U:O2'	32:1a:561:U:OP2	2.21	0.57
1:2A:1647:G:OP1	60:2A:3909:HOH:O	2.17	0.57
1:2A:2641:G:P	9:2N:74:ARG:HH22	2.26	0.57
6:2G:80:PHE:O	6:2G:82:LEU:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.19	0.57
33:2b:77:ALA:O	33:2b:81:VAL:HG12	2.04	0.57
34:2c:151:VAL:HG22	34:2c:200:ALA:HA	1.86	0.57
40:2i:19:LEU:HD23	40:2i:61:ALA:HB2	1.86	0.57
1:1A:675:A:OP2	60:1A:4199:HOH:O	2.16	0.57
1:1A:2223:G:OP1	3:1D:172:TYR:OH	2.18	0.57
40:1i:111:ARG:O	40:1i:113:LYS:NZ	2.36	0.57
7:2H:17:VAL:HG22	7:2H:26:VAL:HG22	1.85	0.57
32:2a:390:C:O3'	47:2p:28:ARG:NH2	2.38	0.57
32:2a:757:U:H2'	32:2a:758:G:O4'	2.04	0.57
32:2a:1162:C:H42	32:2a:1174:G:H1	1.53	0.57
1:1A:307:G:H21	1:1A:330:A:H62	1.53	0.57
1:1A:530:G:N1	1:1A:2023:G:OP1	2.33	0.57
1:1A:1084:A:N3	1:1A:1105:U:O2'	2.29	0.57
1:1A:1176:G:N2	1:1A:1178:C:OP2	2.38	0.57
1:1A:2857:G:N2	1:1A:2860:A:OP2	2.33	0.57
18:1W:67:ASP:N	18:1W:67:ASP:OD1	2.37	0.57
32:1a:67:C:H2'	32:1a:68:G:C8	2.39	0.57
32:1a:447:G:O6	32:1a:485:G:O2'	2.22	0.57
32:2a:442:C:H42	32:2a:492:G:H1	1.51	0.57
32:2a:662:G:H2'	32:2a:663:A:C8	2.39	0.57
32:2a:1129:C:H42	32:2a:1143:G:H1	1.51	0.57
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.69	0.57
34:2c:175:LEU:HD21	34:2c:201:TYR:HE1	1.68	0.57
37:2f:99:ALA:HB2	49:2r:31:LEU:HD11	1.86	0.57
41:2j:6:ILE:HG12	41:2j:98:ILE:HG23	1.87	0.57
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.87	0.57
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	1.85	0.57
32:1a:689:C:OP1	42:1k:44:SER:OG	2.18	0.57
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.05	0.57
1:2A:2235:G:O6	60:2A:3884:HOH:O	2.15	0.57
1:2A:2306:C:N4	6:2G:42:GLY:O	2.31	0.57
8:2I:75:LEU:HD11	8:2I:105:HIS:CG	2.39	0.57
14:2S:67:ARG:HD2	14:2S:71:ARG:HH21	1.69	0.57
40:2i:50:LEU:HB2	40:2i:56:LEU:HD23	1.87	0.57
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.05	0.57
14:1S:59:LYS:HD2	14:1S:60:GLY:H	1.68	0.57
32:1a:142:G:H2'	32:1a:143:A:H8	1.70	0.57
32:1a:1325:C:H4'	52:1u:17:THR:HG21	1.85	0.57
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.20	0.57
40:1i:121:ARG:NH1	40:1i:122:ALA:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1001:A:OP2	60:2A:3914:HOH:O	2.18	0.57
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.23	0.57
6:2G:67:LYS:NZ	60:2G:301:HOH:O	2.36	0.57
10:2O:15:GLY:O	10:2O:47:ILE:HG13	2.05	0.57
33:2b:7:VAL:O	33:2b:217:ARG:NH1	2.38	0.57
42:2k:18:ARG:NH2	42:2k:35:PRO:O	2.31	0.57
46:2o:6:GLU:OE1	46:2o:6:GLU:N	2.34	0.57
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.69	0.57
1:1A:1173:G:O2'	1:1A:1174:A:O5'	2.23	0.57
13:1R:103:ARG:NH1	13:1R:108:GLY:O	2.38	0.57
36:1e:57:LYS:HG2	36:1e:61:TYR:HE2	1.69	0.57
46:1o:16:ALA:HB1	46:1o:21:ASP:HB3	1.87	0.57
32:2a:1112:C:O2	34:2c:179:ARG:N	2.38	0.57
34:2c:131:ARG:HD3	34:2c:166:GLU:HG2	1.85	0.57
36:2e:43:LEU:O	36:2e:65:ASN:ND2	2.27	0.57
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.69	0.56
1:1A:1139:G:OP1	60:1N:301:HOH:O	2.18	0.56
24:12:13:ALA:HA	24:12:16:LEU:HD12	1.87	0.56
1:2A:973:A:H8	1:2A:973:A:OP1	1.87	0.56
1:2A:2821:A:OP2	60:2R:301:HOH:O	2.17	0.56
18:2W:18:ARG:NH1	18:2W:76:VAL:O	2.38	0.56
22:20:10:THR:HG22	22:20:12:ASN:H	1.70	0.56
32:2a:41:G:H2'	32:2a:42:G:C8	2.40	0.56
1:1A:576:U:H2'	1:1A:577:G:C8	2.41	0.56
1:1A:792:G:H5"	1:1A:793:A:H5'	1.85	0.56
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.06	0.56
33:1b:70:PHE:CD1	33:1b:163:PHE:HB3	2.39	0.56
44:1m:40:ASN:O	44:1m:43:THR:OG1	2.22	0.56
1:2A:321:G:O2'	1:2A:340:A:N3	2.36	0.56
1:2A:2144:U:HO2'	1:2A:2147:G:H1	1.49	0.56
1:2A:2498:C:OP1	60:2A:3910:HOH:O	2.17	0.56
12:2Q:109:VAL:HG13	12:2Q:113:GLN:HB2	1.86	0.56
32:2a:683:G:O6	60:2a:3218:HOH:O	2.17	0.56
32:2a:718:G:C8	42:2k:116:HIS:HB3	2.40	0.56
32:2a:1348:U:H2'	32:2a:1349:A:H8	1.71	0.56
1:1A:2747:G:O6	1:1A:2755:C:H5"	2.06	0.56
3:1D:72:LYS:HD2	3:1D:103:ARG:NH1	2.20	0.56
9:1N:33:LEU:HD12	9:1N:38:HIS:ND1	2.20	0.56
19:1X:60:ARG:NH1	29:17:47:ARG:HH22	2.01	0.56
32:1a:661:G:H1	32:1a:744:C:H42	1.54	0.56
1:2A:1223:G:N2	1:2A:1226:A:OP2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2224:G:OP2	60:2A:3916:HOH:O	2.18	0.56
1:2A:2719:G:O6	60:2A:3900:HOH:O	2.16	0.56
45:2n:26:ARG:HD3	45:2n:43:CYS:HB3	1.86	0.56
46:2o:68:ARG:NH2	60:2o:201:HOH:O	2.37	0.56
1:1A:324:A:N6	1:1A:338:G:O2'	2.38	0.56
1:1A:1956:U:OP2	60:1A:4212:HOH:O	2.18	0.56
1:1A:2712:U:OP1	1:1A:2714:G:H4'	2.06	0.56
25:13:8:LEU:HD13	25:13:31:LEU:HD23	1.88	0.56
32:1a:189(K):U:H2'	32:1a:189(L):G:H8	1.70	0.56
36:1e:37:ARG:NH1	36:1e:112:LEU:HD23	2.19	0.56
1:2A:821:A:H2'	1:2A:946:G:H5"	1.87	0.56
1:2A:1081:U:H2'	1:2A:1082:U:O2	2.06	0.56
1:2A:1845:G:OP1	3:2D:258:LYS:NZ	2.35	0.56
2:2B:114:C:H4'	14:2S:46:VAL:HG13	1.87	0.56
50:2s:38:SER:HB2	50:2s:71:LEU:HD22	1.87	0.56
1:1A:1654:A:OP1	13:1R:1:MET:N	2.33	0.56
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.03	0.56
39:1h:4:ASP:OD2	39:1h:85:ARG:NH1	2.39	0.56
1:2A:108:U:H2'	1:2A:109:G:H8	1.71	0.56
1:2A:271(G):C:H2'	1:2A:271(H):G:H8	1.71	0.56
1:2A:888:C:OP1	44:2m:93:ARG:NH1	2.39	0.56
1:2A:1102:C:H2'	1:2A:1103:A:H8	1.70	0.56
5:2F:153:SER:HB2	5:2F:189:THR:HA	1.87	0.56
26:24:46:GLN:O	26:24:48:ARG:N	2.34	0.56
33:2b:78:GLN:O	33:2b:94:ASN:ND2	2.38	0.56
40:2i:54:ASP:O	40:2i:56:LEU:N	2.38	0.56
1:1A:887:A:H2	1:1A:889:C:H2'	1.70	0.56
1:1A:2453:A:OP1	60:1A:4205:HOH:O	2.17	0.56
4:1E:101:ARG:NH2	60:1E:405:HOH:O	2.39	0.56
32:1a:580:U:H2'	32:1a:581:G:O4'	2.06	0.56
40:1i:20:ARG:O	40:1i:60:ASP:N	2.33	0.56
48:1q:67:LYS:O	48:1q:69:LYS:N	2.36	0.56
32:2a:56:U:H2'	32:2a:57:G:H8	1.68	0.56
32:2a:229:U:O2'	47:2p:23:ASP:OD2	2.23	0.56
1:1A:1779:U:H2'	60:1A:4369:HOH:O	2.06	0.56
1:1A:2279:G:O6	22:10:14:ARG:HG3	2.05	0.56
1:1A:2393:A:H5'	11:1P:63:PRO:HB3	1.88	0.56
20:1Y:13:VAL:HB	20:1Y:72:VAL:HG13	1.87	0.56
1:2A:2189:U:H2'	1:2A:2190:G:C8	2.41	0.56
1:1A:2180:U:H2'	1:1A:2181:G:O4'	2.05	0.56
1:2A:1669:A:H5"	1:2A:2550:G:OP1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.41	0.56
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	1.87	0.56
7:2H:46:GLU:HB2	7:2H:49:VAL:HG12	1.88	0.56
23:21:2:SER:HB3	23:21:46:LEU:HD12	1.88	0.56
32:2a:533:A:OP2	60:2a:3219:HOH:O	2.18	0.56
1:1A:1231:G:H2'	1:1A:1232:G:C8	2.41	0.56
2:1B:79:C:OP2	60:1B:306:HOH:O	2.18	0.56
10:1O:63:VAL:HG12	10:1O:106:LEU:HD11	1.87	0.56
1:2A:2058:A:N7	60:2A:4093:HOH:O	2.33	0.56
7:2H:33:LEU:HD21	7:2H:136:ILE:HB	1.87	0.56
32:2a:573:A:N3	32:2a:883:C:O2'	2.38	0.56
32:2a:1255:G:OP1	41:2j:45:ARG:NH2	2.39	0.56
34:2c:124:ILE:HD11	34:2c:189:ALA:HB3	1.88	0.56
43:2l:28:LYS:N	43:2l:29:GLY:HA2	2.20	0.56
1:1A:639:U:H2'	1:1A:640:C:C6	2.41	0.56
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.41	0.56
44:1m:48:LEU:HD13	44:1m:53:VAL:HG22	1.87	0.56
1:2A:637:A:H8	11:2P:117:GLU:HG3	1.71	0.56
1:2A:809:G:OP2	60:2A:3919:HOH:O	2.18	0.56
1:2A:1066:U:O2'	1:2A:1067:A:O3'	2.22	0.56
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.22	0.56
9:2N:28:THR:HG22	9:2N:29:LYS:HG2	1.87	0.56
40:2i:3:GLN:NE2	40:2i:20:ARG:HH21	2.04	0.56
1:1A:1359:A:H61	1:1A:1372:U:H3	1.53	0.55
32:1a:165:C:H2'	32:1a:166:G:C8	2.41	0.55
1:2A:2080:G:OP1	23:21:35:THR:OG1	2.24	0.55
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.88	0.55
21:2Z:99:TYR:HB3	21:2Z:123:ASP:HB2	1.88	0.55
32:2a:748:C:H4'	32:2a:749:C:O5'	2.05	0.55
49:2r:51:LEU:HD22	49:2r:55:ARG:HE	1.71	0.55
1:1A:1659:U:OP1	60:1A:4208:HOH:O	2.17	0.55
6:1G:114:ILE:HB	6:1G:117:PHE:HB2	1.89	0.55
41:1j:61:GLU:OE2	45:1n:58:LYS:NZ	2.31	0.55
1:2A:521:G:N7	60:2A:4097:HOH:O	2.33	0.55
1:2A:2805:G:H2'	1:2A:2807:G:H8	1.71	0.55
19:2X:11:PRO:HB3	19:2X:92:LEU:HD11	1.88	0.55
34:2c:40:ARG:NH2	34:2c:55:VAL:O	2.39	0.55
41:2j:38:ILE:HD11	41:2j:71:LEU:HD22	1.88	0.55
1:1A:1590:U:OP2	60:1A:4211:HOH:O	2.18	0.55
1:1A:1831:G:O6	60:1A:4174:HOH:O	2.13	0.55
6:1G:38:VAL:HG22	6:1G:93:THR:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.41	0.55
48:1q:9:VAL:HG22	48:1q:56:VAL:HG22	1.89	0.55
1:2A:236:C:H2'	1:2A:237:C:H6	1.72	0.55
1:2A:2732:G:O6	60:2A:3920:HOH:O	2.18	0.55
1:1A:674:G:H1'	5:1F:74:ARG:HD2	1.87	0.55
3:2D:77:ALA:HA	3:2D:97:TYR:HA	1.88	0.55
32:2a:1320:C:H1'	50:2s:73:GLU:HG2	1.87	0.55
44:2m:34:LEU:HD13	44:2m:41:PRO:HB3	1.88	0.55
12:1Q:116:GLU:OE2	12:1Q:119:ARG:NH2	2.32	0.55
32:1a:270:A:H2'	32:1a:271:C:C6	2.41	0.55
32:1a:667:G:H4'	46:1o:51:HIS:ND1	2.21	0.55
32:1a:763:G:H2'	32:1a:764:C:C6	2.42	0.55
40:1i:43:ALA:HA	40:1i:74:ILE:HD13	1.88	0.55
1:2A:271(A):A:N1	1:2A:272(D):G:O2'	2.36	0.55
1:2A:2114:A:H3'	1:2A:2115:G:H8	1.71	0.55
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.41	0.55
32:2a:976:G:H5'	32:2a:1358:U:O2'	2.06	0.55
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.21	0.55
39:2h:51:VAL:HG11	39:2h:60:ARG:HD2	1.88	0.55
1:1A:1301:A:O2'	1:1A:1302:A:H3'	2.07	0.55
3:1D:88:ARG:NH1	60:1D:407:HOH:O	2.32	0.55
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.06	0.55
15:1T:127:ALA:C	15:1T:129:ARG:H	2.14	0.55
20:1Y:6:HIS:H	20:1Y:6:HIS:CD2	2.25	0.55
35:1d:65:ARG:HD2	35:1d:72:GLU:HA	1.89	0.55
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.89	0.55
1:2A:271(W):G:O6	60:2A:3898:HOH:O	2.16	0.55
1:2A:509:C:O3'	60:2A:3915:HOH:O	2.18	0.55
1:2A:1058:G:N2	1:2A:1081:U:H1'	2.22	0.55
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.41	0.55
1:2A:1740:G:H2'	1:2A:1741:A:H8	1.71	0.55
1:2A:2141:G:H1	1:2A:2149:G:H22	1.54	0.55
1:2A:2573:C:OP1	1:2A:2574:G:H5"	2.06	0.55
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.07	0.55
20:2Y:87:LYS:HD2	20:2Y:95:LYS:HD2	1.88	0.55
33:2b:158:LEU:HD23	33:2b:182:ILE:HD11	1.89	0.55
53:2y:74:ILE:O	53:2y:78:ILE:HG12	2.06	0.55
7:1H:42:ARG:NH1	7:1H:53:GLU:OE1	2.40	0.55
8:2I:14:ASP:O	8:2I:17:GLN:HB2	2.06	0.55
20:2Y:55:TYR:CZ	20:2Y:61:ILE:HG21	2.41	0.55
32:2a:559:A:H4'	32:2a:560:U:H3'	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1003:G:H2'	32:2a:1004:A:C4'	2.26	0.55
33:2b:112:VAL:HG22	33:2b:149:LEU:HD13	1.89	0.55
33:2b:162:ILE:HD11	33:2b:184:VAL:HG22	1.89	0.55
44:2m:60:VAL:HG23	44:2m:64:TRP:CE3	2.42	0.55
21:1Z:145:GLU:H	21:1Z:148:ASP:HB2	1.71	0.55
33:1b:231:GLU:HB3	33:1b:232:PRO:CD	2.36	0.55
42:1k:27:ASN:OD1	42:1k:28:THR:N	2.40	0.55
1:2A:438:G:H2'	1:2A:440:G:H8	1.70	0.55
1:2A:602:G:O2'	1:2A:655:A:N6	2.40	0.55
21:2Z:179:ASP:HB3	21:2Z:182:LYS:HG2	1.87	0.55
32:2a:1411:C:H2'	32:2a:1412:C:C6	2.41	0.55
32:2a:1498:UR3:O4	60:2a:3222:HOH:O	2.18	0.55
34:2c:6:HIS:HB3	45:2n:49:HIS:ND1	2.22	0.55
1:1A:1671:U:O4	60:1A:4154:HOH:O	2.16	0.55
1:1A:1697:G:OP2	1:1A:1698:A:O2'	2.19	0.55
8:1I:114:LEU:HD12	8:1I:115:ALA:H	1.70	0.55
32:1a:91:C:H2'	32:1a:92:C:C6	2.41	0.55
32:1a:841:U:C5	32:1a:848:C:H1'	2.42	0.55
32:1a:1179:A:O3'	40:1i:103:THR:HB	2.07	0.55
35:1d:190:ASP:N	35:1d:190:ASP:OD1	2.39	0.55
46:1o:6:GLU:OE1	46:1o:6:GLU:N	2.38	0.55
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.89	0.55
12:2Q:111:GLU:OE2	12:2Q:133:ARG:NH2	2.37	0.55
13:2R:19:ALA:O	13:2R:23:ASN:ND2	2.39	0.55
32:2a:192:U:H2'	32:2a:193:C:H6	1.71	0.55
48:2q:64:PRO:HB3	48:2q:70:ARG:NH1	2.22	0.55
1:1A:1578:U:H2'	1:1A:1579:A:H5'	1.88	0.55
1:1A:2285:C:OP2	28:16:6:ARG:NH1	2.40	0.55
2:1B:52:A:N6	14:1S:33:LYS:HG2	2.22	0.55
4:1E:73:GLU:H	4:1E:73:GLU:CD	2.15	0.55
11:1P:42:SER:O	60:1P:301:HOH:O	2.18	0.55
32:1a:890:G:O2'	32:1a:906:G:O6	2.19	0.55
35:1d:196:LEU:O	35:1d:198:VAL:N	2.39	0.55
1:2A:451:C:H5'	60:2A:3951:HOH:O	2.07	0.55
4:2E:1:MET:HE2	4:2E:199:ARG:HB3	1.88	0.55
34:2c:19:GLU:HB3	34:2c:40:ARG:NH2	2.22	0.55
35:2d:79:PHE:HE1	35:2d:204:ILE:HD13	1.72	0.55
1:1A:796:C:H2'	1:1A:797:C:C6	2.43	0.54
1:1A:1634:A:OP2	60:1A:4216:HOH:O	2.18	0.54
3:1D:242:ARG:HG3	3:1D:242:ARG:HH11	1.73	0.54
32:1a:376:G:H4'	47:1p:5:ARG:NH1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1784:A:OP2	60:2A:3818:HOH:O	2.18	0.54
11:2P:2:LYS:NZ	11:2P:4:SER:OG	2.22	0.54
47:2p:75:ARG:HG3	47:2p:80:PHE:HD2	1.72	0.54
53:2y:12:ILE:HG23	53:2y:16:ILE:HG23	1.87	0.54
1:1A:234:C:H2'	1:1A:235:U:H6	1.71	0.54
4:1E:52:LEU:HD12	4:1E:77:ILE:HD11	1.89	0.54
7:1H:40:GLU:OE2	7:1H:60:ARG:NH1	2.41	0.54
13:1R:79:LEU:HD12	13:1R:83:ILE:HB	1.89	0.54
18:1W:25:ARG:NH2	18:1W:74:ALA:O	2.37	0.54
26:24:48:ARG:O	26:24:50:VAL:N	2.39	0.54
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.88	0.54
32:2a:1411:C:H2'	32:2a:1412:C:H6	1.72	0.54
1:1A:100:G:N2	24:12:4:SER:HB3	2.21	0.54
1:1A:615:G:OP1	5:1F:40:GLN:NE2	2.40	0.54
6:1G:114:ILE:HG12	6:1G:140:ILE:HG12	1.90	0.54
32:1a:376:G:H4'	47:1p:5:ARG:HH11	1.73	0.54
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.40	0.54
32:1a:1347:G:H5"	40:1i:107:ARG:HB3	1.89	0.54
1:2A:108:U:H2'	1:2A:109:G:C8	2.43	0.54
32:2a:256:U:H2'	32:2a:257:G:C8	2.42	0.54
37:2f:35:ALA:HA	37:2f:67:MET:HB3	1.89	0.54
1:1A:2492:U:H2'	1:1A:2493:U:C6	2.43	0.54
32:1a:503:C:H2'	32:1a:504:C:H6	1.73	0.54
32:1a:568:G:O2'	32:1a:574:A:N1	2.37	0.54
41:1j:16:LEU:HD21	41:1j:70:ARG:HG2	1.90	0.54
42:1k:54:ARG:O	42:1k:57:THR:OG1	2.25	0.54
43:1l:53:ARG:HB3	43:1l:69:TYR:HE1	1.73	0.54
51:1t:64:ASP:OD1	51:1t:64:ASP:N	2.37	0.54
1:2A:2376:A:N6	60:2A:4178:HOH:O	2.41	0.54
10:2O:76:ALA:HB3	15:2T:75:ILE:HB	1.90	0.54
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.07	0.54
26:24:49:PHE:HB3	26:24:50:VAL:HG22	1.88	0.54
32:2a:1316:G:H4'	45:2n:18:VAL:HG11	1.90	0.54
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.42	0.54
15:1T:35:LYS:HG2	15:1T:40:THR:HG22	1.89	0.54
32:1a:1182:G:H4'	32:1a:1183:A:H5'	1.89	0.54
1:2A:854:G:H2'	1:2A:855:G:C8	2.43	0.54
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.37	0.54
11:2P:121:LYS:O	11:2P:123:LEU:N	2.40	0.54
25:23:6:VAL:HG22	25:23:56:VAL:HG13	1.87	0.54
32:2a:189(K):U:H2'	32:2a:189(L):G:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:166:ASP:HB3	33:2b:169:LYS:HB3	1.88	0.54
38:2g:114:ARG:HB2	38:2g:115:ARG:NH2	2.23	0.54
40:2i:3:GLN:HG2	40:2i:20:ARG:NE	2.21	0.54
1:1A:99:U:O4	20:1Y:8:LYS:NZ	2.41	0.54
7:1H:3:ARG:NH1	7:1H:4:ILE:H	2.05	0.54
15:1T:53:ARG:O	15:1T:59:THR:HB	2.08	0.54
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.89	0.54
36:1e:40:ARG:NH2	36:1e:68:GLU:OE2	2.40	0.54
44:1m:23:TYR:HB3	44:1m:67:GLU:HA	1.90	0.54
1:2A:1637:A:H4'	1:2A:2711:A:O2'	2.08	0.54
32:2a:21:G:H2'	32:2a:22:G:C8	2.43	0.54
32:2a:202:U:H5"	32:2a:203:U:H5	1.72	0.54
32:2a:1122:U:H2'	32:2a:1123:A:H8	1.73	0.54
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.88	0.54
1:1A:1478:G:O2'	1:1A:1558:A:N7	2.40	0.54
1:1A:1920:OMC:HM22	1:1A:1921:G:H5'	1.90	0.54
26:14:56:VAL:O	26:14:60:GLN:HB2	2.08	0.54
32:1a:407:G:H5"	35:1d:115:ARG:HG2	1.89	0.54
32:1a:984:C:H42	32:1a:1221:G:H1	1.53	0.54
46:1o:22:THR:OG1	46:1o:23:GLY:N	2.40	0.54
1:2A:1967:C:OP1	60:2A:3913:HOH:O	2.18	0.54
1:2A:2156:G:N7	1:2A:2157:G:N2	2.56	0.54
4:2E:178:GLU:OE1	4:2E:178:GLU:N	2.35	0.54
30:28:58:ILE:HG12	60:28:209:HOH:O	2.08	0.54
32:2a:560:U:H5'	32:2a:566:G:N2	2.23	0.54
32:2a:674:G:OP1	37:2f:87:ARG:NH2	2.41	0.54
34:2c:124:ILE:HD12	34:2c:196:LEU:HD12	1.90	0.54
1:1A:1083:U:H1'	1:1A:1086:A:N6	2.22	0.54
1:1A:1618:A:OP2	60:1A:4218:HOH:O	2.18	0.54
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.08	0.54
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.90	0.54
36:1e:103:GLY:O	36:1e:107:ARG:HB3	2.08	0.54
43:1l:70:ILE:HG12	43:1l:100:ILE:HD12	1.89	0.54
1:2A:200:U:O2	1:2A:386:G:N2	2.41	0.54
1:2A:588:U:H2'	1:2A:589:C:C6	2.42	0.54
1:2A:2882:A:OP1	13:2R:96:ARG:NH1	2.41	0.54
4:2E:51:PHE:O	4:2E:77:ILE:N	2.28	0.54
1:1A:236:C:H2'	1:1A:237:C:H6	1.73	0.54
1:1A:2526:G:N2	60:1A:4579:HOH:O	2.41	0.54
32:1a:316:G:OP2	32:1a:351:G:O2'	2.26	0.54
41:1j:49:VAL:HG23	45:1n:41:ARG:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:54:HIS:CD2	21:2Z:101:PRO:HG3	2.43	0.54
23:21:80:LEU:O	60:21:201:HOH:O	2.19	0.54
32:2a:109:A:C6	32:2a:326:G:C6	2.95	0.54
32:2a:756:C:H2'	32:2a:757:U:O4'	2.08	0.54
32:2a:854:G:N7	60:2a:3260:HOH:O	2.33	0.54
32:2a:1371:G:O3'	40:2i:69:GLY:HA3	2.07	0.54
1:1A:1381:G:N7	60:1A:4431:HOH:O	2.34	0.54
1:1A:1633:G:OP2	60:1A:4217:HOH:O	2.18	0.54
5:1F:64:ILE:HG21	5:1F:78:ILE:HG23	1.90	0.54
5:1F:195:ASP:HB2	5:1F:198:ALA:H	1.72	0.54
32:1a:446:G:O6	60:1a:3322:HOH:O	2.14	0.54
1:2A:84:A:N1	1:2A:98:G:O2'	2.39	0.54
1:2A:729:G:C6	3:2D:208:LYS:HB2	2.43	0.54
1:2A:2105:C:N4	1:2A:2184:G:H1	2.06	0.54
39:2h:110:ALA:HB3	39:2h:121:ASP:HB3	1.90	0.54
1:1A:2602:A:H4'	1:1A:2603:G:OP1	2.08	0.53
10:1O:8:LEU:HD22	10:1O:82:ASN:HB2	1.89	0.53
32:1a:881:G:OP2	43:1l:12:ARG:NH2	2.41	0.53
32:1a:1256:A:H3'	34:1c:27:LYS:HZ1	1.73	0.53
21:2Z:33:LEU:HD11	21:2Z:90:VAL:HG21	1.89	0.53
21:2Z:104:PHE:HB3	21:2Z:141:VAL:HG11	1.90	0.53
32:2a:1001:A:H2'	32:2a:1001(A):G:C8	2.43	0.53
1:1A:96:G:H4'	24:12:48:HIS:CD2	2.43	0.53
3:1D:221:VAL:HG22	3:1D:226:MET:HE2	1.90	0.53
32:1a:652:U:O4	32:1a:752:G:O2'	2.23	0.53
32:1a:657:G:H21	46:1o:22:THR:HG1	1.56	0.53
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.43	0.53
9:2N:67:LEU:O	9:2N:88:GLU:HG3	2.09	0.53
19:2X:88:LYS:HD2	19:2X:93:GLU:HG3	1.90	0.53
32:2a:297:G:N2	32:2a:300:A:OP2	2.41	0.53
39:2h:82:HIS:N	39:2h:138:TRP:O	2.41	0.53
39:2h:86:ILE:HG21	39:2h:133:LEU:HD22	1.89	0.53
44:2m:60:VAL:HG23	44:2m:64:TRP:HE3	1.72	0.53
51:2t:33:ILE:O	51:2t:37:SER:OG	2.16	0.53
1:1A:271(E):U:H2'	1:1A:271(F):C:C6	2.43	0.53
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.90	0.53
21:1Z:50:GLN:NE2	60:1Z:404:HOH:O	2.42	0.53
32:1a:1358:U:OP2	32:1a:1359:C:N4	2.41	0.53
35:1d:194:LEU:HD13	35:1d:195:ALA:H	1.73	0.53
1:2A:859:G:N2	1:2A:917:A:OP2	2.37	0.53
1:2A:1007:C:H5"	9:2N:35:ARG:NH1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1012:U:C5	9:2N:28:THR:HG21	2.44	0.53
1:2A:1790:C:H5"	1:2A:1791:A:OP1	2.07	0.53
2:2B:66:A:N6	2:2B:108:U:H3'	2.22	0.53
8:2I:84:GLY:O	8:2I:85:GLU:HB2	2.08	0.53
9:2N:58:ASP:OD1	9:2N:58:ASP:N	2.31	0.53
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.91	0.53
31:29:15:LYS:HB3	31:29:26:ILE:HG13	1.89	0.53
32:2a:1320:C:H2'	32:2a:1321:C:O4'	2.07	0.53
1:1A:1040:C:H2'	1:1A:1041:C:O4'	2.07	0.53
1:1A:2406:U:H2'	1:1A:2406:U:OP2	2.09	0.53
2:1B:91:C:H5'	12:1Q:18:LYS:HA	1.90	0.53
19:1X:63:LYS:O	19:1X:64:LYS:HD3	2.09	0.53
31:19:12:ASP:OD1	31:19:12:ASP:N	2.37	0.53
32:1a:1347:G:N1	32:1a:1374:A:OP2	2.24	0.53
1:2A:798:G:O6	60:2A:3902:HOH:O	2.17	0.53
1:2A:2228:G:O6	60:2A:3888:HOH:O	2.15	0.53
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.90	0.53
32:2a:646:U:H2'	32:2a:647:C:C6	2.43	0.53
32:2a:1024:G:H2'	32:2a:1025:U:H5"	1.90	0.53
38:2g:65:ALA:HB1	38:2g:127:ALA:HB3	1.89	0.53
43:2l:24:VAL:HB	43:2l:27:LEU:HD22	1.91	0.53
1:1A:826:U:OP1	60:1A:4156:HOH:O	2.19	0.53
1:1A:2133:G:N2	1:1A:2157:G:H2'	2.24	0.53
35:1d:61:LYS:HD2	35:1d:207:TYR:OH	2.09	0.53
1:2A:699:A:H2'	1:2A:700:G:O4'	2.09	0.53
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.44	0.53
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.90	0.53
33:2b:17:PHE:HB3	33:2b:44:LEU:HD21	1.89	0.53
40:2i:80:GLY:HA2	40:2i:83:ARG:HB2	1.89	0.53
1:1A:1666:G:O6	60:1A:4210:HOH:O	2.17	0.53
32:1a:339:C:H2'	32:1a:340:U:C6	2.44	0.53
35:1d:180:GLY:O	35:1d:182:LYS:NZ	2.41	0.53
1:2A:1533:G:N2	1:2A:1536:C:N3	2.55	0.53
1:1A:784:A:H5'	1:1A:785:G:OP1	2.08	0.53
32:1a:1320:C:H2'	32:1a:1321:C:O4'	2.09	0.53
33:1b:130:ARG:HH21	33:1b:138:LEU:HD11	1.74	0.53
1:2A:824:A:H1'	1:2A:2358:G:N7	2.24	0.53
1:2A:1016:G:H2'	1:2A:1017:G:H8	1.73	0.53
1:2A:2102:U:H2'	1:2A:2103:C:C6	2.43	0.53
1:2A:2615:U:OP1	60:2A:3926:HOH:O	2.19	0.53
7:2H:3:ARG:HE	7:2H:54:ARG:HH12	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:258:G:H2'	32:2a:259:G:C8	2.43	0.53
32:2a:735:C:H2'	32:2a:736:C:H6	1.74	0.53
45:2n:24:CYS:HB3	45:2n:29:ARG:H	1.73	0.53
1:1A:754:C:H2'	1:1A:755:C:C6	2.44	0.53
1:1A:761:A:H5"	60:1A:5736:HOH:O	2.08	0.53
6:1G:82:LEU:HD21	6:1G:88:ILE:HD13	1.91	0.53
32:1a:58:C:O2'	32:1a:388:G:N7	2.35	0.53
32:1a:62:U:O2'	32:1a:379:C:O2	2.23	0.53
32:1a:454:C:OP1	47:1p:75:ARG:NH2	2.41	0.53
32:1a:737:A:H2'	32:1a:738:C:C6	2.43	0.53
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.43	0.53
33:1b:54:THR:HG21	33:1b:201:ILE:HD11	1.90	0.53
5:2F:150:GLY:HA2	5:2F:172:TRP:CE3	2.44	0.53
9:2N:102:ALA:O	9:2N:106:MET:HG3	2.09	0.53
24:22:24:LEU:HD23	24:22:60:LEU:HD21	1.91	0.53
32:2a:914:A:O5'	60:2a:3223:HOH:O	2.18	0.53
32:2a:1073:U:O2'	33:2b:104:ASN:OD1	2.23	0.53
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.08	0.53
32:2a:1391:U:H2'	32:2a:1392:G:C8	2.43	0.53
40:2i:51:ARG:HG2	40:2i:56:LEU:HD21	1.89	0.53
32:1a:656:C:O2'	46:1o:28:GLN:NE2	2.40	0.53
38:1g:113:GLU:HG2	38:1g:119:ARG:HG2	1.91	0.53
1:2A:18:C:OP1	60:2A:3917:HOH:O	2.18	0.53
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	1.91	0.53
32:2a:141:A:H1'	32:2a:182:U:O2	2.09	0.53
32:2a:406:G:H5'	35:2d:5:ILE:HD11	1.90	0.53
32:2a:1502:A:H5'	32:2a:1504:G:N7	2.23	0.53
35:2d:57:ARG:HB3	35:2d:206:PHE:HB2	1.91	0.53
1:1A:1709:U:H2'	1:1A:1710:C:C6	2.44	0.53
32:1a:452:A:O2'	32:1a:453:A:OP2	2.27	0.53
36:1e:57:LYS:HG2	36:1e:61:TYR:CE2	2.43	0.53
39:1h:39:LEU:HB3	39:1h:45:ILE:HG12	1.90	0.53
1:2A:199:A:OP2	60:2A:3925:HOH:O	2.19	0.53
1:2A:458:G:O2'	1:2A:469:G:O6	2.25	0.53
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.44	0.53
4:2E:101:ARG:NH2	4:2E:171:GLU:HB2	2.24	0.53
6:2G:145:THR:HG23	6:2G:147:ASP:H	1.73	0.53
33:2b:102:LEU:HD23	33:2b:182:ILE:HD12	1.89	0.53
1:1A:774:A:N3	1:1A:774:A:H2'	2.24	0.52
1:1A:1094:U:H1'	1:1A:1097:U:H5	1.74	0.52
8:1I:10:GLU:O	8:1I:12:LEU:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:189(A):C:N4	32:1a:189(J):G:O6	2.43	0.52
34:1c:18:TRP:H	34:1c:18:TRP:HE3	1.56	0.52
37:1f:68:PRO:HG2	37:1f:71:ARG:HD2	1.92	0.52
1:2A:530:G:O6	60:2A:3903:HOH:O	2.19	0.52
1:2A:635:C:O2'	1:2A:639:U:OP1	2.27	0.52
1:2A:1068:G:OP1	1:2A:1095:A:O2'	2.25	0.52
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.44	0.52
21:2Z:153:SER:OG	21:2Z:154:ASP:N	2.42	0.52
22:20:27:GLU:HB2	22:20:69:PHE:HD1	1.74	0.52
32:2a:19:C:H5"	36:2e:86:ALA:HB3	1.90	0.52
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.43	0.52
1:1A:1266:G:O2'	1:1A:2012:G:O6	2.18	0.52
32:1a:108:G:N1	51:1t:15:ARG:HG2	2.25	0.52
32:1a:184:G:H2'	32:1a:185:A:H8	1.75	0.52
32:1a:1347:G:C8	40:1i:107:ARG:HB2	2.45	0.52
38:1g:9:VAL:O	38:1g:11:GLN:NE2	2.42	0.52
38:1g:79:ARG:HA	38:1g:84:ASN:HA	1.91	0.52
39:1h:83:ILE:HA	39:1h:136:GLU:O	2.09	0.52
1:2A:18:C:O2'	1:2A:554:U:OP1	2.27	0.52
1:2A:1065:U:H4'	1:2A:1066:U:H5'	1.91	0.52
1:2A:1069:A:H2'	1:2A:1073:A:N7	2.24	0.52
1:2A:1695:G:N7	3:2D:14:ARG:NH2	2.57	0.52
1:2A:2655:G:O2'	1:2A:2664:G:O6	2.23	0.52
5:2F:183:VAL:O	5:2F:187:VAL:HG23	2.09	0.52
12:2Q:11:LYS:HD3	12:2Q:87:LYS:HG2	1.91	0.52
34:2c:36:ASP:O	34:2c:40:ARG:HG3	2.09	0.52
35:2d:78:LEU:HD22	35:2d:96:LEU:HB3	1.91	0.52
42:2k:61:ALA:HB1	42:2k:94:ALA:HB2	1.90	0.52
1:1A:848:G:H2'	1:1A:849:A:C8	2.44	0.52
1:1A:1359:A:N3	1:1A:1359:A:H5'	2.25	0.52
1:1A:1794:U:H2'	1:1A:1795:C:H6	1.74	0.52
1:1A:2181:G:H2'	1:1A:2182:G:C8	2.45	0.52
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.44	0.52
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.09	0.52
32:1a:279:A:C8	48:1q:98:LEU:HD23	2.45	0.52
32:1a:437:U:H5'	35:1d:155:LEU:HD21	1.91	0.52
36:1e:122:GLU:O	36:1e:126:ARG:NH1	2.41	0.52
47:1p:19:ILE:HG13	47:1p:36:ILE:HG13	1.92	0.52
1:2A:116:C:H2'	1:2A:117:G:O4'	2.09	0.52
1:2A:974:G:N2	60:2A:4126:HOH:O	2.38	0.52
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2889:C:H2'	1:2A:2891:G:O4'	2.09	0.52
32:2a:460:G:H2'	32:2a:461:A:H2'	1.91	0.52
1:1A:1227:G:OP2	16:1U:16:LYS:NZ	2.40	0.52
1:1A:1468:C:OP1	60:1A:4227:HOH:O	2.19	0.52
1:1A:2537:U:H2'	1:1A:2538:C:C6	2.44	0.52
4:1E:47:VAL:HG13	4:1E:49:LEU:HD13	1.90	0.52
34:1c:35:GLU:HG2	34:1c:39:ILE:HD11	1.91	0.52
35:1d:60:GLU:OE1	35:1d:199:ASN:N	2.42	0.52
1:2A:600:G:OP1	5:2F:29:ASN:ND2	2.42	0.52
1:2A:1638:C:OP1	1:2A:2710:C:O2'	2.28	0.52
1:2A:1709:U:H2'	1:2A:1710:C:C6	2.45	0.52
1:2A:2286:A:H4'	1:2A:2287:A:O4'	2.09	0.52
1:2A:2815:C:H5'	27:25:29:THR:HG21	1.90	0.52
32:2a:1347:G:C8	40:2i:107:ARG:HB3	2.45	0.52
1:1A:1968:G:OP1	60:1A:4219:HOH:O	2.19	0.52
2:1B:95:C:N4	60:1B:312:HOH:O	2.26	0.52
13:1R:22:ARG:HG2	13:1R:69:ASP:HB3	1.92	0.52
43:1l:24:VAL:HB	43:1l:27:LEU:HD22	1.91	0.52
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.09	0.52
1:2A:2104:G:O6	1:2A:2185:C:C4	2.62	0.52
1:2A:2679:A:H4'	4:2E:165:VAL:HG11	1.92	0.52
2:2B:50:G:OP1	14:2S:63:THR:OG1	2.25	0.52
8:2I:95:LYS:N	60:2I:301:HOH:O	2.29	0.52
32:2a:857:C:H2'	32:2a:858:G:O4'	2.09	0.52
53:2y:82:GLU:OE1	60:2y:301:HOH:O	2.19	0.52
1:1A:251:A:C5	1:1A:252:G:H1'	2.44	0.52
23:11:4:VAL:HG22	23:11:11:ARG:HG3	1.92	0.52
32:1a:299:G:O6	60:1a:3320:HOH:O	2.14	0.52
36:1e:6:PHE:HZ	36:1e:40:ARG:HE	1.57	0.52
41:1j:81:THR:C	41:1j:83:GLU:H	2.17	0.52
44:1m:4:ILE:HG13	44:1m:4:ILE:O	2.10	0.52
51:1t:57:ARG:HH22	51:1t:100:ILE:HD12	1.75	0.52
1:2A:885:C:H2'	1:2A:886:C:O4'	2.10	0.52
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.44	0.52
2:2B:42:C:O2'	6:2G:66:GLN:HG2	2.09	0.52
32:2a:1054:C:OP2	60:2a:3224:HOH:O	2.19	0.52
33:2b:71:VAL:HG23	33:2b:164:VAL:HA	1.91	0.52
35:2d:79:PHE:CE1	35:2d:204:ILE:HD13	2.44	0.52
1:1A:1930:G:OP1	60:1A:4223:HOH:O	2.19	0.52
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.45	0.52
32:1a:524:G:H2'	32:1a:525:C:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1y:85:LEU:O	53:1y:89:GLN:HG2	2.09	0.52
1:2A:372:G:O2'	1:2A:400:G:O6	2.24	0.52
1:2A:1064:C:H3'	1:2A:1065:U:H5'	1.92	0.52
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.25	0.52
1:2A:2105:C:N4	1:2A:2106:G:O6	2.43	0.52
1:2A:2126:A:H4'	1:2A:2127:G:O5'	2.09	0.52
1:2A:2331:G:O2'	22:20:43:THR:HG22	2.10	0.52
21:2Z:125:LEU:HG	21:2Z:164:ALA:HB3	1.91	0.52
32:2a:1080:A:OP1	36:2e:47:LYS:HD3	2.09	0.52
33:2b:168:THR:OG1	33:2b:192:SER:HA	2.09	0.52
36:2e:100:VAL:HA	36:2e:118:ILE:HG22	1.92	0.52
44:2m:49:THR:OG1	44:2m:52:GLU:OE1	2.27	0.52
1:1A:1937:A:H1'	1:1A:1939:5MU:H72	1.92	0.52
12:1Q:57:HIS:HD2	12:1Q:117:ALA:HB2	1.75	0.52
32:1a:690:G:C6	32:1a:691:G:C6	2.98	0.52
37:1f:44:GLY:HA2	37:1f:59:TYR:CE1	2.45	0.52
42:1k:61:ALA:HB1	42:1k:94:ALA:HB2	1.92	0.52
1:2A:531:C:OP2	60:2A:3922:HOH:O	2.18	0.52
1:2A:586:A:N1	1:2A:809:G:O2'	2.39	0.52
1:2A:644:A:H4'	1:2A:645:C:H5	1.74	0.52
1:2A:1740:G:H2'	1:2A:1741:A:C8	2.44	0.52
3:2D:73:VAL:HG13	3:2D:120:GLY:HA3	1.92	0.52
4:2E:38:THR:OG1	4:2E:41:LYS:N	2.43	0.52
7:2H:163:TYR:CE1	7:2H:169:VAL:HG22	2.45	0.52
13:2R:67:LEU:HD12	13:2R:76:VAL:HG21	1.92	0.52
32:2a:517:G:C2	32:2a:531:U:H5'	2.44	0.52
32:2a:598:U:H2'	32:2a:599:C:C6	2.45	0.52
32:2a:1118:C:H1'	32:2a:1179:A:C5	2.45	0.52
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.45	0.52
43:2l:7:ILE:O	43:2l:11:VAL:HG23	2.10	0.52
52:2u:6:ARG:HE	52:2u:15:ARG:HH12	1.57	0.52
1:1A:526:A:OP1	60:1A:4225:HOH:O	2.19	0.52
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.45	0.52
20:1Y:14:LEU:HB2	20:1Y:75:ILE:HD11	1.92	0.52
32:1a:578:C:O2'	32:1a:728:A:N3	2.40	0.52
1:2A:888:C:H2'	1:2A:889:C:C2	2.44	0.52
1:2A:1287:A:H8	13:2R:104:ARG:HD3	1.74	0.52
32:2a:188:C:O4'	51:2t:89:ARG:NH2	2.43	0.52
32:2a:1095:U:H2'	32:2a:1096:C:C6	2.45	0.52
33:2b:127:ILE:C	33:2b:129:GLU:H	2.18	0.52
48:2q:64:PRO:HB3	48:2q:70:ARG:HH11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:2s:58:VAL:HG21	50:2s:75:ALA:HA	1.92	0.52
1:1A:2046:G:H5'	27:15:19:ARG:HG3	1.92	0.52
4:1E:2:LYS:HB2	4:1E:95:ILE:HD12	1.91	0.52
25:13:18:ASP:OD1	25:13:18:ASP:N	2.42	0.52
32:1a:979:C:H42	45:1n:18:VAL:HB	1.74	0.52
39:1h:81:HIS:N	39:1h:138:TRP:O	2.43	0.52
40:1i:8:GLY:HA3	40:1i:76:ALA:O	2.10	0.52
1:2A:315:G:H2'	1:2A:316:C:C6	2.44	0.52
1:2A:641:C:O2'	1:2A:2350:C:OP1	2.17	0.52
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.43	0.52
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.45	0.52
1:2A:2602:A:H1'	1:2A:2603:G:C5'	2.39	0.52
14:2S:62:LYS:HA	14:2S:65:VAL:HB	1.91	0.52
21:2Z:152:ALA:HA	21:2Z:155:LEU:HD22	1.92	0.52
32:2a:255:G:H2'	32:2a:256:U:C6	2.45	0.52
32:2a:992:U:H4'	32:2a:993:G:O5'	2.09	0.52
1:1A:1064:C:H3'	1:1A:1065:U:C5'	2.38	0.51
1:1A:1155:A:OP1	60:1A:4228:HOH:O	2.19	0.51
6:1G:64:THR:HB	6:1G:94:LEU:HD21	1.92	0.51
22:10:10:THR:HA	60:10:214:HOH:O	2.10	0.51
32:1a:116:A:H61	32:1a:313:A:H1'	1.75	0.51
32:1a:160:A:H2'	32:1a:161:A:O4'	2.10	0.51
32:1a:1030(C):G:H2'	32:1a:1030(D):A:C8	2.43	0.51
32:1a:1065:U:H5"	32:1a:1190:G:N2	2.26	0.51
44:1m:90:LEU:HA	44:1m:93:ARG:HG3	1.92	0.51
50:1s:12:ASP:OD1	50:1s:37:ARG:NH1	2.38	0.51
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.92	0.51
1:2A:2115:G:N2	1:2A:2119:A:H5'	2.25	0.51
4:2E:29:GLY:HA3	60:2E:411:HOH:O	2.09	0.51
10:2O:68:GLU:HB3	10:2O:78:ARG:HB2	1.92	0.51
10:2O:75:SER:OG	10:2O:76:ALA:N	2.43	0.51
32:2a:338:A:H2	32:2a:351:G:H22	1.58	0.51
32:2a:1268:A:N3	32:2a:1326:C:O2'	2.43	0.51
32:2a:1457:G:H5"	51:2t:35:THR:HG21	1.92	0.51
36:2e:78:HIS:CD2	36:2e:142:LEU:HD23	2.45	0.51
38:2g:113:GLU:O	38:2g:119:ARG:NH1	2.38	0.51
43:2l:33:ARG:HH11	43:2l:62:SER:HB3	1.75	0.51
1:1A:330:A:HO2'	1:1A:331:A:H8	1.56	0.51
1:1A:1045:A:H1'	1:1A:1047:G:N3	2.24	0.51
1:1A:2846:G:H2'	1:1A:2847:U:O4'	2.10	0.51
2:1B:66:A:H61	2:1B:108:U:H2'	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.22	0.51
6:1G:146:TYR:O	6:1G:149:VAL:HG12	2.09	0.51
8:1I:40:THR:OG1	8:1I:41:GLU:N	2.43	0.51
13:1R:67:LEU:HD22	13:1R:76:VAL:HG21	1.92	0.51
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	1.91	0.51
21:1Z:128:VAL:HG23	21:1Z:161:VAL:HB	1.92	0.51
32:1a:833:U:H2'	32:1a:834:C:C6	2.45	0.51
32:1a:1129:C:H42	32:1a:1143:G:H1	1.57	0.51
40:1i:9:ARG:HB3	40:1i:104:ARG:NH2	2.25	0.51
3:2D:132:PRO:HG2	3:2D:135:PHE:CD2	2.46	0.51
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.83	0.51
32:2a:407:G:H5"	35:2d:115:ARG:HB3	1.93	0.51
53:2y:65:GLY:N	53:2y:77:LEU:HB2	2.24	0.51
1:1A:801:G:OP2	60:1A:4215:HOH:O	2.18	0.51
1:1A:1823:G:OP1	3:1D:54:ARG:NH1	2.44	0.51
1:1A:2111:C:H42	1:1A:2147:G:H22	1.57	0.51
1:1A:2137:C:H42	1:1A:2154:G:H1	1.58	0.51
6:1G:103:LEU:HD23	6:1G:106:LEU:HD23	1.92	0.51
11:1P:140:ALA:O	25:23:38:GLU:HG2	2.10	0.51
16:1U:49:HIS:HA	16:1U:52:ARG:HG2	1.93	0.51
19:1X:35:THR:HG22	19:1X:38:GLU:HB3	1.91	0.51
32:1a:1118:C:H1'	32:1a:1179:A:C5	2.46	0.51
35:1d:116:GLN:NE2	35:1d:157:LEU:HD21	2.25	0.51
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	1.91	0.51
1:2A:871:U:H2'	1:2A:872:A:C8	2.45	0.51
1:2A:944:G:O3'	60:2A:3927:HOH:O	2.19	0.51
1:2A:2533:A:OP1	1:2A:2665:A:O2'	2.23	0.51
1:2A:2647:U:H2'	1:2A:2648:C:C6	2.45	0.51
1:2A:2698:U:H2'	1:2A:2699:C:C6	2.46	0.51
6:2G:113:ARG:NH2	6:2G:141:PHE:O	2.44	0.51
13:2R:42:LYS:HB3	13:2R:45:ARG:NH2	2.25	0.51
21:2Z:5:LEU:HB2	21:2Z:47:VAL:HG21	1.92	0.51
32:2a:920:U:H2'	32:2a:921:U:C6	2.45	0.51
32:2a:973:G:H3'	32:2a:974:A:H5"	1.93	0.51
33:2b:204:ASN:O	33:2b:210:SER:OG	2.20	0.51
38:2g:51:GLN:HB2	38:2g:58:PRO:HD3	1.92	0.51
1:1A:749:C:OP2	60:1A:4224:HOH:O	2.19	0.51
1:1A:1430:C:H2'	1:1A:1431:U:H6	1.76	0.51
1:1A:1798:U:H5'	3:1D:259:THR:CG2	2.41	0.51
1:1A:2689:U:H4'	1:1A:2690:C:H5'	1.91	0.51
13:1R:24:GLN:NE2	60:1R:307:HOH:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:262:A:H2'	32:1a:263:A:C8	2.44	0.51
34:1c:105:GLU:HG2	34:1c:106:VAL:H	1.75	0.51
1:2A:601:C:OP1	5:2F:108:LYS:NZ	2.38	0.51
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.11	0.51
7:2H:3:ARG:HG2	7:2H:6:ARG:CZ	2.41	0.51
12:2Q:109:VAL:O	60:2Q:302:HOH:O	2.19	0.51
18:2W:27:LYS:O	18:2W:71:VAL:HG23	2.10	0.51
38:2g:45:ASP:O	38:2g:49:ILE:HG13	2.10	0.51
1:1A:376:C:OP1	60:1A:4213:HOH:O	2.18	0.51
2:1B:103:G:O6	60:1B:307:HOH:O	2.18	0.51
4:1E:140:SER:O	60:1E:403:HOH:O	2.19	0.51
32:1a:180:U:O2	32:1a:196:A:N6	2.42	0.51
32:1a:198:G:H2'	32:1a:199:G:C8	2.46	0.51
32:1a:922:G:H4'	36:1e:20:GLN:HA	1.92	0.51
49:1r:58:LEU:HD23	49:1r:62:GLU:HB3	1.92	0.51
1:2A:1056:G:H5"	1:2A:1057:A:H5'	1.91	0.51
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.45	0.51
1:2A:2684:U:H1'	10:2O:70:LYS:HD2	1.92	0.51
4:2E:9:VAL:HG22	4:2E:25:VAL:HB	1.93	0.51
6:2G:27:ASN:HB3	6:2G:30:GLU:HB2	1.93	0.51
32:2a:108:G:C6	51:2t:15:ARG:HG2	2.45	0.51
32:2a:1145:C:H5"	32:2a:1146:A:OP1	2.09	0.51
32:2a:1362:C:H2'	32:2a:1363:C:H5"	1.91	0.51
33:2b:11:LEU:HD13	33:2b:217:ARG:HH22	1.76	0.51
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.09	0.51
7:1H:159:GLU:HG2	7:1H:169:VAL:HG11	1.91	0.51
13:1R:12:ARG:O	13:1R:17:ARG:NH1	2.43	0.51
32:1a:254:G:N2	48:1q:16:GLN:OE1	2.37	0.51
32:1a:864:A:OP2	60:1a:3331:HOH:O	2.19	0.51
1:2A:995:C:O2	9:2N:3:THR:OG1	2.25	0.51
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.45	0.51
60:2A:4036:HOH:O	18:2W:18:ARG:HD3	2.10	0.51
3:2D:132:PRO:HD3	3:2D:190:TYR:CZ	2.46	0.51
32:2a:1103:C:OP1	33:2b:96:ARG:NH2	2.44	0.51
35:2d:127:THR:HA	35:2d:132:ARG:HA	1.92	0.51
36:2e:74:GLY:HA3	36:2e:116:THR:HG22	1.91	0.51
3:1D:108:PRO:HG3	3:1D:143:HIS:CE1	2.46	0.51
24:12:28:LYS:HG2	24:12:53:LEU:HD21	1.93	0.51
1:2A:463:G:OP1	60:2A:3933:HOH:O	2.19	0.51
1:2A:848:G:H2'	1:2A:849:A:C8	2.46	0.51
21:2Z:42:VAL:O	21:2Z:46:LYS:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2f:24:GLU:O	37:2f:28:ARG:HB3	2.10	0.51
1:1A:839:U:H1'	1:1A:1191:G:H1'	1.92	0.51
4:1E:1:MET:HE2	4:1E:202:LYS:HE2	1.93	0.51
32:1a:424:G:H2'	32:1a:425:G:C8	2.46	0.51
32:1a:1004:A:O2'	32:1a:1038:C:O2	2.26	0.51
33:1b:207:ALA:O	33:1b:210:SER:N	2.42	0.51
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	1.92	0.51
37:1f:6:VAL:HG22	37:1f:90:VAL:HG22	1.93	0.51
1:2A:1064:C:H3'	1:2A:1065:U:C5'	2.40	0.51
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.10	0.51
1:2A:2250:G:O2'	1:2A:2496:C:OP1	2.23	0.51
21:2Z:39:VAL:HG21	21:2Z:44:PHE:HB2	1.93	0.51
32:2a:148:G:H1	32:2a:174:C:H42	1.59	0.51
32:2a:1279:A:H2'	32:2a:1279:A:N3	2.26	0.51
33:2b:16:HIS:CG	33:2b:210:SER:HB3	2.45	0.51
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.93	0.51
47:2p:48:TRP:CD1	47:2p:48:TRP:H	2.29	0.51
1:1A:1754:C:OP1	15:1T:96:ARG:NH1	2.44	0.51
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.25	0.51
5:1F:30:PRO:HB3	11:1P:1:MET:HE1	1.93	0.51
10:1O:64:ARG:HB2	10:1O:79:PHE:CG	2.45	0.51
32:1a:648:A:H2'	32:1a:649:G:H8	1.75	0.51
35:1d:76:ARG:HD3	35:1d:207:TYR:CE1	2.46	0.51
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.10	0.51
1:2A:1648:C:OP1	60:2A:3909:HOH:O	2.19	0.51
1:2A:1998:G:O2'	1:2A:2724:C:O2'	2.28	0.51
4:2E:11:MET:HG2	4:2E:24:THR:HG23	1.93	0.51
7:2H:113:VAL:HG11	7:2H:151:ILE:HG21	1.93	0.51
10:2O:94:ARG:N	60:2O:306:HOH:O	2.44	0.51
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.93	0.51
26:24:34:GLU:HB2	44:2m:57:ARG:CZ	2.40	0.51
32:2a:102:G:H2'	32:2a:103:C:C6	2.46	0.51
32:2a:943:U:H1'	40:2i:124:GLN:HE22	1.76	0.51
35:2d:31:CYS:SG	35:2d:33:MET:HB2	2.51	0.51
36:2e:12:LEU:HB3	36:2e:31:LEU:HB2	1.92	0.51
36:2e:69:VAL:HG11	36:2e:113:ALA:HB1	1.92	0.51
1:1A:1278:A:OP1	13:1R:36:THR:HG23	2.10	0.51
1:1A:1939:5MU:OP1	1:1A:2604:U:O2'	2.28	0.51
1:1A:2206:G:OP2	1:1A:2206:G:H4'	2.10	0.51
32:1a:17:U:H2'	32:1a:18:C:C6	2.46	0.51
32:1a:266:G:H2'	32:1a:266:G:N3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1356:G:H2'	32:1a:1357:A:H8	1.71	0.51
34:1c:180:ALA:HB1	34:1c:203:PHE:HE1	1.76	0.51
35:1d:65:ARG:NH1	35:1d:70:ILE:O	2.44	0.51
44:1m:11:ARG:C	44:1m:13:LYS:H	2.19	0.51
44:1m:52:GLU:HA	44:1m:55:ARG:HG3	1.93	0.51
1:2A:1079:C:N3	1:2A:1080:C:H1'	2.26	0.51
1:2A:2690:C:N4	1:2A:2713:A:H1'	2.25	0.51
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG11	1.92	0.51
32:2a:1190:G:H5'	34:2c:176:HIS:CE1	2.46	0.51
40:2i:3:GLN:HE21	40:2i:20:ARG:HH21	1.59	0.51
1:1A:614(B):G:OP1	57:1F:317:ARG:N	2.44	0.50
1:1A:768:G:O2'	1:1A:1379:A:N1	2.38	0.50
1:1A:1359:A:N1	1:1A:1372:U:O4	2.44	0.50
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.45	0.50
4:1E:59:VAL:HG21	4:1E:74:PRO:HB3	1.93	0.50
7:1H:88:LEU:HD23	7:1H:130:ARG:HG3	1.93	0.50
9:1N:58:ASP:OD1	9:1N:58:ASP:N	2.44	0.50
26:14:46:GLN:O	26:14:48:ARG:N	2.44	0.50
32:1a:359:U:H2'	32:1a:360:A:C8	2.47	0.50
32:1a:376:G:H2'	32:1a:377:G:C8	2.46	0.50
32:1a:659:U:H2'	32:1a:660:G:C8	2.46	0.50
32:1a:691:G:H2'	32:1a:692:U:C6	2.46	0.50
32:1a:721:G:H4'	32:1a:722:A:O4'	2.11	0.50
32:1a:1157:A:H1'	32:1a:1181:G:N2	2.26	0.50
32:1a:1316:G:H5"	45:1n:17:LYS:NZ	2.25	0.50
1:2A:207:A:H2'	1:2A:208:C:O4'	2.11	0.50
1:2A:1063:G:N2	1:2A:1075:C:H42	2.03	0.50
1:2A:1966:A:N3	1:2A:2592:G:O2'	2.37	0.50
3:2D:71:ASP:HB3	3:2D:103:ARG:HH22	1.76	0.50
4:2E:105:THR:HG21	4:2E:164:ARG:NH1	2.26	0.50
23:21:77:ALA:HA	23:21:80:LEU:HD22	1.92	0.50
26:24:47:GLN:C	26:24:49:PHE:H	2.19	0.50
32:2a:741:G:H5"	46:2o:59:MET:HE1	1.93	0.50
42:2k:62:GLN:HG3	42:2k:97:ALA:HB2	1.93	0.50
44:2m:10:PRO:HG2	44:2m:13:LYS:HD2	1.93	0.50
44:2m:13:LYS:HE3	44:2m:21:TYR:CZ	2.46	0.50
1:1A:2572:A:N7	4:1E:144:ARG:HD2	2.25	0.50
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.46	0.50
8:1I:57:ARG:HA	8:1I:60:GLU:HB3	1.92	0.50
12:1Q:21:THR:HG21	12:1Q:101:ARG:N	2.26	0.50
15:1T:13:ARG:HB3	15:1T:13:ARG:HH11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1003:G:O2'	32:1a:1004:A:H4'	2.11	0.50
32:1a:1320:C:H1'	50:1s:73:GLU:HG2	1.93	0.50
32:1a:1417:G:H2'	32:1a:1482:G:N2	2.26	0.50
36:1e:74:GLY:HA3	36:1e:116:THR:HG22	1.92	0.50
38:1g:54:THR:O	38:1g:56:GLN:NE2	2.44	0.50
40:1i:9:ARG:HB3	40:1i:104:ARG:HH21	1.76	0.50
1:2A:107:C:H2'	1:2A:108:U:H6	1.76	0.50
1:2A:1657:C:H2'	1:2A:1658:C:H6	1.76	0.50
1:2A:1998:G:HO2'	1:2A:2724:C:HO2'	1.60	0.50
1:2A:2342:C:O2'	1:2A:2374:C:H5"	2.12	0.50
6:2G:54:GLU:O	6:2G:58:GLN:N	2.43	0.50
7:2H:9:ILE:HB	7:2H:50:VAL:HB	1.92	0.50
7:2H:101:ARG:NH2	7:2H:117:PRO:O	2.44	0.50
32:2a:23:C:H5	32:2a:561:U:O4	1.94	0.50
43:2l:110:VAL:O	43:2l:122:THR:OG1	2.27	0.50
1:1A:2001:A:H2'	1:1A:2002:G:C8	2.45	0.50
1:1A:2405:G:O2'	1:1A:2406:U:OP1	2.25	0.50
24:12:65:ASN:ND2	60:12:103:HOH:O	2.44	0.50
25:13:55:ARG:NH1	60:13:202:HOH:O	2.34	0.50
32:1a:64:G:H4'	32:1a:65:U:H3'	1.93	0.50
53:1y:37:PRO:HB3	53:1y:54:ILE:HG12	1.93	0.50
1:2A:1027:A:C2	1:2A:2488:A:H5'	2.47	0.50
1:2A:2305:A:H5"	6:2G:134:GLY:HA3	1.93	0.50
6:2G:32:PRO:HB3	6:2G:163:ALA:HB2	1.94	0.50
32:2a:266:G:N3	32:2a:266:G:H5"	2.26	0.50
32:2a:1083:U:OP2	60:2a:3220:HOH:O	2.18	0.50
1:1A:2557:G:H2'	1:1A:2558:C:C6	2.46	0.50
5:2F:126:VAL:HG21	5:2F:129:PHE:CZ	2.47	0.50
10:2O:120:GLU:HG2	10:2O:122:LEU:HG	1.93	0.50
32:2a:952:U:H2'	32:2a:953:G:C8	2.43	0.50
32:2a:1172:C:H2'	32:2a:1173:G:C8	2.46	0.50
33:2b:178:ARG:HH12	39:2h:68:ARG:HH22	1.59	0.50
41:2j:11:PHE:HE1	41:2j:67:THR:HG22	1.75	0.50
1:1A:61:G:H5'	24:12:50:ILE:HG21	1.94	0.50
1:1A:1833:U:O2'	1:1A:1969:A:N1	2.35	0.50
1:1A:2004:G:OP2	60:1A:4221:HOH:O	2.19	0.50
3:1D:67:PHE:HE1	3:1D:106:ILE:HD11	1.75	0.50
32:1a:262:A:C6	32:1a:263:A:C6	2.99	0.50
32:1a:487:A:H2'	32:1a:488:C:O4'	2.11	0.50
32:1a:598:U:H4'	39:1h:94:TYR:CD2	2.46	0.50
32:1a:927:G:O2'	32:1a:1503:A:N7	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.25	0.50
1:2A:249:C:OP2	60:2A:3936:HOH:O	2.20	0.50
1:2A:1627:G:OP1	60:2A:3928:HOH:O	2.19	0.50
1:2A:2000:G:OP1	13:2R:5:LYS:NZ	2.40	0.50
1:2A:2035:G:OP1	60:2A:3935:HOH:O	2.20	0.50
1:2A:2482:G:OP2	60:2A:3934:HOH:O	2.20	0.50
1:2A:2785:C:OP1	4:2E:41:LYS:NZ	2.34	0.50
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	1.94	0.50
5:2F:85:GLY:O	60:2F:401:HOH:O	2.20	0.50
7:2H:54:ARG:HB3	7:2H:65:HIS:CD2	2.47	0.50
32:2a:1314:C:H2'	32:2a:1315:U:C6	2.47	0.50
38:2g:75:VAL:HG13	38:2g:145:ALA:HA	1.92	0.50
43:2l:70:ILE:HG12	43:2l:100:ILE:HD12	1.94	0.50
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.47	0.50
6:1G:101:ILE:HD13	26:14:25:TYR:HB2	1.94	0.50
11:1P:65:ARG:HG2	56:18:105:MPD:O2	2.11	0.50
14:1S:103:GLU:O	14:1S:107:GLU:HG3	2.12	0.50
32:1a:835:U:OP1	49:1r:64:ARG:NH1	2.41	0.50
32:1a:1297:C:O2	38:1g:114:ARG:NH1	2.45	0.50
42:1k:46:GLY:HA2	42:1k:50:TYR:O	2.11	0.50
1:2A:1464:C:H2'	1:2A:1465:G:C8	2.47	0.50
1:2A:1891:G:O6	60:2A:3918:HOH:O	2.18	0.50
6:2G:171:ALA:O	6:2G:175:LEU:N	2.34	0.50
32:2a:536:C:H2'	32:2a:537:G:C8	2.47	0.50
32:2a:1220:G:H2'	32:2a:1221:G:C8	2.47	0.50
33:2b:146:GLN:O	33:2b:150:SER:HB2	2.11	0.50
37:2f:68:PRO:HB2	37:2f:71:ARG:HD2	1.94	0.50
44:2m:39:ILE:HG12	44:2m:52:GLU:HG2	1.92	0.50
44:2m:80:ARG:O	44:2m:84:ILE:HG23	2.10	0.50
46:2o:24:SER:OG	46:2o:25:THR:N	2.43	0.50
47:2p:43:LYS:HG2	47:2p:48:TRP:CG	2.47	0.50
1:1A:832:G:OP1	60:1A:4230:HOH:O	2.19	0.50
1:1A:2099:U:H3	1:1A:2190:G:H1	1.58	0.50
4:1E:174:ASP:OD1	4:1E:175:VAL:N	2.45	0.50
9:1N:9:VAL:HG21	9:1N:39:ARG:HH22	1.77	0.50
19:1X:11:PRO:HB3	19:1X:92:LEU:HD11	1.93	0.50
1:2A:205:G:O6	23:21:39:LYS:NZ	2.27	0.50
1:2A:858:U:OP2	22:20:77:ARG:NH2	2.44	0.50
1:2A:2144:U:O2'	1:2A:2147:G:N1	2.38	0.50
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.75	0.50
2:2B:75:G:N7	60:2B:313:HOH:O	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:32:LEU:HD11	5:2F:105:VAL:HG13	1.94	0.50
5:2F:164:ARG:HD2	5:2F:175:THR:HG23	1.93	0.50
11:2P:55:ARG:HA	60:2P:301:HOH:O	2.10	0.50
15:2T:105:LEU:HD22	15:2T:109:GLU:HB3	1.94	0.50
21:2Z:10:ARG:NH1	21:2Z:26:GLY:O	2.45	0.50
30:28:34:TRP:CG	30:28:35:GLN:N	2.80	0.50
33:2b:197:VAL:HG12	33:2b:200:ILE:HG13	1.94	0.50
39:2h:81:HIS:ND1	39:2h:138:TRP:OXT	2.27	0.50
47:2p:53:VAL:HG13	47:2p:79:VAL:HG22	1.92	0.50
1:1A:228:A:H8	1:1A:229:A:H5'	1.76	0.50
1:1A:644:A:H4'	1:1A:645:C:H5	1.77	0.50
1:1A:2597:G:OP1	60:1A:4226:HOH:O	2.19	0.50
1:1A:2815:C:H5'	27:15:29:THR:HG21	1.93	0.50
7:1H:25:LYS:NZ	7:1H:32:GLU:OE2	2.44	0.50
9:1N:91:LEU:HG	9:1N:98:VAL:HG21	1.93	0.50
32:1a:175:C:H2'	32:1a:176:C:C6	2.46	0.50
32:1a:596:C:OP2	60:1a:3329:HOH:O	2.19	0.50
32:1a:950:U:OP2	44:1m:102:ARG:HD2	2.12	0.50
1:2A:202:U:OP1	60:2A:3932:HOH:O	2.19	0.50
1:2A:2454:G:O6	60:2A:3931:HOH:O	2.19	0.50
8:2I:27:ARG:HG2	23:21:71:TYR:CZ	2.46	0.50
13:2R:13:HIS:CE1	13:2R:16:HIS:HB2	2.47	0.50
19:2X:35:THR:HG22	19:2X:37:THR:N	2.26	0.50
23:21:64:ALA:HA	23:21:67:ILE:HG13	1.94	0.50
26:24:59:PHE:HA	26:24:61:ARG:N	2.26	0.50
32:2a:715:A:H2'	32:2a:716:A:C8	2.47	0.50
32:2a:973:G:O3'	45:2n:41:ARG:NH2	2.45	0.50
32:2a:986:A:H1'	50:2s:54:GLY:O	2.11	0.50
32:2a:1125:U:O2'	32:2a:1126:U:O5'	2.26	0.50
32:2a:1203:C:H2'	32:2a:1204:A:C8	2.46	0.50
1:1A:2627:G:O2'	1:1A:2781:A:N1	2.44	0.50
32:1a:289:G:OP2	60:1a:3306:HOH:O	2.20	0.50
1:2A:249:C:O2	30:28:12:LYS:NZ	2.37	0.50
1:2A:584:C:OP2	16:2U:6:THR:OG1	2.24	0.50
1:2A:740:U:O3'	60:2A:3937:HOH:O	2.20	0.50
1:2A:1613:G:O2'	60:2A:3939:HOH:O	2.20	0.50
1:2A:2853:C:H2'	1:2A:2854:G:C8	2.47	0.50
6:2G:179:PRO:HB3	26:24:43:TYR:HE1	1.77	0.50
7:2H:11:VAL:HG13	7:2H:15:VAL:HG23	1.94	0.50
17:2V:52:VAL:HG23	17:2V:55:ALA:HB3	1.94	0.50
25:23:4:LEU:HD23	25:23:58:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:192:U:H2'	32:2a:193:C:C6	2.47	0.50
32:2a:1248:A:O2'	40:2i:70:LYS:NZ	2.43	0.50
41:2j:7:LYS:HB3	41:2j:97:GLU:HB2	1.94	0.50
45:2n:29:ARG:HB3	45:2n:40:CYS:HB3	1.93	0.50
1:1A:889:C:O2'	1:1A:890:A:O5'	2.28	0.49
1:1A:2065:C:H2'	1:1A:2066:C:C6	2.47	0.49
33:1b:134:GLU:HG3	33:1b:137:ARG:HH21	1.77	0.49
35:1d:173:TRP:CE3	35:1d:174:LEU:HG	2.47	0.49
1:2A:463:G:H5"	60:2A:3933:HOH:O	2.12	0.49
1:2A:579:G:O2'	1:2A:2019:A:OP1	2.27	0.49
1:2A:1171:G:N2	1:2A:1179:C:N3	2.58	0.49
1:2A:2094:G:OP1	8:2I:22:LYS:HD2	2.11	0.49
1:2A:2128:C:H5'	1:2A:2129:C:OP2	2.12	0.49
1:2A:2427:C:OP2	60:2A:3930:HOH:O	2.19	0.49
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.47	0.49
1:2A:2823:A:OP1	4:2E:113:PHE:HB2	2.12	0.49
32:2a:932:C:H2'	32:2a:933:G:C8	2.47	0.49
32:2a:966:M2G:H8	32:2a:966:M2G:O5'	1.95	0.49
32:2a:1122:U:H2'	32:2a:1123:A:C8	2.46	0.49
32:2a:1186:G:O3'	40:2i:113:LYS:NZ	2.42	0.49
32:2a:1318:A:H5"	50:2s:3:ARG:HH22	1.77	0.49
37:2f:3:ARG:HD3	37:2f:64:GLN:HE21	1.76	0.49
1:1A:2111:C:H42	1:1A:2147:G:N2	2.10	0.49
5:1F:132:VAL:HA	5:1F:138:GLU:HB3	1.93	0.49
26:14:62:ARG:C	26:14:64:GLY:HA2	2.38	0.49
32:1a:1326:C:H5"	52:1u:18:TYR:O	2.13	0.49
37:1f:22:GLU:OE2	37:1f:82:ARG:NH2	2.46	0.49
4:2E:77:ILE:HG21	4:2E:195:LEU:HD22	1.92	0.49
6:2G:112:PRO:HG3	26:24:43:TYR:CE2	2.39	0.49
7:2H:20:ALA:HB3	7:2H:23:ARG:HB3	1.94	0.49
12:2Q:17:LEU:HB3	12:2Q:39:PRO:HB2	1.94	0.49
32:2a:451:A:N6	32:2a:480:U:H2'	2.28	0.49
32:2a:999:C:N4	32:2a:1042:G:H1	2.10	0.49
1:1A:424:G:N7	56:1A:4013:MPD:H52	2.27	0.49
1:1A:1623:G:OP1	60:1A:4233:HOH:O	2.20	0.49
13:1R:44:LEU:HD22	13:1R:48:VAL:HG23	1.94	0.49
32:1a:623:C:H2'	32:1a:624:C:O4'	2.13	0.49
33:1b:21:ARG:HB3	33:1b:39:ILE:HD13	1.94	0.49
35:1d:142:PRO:HA	35:1d:185:PHE:HD2	1.77	0.49
36:1e:45:PHE:CD2	36:1e:47:LYS:HE2	2.47	0.49
40:1i:33:PHE:CZ	40:1i:47:LEU:HD21	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1j:78:ASN:O	41:1j:80:LYS:N	2.45	0.49
1:2A:571:A:N6	1:2A:2499:C:O3'	2.44	0.49
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.47	0.49
1:2A:2424:C:O2	1:2A:2429:G:O2'	2.25	0.49
32:2a:1232:U:H5"	40:2i:124:GLN:O	2.12	0.49
40:2i:43:ALA:C	40:2i:45:ALA:H	2.20	0.49
44:2m:17:VAL:HG12	44:2m:27:LYS:HD3	1.95	0.49
44:2m:82:MET:SD	44:2m:93:ARG:HG2	2.52	0.49
1:1A:1138:G:N3	9:1N:106:MET:HE2	2.26	0.49
1:1A:1358:G:OP2	60:1A:4214:HOH:O	2.18	0.49
1:1A:2820:A:N6	60:1A:4668:HOH:O	2.45	0.49
3:1D:71:ASP:OD2	3:1D:103:ARG:NH2	2.45	0.49
30:18:56:GLU:HG2	60:18:226:HOH:O	2.13	0.49
32:1a:507:C:OP2	32:1a:508:C:O2'	2.24	0.49
32:1a:1367:C:H5'	41:1j:60:ARG:NH1	2.27	0.49
1:2A:752:A:H4'	1:2A:753:C:O5'	2.12	0.49
1:2A:1153:C:H2'	1:2A:1154:G:O4'	2.12	0.49
32:2a:45:U:H2'	32:2a:46:G:H8	1.73	0.49
32:2a:164:U:H2'	32:2a:165:C:C6	2.48	0.49
32:2a:1446:U:H4'	32:2a:1447:A:C6	2.47	0.49
44:2m:108:ARG:HE	44:2m:114:ARG:HG3	1.78	0.49
49:2r:47:THR:HG21	49:2r:49:LYS:HE2	1.94	0.49
1:1A:279:C:H42	1:1A:361:G:H1	1.60	0.49
1:1A:910:A:N3	1:1A:2264:C:O2'	2.41	0.49
1:1A:2584:U:H2'	1:1A:2585:U:H2'	1.94	0.49
2:1B:77:U:OP1	21:1Z:19:ARG:NH2	2.46	0.49
32:1a:583:A:N6	32:1a:758:G:O2'	2.45	0.49
42:1k:33:THR:HA	42:1k:39:PRO:HA	1.95	0.49
46:1o:74:ASP:CG	46:1o:77:ARG:HB2	2.38	0.49
1:2A:597:U:H2'	1:2A:598:G:H8	1.75	0.49
1:2A:1012:U:OP1	16:2U:75:ASN:ND2	2.42	0.49
1:2A:1053:C:H2'	1:2A:1054:A:H8	1.76	0.49
1:2A:1428:C:N4	1:2A:1570:A:OP2	2.37	0.49
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.47	0.49
14:2S:28:VAL:HG13	14:2S:101:LEU:HD13	1.94	0.49
19:2X:46:ALA:HB1	24:22:33:MET:HE1	1.94	0.49
32:2a:399:G:H2'	32:2a:400:C:C6	2.47	0.49
32:2a:1058:G:N2	41:2j:53:PRO:HG3	2.26	0.49
33:2b:124:SER:HB2	33:2b:125:PRO:HD3	1.94	0.49
37:2f:50:TYR:CE2	49:2r:77:GLY:HA2	2.48	0.49
1:1A:2228:G:OP1	3:1D:261:LYS:NZ	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2314:C:H2'	1:1A:2315:G:H8	1.78	0.49
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.48	0.49
3:1D:16:MET:HG2	3:1D:211:ARG:HH21	1.78	0.49
3:1D:108:PRO:HD2	3:1D:111:LEU:HG	1.95	0.49
20:1Y:92:ASN:H	20:1Y:92:ASN:HD22	1.61	0.49
32:1a:1075:C:OP1	33:1b:179:LYS:NZ	2.30	0.49
33:1b:55:PHE:HA	33:1b:58:ILE:HB	1.94	0.49
33:1b:88:ALA:HB2	33:1b:219:VAL:HG13	1.95	0.49
35:1d:105:VAL:HG13	35:1d:110:PHE:HB2	1.95	0.49
1:2A:2051:A:H5'	1:2A:2578:G:O4'	2.13	0.49
1:2A:2104:G:N2	1:2A:2105:C:C4	2.80	0.49
1:2A:2400:G:H4'	28:26:18:ARG:HG2	1.93	0.49
6:2G:39:ILE:HG23	6:2G:155:MET:HG3	1.94	0.49
16:2U:102:GLU:HG3	17:2V:2:PHE:CZ	2.47	0.49
20:2Y:92:ASN:ND2	20:2Y:94:LYS:HG2	2.27	0.49
32:2a:1427:U:H2'	32:2a:1428:A:C8	2.47	0.49
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.28	0.49
6:1G:110:ALA:O	6:1G:140:ILE:HG23	2.13	0.49
32:1a:403:C:N4	60:1a:3413:HOH:O	2.46	0.49
32:1a:673:G:O3'	37:1f:87:ARG:NH2	2.45	0.49
32:1a:966:M2G:C1'	53:1y:53:THR:HG21	2.43	0.49
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.47	0.49
34:1c:116:VAL:HG21	34:1c:202:ILE:HD11	1.93	0.49
36:1e:78:HIS:CD2	36:1e:78:HIS:H	2.30	0.49
38:1g:27:ILE:HD12	38:1g:40:ALA:HA	1.93	0.49
49:1r:33:ASP:OD2	49:1r:36:ASN:N	2.44	0.49
1:2A:754:C:H2'	1:2A:755:C:C6	2.47	0.49
1:2A:1050:A:H2'	1:2A:1051:G:C8	2.47	0.49
1:2A:1408:C:H2'	1:2A:1409:C:C6	2.48	0.49
1:2A:2131:G:H5"	1:2A:2132:U:H5'	1.94	0.49
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.12	0.49
14:2S:67:ARG:HD2	14:2S:71:ARG:NH2	2.28	0.49
25:23:3:ARG:HD2	25:23:36:VAL:HG12	1.95	0.49
32:2a:130:A:O2'	32:2a:131:C:O5'	2.28	0.49
32:2a:457:C:H2'	32:2a:458:C:H6	1.76	0.49
32:2a:1272:G:H2'	32:2a:1273:G:O4'	2.12	0.49
33:2b:193:ASP:OD2	33:2b:196:LEU:HB2	2.12	0.49
35:2d:191:ARG:HH21	35:2d:200:GLU:CD	2.20	0.49
1:1A:2138:C:H2'	1:1A:2139:C:C5	2.48	0.49
8:1I:4:ILE:HD11	8:1I:44:LEU:HD13	1.93	0.49
32:1a:198:G:H2'	32:1a:199:G:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:922:G:C6	32:1a:923:A:C6	3.00	0.49
32:1a:1183:A:H3'	32:1a:1184:G:H5"	1.95	0.49
33:1b:155:LEU:HD21	33:1b:159:PRO:HD3	1.93	0.49
35:1d:33:MET:SD	35:1d:37:PRO:HA	2.53	0.49
1:2A:345:A:N3	1:2A:346:A:N6	2.60	0.49
1:2A:428:A:OP2	1:2A:428:A:H8	1.96	0.49
1:2A:1313:U:OP1	60:2A:3929:HOH:O	2.19	0.49
1:2A:1789:A:N6	60:2A:4254:HOH:O	2.46	0.49
2:2B:58:A:OP2	60:2B:307:HOH:O	2.20	0.49
6:2G:170:ARG:NH2	6:2G:174:GLU:OE2	2.40	0.49
32:2a:255:G:H2'	32:2a:256:U:H6	1.77	0.49
32:2a:514:C:H2'	32:2a:515:G:H8	1.78	0.49
32:2a:653:A:OP1	39:2h:56:LYS:NZ	2.42	0.49
32:2a:936:C:H2'	32:2a:937:A:O4'	2.12	0.49
42:2k:56:GLY:O	42:2k:89:ALA:HB3	2.13	0.49
42:2k:83:ILE:HD13	42:2k:109:VAL:HG13	1.94	0.49
51:2t:29:LYS:O	51:2t:33:ILE:HG12	2.13	0.49
53:2y:32:THR:HB	53:2y:89:GLN:HE22	1.77	0.49
1:1A:365:C:H5"	60:1A:4545:HOH:O	2.13	0.49
1:1A:2294:C:H2'	1:1A:2295:C:H6	1.77	0.49
28:16:9:LEU:HD13	28:16:51:GLU:HG3	1.95	0.49
32:1a:107:G:H2'	32:1a:108:G:O4'	2.13	0.49
32:1a:1121:U:H2'	32:1a:1122:U:C6	2.48	0.49
32:1a:1243:C:H2'	32:1a:1244:C:C6	2.48	0.49
33:1b:27:LYS:HB2	33:1b:194:PRO:HD2	1.94	0.49
50:1s:43:GLU:OE1	50:1s:43:GLU:N	2.45	0.49
1:2A:184:C:H2'	1:2A:185:U:C6	2.48	0.49
1:2A:637:A:OP1	11:2P:133:SER:OG	2.15	0.49
1:2A:667:U:O2	30:28:2:PRO:HD2	2.13	0.49
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.47	0.49
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.13	0.49
6:2G:39:ILE:HG21	6:2G:60:LEU:HD11	1.95	0.49
8:2I:92:VAL:HG23	8:2I:120:ILE:HB	1.95	0.49
18:2W:78:GLU:OE2	18:2W:99:ARG:HD3	2.13	0.49
19:2X:50:LYS:HB3	19:2X:84:ALA:HB2	1.93	0.49
22:20:32:ARG:H	22:20:35:ASN:ND2	2.10	0.49
32:2a:992:U:H5"	32:2a:993:G:C8	2.48	0.49
1:1A:2774:C:H2'	1:1A:2775:A:O4'	2.12	0.49
10:1O:98:VAL:HG22	10:1O:118:ALA:HA	1.94	0.49
32:1a:169:C:H2'	32:1a:170:U:C6	2.48	0.49
32:1a:376:G:H2'	32:1a:377:G:H8	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1316:G:H5"	45:1n:17:LYS:HZ3	1.78	0.49
42:1k:84:VAL:HG11	42:1k:91:ARG:HD2	1.95	0.49
1:2A:209:C:OP1	60:2A:3940:HOH:O	2.20	0.49
1:2A:309:G:N3	1:2A:329:G:O2'	2.46	0.49
1:2A:1079:C:C2	1:2A:1080:C:H1'	2.47	0.49
1:2A:1196:C:H2'	1:2A:1197:G:H8	1.78	0.49
1:2A:2153:G:H2'	1:2A:2154:G:C8	2.48	0.49
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.46	0.49
12:2Q:57:HIS:HD2	12:2Q:117:ALA:HB2	1.78	0.49
30:28:28:GLY:N	60:28:202:HOH:O	2.43	0.49
32:2a:103:C:P	51:2t:17:ARG:HH21	2.34	0.49
32:2a:390:C:H2'	32:2a:391:G:C8	2.48	0.49
32:2a:401:C:O2'	32:2a:621:A:N3	2.38	0.49
32:2a:1400:5MC:N3	53:2y:63:ALA:HA	2.28	0.49
44:2m:88:ARG:HG2	44:2m:98:VAL:HG12	1.94	0.49
1:1A:234:C:H2'	1:1A:235:U:C6	2.48	0.48
1:1A:1858:G:N2	1:1A:1883:G:H2'	2.28	0.48
1:1A:2074:U:H2'	1:1A:2075:U:C6	2.47	0.48
1:1A:2189:U:C2'	1:1A:2190:G:H5'	2.43	0.48
3:1D:147:LEU:HD13	3:1D:155:LEU:HD11	1.96	0.48
8:1I:48:GLU:HG2	8:1I:52:ARG:HH22	1.78	0.48
10:1O:43:VAL:HG12	10:1O:54:GLU:HA	1.94	0.48
18:1W:9:TYR:HA	18:1W:100:THR:HG23	1.95	0.48
32:1a:7:G:H5"	32:1a:298:A:O4'	2.13	0.48
32:1a:173:U:OP1	60:1a:3332:HOH:O	2.20	0.48
33:1b:55:PHE:CG	33:1b:221:LEU:HD11	2.48	0.48
42:1k:99:GLN:HG2	42:1k:105:VAL:HG21	1.94	0.48
53:1y:53:THR:HG22	53:1y:62:VAL:HG22	1.94	0.48
1:2A:779:U:OP1	3:2D:49:ILE:HG13	2.12	0.48
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.12	0.48
1:2A:2591:C:OP1	60:2A:3870:HOH:O	2.19	0.48
5:2F:74:ARG:H	5:2F:74:ARG:HG3	1.44	0.48
6:2G:39:ILE:HG12	6:2G:157:ILE:HG12	1.95	0.48
32:2a:337:C:H2'	32:2a:338:A:H8	1.77	0.48
32:2a:499:A:H4'	32:2a:500:G:OP1	2.12	0.48
32:2a:649:G:O6	60:2a:3221:HOH:O	2.18	0.48
32:2a:983:A:H3'	32:2a:983:A:N3	2.28	0.48
36:2e:6:PHE:HB2	36:2e:34:VAL:HG22	1.94	0.48
43:2l:103:GLY:N	43:2l:107:ALA:O	2.44	0.48
1:1A:807:U:OP2	11:1P:41:ARG:NH2	2.44	0.48
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1678:G:OP2	1:1A:1678:G:N2	2.40	0.48
6:1G:59:GLU:OE1	6:1G:153:ARG:NH2	2.45	0.48
32:1a:141:A:H1'	32:1a:182:U:O2	2.13	0.48
32:1a:1503:A:H5'	32:1a:1531:A:H1'	1.95	0.48
35:1d:159:ARG:HB3	35:1d:159:ARG:CZ	2.43	0.48
48:1q:86:GLU:O	48:1q:90:ILE:HG12	2.12	0.48
1:2A:296:C:H2'	1:2A:297:C:H6	1.78	0.48
1:2A:568:U:H5'	1:2A:945:A:H62	1.78	0.48
1:2A:854:G:H2'	1:2A:855:G:H8	1.77	0.48
1:2A:1116:C:H2'	1:2A:1117:G:H8	1.78	0.48
1:2A:1250:G:H5"	60:2A:4848:HOH:O	2.12	0.48
1:2A:1849:G:H2'	1:2A:1850:G:C8	2.47	0.48
1:2A:2695:C:H2'	1:2A:2696:U:H6	1.78	0.48
12:2Q:59:ARG:NH1	12:2Q:60:ARG:HE	2.11	0.48
23:21:8:SER:HB3	23:21:66:HIS:CD2	2.49	0.48
32:2a:134:A:H61	47:2p:25:ARG:HH22	1.60	0.48
33:2b:101:MET:HG2	33:2b:108:ILE:HG21	1.95	0.48
1:1A:29:U:H2'	1:1A:30:G:C8	2.47	0.48
1:1A:919:G:H2'	1:1A:920:G:O4'	2.14	0.48
1:1A:1007:C:H5"	9:1N:35:ARG:NH1	2.28	0.48
1:1A:1226:A:OP1	17:1V:84:LYS:NZ	2.40	0.48
1:1A:1230:C:H2'	1:1A:1231:G:C8	2.49	0.48
1:1A:2822:G:O2'	1:1A:2824:C:OP2	2.23	0.48
32:1a:916:G:N7	60:1a:3374:HOH:O	2.34	0.48
33:1b:80:ILE:HD12	33:1b:208:ILE:HG22	1.95	0.48
39:1h:124:ALA:O	39:1h:128:GLY:N	2.42	0.48
2:2B:3:C:H2'	2:2B:4:C:C6	2.48	0.48
2:2B:8:U:O3'	14:2S:25:ARG:NH2	2.41	0.48
13:2R:95:THR:HG22	13:2R:116:LEU:HD23	1.95	0.48
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.94	0.48
34:2c:186:PHE:CZ	34:2c:188:LEU:HB2	2.49	0.48
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.48	0.48
1:1A:2050:C:H1'	4:1E:156:MET:HE2	1.94	0.48
1:1A:2615:U:H2'	1:1A:2616:C:H6	1.78	0.48
33:1b:9:GLU:HG3	33:1b:217:ARG:HH22	1.78	0.48
43:1l:7:ILE:O	43:1l:11:VAL:HG23	2.12	0.48
1:2A:639:U:H2'	1:2A:640:C:C6	2.48	0.48
1:2A:2105:C:N3	1:2A:2184:G:N2	2.58	0.48
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.49	0.48
60:2B:340:HOH:O	21:2Z:31:ARG:HG2	2.13	0.48
5:2F:32:LEU:O	5:2F:36:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:77:ILE:HG21	6:2G:80:PHE:CD2	2.49	0.48
8:2I:5:LEU:HG	8:2I:9:LEU:HD12	1.95	0.48
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	1.94	0.48
18:2W:76:VAL:HG22	18:2W:103:ILE:HG23	1.95	0.48
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.96	0.48
32:2a:1401:G:OP1	53:2y:80:LYS:HE2	2.13	0.48
34:2c:131:ARG:HD2	34:2c:131:ARG:HA	1.62	0.48
40:2i:79:LEU:HD22	40:2i:104:ARG:HB2	1.95	0.48
1:1A:1277:G:OP1	60:1A:4234:HOH:O	2.20	0.48
1:1A:1802:A:N1	1:1A:1822:G:H1'	2.29	0.48
1:1A:1843:C:H5'	3:1D:253:GLN:NE2	2.29	0.48
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.49	0.48
4:1E:12:THR:OG1	4:1E:13:ARG:N	2.47	0.48
5:1F:95:ARG:HD3	5:1F:97:TYR:CZ	2.48	0.48
32:1a:863:U:O2'	32:1a:865:A:N7	2.42	0.48
32:1a:971:G:OP1	32:1a:972:C:H5"	2.14	0.48
32:1a:1189:C:OP1	41:1j:51:ARG:NH2	2.43	0.48
39:1h:51:VAL:HG11	39:1h:60:ARG:HH12	1.78	0.48
47:1p:74:LEU:HB3	47:1p:79:VAL:HG21	1.95	0.48
49:1r:40:LEU:HD22	49:1r:70:ILE:HG12	1.96	0.48
1:2A:1059:G:OP2	1:2A:1060:U:H3'	2.13	0.48
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.48	0.48
1:2A:2748:A:O2'	7:2H:63:SER:O	2.22	0.48
1:2A:2812:G:H1	1:2A:2888:C:H42	1.61	0.48
5:2F:60:SER:OG	5:2F:61:GLY:N	2.46	0.48
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.94	0.48
32:2a:433:C:H2'	32:2a:434:U:H6	1.78	0.48
1:1A:456:C:H4'	60:1A:6124:HOH:O	2.12	0.48
1:1A:762:U:H5"	60:1A:5736:HOH:O	2.14	0.48
12:1Q:137:TYR:O	12:1Q:141:GLN:HG2	2.13	0.48
32:1a:1124:G:OP1	41:1j:36:GLY:N	2.44	0.48
32:1a:1519:MA6:H8	32:1a:1519:MA6:O5'	2.13	0.48
34:1c:66:VAL:HB	34:1c:101:LEU:HD12	1.94	0.48
44:1m:40:ASN:HB3	44:1m:43:THR:HG23	1.95	0.48
1:2A:1359:A:N3	1:2A:1359:A:H5'	2.29	0.48
19:2X:1:MET:HE1	24:22:26:ARG:HH21	1.78	0.48
32:2a:585:G:OP1	48:2q:37:LYS:NZ	2.39	0.48
35:2d:118:ARG:O	35:2d:122:ARG:N	2.40	0.48
38:2g:26:PHE:HE1	38:2g:105:VAL:HG22	1.77	0.48
39:2h:73:ASP:OD1	39:2h:75:ARG:NH1	2.47	0.48
50:2s:66:MET:HB3	50:2s:74:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:38:A:H2'	1:1A:39:C:C6	2.49	0.48
1:1A:82:G:O6	60:1A:4235:HOH:O	2.20	0.48
1:1A:729:G:C5	3:1D:208:LYS:HB2	2.49	0.48
7:1H:125:VAL:HG12	7:1H:127:GLU:O	2.13	0.48
23:11:3:LYS:O	23:11:12:PRO:HD3	2.13	0.48
32:1a:44:G:C2	32:1a:45:U:H1'	2.49	0.48
32:1a:50:A:H1'	32:1a:52:G:C8	2.48	0.48
32:1a:664:G:N2	32:1a:741:G:H1	2.06	0.48
36:1e:102:ALA:HB1	36:1e:106:PRO:HG2	1.95	0.48
37:1f:19:LEU:HD21	37:1f:59:TYR:CE2	2.49	0.48
38:1g:110:GLN:HA	38:1g:110:GLN:HE21	1.79	0.48
43:1l:71:PRO:O	43:1l:102:ARG:HD3	2.13	0.48
1:2A:863:A:H2'	1:2A:864:G:C8	2.49	0.48
1:2A:1087:G:H22	1:2A:1102:C:N4	2.12	0.48
1:2A:2104:G:O6	1:2A:2186:G:C5	2.67	0.48
7:2H:41:MET:HE2	7:2H:55:PRO:HD2	1.96	0.48
32:2a:41:G:H2'	32:2a:42:G:H8	1.79	0.48
32:2a:1014:A:H2	32:2a:1219:U:H1'	1.78	0.48
32:2a:1071:C:H2'	32:2a:1072:G:C8	2.48	0.48
1:1A:857:C:N4	1:1A:858:U:O4	2.47	0.48
1:1A:2543:G:H2'	1:1A:2544:G:C8	2.48	0.48
1:1A:2662:A:H2'	1:1A:2663:G:O4'	2.13	0.48
22:10:17:GLN:O	22:10:19:LYS:NZ	2.47	0.48
32:1a:1367:C:H5'	41:1j:60:ARG:HH12	1.78	0.48
33:1b:15:VAL:HG11	33:1b:213:LEU:HD22	1.96	0.48
1:2A:211:A:H2'	1:2A:212:G:O4'	2.14	0.48
7:2H:80:SER:OG	7:2H:81:GLU:N	2.41	0.48
10:2O:29:ASN:N	10:2O:29:ASN:OD1	2.46	0.48
18:2W:27:LYS:NZ	60:2W:306:HOH:O	2.46	0.48
20:2Y:86:ARG:HB2	20:2Y:98:VAL:HG23	1.95	0.48
25:23:57:GLU:HG2	25:23:59:VAL:HG22	1.95	0.48
32:2a:67:C:H2'	32:2a:68:G:C8	2.48	0.48
32:2a:442:C:N4	32:2a:492:G:H1	2.11	0.48
32:2a:509:A:N3	32:2a:543:C:O2'	2.39	0.48
32:2a:841:U:OP1	32:2a:841:U:H6	1.97	0.48
32:2a:1014:A:C2	32:2a:1219:U:H1'	2.49	0.48
1:1A:813:U:H2'	1:1A:814:C:C6	2.49	0.48
1:1A:2753:A:N3	31:19:15:LYS:NZ	2.62	0.48
6:1G:20:ILE:O	6:1G:24:GLY:N	2.37	0.48
6:1G:101:ILE:HG22	6:1G:105:LYS:HE2	1.96	0.48
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:7:G:O2'	36:1e:120:THR:O	2.32	0.48
32:1a:584:G:H1	32:1a:757:U:H3	1.62	0.48
32:1a:1316:G:N2	32:1a:1319:A:OP2	2.47	0.48
33:1b:215:LEU:O	33:1b:219:VAL:HG23	2.14	0.48
35:1d:57:ARG:HE	35:1d:205:GLU:HB3	1.78	0.48
1:2A:14:A:OP2	60:2A:3943:HOH:O	2.20	0.48
1:2A:224:G:H2'	1:2A:225:A:O4'	2.14	0.48
1:2A:631:A:H2'	1:2A:632:A:O4'	2.14	0.48
1:2A:1020:A:N1	1:2A:1141:U:O2'	2.44	0.48
1:2A:1062:G:N7	1:2A:1070:A:H1'	2.29	0.48
3:2D:58:HIS:HD1	3:2D:59:LYS:N	2.11	0.48
32:2a:176:C:H2'	32:2a:177:C:C6	2.48	0.48
32:2a:675:A:O2'	42:2k:114:VAL:O	2.29	0.48
32:2a:979:C:OP1	32:2a:1223:C:N4	2.47	0.48
32:2a:1246:C:H2'	32:2a:1247:U:C6	2.49	0.48
36:2e:33:VAL:HA	36:2e:42:GLY:O	2.14	0.48
38:2g:48:LYS:O	38:2g:52:GLU:HG2	2.13	0.48
46:2o:5:LYS:O	46:2o:9:GLN:HG2	2.14	0.48
1:1A:1166:C:H2'	1:1A:1167:U:C6	2.48	0.48
1:1A:1509(B):A:H2'	1:1A:1510:G:O4'	2.14	0.48
1:1A:1904:G:O2'	1:1A:1928:A:N1	2.42	0.48
1:1A:2147:G:H2'	1:1A:2148:G:O4'	2.13	0.48
1:1A:2314:C:H2'	1:1A:2315:G:C8	2.48	0.48
1:1A:2743:C:OP1	31:19:33:LYS:NZ	2.45	0.48
12:1Q:38:GLU:HG3	12:1Q:127:ILE:HG22	1.96	0.48
32:1a:100:C:H2'	32:1a:101:A:C8	2.48	0.48
32:1a:502:G:OP1	43:1l:118:SER:HB3	2.13	0.48
41:1j:45:ARG:HB3	41:1j:65:LEU:HD23	1.95	0.48
1:2A:479:A:N3	1:2A:481:G:H5"	2.29	0.48
4:2E:50:GLY:O	4:2E:51:PHE:HB2	2.13	0.48
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.32	0.48
18:2W:14:PRO:HA	18:2W:17:VAL:HG23	1.96	0.48
32:2a:1034:G:C2	32:2a:1035:A:H1'	2.49	0.48
32:2a:1246:C:H2'	32:2a:1247:U:H6	1.78	0.48
49:2r:70:ILE:HG22	49:2r:74:ARG:HD2	1.96	0.48
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.49	0.47
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.49	0.47
6:1G:143:GLU:HB3	26:14:28:LYS:HE2	1.96	0.47
16:1U:59:ARG:O	16:1U:63:VAL:HG23	2.13	0.47
27:15:15:ARG:NH1	60:15:201:HOH:O	2.22	0.47
32:1a:1343:G:H4'	40:1i:122:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1f:41:GLU:HG2	37:1f:43:LEU:HD11	1.96	0.47
44:1m:4:ILE:HA	44:1m:5:ALA:HA	1.63	0.47
44:1m:16:ASP:OD1	44:1m:16:ASP:N	2.46	0.47
1:2A:858:U:O2	1:2A:2268:A:H2'	2.14	0.47
1:2A:1259:G:N7	60:2A:4117:HOH:O	2.35	0.47
1:2A:1772:G:OP1	60:2A:3947:HOH:O	2.20	0.47
1:2A:2584:U:H2'	1:2A:2585:U:H2'	1.96	0.47
27:25:49:CYS:SG	27:25:51:TYR:HB2	2.54	0.47
32:2a:403:C:O2'	32:2a:404:U:H5'	2.14	0.47
32:2a:500:G:N2	32:2a:546:G:H1'	2.29	0.47
35:2d:72:GLU:OE2	35:2d:207:TYR:OH	2.32	0.47
1:1A:34:C:O2'	1:1A:35:G:H5'	2.14	0.47
1:1A:154(A):C:H3'	60:1A:7579:HOH:O	2.14	0.47
1:1A:1250:G:H5"	60:1U:328:HOH:O	2.14	0.47
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.13	0.47
1:1A:2649:U:H2'	1:1A:2650:U:C6	2.48	0.47
4:1E:29:GLY:HA3	60:1E:406:HOH:O	2.12	0.47
21:1Z:53:ILE:HG13	21:1Z:54:HIS:CD2	2.49	0.47
23:11:3:LYS:HB3	23:11:61:ARG:HH22	1.78	0.47
32:1a:41:G:H2'	32:1a:42:G:C8	2.49	0.47
32:1a:199:G:H2'	32:1a:200:G:C8	2.50	0.47
33:1b:16:HIS:HB3	33:1b:210:SER:CB	2.38	0.47
1:2A:660:G:O3'	5:2F:38:ARG:NH2	2.47	0.47
1:2A:784:A:H5'	1:2A:785:G:OP1	2.14	0.47
1:2A:984:A:H5"	1:2A:985:C:H5	1.78	0.47
1:2A:2145:C:O2'	1:2A:2147:G:N2	2.46	0.47
4:2E:111:ARG:HD3	4:2E:160:TYR:CE2	2.49	0.47
7:2H:144:VAL:O	7:2H:148:ILE:HG12	2.13	0.47
14:2S:36:TYR:N	14:2S:36:TYR:CD1	2.82	0.47
26:24:59:PHE:HE2	50:2s:64:GLU:HB2	1.79	0.47
32:2a:19:C:H2'	32:2a:20:U:C6	2.50	0.47
32:2a:385:C:H2'	32:2a:386:C:H6	1.79	0.47
35:2d:119:GLN:HG3	35:2d:123:HIS:ND1	2.29	0.47
36:2e:102:ALA:HB1	36:2e:106:PRO:HG2	1.96	0.47
40:2i:111:ARG:HG2	40:2i:113:LYS:HG3	1.96	0.47
41:2j:35:SER:HB3	41:2j:73:ASP:HB2	1.95	0.47
50:2s:12:ASP:OD2	50:2s:38:SER:OG	2.27	0.47
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.13	0.47
1:1A:2123:G:H1	1:1A:2175:C:H42	1.61	0.47
32:1a:1239:A:H4'	32:1a:1240:U:H5"	1.96	0.47
51:1t:79:ARG:HD2	51:1t:83:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:863:A:H2'	1:2A:864:G:H8	1.79	0.47
1:2A:1047:G:H2'	1:2A:1110:G:N2	2.21	0.47
1:2A:1292:U:H2'	1:2A:1293:C:H6	1.78	0.47
2:2B:90:A:N7	2:2B:91:C:H1'	2.29	0.47
12:2Q:138:ASP:OD1	12:2Q:138:ASP:N	2.46	0.47
26:24:58:ARG:HH21	50:2s:68:GLY:H	1.62	0.47
32:2a:1372:U:H2'	32:2a:1373:G:O4'	2.12	0.47
38:2g:15:ASP:OD2	38:2g:44:TYR:OH	2.31	0.47
47:2p:9:PHE:CE1	47:2p:18:ARG:HD2	2.48	0.47
53:2y:34:LEU:HD23	53:2y:56:THR:HG22	1.96	0.47
1:1A:207:A:H2'	1:1A:208:C:O4'	2.14	0.47
1:1A:1279:G:H4'	13:1R:31:HIS:CD2	2.49	0.47
1:1A:2512:C:H2'	1:1A:2513:G:O4'	2.14	0.47
5:1F:160:ASN:OD1	5:1F:162:LEU:HB2	2.15	0.47
24:12:51:ARG:HD3	24:12:55:ARG:NH1	2.29	0.47
30:18:26:LYS:HD2	30:18:48:PHE:CD2	2.49	0.47
32:1a:148:G:H2'	32:1a:149:A:C8	2.50	0.47
32:1a:598:U:O4	60:1a:3329:HOH:O	2.19	0.47
33:1b:207:ALA:O	33:1b:211:ILE:HG13	2.14	0.47
1:2A:2114:A:H61	1:2A:2119:A:H8	1.61	0.47
1:2A:2895:U:H2'	1:2A:2896:C:O4'	2.14	0.47
18:2W:71:VAL:HA	18:2W:107:LEU:HD12	1.95	0.47
32:2a:554:C:H2'	32:2a:555:C:C6	2.50	0.47
32:2a:1052:U:O2'	32:2a:1055:A:OP2	2.28	0.47
32:2a:1320:C:N3	50:2s:36:ARG:NH2	2.62	0.47
39:2h:7:ALA:HA	39:2h:10:LEU:HD12	1.97	0.47
50:2s:58:VAL:HG21	50:2s:76:PRO:HD2	1.95	0.47
51:2t:13:LEU:O	51:2t:17:ARG:HG3	2.15	0.47
1:1A:827:U:O2'	1:1A:2068:U:C2	2.61	0.47
1:1A:1065:U:O2	1:1A:1066:U:N3	2.47	0.47
1:1A:2065:C:H2'	1:1A:2066:C:H6	1.79	0.47
1:1A:2681:C:H5"	60:1A:4945:HOH:O	2.14	0.47
1:1A:2801(A):A:N3	1:1A:2895:U:H1'	2.30	0.47
18:1W:27:LYS:HD2	18:1W:31:GLU:CD	2.40	0.47
1:2A:463:G:O6	60:2A:3948:HOH:O	2.21	0.47
1:2A:2203:U:H2'	1:2A:2205:C:C6	2.49	0.47
1:2A:2610:C:O2'	60:2A:3837:HOH:O	2.07	0.47
2:2B:102:A:OP2	60:2B:306:HOH:O	2.20	0.47
7:2H:164:TYR:HB2	7:2H:167:GLU:HB2	1.95	0.47
8:2I:26:ALA:HB1	8:2I:31:LEU:HD13	1.95	0.47
17:2V:5:VAL:HG21	17:2V:35:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:2V:24:LYS:HA	17:2V:92:THR:OG1	2.15	0.47
32:2a:438:G:H4'	35:2d:123:HIS:HD2	1.80	0.47
36:2e:87:SER:HB3	36:2e:131:ILE:HD13	1.95	0.47
37:2f:70:ASP:OD1	37:2f:70:ASP:N	2.33	0.47
1:1A:535:C:O3'	16:1U:53:ARG:NH1	2.48	0.47
32:1a:148:G:H2'	32:1a:149:A:H8	1.80	0.47
32:1a:1252:A:H2'	32:1a:1253:G:O4'	2.15	0.47
1:2A:1171:G:H1	1:2A:1179:C:N4	2.12	0.47
1:2A:1464:C:O2'	1:2A:1528:A:N3	2.40	0.47
1:2A:2184:G:C2	1:2A:2185:C:H1'	2.48	0.47
1:2A:2365:G:H5"	60:2A:4133:HOH:O	2.15	0.47
7:2H:15:VAL:HG12	7:2H:28:GLY:HA2	1.95	0.47
18:2W:12:ILE:O	18:2W:101:SER:OG	2.33	0.47
32:2a:15:G:H21	36:2e:18:ARG:HA	1.79	0.47
32:2a:303:A:O2'	32:2a:555:C:O2'	2.28	0.47
32:2a:404:U:H2'	32:2a:405:U:C6	2.49	0.47
32:2a:974:A:P	45:2n:41:ARG:HH21	2.38	0.47
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.30	0.47
38:2g:77:SER:HA	38:2g:85:TYR:O	2.15	0.47
44:2m:3:ARG:HB2	44:2m:9:ILE:H	1.80	0.47
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.97	0.47
46:2o:87:ILE:HG22	46:2o:88:ARG:H	1.80	0.47
1:1A:446:G:H5"	60:1A:4400:HOH:O	2.15	0.47
1:1A:644:A:H4'	1:1A:645:C:C5	2.50	0.47
1:1A:878:A:H2'	1:1A:879:G:H5'	1.96	0.47
1:1A:1171:G:H3'	1:1A:1173:G:H5'	1.97	0.47
1:1A:1176:G:H1'	1:1A:1177:A:C5'	2.44	0.47
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.15	0.47
1:1A:2406:U:C2	11:1P:72:PRO:HG2	2.50	0.47
1:1A:2483:C:N3	12:1Q:124:LYS:NZ	2.63	0.47
1:1A:2721:A:H5"	60:1A:4356:HOH:O	2.14	0.47
2:1B:41:U:H5	6:1G:70:VAL:H	1.61	0.47
7:1H:9:ILE:HD11	7:1H:69:ARG:HG2	1.97	0.47
10:1O:7:TYR:HE1	10:1O:20:MET:HE3	1.79	0.47
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.15	0.47
14:1S:99:LYS:O	14:1S:103:GLU:HG3	2.14	0.47
15:1T:127:ALA:C	15:1T:129:ARG:N	2.73	0.47
32:1a:235:C:H2'	32:1a:236:G:C8	2.49	0.47
32:1a:452:A:H4'	47:1p:72:ARG:NH1	2.29	0.47
32:1a:818:G:HO2'	32:1a:820:U:H6	1.61	0.47
32:1a:861:G:O6	32:1a:869:G:N2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1065:U:H5”	32:1a:1190:G:H22	1.79	0.47
32:1a:1124:G:H5”	41:1j:35:SER:OG	2.15	0.47
32:1a:1260:C:H4’	32:1a:1284:C:H5’	1.97	0.47
34:1c:58:GLU:HB3	41:1j:92:THR:HG21	1.95	0.47
34:1c:71:ALA:O	34:1c:73:PRO:HD3	2.14	0.47
35:1d:29:PRO:HA	35:1d:34:GLU:HG2	1.96	0.47
35:1d:182:LYS:NZ	35:1d:182:LYS:HB3	2.30	0.47
37:1f:60:PHE:CE2	49:1r:78:LEU:HD21	2.50	0.47
41:1j:81:THR:O	41:1j:83:GLU:N	2.47	0.47
1:2A:1065:U:H4’	1:2A:1066:U:C5’	2.45	0.47
1:2A:1069:A:H2’	1:2A:1073:A:C8	2.49	0.47
1:2A:1503:U:H2’	1:2A:1504:C:C6	2.49	0.47
1:2A:1579:A:H2’	1:2A:1580:A:C8	2.50	0.47
1:2A:1991:U:H2’	1:2A:1992:G:H5”	1.95	0.47
4:2E:1:MET:HE1	4:2E:199:ARG:HD2	1.97	0.47
4:2E:52:LEU:HB3	4:2E:53:PRO:HD2	1.97	0.47
7:2H:3:ARG:HH21	7:2H:54:ARG:NH1	2.13	0.47
9:2N:57:ALA:O	9:2N:60:ILE:HG22	2.15	0.47
20:2Y:21:LYS:HB2	20:2Y:21:LYS:HE3	1.72	0.47
30:28:22:VAL:HG21	30:28:59:LYS:HG2	1.97	0.47
32:2a:102:G:H2’	32:2a:103:C:H6	1.80	0.47
32:2a:186:C:H2’	32:2a:187:C:C6	2.50	0.47
32:2a:501:C:H2’	32:2a:502:G:C8	2.47	0.47
32:2a:552:U:H4’	43:2l:87:GLY:HA2	1.96	0.47
32:2a:605:U:H2’	32:2a:606:G:O4’	2.15	0.47
32:2a:947:G:O3’	44:2m:109:THR:OG1	2.33	0.47
32:2a:1262:C:H2’	32:2a:1263:C:H6	1.79	0.47
32:2a:1427:U:H2’	32:2a:1428:A:H8	1.79	0.47
33:2b:82:ARG:HG3	33:2b:92:TYR:CZ	2.49	0.47
35:2d:172:PRO:HB2	35:2d:187:ARG:NH2	2.30	0.47
37:2f:2:ARG:NE	37:2f:69:GLU:HG2	2.29	0.47
37:2f:89:MET:HE1	49:2r:72:ARG:HB3	1.95	0.47
1:1A:1422:G:H1’	1:1A:1496:A:N1	2.30	0.47
1:1A:1942:5MC:OP2	1:1A:1943:U:O2’	2.24	0.47
1:1A:2723:C:N4	60:1A:4730:HOH:O	2.48	0.47
3:1D:26:LYS:HE2	3:1D:28:GLU:O	2.15	0.47
7:1H:126:PRO:HG2	7:1H:130:ARG:HH21	1.80	0.47
7:1H:127:GLU:OE2	7:1H:130:ARG:NH1	2.48	0.47
7:1H:150:ALA:HA	7:1H:153:LYS:HE2	1.97	0.47
8:1I:65:ALA:O	8:1I:69:LYS:N	2.47	0.47
19:1X:25:LYS:HA	19:1X:81:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:114:U:O2'	32:1a:115:G:H5'	2.15	0.47
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.97	0.47
32:1a:1347:G:N2	32:1a:1373:G:H2'	2.29	0.47
1:2A:247:G:H4'	1:2A:386:G:C5	2.50	0.47
1:2A:628:G:H2'	1:2A:629:G:C8	2.49	0.47
1:2A:807:U:OP2	11:2P:41:ARG:NH2	2.45	0.47
1:2A:1891:G:N7	60:2A:4120:HOH:O	2.36	0.47
1:2A:2572:A:N7	4:2E:145:LYS:HB2	2.29	0.47
4:2E:101:ARG:HD3	4:2E:170:LEU:O	2.15	0.47
5:2F:117:ARG:HH21	5:2F:187:VAL:HA	1.80	0.47
6:2G:84:LYS:HG2	6:2G:85:GLY:N	2.30	0.47
23:21:83:GLU:HA	23:21:84:GLY:HA2	1.60	0.47
28:26:14:THR:OG1	28:26:48:VAL:O	2.27	0.47
32:2a:632:A:H5'	32:2a:633:G:OP2	2.15	0.47
34:2c:32:LEU:O	34:2c:36:ASP:HB2	2.15	0.47
39:2h:9:MET:HG3	39:2h:26:VAL:HG11	1.96	0.47
1:1A:7:G:H2'	1:1A:8:A:C8	2.49	0.47
1:1A:2691:C:O3'	1:1A:2871:C:H4'	2.15	0.47
32:1a:56:U:H2'	32:1a:57:G:C8	2.50	0.47
32:1a:965:A:C8	53:1y:8:LYS:HD2	2.50	0.47
32:1a:1329:A:P	44:1m:28:ALA:HB3	2.54	0.47
32:1a:1458:G:OP1	51:1t:35:THR:OG1	2.28	0.47
4:2E:143:ASN:HB2	4:2E:147:PRO:HD2	1.96	0.47
10:2O:23:ARG:HG3	10:2O:24:VAL:N	2.29	0.47
20:2Y:6:HIS:H	20:2Y:6:HIS:CD2	2.33	0.47
32:2a:398:C:OP2	60:2a:3227:HOH:O	2.21	0.47
32:2a:1008:C:H2'	32:2a:1009:G:H8	1.77	0.47
1:1A:715:G:O6	46:1o:53:HIS:NE2	2.45	0.47
1:1A:1486:A:H2'	1:1A:1487:G:C8	2.48	0.47
1:1A:2657:A:O2'	7:1H:160:LYS:NZ	2.33	0.47
11:1P:90:ARG:HG3	11:1P:91:PHE:CD2	2.49	0.47
12:1Q:141:GLN:NE2	21:1Z:74:VAL:O	2.43	0.47
15:1T:11:GLU:O	15:1T:15:VAL:HG23	2.15	0.47
32:1a:1340:A:OP2	60:1a:3333:HOH:O	2.20	0.47
33:1b:116:GLU:HA	33:1b:119:GLU:HG3	1.96	0.47
35:1d:156:GLU:HA	35:1d:159:ARG:HD2	1.96	0.47
36:1e:102:ALA:O	36:1e:107:ARG:NH1	2.48	0.47
37:1f:69:GLU:O	37:1f:72:VAL:HG12	2.15	0.47
38:1g:89:MET:SD	38:1g:155:ARG:HB2	2.55	0.47
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.50	0.47
1:2A:557:U:H2'	1:2A:558:G:H8	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:568:U:H5'	1:2A:945:A:N6	2.30	0.47
1:2A:1011:G:OP1	16:2U:77:SER:OG	2.29	0.47
1:2A:1092:C:H2'	1:2A:1092:C:O2	2.15	0.47
1:2A:1683:C:H2'	1:2A:1684:C:C6	2.50	0.47
1:2A:2206:G:OP2	1:2A:2206:G:H4'	2.15	0.47
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.30	0.47
4:2E:48:GLN:HA	4:2E:80:GLU:HA	1.97	0.47
6:2G:53:LEU:HD23	6:2G:53:LEU:HA	1.70	0.47
12:2Q:4:PRO:HG3	12:2Q:69:PHE:HE2	1.78	0.47
13:2R:28:LEU:HD13	13:2R:114:VAL:HG23	1.97	0.47
15:2T:41:ARG:NH1	32:2a:346:G:OP1	2.38	0.47
21:2Z:80:ARG:HB2	21:2Z:80:ARG:HH11	1.80	0.47
32:2a:1128:C:H5"	40:2i:66:ARG:NH1	2.30	0.47
32:2a:1163:C:H2'	32:2a:1164:G:C8	2.50	0.47
34:2c:60:ALA:HB3	34:2c:63:ASN:OD1	2.15	0.47
41:2j:77:PRO:O	41:2j:81:THR:OG1	2.28	0.47
46:2o:55:GLY:O	46:2o:59:MET:HB2	2.15	0.47
50:2s:53:ASN:HB3	50:2s:75:ALA:HB1	1.96	0.47
1:1A:886:C:H2'	1:1A:887:A:H5"	1.97	0.46
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.15	0.46
1:1A:1316:U:H2'	1:1A:1317:A:C8	2.50	0.46
1:1A:2010:G:OP1	60:1A:4238:HOH:O	2.20	0.46
6:1G:15:VAL:HG22	6:1G:175:LEU:HB3	1.97	0.46
8:1I:72:LEU:C	8:1I:74:ASN:H	2.23	0.46
18:1W:19:LEU:HB3	27:15:25:LEU:HD11	1.97	0.46
25:13:6:VAL:HG12	25:13:54:VAL:HG21	1.97	0.46
32:1a:177:C:OP1	51:1t:65:LYS:NZ	2.31	0.46
32:1a:458:C:H2'	32:1a:460:G:O4'	2.15	0.46
32:1a:474:G:H2'	32:1a:475:G:C8	2.50	0.46
32:1a:1131:G:H8	32:1a:1131:G:O5'	1.98	0.46
1:2A:601:C:O2'	1:2A:605:C:H5"	2.16	0.46
1:2A:1003:G:H4'	60:2A:5493:HOH:O	2.15	0.46
1:2A:2103:C:H42	1:2A:2185:C:H42	1.61	0.46
1:2A:2140:C:H2'	1:2A:2141:G:H8	1.80	0.46
1:2A:2167:U:H2'	1:2A:2168:G:C4	2.49	0.46
1:2A:2373:G:OP1	60:2A:3949:HOH:O	2.21	0.46
2:2B:24:G:H4'	2:2B:25:A:N7	2.30	0.46
3:2D:145:VAL:HB	3:2D:155:LEU:HB2	1.97	0.46
6:2G:110:ALA:HB1	6:2G:140:ILE:HG22	1.97	0.46
8:2I:4:ILE:HD11	8:2I:44:LEU:HD13	1.97	0.46
17:2V:52:VAL:CG2	17:2V:55:ALA:HB3	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:23:7:LYS:NZ	25:23:32:GLN:O	2.46	0.46
30:28:16:ILE:HG12	30:28:22:VAL:HG22	1.96	0.46
32:2a:560:U:H4'	32:2a:561:U:O5'	2.15	0.46
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.50	0.46
34:2c:10:PHE:CZ	34:2c:178:LEU:HD11	2.50	0.46
1:1A:1632:A:OP2	60:1A:4236:HOH:O	2.20	0.46
1:1A:2164:C:H5"	1:1A:2165:G:OP2	2.14	0.46
1:1A:2593:U:H2'	1:1A:2594:C:C6	2.51	0.46
1:1A:2719:G:OP2	60:1A:4239:HOH:O	2.21	0.46
1:1A:2723:C:OP1	13:1R:3:HIS:ND1	2.27	0.46
4:1E:120:TRP:CE3	4:1E:155:LYS:HD3	2.50	0.46
5:1F:178:PRO:HB2	5:1F:201:VAL:HG21	1.96	0.46
6:1G:135:LEU:O	6:1G:154:GLY:HA3	2.15	0.46
21:1Z:67:LEU:HD23	21:1Z:67:LEU:HA	1.75	0.46
32:1a:1127:G:H5'	32:1a:1280:A:O2'	2.15	0.46
32:1a:1315:U:C4	32:1a:1316:G:C6	3.03	0.46
36:1e:57:LYS:O	36:1e:61:TYR:HD2	1.98	0.46
1:2A:2586:C:H1'	60:2A:4255:HOH:O	2.14	0.46
3:2D:132:PRO:HA	3:2D:190:TYR:HA	1.97	0.46
7:2H:24:VAL:HG13	7:2H:37:VAL:HG21	1.98	0.46
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.97	0.46
9:2N:34:LEU:O	9:2N:49:GLY:HA3	2.16	0.46
14:2S:36:TYR:N	14:2S:36:TYR:HD1	2.14	0.46
32:2a:1151:A:O2'	32:2a:1152:A:H8	1.98	0.46
33:2b:76:GLN:HG3	33:2b:206:ASP:O	2.16	0.46
33:2b:121:LEU:O	33:2b:125:PRO:HD2	2.14	0.46
34:2c:13:GLY:HA3	45:2n:57:ARG:NH2	2.31	0.46
1:1A:492:A:H2'	1:1A:493:G:O4'	2.14	0.46
1:1A:2343:C:HO2'	1:1A:2373:G:HO2'	1.60	0.46
32:1a:222:U:H2'	32:1a:223:U:C6	2.49	0.46
32:1a:1270:C:H2'	32:1a:1271:G:C8	2.50	0.46
32:1a:1343:G:H2'	32:1a:1344:C:C6	2.51	0.46
46:1o:29:VAL:HG13	46:1o:63:ARG:HG3	1.97	0.46
1:2A:1227:G:OP2	16:2U:16:LYS:NZ	2.41	0.46
9:2N:96:GLU:OE1	9:2N:96:GLU:N	2.44	0.46
12:2Q:4:PRO:HB2	12:2Q:7:MET:HE2	1.95	0.46
32:2a:44:G:H2'	32:2a:45:U:O4'	2.15	0.46
32:2a:132:C:H2'	32:2a:133:U:O4'	2.15	0.46
32:2a:1500:A:H5"	32:2a:1508:G:H5"	1.97	0.46
35:2d:3:ARG:HD3	35:2d:118:ARG:NE	2.30	0.46
38:2g:62:PHE:HA	38:2g:124:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2g:68:ASN:HD22	38:2g:128:ALA:HA	1.81	0.46
38:2g:148:ASN:HD22	38:2g:151:TYR:HD2	1.63	0.46
39:2h:72:PRO:O	39:2h:74:PRO:HD3	2.16	0.46
43:2l:83:VAL:HG22	43:2l:84:LEU:H	1.79	0.46
51:2t:25:ARG:O	51:2t:29:LYS:HG3	2.15	0.46
53:2y:38:HIS:HB3	53:2y:53:THR:OG1	2.15	0.46
1:1A:1045:A:H1'	1:1A:1047:G:C2	2.51	0.46
5:1F:52:LYS:NZ	60:1F:413:HOH:O	2.46	0.46
6:1G:36:LYS:HD3	6:1G:95:ARG:HH12	1.80	0.46
25:13:7:LYS:HB2	25:13:34:GLU:HG2	1.98	0.46
32:1a:476:G:H2'	32:1a:477:A:O4'	2.15	0.46
32:1a:1263:C:H2'	32:1a:1264:C:C6	2.50	0.46
32:1a:1340:A:OP1	53:1y:57:PRO:HB3	2.15	0.46
39:1h:17:THR:O	39:1h:78:GLN:NE2	2.35	0.46
46:1o:61:GLY:O	46:1o:65:ARG:HG3	2.16	0.46
1:2A:1016:G:C4	1:2A:1017:G:C8	3.03	0.46
1:2A:1062:G:C8	1:2A:1070:A:H1'	2.50	0.46
1:2A:1826:G:H4'	3:2D:242:ARG:CZ	2.45	0.46
1:2A:2134:A:H5"	1:2A:2156:G:N2	2.30	0.46
1:2A:2478:A:H5'	31:29:31:LYS:HE2	1.95	0.46
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.50	0.46
19:2X:40:LYS:HG3	19:2X:51:VAL:HB	1.97	0.46
26:24:59:PHE:HB3	26:24:61:ARG:HG2	1.98	0.46
32:2a:93:G:H2'	32:2a:96:U:O4'	2.16	0.46
32:2a:176:C:H2'	32:2a:177:C:H6	1.81	0.46
32:2a:179:A:H2'	32:2a:180:U:C6	2.51	0.46
32:2a:570:G:H2'	32:2a:571:U:C6	2.51	0.46
32:2a:614:A:H2'	32:2a:615:C:C6	2.50	0.46
32:2a:1057:G:H2'	32:2a:1058:G:O4'	2.15	0.46
34:2c:5:ILE:HG12	45:2n:49:HIS:HE1	1.79	0.46
47:2p:54:GLU:HG3	47:2p:55:ARG:N	2.31	0.46
1:1A:587:C:OP2	11:1P:21:ARG:NH1	2.38	0.46
1:1A:2322:A:H2'	1:1A:2323:G:O4'	2.16	0.46
1:1A:2464:C:O2'	60:1A:4172:HOH:O	2.13	0.46
5:1F:172:TRP:CD1	5:1F:172:TRP:H	2.33	0.46
7:1H:111:HIS:CD2	7:1H:111:HIS:H	2.32	0.46
15:1T:24:PRO:HA	15:1T:49:VAL:HG22	1.97	0.46
15:1T:54:ARG:HA	15:1T:59:THR:HB	1.98	0.46
21:1Z:4:ARG:NE	21:1Z:60:GLU:OE2	2.36	0.46
25:13:43:ILE:O	25:13:47:VAL:HG23	2.16	0.46
32:1a:174:C:H2'	32:1a:175:C:H6	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1216:G:H5”	45:1n:5:ALA:HB2	1.98	0.46
51:1t:63:ILE:HD13	51:1t:80:ARG:HB3	1.97	0.46
53:1y:76:GLU:HA	53:1y:79:ASN:HD22	1.80	0.46
1:2A:2206:G:H5”	1:2A:2207:G:C5	2.50	0.46
7:2H:56:SER:OG	7:2H:57:ASP:N	2.49	0.46
32:2a:59:A:O2’	60:2a:3228:HOH:O	2.21	0.46
32:2a:110:C:H2’	32:2a:111:G:O4’	2.14	0.46
32:2a:222:U:H2’	32:2a:223:U:C6	2.51	0.46
32:2a:735:C:H2’	32:2a:736:C:C6	2.50	0.46
32:2a:1040:U:H2’	32:2a:1041:A:O4’	2.15	0.46
32:2a:1505:G:H4’	32:2a:1506:U:H5”	1.97	0.46
39:2h:112:LEU:HB3	39:2h:133:LEU:HA	1.97	0.46
40:2i:8:GLY:HA2	40:2i:79:LEU:HD23	1.98	0.46
42:2k:48:ILE:HD11	42:2k:64:ALA:HA	1.97	0.46
46:2o:43:LEU:HD12	46:2o:56:LEU:HD22	1.98	0.46
50:2s:61:TYR:CE2	50:2s:63:THR:HG22	2.50	0.46
1:1A:330:A:H2	1:1A:1210:A:O2’	1.98	0.46
1:1A:817:C:O2’	1:1A:839:U:H5”	2.15	0.46
1:1A:911:A:H2’	12:1Q:9:TYR:OH	2.15	0.46
1:1A:2348:U:O4	1:1A:2382:G:C2	2.69	0.46
1:1A:2756:U:H1’	1:1A:2757:A:H5”	1.96	0.46
4:1E:9:VAL:HG13	4:1E:25:VAL:O	2.16	0.46
12:1Q:109:VAL:HG22	12:1Q:113:GLN:OE1	2.16	0.46
13:1R:70:LEU:O	13:1R:72:ASP:N	2.47	0.46
15:1T:117:ASP:O	15:1T:121:ILE:HG13	2.16	0.46
32:1a:731:G:OP1	32:1a:766:A:H1’	2.16	0.46
32:1a:936:C:H2’	32:1a:937:A:O4’	2.15	0.46
41:1j:47:PHE:CZ	45:1n:37:PHE:HE2	2.34	0.46
45:1n:26:ARG:HD3	45:1n:43:CYS:HB3	1.98	0.46
1:2A:1803:A:O2’	3:2D:259:THR:HG21	2.15	0.46
3:2D:77:ALA:HB2	3:2D:97:TYR:CD1	2.51	0.46
7:2H:64:LEU:O	7:2H:68:THR:OG1	2.32	0.46
21:2Z:24:LEU:HD12	21:2Z:25:PRO:HD2	1.98	0.46
32:2a:565:U:H3’	32:2a:566:G:H2’	1.98	0.46
35:2d:70:ILE:HG12	35:2d:74:GLN:HB2	1.97	0.46
40:2i:15:ALA:HB2	40:2i:65:VAL:HG23	1.98	0.46
40:2i:37:PHE:HD1	40:2i:40:LEU:HD12	1.80	0.46
40:2i:100:GLY:O	40:2i:103:THR:HG22	2.15	0.46
1:1A:2061:G:OP1	5:1F:68:LYS:NZ	2.29	0.46
1:1A:2286:A:H4’	1:1A:2287:A:O4’	2.16	0.46
8:1I:30:LEU:HA	8:1I:35:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:86:LYS:HB3	11:1P:118:GLY:HA3	1.97	0.46
32:1a:108:G:C6	51:1t:15:ARG:HG2	2.51	0.46
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.98	0.46
1:2A:154(A):C:N4	1:2A:171:G:H1	2.09	0.46
1:2A:671:C:H2'	1:2A:672:C:C6	2.51	0.46
1:2A:2291:U:OP1	1:2A:2380:C:O2'	2.23	0.46
2:2B:32:C:H2'	2:2B:33:G:H8	1.81	0.46
5:2F:122:LYS:HD2	5:2F:191:ARG:HD2	1.97	0.46
7:2H:8:PRO:HB3	7:2H:51:ARG:HG2	1.98	0.46
10:2O:68:GLU:CD	10:2O:68:GLU:H	2.24	0.46
14:2S:26:LEU:HD22	14:2S:87:PHE:CD1	2.51	0.46
32:2a:1128:C:H5"	40:2i:66:ARG:HH12	1.79	0.46
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.51	0.46
34:2c:57:ILE:HG12	34:2c:66:VAL:HG22	1.98	0.46
39:2h:11:THR:HG22	39:2h:15:ASN:ND2	2.29	0.46
40:2i:16:ARG:N	40:2i:64:THR:O	2.48	0.46
1:1A:229:A:H3'	1:1A:230:U:H5'	1.97	0.46
1:1A:897:C:H2'	1:1A:898:C:C6	2.51	0.46
1:1A:1048:A:OP2	1:1A:1109:C:N4	2.49	0.46
1:1A:2320:A:H2'	1:1A:2320:A:N3	2.31	0.46
1:1A:2445:G:OP1	5:1F:74:ARG:NH2	2.49	0.46
1:1A:2544:G:H1'	1:1A:2646:C:H4'	1.96	0.46
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.49	0.46
6:1G:98:ARG:CZ	26:14:1:MET:HE3	2.46	0.46
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.31	0.46
32:1a:532:A:H2	32:1a:1206:G:H21	1.63	0.46
32:1a:625:G:H4'	47:1p:16:HIS:CD2	2.51	0.46
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.97	0.46
32:1a:1498:UR3:H4'	32:1a:1519:MA6:H2	1.98	0.46
33:1b:127:ILE:HG22	33:1b:130:ARG:HG2	1.96	0.46
47:1p:29:ASP:OD1	47:1p:29:ASP:N	2.49	0.46
1:2A:41:C:H2'	1:2A:42:G:H8	1.79	0.46
1:2A:1349:A:OP1	60:2A:3945:HOH:O	2.20	0.46
1:2A:1800:C:P	3:2D:183:ARG:HH12	2.38	0.46
1:2A:1973:G:H2'	1:2A:1974:C:C6	2.51	0.46
16:2U:97:ASP:OD2	60:2U:301:HOH:O	2.21	0.46
19:2X:94:GLY:HA3	19:2X:95:LEU:C	2.41	0.46
25:23:23:LEU:HD13	25:23:50:VAL:HG11	1.96	0.46
32:2a:258:G:H1	32:2a:268:C:N4	2.12	0.46
32:2a:1151:A:N3	41:2j:39:PRO:HG3	2.31	0.46
46:2o:7:GLU:O	46:2o:11:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:2o:79:ARG:O	46:2o:83:GLU:HB3	2.16	0.46
48:2q:66:SER:HB3	48:2q:69:LYS:HD3	1.97	0.46
1:1A:264:C:O2'	1:1A:265:A:H2'	2.15	0.46
1:1A:466:A:N3	1:1A:683:C:H1'	2.31	0.46
1:1A:1416:G:O2'	1:1A:1417:C:OP2	2.30	0.46
1:1A:2065:C:H4'	1:1A:2251:OMG:HM22	1.98	0.46
21:1Z:3:TYR:O	21:1Z:58:VAL:HG22	2.16	0.46
30:18:62:LEU:HB3	30:18:65:GLU:HG3	1.97	0.46
32:1a:945:G:C2	32:1a:946:A:C8	3.03	0.46
40:1i:21:PRO:HA	40:1i:59:PHE:HA	1.97	0.46
1:2A:1079:C:H6	1:2A:1088:A:N1	2.14	0.46
1:2A:2104:G:N1	1:2A:2185:C:O2	2.49	0.46
1:2A:2134:A:P	1:2A:2156:G:H22	2.39	0.46
1:2A:2171:A:H4'	1:2A:2172:U:OP1	2.13	0.46
10:2O:70:LYS:HB3	10:2O:70:LYS:HE2	1.71	0.46
18:2W:1:MET:HE3	18:2W:62:HIS:HB3	1.98	0.46
32:2a:690:G:H2'	32:2a:691:G:O4'	2.16	0.46
32:2a:1441:G:H1'	32:2a:1461:G:N2	2.30	0.46
1:1A:127:A:H5"	1:1A:128:C:C6	2.50	0.46
1:1A:271(H):G:HO2'	1:1A:271(I):G:H8	1.61	0.46
1:1A:582:G:H2'	1:1A:583:G:C8	2.51	0.46
1:1A:848:G:O6	1:1A:928:G:H2'	2.15	0.46
1:1A:1710:C:O2'	1:1A:2858:C:N3	2.49	0.46
1:1A:2233:U:H2'	1:1A:2234:G:C8	2.51	0.46
1:1A:2336:A:H61	22:10:43:THR:CG2	2.28	0.46
2:1B:7:G:H5"	2:1B:7:G:H8	1.80	0.46
4:1E:49:LEU:HD12	4:1E:49:LEU:HA	1.72	0.46
17:1V:61:VAL:HA	17:1V:94:LEU:HD23	1.98	0.46
21:1Z:128:VAL:HG22	21:1Z:132:ASN:HB3	1.97	0.46
32:1a:108:G:H1	51:1t:15:ARG:HG2	1.81	0.46
32:1a:132:C:OP1	51:1t:75:ASN:ND2	2.48	0.46
32:1a:911:U:H2'	32:1a:912:C:C6	2.51	0.46
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.46	0.46
32:1a:1299:A:N3	32:1a:1299:A:H5"	2.31	0.46
36:1e:50:GLU:HB2	36:1e:53:LEU:HD13	1.98	0.46
41:1j:84:GLN:HE21	41:1j:85:LEU:HG	1.81	0.46
48:1q:9:VAL:HG21	48:1q:84:LEU:HD12	1.99	0.46
48:1q:59:ILE:HG22	48:1q:73:VAL:HA	1.97	0.46
51:1t:59:ALA:O	51:1t:63:ILE:HG13	2.15	0.46
51:1t:63:ILE:HG22	51:1t:77:ALA:HB1	1.98	0.46
1:2A:839:U:O2'	1:2A:1191:G:N3	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1341:U:C5	1:2A:1395:A:H2	2.33	0.46
1:2A:1366:A:OP1	23:21:3:LYS:NZ	2.38	0.46
1:2A:1702:G:H2'	1:2A:1703:G:O4'	2.16	0.46
1:2A:2281:C:O2'	1:2A:2282:G:H5'	2.16	0.46
1:2A:2816:C:O2	1:2A:2883:A:O2'	2.34	0.46
4:2E:96:PHE:O	4:2E:175:VAL:HG11	2.16	0.46
53:2y:63:ALA:HB2	53:2y:84:GLN:NE2	2.30	0.46
1:1A:875:G:H1	1:1A:902:C:H42	1.63	0.45
1:1A:1745(A):C:H2'	1:1A:1746:G:O4'	2.15	0.45
1:1A:2114:A:O2'	1:1A:2168:G:OP1	2.34	0.45
4:1E:144:ARG:HB3	4:1E:145:LYS:H	1.47	0.45
14:1S:15:ARG:NE	14:1S:88:ASP:OD2	2.48	0.45
21:1Z:157:LEU:HD11	21:1Z:163:LEU:HD13	1.98	0.45
26:14:69:LYS:HB2	50:1s:20:LEU:HD13	1.98	0.45
32:1a:108:G:H5"	32:1a:109:A:H5"	1.97	0.45
32:1a:292:G:C5	32:1a:293:G:H1'	2.51	0.45
32:1a:509:A:O2'	32:1a:510:A:OP1	2.32	0.45
32:1a:946:A:H2'	32:1a:947:G:C8	2.51	0.45
32:1a:1028:C:H2'	32:1a:1029:C:H4'	1.98	0.45
32:1a:1296:C:H5"	44:1m:44:ARG:HH22	1.80	0.45
32:1a:1328:C:H5"	44:1m:28:ALA:HB1	1.97	0.45
34:1c:131:ARG:HE	34:1c:135:LYS:HE3	1.80	0.45
53:1y:27:LEU:HB2	53:1y:34:LEU:HD11	1.98	0.45
1:2A:76:C:O3'	24:22:59:ARG:HG3	2.16	0.45
1:2A:196:A:N3	1:2A:196:A:H2'	2.31	0.45
1:2A:271(T):C:N4	60:2A:4261:HOH:O	2.47	0.45
1:2A:312:G:H4'	1:2A:331:A:N3	2.31	0.45
1:2A:2006:C:OP2	60:2A:3944:HOH:O	2.20	0.45
1:2A:2283:C:C2	1:2A:2389:G:C2	3.04	0.45
6:2G:98:ARG:CZ	26:24:1:MET:HE3	2.46	0.45
8:2I:14:ASP:OD1	8:2I:15:VAL:N	2.47	0.45
9:2N:96:GLU:HB2	9:2N:122:VAL:HG12	1.98	0.45
11:2P:90:ARG:NH1	11:2P:105:LEU:HD11	2.31	0.45
32:2a:45:U:O2'	60:2a:3230:HOH:O	2.21	0.45
32:2a:129:U:O4	60:2a:3229:HOH:O	2.21	0.45
35:2d:76:ARG:HD3	35:2d:207:TYR:CE1	2.51	0.45
41:2j:11:PHE:CE1	41:2j:67:THR:HG22	2.51	0.45
42:2k:85:ARG:HE	42:2k:111:ASP:HB3	1.81	0.45
1:1A:186:G:H2'	1:1A:187:G:H8	1.82	0.45
2:1B:90:A:N7	2:1B:91:C:H1'	2.31	0.45
11:1P:17:LYS:HE3	11:1P:27:HIS:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1S:20:ARG:NH2	22:10:51:VAL:O	2.48	0.45
32:1a:503:C:H2'	32:1a:504:C:C6	2.51	0.45
32:1a:828:A:H2'	32:1a:829:G:O4'	2.16	0.45
32:1a:865:A:C2	32:1a:918:A:H4'	2.51	0.45
32:1a:977:A:H2'	32:1a:978:A:H5"	1.98	0.45
32:1a:1030(C):G:H8	32:1a:1030(D):A:C8	2.35	0.45
33:1b:124:SER:HA	33:1b:125:PRO:HA	1.61	0.45
37:1f:76:ALA:HB1	37:1f:80:ARG:NH2	2.31	0.45
41:1j:5:ARG:HD3	41:1j:71:LEU:HD11	1.98	0.45
50:1s:18:LYS:O	50:1s:22:LEU:HG	2.16	0.45
51:1t:90:GLN:HA	51:1t:93:GLU:HG2	1.97	0.45
1:2A:761:A:OP1	60:2A:3861:HOH:O	2.21	0.45
1:2A:862:G:H2'	1:2A:863:A:O4'	2.16	0.45
1:2A:2254:C:OP2	60:2A:3942:HOH:O	2.20	0.45
1:2A:2350:C:H2'	1:2A:2351:G:O4'	2.16	0.45
5:2F:139:PHE:HB2	5:2F:166:ALA:HB1	1.98	0.45
6:2G:36:LYS:HE2	6:2G:160:VAL:HG21	1.98	0.45
15:2T:23:ARG:N	15:2T:26:ASP:OD2	2.42	0.45
20:2Y:23:ARG:HA	20:2Y:23:ARG:HD3	1.70	0.45
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.49	0.45
32:2a:352:C:H4'	32:2a:354:G:OP1	2.16	0.45
32:2a:501:C:OP1	43:2l:117:ARG:NH2	2.49	0.45
32:2a:724:G:C2	32:2a:725:G:C8	3.04	0.45
32:2a:1320:C:H42	50:2s:36:ARG:HE	1.64	0.45
38:2g:108:ALA:O	38:2g:119:ARG:HD2	2.15	0.45
1:1A:222:A:H5"	1:1A:421:U:OP1	2.17	0.45
1:1A:1652:A:O2'	1:1A:1653:G:H5'	2.16	0.45
1:1A:1706:U:OP1	60:1A:4237:HOH:O	2.20	0.45
1:1A:2096:U:H3	1:1A:2193:G:H1	1.64	0.45
3:1D:26:LYS:HD3	3:1D:83:GLU:OE2	2.17	0.45
32:1a:738:C:H2'	32:1a:739:C:C6	2.51	0.45
32:1a:779:C:H2'	32:1a:780:A:O4'	2.16	0.45
32:1a:920:U:H2'	32:1a:921:U:C6	2.51	0.45
33:1b:84:GLU:HB2	33:1b:215:LEU:HD13	1.97	0.45
33:1b:97:TRP:HH2	33:1b:176:GLU:CD	2.23	0.45
35:1d:178:VAL:C	35:1d:180:GLY:H	2.24	0.45
1:2A:271(G):C:H2'	1:2A:271(H):G:C8	2.51	0.45
1:2A:519:U:H2'	1:2A:520:G:C8	2.52	0.45
1:2A:888:C:H2'	1:2A:889:C:N3	2.31	0.45
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.51	0.45
1:2A:2635:C:H5"	4:2E:78:LEU:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:139:PHE:O	5:2F:143:ALA:N	2.40	0.45
7:2H:117:PRO:HA	7:2H:118:PRO:HD3	1.84	0.45
11:2P:1:MET:HE2	11:2P:5:ASP:HB3	1.99	0.45
15:2T:16:ARG:HG3	15:2T:18:ASP:OD1	2.17	0.45
15:2T:24:PRO:HD3	15:2T:52:ILE:HD12	1.99	0.45
32:2a:814:A:H2'	32:2a:816:A:C5'	2.46	0.45
32:2a:1490:C:H2'	32:2a:1491:G:C8	2.51	0.45
1:1A:918:A:H5"	2:1B:98:G:O2'	2.16	0.45
1:1A:1213:A:N3	1:1A:1238:G:O2'	2.42	0.45
1:1A:2079:U:O3'	23:11:35:THR:OG1	2.33	0.45
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.51	0.45
13:1R:24:GLN:HE21	13:1R:44:LEU:HG	1.80	0.45
19:1X:76:ARG:HG3	60:1X:106:HOH:O	2.16	0.45
32:1a:364:A:H2'	32:1a:365:U:O2	2.16	0.45
32:1a:418:C:H2'	32:1a:419:C:H6	1.81	0.45
32:1a:619:U:N3	35:1d:134:ASP:OD1	2.36	0.45
32:1a:1260:C:O5'	32:1a:1284:C:H4'	2.16	0.45
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.52	0.45
33:1b:35:GLU:OE1	33:1b:38:GLY:HA2	2.16	0.45
33:1b:101:MET:HA	33:1b:108:ILE:HD12	1.99	0.45
40:1i:29:ASN:ND2	40:1i:65:VAL:H	2.15	0.45
40:1i:50:LEU:HD13	40:1i:56:LEU:HA	1.99	0.45
1:2A:2336:A:H61	22:20:43:THR:CG2	2.30	0.45
1:2A:2376:A:H8	1:2A:2376:A:OP1	1.99	0.45
1:2A:2395:C:O2'	23:21:30:VAL:HG22	2.17	0.45
6:2G:15:VAL:HG13	6:2G:175:LEU:HD23	1.98	0.45
7:2H:3:ARG:HG2	7:2H:6:ARG:NH1	2.31	0.45
13:2R:87:TYR:OH	13:2R:117:VAL:O	2.28	0.45
14:2S:3:ARG:HD2	14:2S:3:ARG:HA	1.59	0.45
32:2a:35:G:O2'	43:2l:118:SER:O	2.34	0.45
32:2a:538:G:H2'	32:2a:539:A:H8	1.81	0.45
32:2a:789:U:O2'	32:2a:791:G:N7	2.48	0.45
32:2a:790:A:N6	32:2a:1498:UR3:OP1	2.49	0.45
32:2a:1323:G:H4'	32:2a:1363:C:C2	2.52	0.45
37:2f:19:LEU:HD11	37:2f:59:TYR:CZ	2.51	0.45
39:2h:86:ILE:HG12	39:2h:135:CYS:HA	1.98	0.45
1:1A:2870:C:OP1	13:1R:57:ARG:NH1	2.34	0.45
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.17	0.45
6:1G:109:VAL:C	6:1G:112:PRO:HD2	2.41	0.45
32:1a:131:C:O2'	32:1a:262:A:N3	2.37	0.45
32:1a:421:U:O2'	32:1a:422:C:H5'	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:632:A:H3'	32:1a:633:G:H8	1.80	0.45
32:1a:692:U:O2'	32:1a:694:A:N7	2.40	0.45
33:1b:12:GLU:O	33:1b:15:VAL:N	2.48	0.45
39:1h:7:ALA:HB2	39:1h:85:ARG:HG3	1.98	0.45
41:1j:31:GLY:HA2	41:1j:32:ALA:HA	1.61	0.45
47:1p:47:ASP:O	47:1p:49:LEU:N	2.41	0.45
1:2A:131:G:OP1	60:2A:3950:HOH:O	2.21	0.45
1:2A:328:U:H4'	20:2Y:68:HIS:CE1	2.51	0.45
1:2A:1419:A:N6	1:2A:1494:A:N1	2.52	0.45
1:2A:2061:G:H2'	1:2A:2501:C:O2'	2.16	0.45
7:2H:109:PHE:C	7:2H:111:HIS:H	2.25	0.45
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.17	0.45
30:28:29:LYS:N	60:28:202:HOH:O	2.27	0.45
32:2a:40:C:N4	32:2a:402:G:H1	2.11	0.45
32:2a:540:G:H2'	32:2a:541:G:C8	2.52	0.45
32:2a:545:C:H5'	35:2d:72:GLU:CB	2.47	0.45
32:2a:615:C:H2'	32:2a:616:G:O4'	2.16	0.45
32:2a:1004:A:N7	32:2a:1037:C:H2'	2.31	0.45
33:2b:24:TRP:CD1	33:2b:24:TRP:H	2.35	0.45
34:2c:131:ARG:HD3	34:2c:166:GLU:CG	2.47	0.45
35:2d:76:ARG:HD2	35:2d:76:ARG:HA	1.61	0.45
1:1A:446:G:OP1	16:1U:3:ARG:NH1	2.50	0.45
1:1A:1180:C:H2'	1:1A:1181:C:C6	2.52	0.45
1:1A:1919:A:N1	32:1a:1495:U:O2'	2.42	0.45
1:1A:2563:U:H5'	60:1A:4500:HOH:O	2.17	0.45
1:1A:2667:C:H2'	1:1A:2668:G:O4'	2.17	0.45
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.16	0.45
6:1G:2:PRO:HB3	6:1G:8:LYS:NZ	2.32	0.45
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.53	0.45
9:1N:38:HIS:CD2	9:1N:39:ARG:HG2	2.52	0.45
14:1S:87:PHE:CE1	14:1S:102:ALA:HB2	2.52	0.45
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.60	0.45
32:1a:155:C:H2'	32:1a:156:G:O4'	2.16	0.45
32:1a:901:A:OP2	60:1a:3335:HOH:O	2.21	0.45
32:1a:1121:U:H2'	32:1a:1122:U:H6	1.82	0.45
37:1f:15:ASP:OD1	37:1f:17:SER:N	2.49	0.45
37:1f:15:ASP:OD1	37:1f:18:GLN:N	2.29	0.45
41:1j:37:PRO:HA	41:1j:72:VAL:HG12	1.97	0.45
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.98	0.45
50:1s:35:SER:O	50:1s:71:LEU:HD12	2.16	0.45
1:2A:26:G:C6	1:2A:27:G:N1	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.51	0.45
1:2A:1866:C:H2'	1:2A:1876:A:O4'	2.17	0.45
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.35	0.45
1:2A:2127:G:H2'	1:2A:2128:C:O4'	2.16	0.45
1:2A:2197:U:H1'	1:2A:2198:A:C8	2.51	0.45
4:2E:82:ARG:HG3	4:2E:83:ASP:N	2.31	0.45
10:2O:120:GLU:HB2	15:2T:68:TYR:HE2	1.81	0.45
32:2a:1326:C:H2'	32:2a:1327:C:C6	2.51	0.45
32:2a:1512:U:H2'	32:2a:1513:A:C8	2.51	0.45
34:2c:119:ARG:HH11	34:2c:140:ARG:CZ	2.30	0.45
38:2g:49:ILE:HA	38:2g:52:GLU:HG2	1.98	0.45
48:2q:6:LEU:O	48:2q:58:GLU:HA	2.16	0.45
1:1A:300:A:OP2	20:1Y:86:ARG:NH2	2.50	0.45
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.52	0.45
1:1A:1792:G:O2'	1:1A:1830:C:OP1	2.31	0.45
1:1A:2193:G:H2'	1:1A:2194:G:H8	1.82	0.45
3:1D:102:LYS:C	3:1D:103:ARG:HG2	2.41	0.45
7:1H:41:MET:HE2	7:1H:65:HIS:HA	1.99	0.45
15:1T:8:LYS:NZ	60:1T:304:HOH:O	2.50	0.45
17:1V:97:LYS:HD3	17:1V:97:LYS:HA	1.83	0.45
20:1Y:28:LYS:HG3	20:1Y:40:GLU:HG2	1.98	0.45
32:1a:1263:C:H2'	32:1a:1264:C:H6	1.82	0.45
32:1a:1314:C:H2'	32:1a:1315:U:C6	2.51	0.45
33:1b:71:VAL:O	33:1b:165:VAL:HG23	2.17	0.45
33:1b:80:ILE:HG21	33:1b:211:ILE:HG22	1.98	0.45
34:1c:8:ILE:HD12	34:1c:16:ARG:NE	2.32	0.45
43:1l:70:ILE:HD13	43:1l:77:LEU:HD12	1.98	0.45
50:1s:63:THR:OG1	50:1s:65:ASN:OD1	2.26	0.45
1:2A:969:U:H2'	1:2A:970:C:C6	2.52	0.45
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.42	0.45
30:28:22:VAL:HG12	30:28:50:LEU:HD12	1.99	0.45
32:2a:353:A:H5'	32:2a:353:A:H8	1.82	0.45
32:2a:931:C:H42	32:2a:1386:G:H1	1.64	0.45
32:2a:1305:G:H22	32:2a:1331:G:H1'	1.81	0.45
37:2f:3:ARG:HD3	37:2f:64:GLN:NE2	2.31	0.45
53:2y:54:ILE:O	53:2y:61:LEU:N	2.41	0.45
1:1A:645:C:H5'	1:1A:646:A:OP2	2.17	0.45
1:1A:1217:C:OP1	60:1A:4240:HOH:O	2.21	0.45
3:1D:145:VAL:HG12	3:1D:146:GLU:O	2.16	0.45
4:1E:2:LYS:HA	4:1E:84:PHE:CD1	2.51	0.45
5:1F:9:ILE:HG21	5:1F:125:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:65:TRP:CZ2	5:1F:75:HIS:HD2	2.33	0.45
6:1G:96:ARG:N	6:1G:99:MET:HE2	2.32	0.45
12:1Q:1:MET:HE2	12:1Q:1:MET:HB3	1.84	0.45
32:1a:445:G:C6	32:1a:490:G:C6	3.04	0.45
32:1a:585:G:N3	32:1a:879:C:H4'	2.31	0.45
32:1a:648:A:H2'	32:1a:649:G:C8	2.52	0.45
32:1a:985:C:H2'	32:1a:986:A:H8	1.81	0.45
32:1a:1256:A:H3'	34:1c:27:LYS:NZ	2.32	0.45
32:1a:1272:G:H2'	32:1a:1273:G:O4'	2.15	0.45
32:1a:1346:A:O3'	32:1a:1347:G:H4'	2.17	0.45
32:1a:1500:A:N7	60:1a:3379:HOH:O	2.36	0.45
33:1b:17:PHE:HB3	33:1b:44:LEU:HD21	1.99	0.45
48:1q:45:HIS:HB2	48:1q:65:ILE:HD13	1.98	0.45
52:1u:18:TYR:CE1	52:1u:24:ARG:HB3	2.52	0.45
1:2A:800:A:O4'	1:2A:801:G:H3'	2.16	0.45
1:2A:861:A:C2	1:2A:917:A:C4	3.05	0.45
1:2A:2134:A:N7	1:2A:2157:G:H5'	2.32	0.45
1:2A:2811:G:OP1	4:2E:60:ASN:HB2	2.17	0.45
3:2D:20:ASP:OD1	3:2D:20:ASP:N	2.40	0.45
6:2G:96:ARG:O	6:2G:99:MET:HB3	2.17	0.45
7:2H:124:GLU:HB2	7:2H:132:ARG:HB3	1.99	0.45
7:2H:144:VAL:HA	7:2H:147:ASN:HB2	1.99	0.45
9:2N:34:LEU:HD12	9:2N:34:LEU:HA	1.82	0.45
14:2S:74:ALA:HB3	14:2S:108:GLY:HA3	1.99	0.45
32:2a:224:C:H2'	32:2a:225:C:C6	2.52	0.45
32:2a:836:G:C6	32:2a:851:G:C6	3.05	0.45
32:2a:1305:G:OP1	52:2u:2:GLY:N	2.50	0.45
34:2c:199:LYS:HB3	34:2c:201:TYR:HE2	1.81	0.45
35:2d:88:VAL:HG22	36:2e:96:PRO:HB2	1.98	0.45
38:2g:42:ILE:HD13	38:2g:116:ALA:HB3	1.99	0.45
38:2g:78:ARG:HB2	38:2g:156:TRP:CZ3	2.52	0.45
39:2h:39:LEU:HD21	39:2h:137:VAL:HG21	1.98	0.45
40:2i:16:ARG:HH11	40:2i:64:THR:HG21	1.81	0.45
45:2n:23:ARG:NH1	45:2n:30:ALA:HB2	2.32	0.45
47:2p:39:TYR:HB2	47:2p:49:LEU:HD13	1.98	0.45
1:1A:143:G:H2'	1:1A:143(A):C:C6	2.52	0.45
1:1A:715:G:C2	46:1o:56:LEU:HD21	2.51	0.45
1:1A:1166:C:H2'	1:1A:1167:U:H6	1.82	0.45
1:1A:2174:C:H2'	1:1A:2175:C:C6	2.52	0.45
1:1A:2422:A:H2'	60:1A:7353:HOH:O	2.16	0.45
7:1H:62:LYS:HE2	7:1H:62:LYS:HB3	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1N:33:LEU:HA	9:1N:38:HIS:CE1	2.52	0.45
19:1X:41:ASN:O	19:1X:45:THR:HG23	2.17	0.45
32:1a:110:C:H2'	32:1a:111:G:O4'	2.16	0.45
32:1a:164:U:H2'	32:1a:165:C:C6	2.52	0.45
32:1a:677:U:H3	32:1a:713:G:H22	1.65	0.45
32:1a:976:G:N2	32:1a:1363:C:OP2	2.44	0.45
32:1a:991:U:H1'	32:1a:992:U:OP2	2.17	0.45
33:1b:15:VAL:HG21	33:1b:213:LEU:HD13	1.99	0.45
39:1h:28:ALA:HA	39:1h:59:LEU:HG	1.98	0.45
45:1n:46:GLU:O	45:1n:50:LYS:HG3	2.17	0.45
1:2A:2099:U:H3	1:2A:2190:G:H1	1.65	0.45
1:2A:2109:U:H2'	1:2A:2110:G:C8	2.52	0.45
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.17	0.45
6:2G:63:ILE:HG22	6:2G:64:THR:HG23	1.99	0.45
32:2a:134:A:N6	47:2p:25:ARG:HH22	2.15	0.45
32:2a:1142:G:H2'	32:2a:1143:G:O4'	2.17	0.45
32:2a:1172:C:H2'	32:2a:1173:G:H8	1.80	0.45
32:2a:1289:A:N1	32:2a:1371:G:O2'	2.41	0.45
32:2a:1333:A:H2'	32:2a:1334:G:O4'	2.17	0.45
32:2a:1443:G:N2	32:2a:1460:A:H1'	2.32	0.45
32:2a:1468:A:H2'	32:2a:1469:G:O4'	2.17	0.45
33:2b:155:LEU:HD21	33:2b:159:PRO:HG3	1.99	0.45
34:2c:17:ASP:OD1	34:2c:18:TRP:N	2.48	0.45
42:2k:102:GLY:O	42:2k:103:LEU:HD12	2.16	0.45
47:2p:55:ARG:HD2	47:2p:55:ARG:HA	1.73	0.45
51:2t:57:ARG:HH12	51:2t:100:ILE:HB	1.81	0.45
1:1A:719:C:H2'	1:1A:720:C:H6	1.81	0.45
1:1A:808:G:OP1	60:1A:4241:HOH:O	2.21	0.45
1:1A:1301:A:C8	1:1A:1303:G:C8	3.04	0.45
3:1D:4:LYS:HB3	3:1D:18:VAL:HG22	1.99	0.45
9:1N:99:LEU:HB2	60:1N:309:HOH:O	2.17	0.45
16:1U:17:ILE:HG23	16:1U:39:LEU:HD12	1.99	0.45
32:1a:1073:U:H2'	32:1a:1074:G:C8	2.52	0.45
32:1a:1314:C:OP2	50:1s:4:SER:OG	2.28	0.45
35:1d:159:ARG:O	35:1d:163:GLU:N	2.46	0.45
45:1n:3:ARG:O	45:1n:6:LEU:HB2	2.17	0.45
1:2A:139:G:H2'	1:2A:140:G:N7	2.32	0.45
1:2A:1053:C:H2'	1:2A:1054:A:C8	2.51	0.45
1:2A:1224:C:O2'	17:2V:85:LYS:HA	2.16	0.45
1:2A:1568:G:H4'	3:2D:59:LYS:HG2	1.99	0.45
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:140:LEU:HA	5:2F:143:ALA:HB3	1.98	0.45
6:2G:63:ILE:HG12	6:2G:141:PHE:CD2	2.52	0.45
10:2O:15:GLY:HA2	10:2O:47:ILE:HD11	1.98	0.45
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	1.98	0.45
19:2X:44:GLU:O	19:2X:48:LYS:N	2.41	0.45
32:2a:495:A:H4'	32:2a:496:A:OP1	2.16	0.45
32:2a:1452:C:H4'	32:2a:1457:G:C8	2.51	0.45
33:2b:63:MET:HG3	33:2b:225:ALA:HB1	1.99	0.45
39:2h:51:VAL:HG21	39:2h:60:ARG:HH11	1.82	0.45
1:1A:247:G:H4'	1:1A:386:G:C5	2.52	0.44
1:1A:747:U:O2	1:1A:2014:A:H1'	2.18	0.44
1:1A:1224:C:H2'	1:1A:1225:G:O4'	2.17	0.44
1:1A:1790:C:H5"	1:1A:1791:A:OP1	2.17	0.44
4:1E:67:PHE:HB3	4:1E:72:VAL:O	2.18	0.44
6:1G:5:VAL:HG22	6:1G:8:LYS:H	1.82	0.44
32:1a:165:C:H2'	32:1a:166:G:H8	1.80	0.44
32:1a:272:C:H2'	32:1a:273:A:H8	1.82	0.44
32:1a:534:U:O3'	60:1a:3336:HOH:O	2.21	0.44
39:1h:24:THR:O	39:1h:61:VAL:N	2.35	0.44
39:1h:96:GLY:O	39:1h:99:GLU:HG2	2.18	0.44
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.18	0.44
48:1q:22:LEU:HD11	48:1q:39:SER:HB2	1.98	0.44
1:2A:184:C:H2'	1:2A:185:U:H6	1.82	0.44
1:2A:859:G:O2'	1:2A:916:G:O6	2.32	0.44
1:2A:996:A:H1'	17:2V:9:GLY:O	2.17	0.44
1:2A:1052:C:N4	1:2A:1053:C:H41	2.16	0.44
1:2A:2570:G:H2'	1:2A:2571:C:O4'	2.17	0.44
8:2I:75:LEU:HD11	8:2I:105:HIS:ND1	2.32	0.44
11:2P:100:LEU:HD12	11:2P:112:LEU:HD11	1.98	0.44
13:2R:83:ILE:O	13:2R:86:ARG:HG2	2.17	0.44
17:2V:31:ALA:O	17:2V:61:VAL:HG22	2.17	0.44
32:2a:866:C:H4'	32:2a:919:A:H5'	1.99	0.44
32:2a:1236:A:O2'	32:2a:1304:G:H4'	2.17	0.44
32:2a:1343:G:H2'	32:2a:1344:C:C6	2.51	0.44
32:2a:1400:5MC:C2	53:2y:63:ALA:HA	2.52	0.44
35:2d:53:ASP:O	35:2d:57:ARG:NH1	2.50	0.44
1:1A:1377:G:OP2	60:1A:4243:HOH:O	2.21	0.44
1:1A:1600:C:OP1	19:1X:77:LYS:NZ	2.50	0.44
1:1A:1877:A:H3'	1:1A:1878:G:O4'	2.18	0.44
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.17	0.44
1:1A:2511:U:O2'	4:1E:138:PRO:O	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2712:U:H1'	1:1A:2712(A):A:C8	2.53	0.44
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.50	0.44
9:1N:138:LEU:HD23	9:1N:138:LEU:HA	1.65	0.44
10:1O:21:CYS:HB2	10:1O:39:ILE:HD12	1.98	0.44
11:1P:112:LEU:HD13	11:1P:127:ALA:HB2	1.99	0.44
32:1a:865:A:H2	32:1a:918:A:H4'	1.82	0.44
32:1a:1034:G:H2'	32:1a:1035:A:O4'	2.16	0.44
32:1a:1112:C:O2	34:1c:179:ARG:HG2	2.17	0.44
35:1d:98:GLU:OE1	35:1d:103:ASN:ND2	2.41	0.44
1:2A:898:C:H2'	1:2A:899:A:O4'	2.17	0.44
1:2A:1087:G:H2'	1:2A:1089:G:H5'	1.99	0.44
1:2A:2050:C:H1'	4:2E:156:MET:HE1	1.98	0.44
1:2A:2819:G:H2'	1:2A:2821:A:N7	2.31	0.44
2:2B:24:G:H4'	2:2B:25:A:C8	2.52	0.44
5:2F:39:TRP:CH2	5:2F:106:ARG:HD3	2.52	0.44
11:2P:98:GLU:O	11:2P:101:VAL:HG12	2.16	0.44
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.98	0.44
16:2U:29:SER:C	16:2U:30:LYS:HD2	2.42	0.44
19:2X:12:VAL:HG21	19:2X:27:THR:HG22	1.99	0.44
21:2Z:40:ASP:OD2	21:2Z:42:VAL:HG13	2.17	0.44
24:22:35:LEU:HD22	24:22:44:LEU:HD21	1.98	0.44
32:2a:114:U:O2'	32:2a:115:G:H5'	2.18	0.44
32:2a:636:U:H5'	48:2q:2:PRO:HD3	1.99	0.44
32:2a:1057:G:O3'	34:2c:197:GLY:HA3	2.17	0.44
32:2a:1149:C:O2'	32:2a:1280:A:N1	2.42	0.44
33:2b:15:VAL:HB	33:2b:209:ARG:HB3	1.99	0.44
43:2l:36:VAL:O	43:2l:58:VAL:HA	2.17	0.44
1:1A:49:A:H5"	1:1A:51:G:O4'	2.18	0.44
1:1A:184:C:H2'	1:1A:185:U:H6	1.82	0.44
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.52	0.44
1:1A:2474:C:O2'	1:1A:2475:C:OP1	2.32	0.44
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.18	0.44
2:1B:16:G:C6	2:1B:69:G:C2	3.05	0.44
12:1Q:75:THR:HG22	60:1Q:317:HOH:O	2.17	0.44
21:1Z:75:ASN:O	21:1Z:84:GLU:HG2	2.17	0.44
32:1a:235:C:H2'	32:1a:236:G:H8	1.83	0.44
32:1a:1005:A:OP2	32:1a:1024:G:N1	2.45	0.44
32:1a:1516:G:H2'	32:1a:1518:MA6:OP2	2.18	0.44
33:1b:189:ASP:HB3	33:1b:203:GLY:O	2.17	0.44
35:1d:107:ARG:HD3	35:1d:107:ARG:HA	1.80	0.44
39:1h:64:LYS:HG2	39:1h:79:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1k:31:THR:HA	42:1k:42:TRP:HA	1.99	0.44
48:1q:43:LEU:HD12	48:1q:68:ARG:HG2	2.00	0.44
1:2A:271(O):C:H2'	1:2A:271(P):C:C6	2.52	0.44
1:2A:1356:G:H2'	1:2A:1357:U:O4'	2.17	0.44
1:2A:1470:G:O2'	1:2A:1520:G:O6	2.27	0.44
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.82	0.44
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.52	0.44
1:2A:2375:G:N1	60:2A:4069:HOH:O	2.31	0.44
1:2A:2512:C:H2'	1:2A:2513:G:O4'	2.16	0.44
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.52	0.44
3:2D:177:LEU:HD12	3:2D:181:GLU:HB3	1.99	0.44
7:2H:30:LYS:HG3	7:2H:80:SER:O	2.17	0.44
26:24:61:ARG:HD3	50:2s:67:VAL:HG12	1.98	0.44
32:2a:477:A:H2'	32:2a:479:C:H6	1.83	0.44
32:2a:524:G:H2'	32:2a:525:C:C6	2.51	0.44
32:2a:1352:C:H2'	32:2a:1353:G:C8	2.52	0.44
32:2a:1369:C:OP2	40:2i:112:LYS:HB3	2.18	0.44
1:1A:858:U:O2	1:1A:2268:A:H2'	2.17	0.44
1:1A:2119:A:O2'	1:1A:2120:G:H5'	2.18	0.44
1:1A:2815:C:HO2'	27:15:43:HIS:HD1	1.61	0.44
6:1G:16:ARG:HD2	6:1G:16:ARG:HA	1.79	0.44
6:1G:67:LYS:HD3	26:14:5:ILE:HB	1.98	0.44
9:1N:99:LEU:O	9:1N:103:VAL:HG23	2.18	0.44
12:1Q:21:THR:HG23	12:1Q:99:PRO:O	2.17	0.44
21:1Z:70:LEU:HG	21:1Z:91:LEU:HD21	2.00	0.44
32:1a:434:U:H2'	32:1a:435:C:C6	2.52	0.44
32:1a:719:C:N4	49:1r:71:LYS:HE2	2.32	0.44
47:1p:67:THR:H	47:1p:70:ALA:HB3	1.82	0.44
47:1p:70:ALA:O	47:1p:74:LEU:HD12	2.17	0.44
1:2A:41:C:H2'	1:2A:42:G:C8	2.52	0.44
1:2A:757:U:H2'	1:2A:758:C:O4'	2.18	0.44
1:2A:996:A:H4'	16:2U:91:ASP:OD2	2.17	0.44
1:2A:1063:G:C8	1:2A:1065:U:H5	2.35	0.44
1:2A:1131:G:C2	1:2A:1132:A:C4	3.06	0.44
1:2A:1916:A:H2'	1:2A:1917:PSU:O4'	2.17	0.44
1:2A:2541:A:N7	60:2A:4129:HOH:O	2.36	0.44
1:2A:2839:G:H5'	13:2R:46:GLY:CA	2.48	0.44
4:2E:111:ARG:HA	13:2R:1:MET:SD	2.57	0.44
7:2H:173:PRO:O	60:2H:201:HOH:O	2.21	0.44
11:2P:114:ILE:HG13	11:2P:130:PHE:CE1	2.52	0.44
32:2a:474:G:H2'	32:2a:475:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:677:U:H3	32:2a:713:G:N2	2.12	0.44
32:2a:1131:G:H2'	32:2a:1132:C:C6	2.53	0.44
32:2a:1297:C:O2'	38:2g:114:ARG:NH1	2.50	0.44
36:2e:91:LEU:HD11	36:2e:110:LEU:HD11	2.00	0.44
39:2h:32:LYS:O	39:2h:36:LEU:HG	2.17	0.44
50:2s:39:THR:HG23	50:2s:69:HIS:O	2.17	0.44
50:2s:64:GLU:H	50:2s:64:GLU:HG2	1.67	0.44
1:1A:9:U:OP1	9:1N:115:ARG:NH2	2.50	0.44
1:1A:1637:A:OP2	60:1A:4245:HOH:O	2.21	0.44
1:1A:1965:C:OP1	1:1A:1966:A:O2'	2.34	0.44
1:1A:2308:G:O2'	1:1A:2310:A:N7	2.44	0.44
1:1A:2370:G:H2'	1:1A:2371:G:C8	2.53	0.44
5:1F:135:LYS:HB2	5:1F:138:GLU:CD	2.42	0.44
32:1a:984:C:N4	32:1a:1221:G:H1	2.16	0.44
32:1a:1187:G:H2'	32:1a:1188:A:C8	2.53	0.44
32:1a:1446:U:O2'	32:1a:1447:A:H3'	2.16	0.44
33:1b:163:PHE:HA	33:1b:185:ILE:O	2.17	0.44
38:1g:31:MET:HE2	38:1g:31:MET:HB3	1.83	0.44
1:2A:536:A:H4'	16:2U:57:PHE:HZ	1.83	0.44
1:2A:1686:C:H2'	1:2A:1687:G:O4'	2.17	0.44
1:2A:1848:A:H2'	1:2A:1849:G:O4'	2.18	0.44
1:2A:2115:G:N1	1:2A:2117:A:N7	2.66	0.44
1:2A:2159:G:H2'	1:2A:2160:G:H8	1.82	0.44
1:2A:2336:A:H61	22:20:43:THR:HG22	1.82	0.44
1:2A:2359:C:H2'	1:2A:2360:A:O4'	2.18	0.44
1:2A:2711:A:OP1	1:2A:2712:U:H3'	2.17	0.44
32:2a:728:A:H2'	32:2a:729:A:C8	2.52	0.44
32:2a:737:A:H2'	32:2a:738:C:C6	2.53	0.44
32:2a:1035:A:H2'	32:2a:1037:C:N4	2.29	0.44
33:2b:27:LYS:HD2	33:2b:193:ASP:OD1	2.17	0.44
33:2b:178:ARG:NH2	39:2h:74:PRO:HB3	2.33	0.44
35:2d:61:LYS:HG3	35:2d:203:VAL:HG13	1.99	0.44
35:2d:61:LYS:HA	35:2d:203:VAL:HG22	1.99	0.44
37:2f:11:ASN:N	37:2f:84:ASN:O	2.50	0.44
37:2f:19:LEU:HD11	37:2f:59:TYR:CE1	2.52	0.44
42:2k:85:ARG:HG2	42:2k:111:ASP:C	2.42	0.44
51:2t:14:LYS:HA	51:2t:17:ARG:CZ	2.48	0.44
1:1A:271(Q):G:O6	60:1A:4232:HOH:O	2.20	0.44
1:1A:771:G:OP1	29:17:10:ARG:NH1	2.50	0.44
1:1A:1570:A:H2'	1:1A:1571:A:C8	2.52	0.44
1:1A:2661:G:H2'	1:1A:2662:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2820:A:OP1	13:1R:2:ARG:NH2	2.50	0.44
8:1I:104:GLN:HG3	8:1I:105:HIS:CE1	2.53	0.44
13:1R:2:ARG:HA	13:1R:5:LYS:HD2	1.99	0.44
27:15:16:ARG:O	27:15:20:ARG:HG3	2.17	0.44
36:1e:81:GLU:HG2	36:1e:90:VAL:HG22	1.99	0.44
1:2A:36:G:N3	1:2A:450:G:O2'	2.48	0.44
1:2A:1771:C:O2'	60:2A:3941:HOH:O	2.20	0.44
1:2A:1839:G:N7	1:2A:1927:A:H1'	2.32	0.44
1:2A:2030:A:H4'	1:2A:2031:A:C8	2.53	0.44
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.49	0.44
1:2A:2722:G:H2'	1:2A:2723:C:C6	2.52	0.44
3:2D:8:PRO:HB3	3:2D:14:ARG:HA	1.99	0.44
7:2H:20:ALA:HB1	7:2H:21:PRO:HD2	1.99	0.44
7:2H:102:ALA:HA	7:2H:117:PRO:HD3	1.99	0.44
21:2Z:108:PRO:HB3	21:2Z:144:LEU:HB2	1.98	0.44
32:2a:4:U:N3	39:2h:105:ARG:HD3	2.31	0.44
32:2a:376:G:O3'	47:2p:5:ARG:HD2	2.16	0.44
32:2a:629:G:H2'	32:2a:630:G:O4'	2.18	0.44
32:2a:926:G:O4'	53:2y:91:LYS:HE3	2.17	0.44
32:2a:1236:A:OP1	52:2u:2:GLY:HA3	2.17	0.44
35:2d:119:GLN:HG3	35:2d:123:HIS:CE1	2.52	0.44
36:2e:80:ILE:HD13	39:2h:104:ARG:HH12	1.83	0.44
51:2t:65:LYS:HA	51:2t:68:LYS:HD3	2.00	0.44
1:1A:272(C):G:H2'	1:1A:272(D):G:O4'	2.17	0.44
1:1A:566:U:H5"	11:1P:29:LYS:HE3	2.00	0.44
1:1A:1216:G:P	16:1U:12:ARG:HH21	2.41	0.44
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.53	0.44
1:1A:2593:U:H2'	1:1A:2594:C:H6	1.83	0.44
6:1G:7:LEU:HD23	6:1G:7:LEU:HA	1.82	0.44
6:1G:41:GLN:HB3	6:1G:43:LEU:HD22	1.99	0.44
8:1I:88:ILE:O	8:1I:121:LYS:NZ	2.51	0.44
12:1Q:17:LEU:HD13	12:1Q:39:PRO:HB2	2.00	0.44
19:1X:72:LYS:NZ	19:1X:75:ASP:OD1	2.46	0.44
22:10:70:GLN:HG2	22:10:72:ARG:HG3	2.00	0.44
24:12:3:LEU:HD23	24:12:3:LEU:HA	1.83	0.44
32:1a:186:C:H2'	32:1a:187:C:C6	2.53	0.44
32:1a:957:U:H3	32:1a:960:U:H5"	1.83	0.44
32:1a:1264:C:H2'	32:1a:1265:G:C8	2.52	0.44
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.50	0.44
43:1l:62:SER:C	43:1l:64:TYR:H	2.24	0.44
46:1o:25:THR:O	46:1o:29:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1s:3:ARG:HH21	50:1s:7:LYS:HD3	1.83	0.44
50:1s:12:ASP:HB3	50:1s:14:HIS:CD2	2.53	0.44
50:1s:50:ALA:HA	50:1s:59:PRO:HA	2.00	0.44
1:2A:452:G:OP2	60:2A:3951:HOH:O	2.21	0.44
1:2A:673:C:OP1	5:2F:54:ARG:NH1	2.38	0.44
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.52	0.44
1:2A:1648:C:H2'	1:2A:1649:G:O4'	2.18	0.44
1:2A:2162:G:HO2'	1:2A:2172:U:HO2'	1.63	0.44
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.53	0.44
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.17	0.44
32:2a:194:C:H2'	32:2a:195:A:H5"	2.00	0.44
32:2a:359:U:H2'	32:2a:360:A:C8	2.53	0.44
32:2a:438:G:C4'	35:2d:123:HIS:HD2	2.31	0.44
32:2a:444:C:H2'	32:2a:445:G:H8	1.82	0.44
32:2a:1030(C):G:H2'	32:2a:1030(D):A:C8	2.52	0.44
33:2b:74:LYS:O	33:2b:78:GLN:N	2.45	0.44
35:2d:19:LEU:HD23	35:2d:67:ILE:HG13	1.99	0.44
1:1A:68:G:H2'	1:1A:69:C:O4'	2.18	0.44
1:1A:526:A:H2'	60:1A:5019:HOH:O	2.17	0.44
1:1A:571:A:O2'	17:1V:78:LYS:HE2	2.18	0.44
1:1A:2319:G:N2	14:1S:3:ARG:HA	2.33	0.44
1:1A:2362:G:OP1	30:18:44:LYS:NZ	2.34	0.44
17:1V:19:LYS:HA	17:1V:94:LEU:O	2.18	0.44
32:1a:688:G:H2'	32:1a:689:C:H6	1.83	0.44
32:1a:965:A:OP2	53:1y:8:LYS:NZ	2.51	0.44
32:1a:1002:G:H2'	32:1a:1003:G:C1'	2.48	0.44
32:1a:1149:C:P	40:1i:9:ARG:HH21	2.40	0.44
32:1a:1298:C:H4'	32:1a:1299:A:C4	2.52	0.44
35:1d:147:ALA:HB2	35:1d:182:LYS:HB2	1.99	0.44
35:1d:177:ASP:OD2	35:1d:180:GLY:HA3	2.17	0.44
40:1i:5:TYR:HE1	40:1i:16:ARG:HB3	1.82	0.44
41:1j:5:ARG:HE	41:1j:73:ASP:CG	2.26	0.44
52:1u:18:TYR:CD1	52:1u:24:ARG:HB3	2.53	0.44
1:2A:438:G:H2'	1:2A:440:G:C8	2.50	0.44
1:2A:443:A:H5"	1:2A:444:C:OP1	2.18	0.44
1:2A:1289:C:H2'	1:2A:1290:C:H6	1.83	0.44
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.18	0.44
7:2H:133:VAL:HG12	7:2H:141:VAL:HG13	2.00	0.44
26:24:48:ARG:HD3	26:24:48:ARG:HA	1.81	0.44
32:2a:685:G:O2'	32:2a:686:U:H5'	2.18	0.44
32:2a:939:G:H5'	38:2g:102:ARG:CZ	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1220:G:H21	50:2s:54:GLY:HA2	1.83	0.44
41:2j:32:ALA:HB1	41:2j:33:GLN:CD	2.43	0.44
42:2k:99:GLN:HG3	42:2k:105:VAL:HG21	2.00	0.44
45:2n:51:GLY:C	45:2n:53:LEU:H	2.25	0.44
1:1A:678:C:H5"	60:1A:6240:HOH:O	2.16	0.44
1:1A:748:G:O6	18:1W:90:ARG:NH1	2.50	0.44
1:1A:1173:G:C2	1:1A:1175:U:H4'	2.52	0.44
1:1A:2334:G:O6	22:10:74:ARG:NH1	2.41	0.44
1:1A:2785:C:H2'	1:1A:2786:U:O4'	2.18	0.44
5:1F:32:LEU:HD11	5:1F:105:VAL:HG13	1.99	0.44
9:1N:42:TRP:HA	9:1N:48:MET:SD	2.58	0.44
21:1Z:183:LEU:HA	21:1Z:183:LEU:HD23	1.70	0.44
32:1a:226:G:H2'	32:1a:227:G:C8	2.53	0.44
32:1a:258:G:H2'	32:1a:259:G:C8	2.53	0.44
32:1a:1008:C:H2'	32:1a:1009:G:O4'	2.18	0.44
32:1a:1010:G:N2	32:1a:1020:U:H1'	2.33	0.44
32:1a:1236:A:H4'	32:1a:1304:G:H4'	1.98	0.44
34:1c:26:LYS:HA	45:1n:36:PHE:HE1	1.83	0.44
34:1c:87:LEU:O	34:1c:91:LEU:N	2.23	0.44
34:1c:120:VAL:HB	34:1c:198:VAL:HG11	1.99	0.44
1:2A:111:A:H4'	24:22:69:ARG:NH1	2.33	0.44
1:2A:290:G:H2'	1:2A:291:C:O4'	2.18	0.44
1:2A:370:G:OP2	1:2A:370:G:H8	2.01	0.44
1:2A:484:C:H2'	1:2A:485:C:C6	2.52	0.44
1:2A:601:C:O2	1:2A:605:C:H4'	2.18	0.44
1:2A:1167:U:O2	1:2A:1183:G:N2	2.51	0.44
1:2A:2115:G:H4'	1:2A:2167:U:H4'	1.98	0.44
1:2A:2728:U:H5'	10:2O:70:LYS:NZ	2.33	0.44
3:2D:6:PHE:HE2	3:2D:18:VAL:HG13	1.82	0.44
5:2F:36:VAL:O	5:2F:40:GLN:HG3	2.18	0.44
7:2H:149:ARG:NH1	7:2H:167:GLU:OE1	2.51	0.44
15:2T:102:ILE:HA	15:2T:105:LEU:HD12	2.00	0.44
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.18	0.44
32:2a:1320:C:C1'	50:2s:73:GLU:HG2	2.48	0.44
34:2c:6:HIS:ND1	45:2n:49:HIS:HB3	2.33	0.44
34:2c:91:LEU:C	34:2c:93:LYS:H	2.26	0.44
35:2d:36:ARG:HB3	35:2d:38:TYR:CE2	2.53	0.44
39:2h:11:THR:HG22	39:2h:15:ASN:HD21	1.83	0.44
39:2h:109:ILE:HG12	39:2h:137:VAL:HB	2.00	0.44
40:2i:25:LYS:O	40:2i:60:ASP:HB2	2.18	0.44
44:2m:92:HIS:CE1	44:2m:98:VAL:HG11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1550:C:H2'	1:1A:1551:C:H6	1.83	0.43
1:1A:1935:G:H1'	1:1A:1964:G:N2	2.33	0.43
1:1A:2051:A:OP2	60:1A:4244:HOH:O	2.21	0.43
1:1A:2336:A:H61	22:10:43:THR:HG22	1.82	0.43
15:1T:16:ARG:NH2	15:1T:83:ILE:O	2.45	0.43
32:1a:197:A:C6	32:1a:221:C:H4'	2.52	0.43
32:1a:335:C:H2'	32:1a:336:C:C6	2.52	0.43
32:1a:453:A:C6	32:1a:454:C:C4	3.06	0.43
32:1a:1030(C):G:N7	32:1a:1031:G:N2	2.65	0.43
34:1c:52:LEU:HD12	34:1c:53:ALA:N	2.32	0.43
36:1e:80:ILE:HG23	36:1e:91:LEU:HB2	2.00	0.43
1:2A:14:A:H5"	1:2A:15:G:OP2	2.18	0.43
1:2A:444:C:H5"	60:2A:4432:HOH:O	2.18	0.43
1:2A:539:G:H2'	1:2A:540:C:H6	1.83	0.43
1:2A:746:A:H8	60:2A:4124:HOH:O	2.01	0.43
1:2A:2619:C:H4'	4:2E:151:TYR:O	2.18	0.43
2:2B:24:G:N3	2:2B:26:A:N6	2.66	0.43
5:2F:178:PRO:HB2	5:2F:201:VAL:HG21	1.98	0.43
11:2P:76:LYS:HE3	11:2P:76:LYS:HB2	1.75	0.43
11:2P:84:ASN:OD1	11:2P:117:GLU:HB2	2.18	0.43
12:2Q:39:PRO:HD3	12:2Q:99:PRO:HG3	2.00	0.43
14:2S:11:LYS:HE3	14:2S:15:ARG:NH2	2.32	0.43
14:2S:49:VAL:HG22	14:2S:80:LEU:HD22	2.00	0.43
32:2a:865:A:H2'	32:2a:866:C:O4'	2.18	0.43
32:2a:1093:A:N3	32:2a:1109:C:O2'	2.44	0.43
32:2a:1324:A:OP1	32:2a:1363:C:H1'	2.18	0.43
33:2b:81:VAL:HG13	33:2b:94:ASN:OD1	2.18	0.43
34:2c:74:GLY:HA2	34:2c:77:ILE:HD11	2.00	0.43
34:2c:182:ILE:HG12	34:2c:203:PHE:CD1	2.49	0.43
1:1A:1557:C:H5"	1:1A:1558:A:OP2	2.18	0.43
1:1A:2441:C:OP2	1:1A:2586:C:O2'	2.35	0.43
1:1A:2592:G:N7	60:1A:4474:HOH:O	2.36	0.43
1:1A:2659:G:O6	60:1A:4167:HOH:O	2.12	0.43
3:1D:127:VAL:HA	3:1D:193:VAL:HG22	2.00	0.43
6:1G:165:THR:OG1	6:1G:168:GLU:HG3	2.18	0.43
10:1O:104:ARG:HD3	15:1T:36:GLU:HG2	2.00	0.43
15:1T:55:ASN:N	15:1T:59:THR:HG22	2.14	0.43
30:18:23:VAL:CG1	30:18:47:LYS:HB3	2.48	0.43
32:1a:741:G:H2'	32:1a:742:G:O4'	2.18	0.43
32:1a:901:A:C5	32:1a:902:G:H1'	2.53	0.43
32:1a:1287:A:H2	32:1a:1353:G:N3	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1372:U:H5”	40:1i:71:SER:HB3	1.99	0.43
33:1b:132:LYS:HA	33:1b:135:GLN:CD	2.43	0.43
47:1p:67:THR:HG22	47:1p:68:ASP:H	1.82	0.43
1:2A:271(Q):G:H2’	1:2A:271(R):G:H8	1.83	0.43
1:2A:536:A:H2’	1:2A:537:C:C6	2.53	0.43
1:2A:1338:G:O2’	1:2A:1393:A:N1	2.49	0.43
1:2A:1902:C:H5’	3:2D:246:PRO:HD3	2.00	0.43
1:2A:2061:G:H5”	1:2A:2503:2MA:C2	2.48	0.43
1:2A:2191:G:H2’	1:2A:2192:G:O4’	2.18	0.43
27:25:16:ARG:HG2	27:25:17:ASP:OD1	2.19	0.43
32:2a:114:U:H2’	32:2a:115:G:C8	2.53	0.43
32:2a:859:A:H2’	32:2a:860:A:O4’	2.19	0.43
32:2a:1123:A:O3’	41:2j:36:GLY:HA3	2.18	0.43
32:2a:1327:C:H2’	32:2a:1328:C:H6	1.83	0.43
33:2b:17:PHE:HD1	33:2b:18:GLY:H	1.66	0.43
33:2b:213:LEU:O	33:2b:217:ARG:HG2	2.18	0.43
34:2c:12:LEU:HD23	34:2c:12:LEU:HA	1.87	0.43
47:2p:3:LYS:NZ	47:2p:65:GLN:O	2.42	0.43
1:1A:26:G:C6	1:1A:27:G:N1	2.86	0.43
1:1A:476:G:H4’	1:1A:502:A:N1	2.33	0.43
1:1A:753:C:H3’	60:1A:4471:HOH:O	2.17	0.43
1:1A:1448:G:O2’	1:1A:1528(A):A:N1	2.50	0.43
1:1A:1651:G:OP1	13:1R:40:LYS:HE3	2.18	0.43
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	2.00	0.43
26:14:40:HIS:CE1	26:14:42:PHE:HB3	2.54	0.43
32:1a:78:G:H1	32:1a:91:C:H42	1.66	0.43
32:1a:284:G:H2’	32:1a:285:G:H8	1.83	0.43
32:1a:383:A:C5	32:1a:384:G:H1’	2.53	0.43
32:1a:412:A:C5	35:1d:35:ARG:HD3	2.53	0.43
32:1a:1030(C):G:H8	32:1a:1030(D):A:N7	2.16	0.43
32:1a:1109:C:H2’	32:1a:1110:A:O4’	2.17	0.43
32:1a:1118:C:H1’	32:1a:1179:A:C4	2.53	0.43
32:1a:1394:A:C5	32:1a:1501:C:H4’	2.53	0.43
33:1b:100:GLY:O	33:1b:104:ASN:N	2.42	0.43
39:1h:21:LYS:N	39:1h:65:TYR:OH	2.50	0.43
44:1m:11:ARG:O	44:1m:13:LYS:N	2.50	0.43
1:2A:248:G:OP1	60:2A:3952:HOH:O	2.21	0.43
1:2A:813:U:H2’	1:2A:814:C:C6	2.54	0.43
1:2A:817:C:O2’	1:2A:839:U:H5”	2.18	0.43
1:2A:1354:A:H2’	1:2A:1355:G:O4’	2.18	0.43
7:2H:67:LEU:O	7:2H:71:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2R:104:ARG:HD2	13:2R:107:ASP:OD1	2.19	0.43
21:2Z:27:VAL:HG12	21:2Z:85:HIS:HE1	1.83	0.43
21:2Z:150:LEU:HB3	21:2Z:171:ILE:HD11	2.00	0.43
32:2a:189(E):U:O2'	32:2a:189(F):U:H5'	2.18	0.43
32:2a:1087:G:N2	32:2a:1099:G:H1'	2.34	0.43
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.52	0.43
32:2a:1318:A:H5"	50:2s:3:ARG:NH2	2.34	0.43
32:2a:1360:A:H8	32:2a:1360:A:OP1	2.00	0.43
32:2a:1465:C:H2'	32:2a:1466:C:O4'	2.18	0.43
33:2b:69:LEU:HD12	33:2b:70:PHE:H	1.83	0.43
33:2b:105:PHE:HE1	33:2b:155:LEU:HD23	1.82	0.43
35:2d:64:LEU:HA	35:2d:67:ILE:HD12	2.00	0.43
35:2d:172:PRO:HB2	35:2d:187:ARG:HH22	1.82	0.43
38:2g:33:ASP:HB2	38:2g:35:LYS:HG3	2.00	0.43
39:2h:86:ILE:HD11	39:2h:136:GLU:HG2	1.99	0.43
41:2j:30:SER:OG	41:2j:81:THR:HG22	2.18	0.43
44:2m:108:ARG:HH12	44:2m:111:LYS:HD2	1.82	0.43
49:2r:35:ARG:HE	49:2r:35:ARG:HB2	1.65	0.43
1:1A:228:A:C8	1:1A:229:A:H5'	2.52	0.43
1:1A:250:G:H2'	1:1A:251:A:C8	2.53	0.43
1:1A:819:A:C4	1:1A:1189:A:C2	3.06	0.43
1:1A:1086:A:H3'	1:1A:1086:A:N3	2.33	0.43
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.52	0.43
1:1A:1824:G:N3	3:1D:254:THR:OG1	2.51	0.43
1:1A:1832:C:OP1	60:1A:4242:HOH:O	2.21	0.43
1:1A:2187:G:H5'	1:1A:2188:C:OP2	2.18	0.43
1:1A:2273:A:H2'	1:1A:2274:A:C8	2.53	0.43
3:1D:35:LYS:HB2	3:1D:36:PRO:HD2	2.00	0.43
4:1E:11:MET:HE2	4:1E:11:MET:HB3	1.85	0.43
4:1E:13:ARG:HD2	4:1E:20:ALA:HB1	2.00	0.43
6:1G:43:LEU:HD11	6:1G:153:ARG:HD3	2.00	0.43
28:16:12:GLU:OE1	28:16:52:VAL:HG21	2.19	0.43
32:1a:1232:U:H5"	40:1i:124:GLN:O	2.18	0.43
34:1c:182:ILE:HG12	34:1c:203:PHE:HD1	1.83	0.43
42:1k:82:VAL:HB	42:1k:108:ILE:HG13	1.99	0.43
1:2A:404:C:OP1	60:2A:3956:HOH:O	2.21	0.43
1:2A:576:U:H2'	1:2A:577:G:C8	2.53	0.43
1:2A:1101:U:H2'	1:2A:1102:C:C6	2.54	0.43
1:2A:1614:A:C2	18:2W:93:ALA:HB2	2.54	0.43
13:2R:79:LEU:HD23	13:2R:83:ILE:HB	2.01	0.43
17:2V:62:LEU:CD1	17:2V:95:LEU:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:23:11:SER:HA	25:23:31:LEU:HD21	2.00	0.43
32:2a:937:A:H1'	32:2a:1379:G:N2	2.33	0.43
32:2a:1030(B):C:H5	32:2a:1030(C):G:N3	2.15	0.43
32:2a:1348:U:H4'	40:2i:120:ARG:HD2	1.99	0.43
32:2a:1375:A:H4'	38:2g:29:LYS:NZ	2.33	0.43
33:2b:98:LEU:HB2	33:2b:101:MET:HE3	2.01	0.43
36:2e:51:VAL:O	36:2e:55:VAL:HG23	2.18	0.43
37:2f:68:PRO:HG2	37:2f:71:ARG:NH1	2.34	0.43
40:2i:23:ASN:OD1	40:2i:23:ASN:N	2.49	0.43
48:2q:27:PHE:CZ	48:2q:36:ILE:HD11	2.54	0.43
1:1A:244:A:C2	1:1A:255:A:C4	3.07	0.43
1:1A:581:C:OP1	16:1U:33:ARG:HG3	2.18	0.43
1:1A:1611:C:OP1	60:1A:4246:HOH:O	2.21	0.43
1:1A:1649:G:O2'	13:1R:107:ASP:OD2	2.36	0.43
1:1A:2127:G:C6	1:1A:2128:C:C4	3.06	0.43
2:1B:33:G:C2	2:1B:50:G:C2	3.06	0.43
16:1U:39:LEU:HD23	16:1U:39:LEU:HA	1.81	0.43
28:16:19:ARG:NH1	28:16:52:VAL:HG11	2.34	0.43
32:1a:738:C:H2'	32:1a:739:C:H6	1.83	0.43
32:1a:820:U:H4'	32:1a:821:G:OP2	2.18	0.43
32:1a:1053:G:N7	32:1a:1200:C:H5'	2.34	0.43
33:1b:135:GLN:H	33:1b:135:GLN:HG3	1.55	0.43
38:1g:116:ALA:O	38:1g:120:ILE:HG12	2.18	0.43
47:1p:47:ASP:C	47:1p:49:LEU:H	2.24	0.43
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.53	0.43
1:2A:579:G:H2'	1:2A:580:C:C6	2.54	0.43
1:2A:657:U:H2'	1:2A:658:C:C6	2.53	0.43
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.53	0.43
1:2A:2182:G:O2'	1:2A:2183:C:H5'	2.18	0.43
1:2A:2305:A:H2'	1:2A:2306:C:O4'	2.18	0.43
1:2A:2392:A:O2'	60:2A:3955:HOH:O	2.21	0.43
1:2A:2750:A:H8	1:2A:2750:A:OP1	2.00	0.43
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.19	0.43
19:2X:5:TYR:CZ	24:22:30:ARG:HG3	2.54	0.43
32:2a:540:G:H2'	32:2a:541:G:H8	1.84	0.43
32:2a:564:C:C4	48:2q:31:LEU:HD11	2.53	0.43
32:2a:1031:G:H2'	32:2a:1032:G:C8	2.54	0.43
32:2a:1128:C:H1'	32:2a:1147:C:N4	2.31	0.43
32:2a:1256:A:N6	32:2a:1278:U:O2	2.52	0.43
33:2b:11:LEU:HD13	33:2b:217:ARG:NH2	2.34	0.43
38:2g:60:LYS:O	38:2g:64:GLN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:2s:31:ILE:O	50:2s:49:ILE:HG23	2.18	0.43
51:2t:50:GLU:HB2	51:2t:99:LEU:HD22	2.00	0.43
53:2y:27:LEU:HD11	53:2y:81:LEU:HB3	2.01	0.43
1:1A:311:A:C6	1:1A:328:U:C4	3.07	0.43
1:1A:614:U:H5'	1:1A:614(C):A:N6	2.34	0.43
1:1A:811:U:H2'	11:1P:21:ARG:HA	2.01	0.43
1:1A:1639:U:O2'	1:1A:1640:C:H5'	2.19	0.43
1:1A:1720:U:H3	1:1A:1742:G:H1	1.66	0.43
1:1A:2849:U:OP2	15:1T:95:ARG:NH1	2.51	0.43
10:1O:92:GLU:HG2	10:1O:113:LYS:HD3	2.01	0.43
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.54	0.43
18:1W:78:GLU:OE2	18:1W:99:ARG:NH1	2.48	0.43
20:1Y:81:LYS:HE2	20:1Y:81:LYS:HB3	1.77	0.43
20:1Y:90:LEU:HD12	20:1Y:90:LEU:HA	1.81	0.43
22:10:10:THR:HG22	22:10:12:ASN:N	2.28	0.43
32:1a:1220:G:H21	50:1s:54:GLY:C	2.21	0.43
40:1i:45:ALA:O	40:1i:48:GLU:HB2	2.18	0.43
43:1l:77:LEU:HD21	43:1l:107:ALA:HA	1.99	0.43
45:1n:27:CYS:SG	45:1n:28:GLY:N	2.91	0.43
46:1o:82:ILE:O	46:1o:86:GLY:N	2.51	0.43
1:2A:478:A:C6	1:2A:480:A:C6	3.07	0.43
1:2A:534:U:H2'	1:2A:535:C:C6	2.54	0.43
1:2A:885:C:H1'	1:2A:892:G:N2	2.34	0.43
1:2A:1638:C:O3'	1:2A:2709:G:N2	2.52	0.43
1:2A:1857:G:C6	1:2A:1858:G:N1	2.87	0.43
1:2A:2649:U:H2'	1:2A:2650:U:C6	2.54	0.43
11:2P:86:LYS:HE3	11:2P:86:LYS:HB2	1.54	0.43
14:2S:25:ARG:NH1	14:2S:40:ILE:HD12	2.34	0.43
22:20:17:GLN:O	22:20:19:LYS:NZ	2.49	0.43
32:2a:380:G:C2	32:2a:384:G:C6	3.07	0.43
32:2a:692:U:O2'	32:2a:694:A:N7	2.38	0.43
32:2a:957:U:O2'	32:2a:959:A:N7	2.44	0.43
32:2a:1002:G:N3	32:2a:1003:G:H8	2.16	0.43
32:2a:1348:U:H2'	32:2a:1349:A:C8	2.52	0.43
34:2c:148:GLY:HA3	34:2c:172:ARG:O	2.18	0.43
35:2d:102:ASP:OD1	35:2d:102:ASP:N	2.52	0.43
38:2g:18:TYR:CE1	38:2g:59:LEU:HB2	2.54	0.43
40:2i:7:THR:OG1	40:2i:83:ARG:NH1	2.51	0.43
1:1A:1051:G:H2'	1:1A:1052:C:O4'	2.18	0.43
1:1A:1359:A:H2'	1:1A:1360:A:H5'	2.01	0.43
1:1A:1586:A:H2'	1:1A:1587:A:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2078:C:C4	1:1A:2079:U:C4	3.07	0.43
1:1A:2186:G:C2	1:1A:2187:G:C8	3.07	0.43
32:1a:1262:C:H2'	32:1a:1263:C:C6	2.54	0.43
32:1a:1399:C:C2	32:1a:1401:G:C5	3.07	0.43
37:1f:19:LEU:O	37:1f:23:LYS:HG3	2.19	0.43
44:1m:3:ARG:HG2	44:1m:8:GLU:HA	2.01	0.43
1:2A:265:A:N6	1:2A:428:A:H1'	2.34	0.43
1:2A:411:G:C5	11:2P:72:PRO:HB3	2.54	0.43
1:2A:539:G:H2'	1:2A:540:C:C6	2.54	0.43
1:2A:842:G:N2	1:2A:937:U:C2	2.86	0.43
1:2A:1196:C:H2'	1:2A:1197:G:C8	2.54	0.43
1:2A:2579:C:H4'	4:2E:134:ILE:HG12	1.99	0.43
1:2A:2680:C:H5'	4:2E:189:PRO:HA	2.01	0.43
2:2B:59:A:H2'	2:2B:60:C:O4'	2.19	0.43
5:2F:155:LEU:HB2	5:2F:189:THR:HG21	2.00	0.43
9:2N:72:TYR:O	9:2N:85:ILE:N	2.44	0.43
13:2R:10:LEU:O	13:2R:12:ARG:NH1	2.51	0.43
13:2R:118:GLU:CD	13:2R:118:GLU:H	2.26	0.43
32:2a:404:U:H2'	32:2a:405:U:H6	1.82	0.43
32:2a:972:C:H4'	41:2j:57:LYS:HB2	2.01	0.43
32:2a:986:A:N3	50:2s:52:TYR:OH	2.50	0.43
32:2a:991:U:H2'	32:2a:1212:U:C4	2.53	0.43
32:2a:1324:A:H4'	32:2a:1362:C:H4'	2.00	0.43
34:2c:44:GLU:HA	34:2c:52:LEU:HD12	2.00	0.43
50:2s:65:ASN:OD1	50:2s:65:ASN:N	2.51	0.43
1:1A:372:G:OP2	23:11:69:LYS:NZ	2.52	0.43
1:1A:620:G:H2'	1:1A:620:G:N3	2.33	0.43
1:1A:1580:A:OP2	1:1A:1580:A:H8	2.02	0.43
1:1A:2092:U:H4'	1:1A:2093:G:O5'	2.19	0.43
1:1A:2168:G:C2	1:1A:2171:A:C8	3.07	0.43
1:1A:2420:C:H5'	28:16:54:ILE:HD11	2.00	0.43
1:1A:2690:C:N4	1:1A:2713:A:H1'	2.34	0.43
4:1E:51:PHE:CD2	4:1E:52:LEU:HG	2.53	0.43
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.53	0.43
17:1V:76:LYS:HD2	17:1V:81:TYR:CD2	2.53	0.43
32:1a:601:C:H2'	32:1a:602:A:C8	2.54	0.43
1:2A:272:G:N7	1:2A:421:U:H2'	2.33	0.43
1:2A:668:G:H5'	1:2A:669:G:OP2	2.18	0.43
1:2A:2206:G:H8	1:2A:2207:G:N7	2.17	0.43
1:2A:2262:U:H4'	1:2A:2328:A:C2	2.54	0.43
1:2A:2360:A:H2'	1:2A:2361:A:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:117:G:O6	60:2B:305:HOH:O	2.19	0.43
14:2S:64:GLU:H	14:2S:64:GLU:HG2	1.56	0.43
32:2a:1292:U:OP2	38:2g:41:ARG:NH2	2.52	0.43
36:2e:82:VAL:HG21	36:2e:138:ALA:HA	2.01	0.43
49:2r:58:LEU:HB3	49:2r:62:GLU:HG3	2.00	0.43
1:1A:2886:G:H2'	1:1A:2887:U:H6	1.82	0.43
31:19:25:VAL:HB	31:19:34:GLN:HB2	2.01	0.43
32:1a:9:G:N7	32:1a:558:G:O2'	2.48	0.43
32:1a:189(D):C:H2'	32:1a:189(E):U:O4'	2.19	0.43
32:1a:284:G:H2'	32:1a:285:G:C8	2.53	0.43
32:1a:292:G:O2'	32:1a:608:A:N6	2.50	0.43
32:1a:304:U:H2'	32:1a:305:G:C8	2.54	0.43
32:1a:1217:C:OP1	45:1n:9:LYS:NZ	2.51	0.43
32:1a:1227:A:O3'	44:1m:115:LYS:HE3	2.18	0.43
32:1a:1270:C:H2'	32:1a:1271:G:H8	1.83	0.43
32:1a:1429:C:H2'	32:1a:1430:C:C6	2.54	0.43
35:1d:22:LYS:HB2	35:1d:26:CYS:SG	2.58	0.43
37:1f:44:GLY:HA2	37:1f:59:TYR:CZ	2.53	0.43
42:1k:20:TYR:CE1	42:1k:83:ILE:HD12	2.53	0.43
53:1y:39:ILE:HD13	53:1y:52:ALA:HB2	2.01	0.43
1:2A:962:G:O2'	1:2A:2496:C:H4'	2.18	0.43
1:2A:1080:C:H2'	1:2A:1081:U:H6	1.84	0.43
1:2A:1698:A:C8	1:2A:1700:A:O4'	2.72	0.43
1:2A:2206:G:H3'	1:2A:2207:G:N7	2.33	0.43
1:2A:2489:G:C6	1:2A:2490:G:C6	3.07	0.43
1:2A:2564:A:C2	1:2A:2647:U:H4'	2.54	0.43
2:2B:56:G:H4'	2:2B:57:A:C8	2.53	0.43
6:2G:12:TYR:HA	6:2G:16:ARG:CG	2.47	0.43
10:2O:9:GLU:O	10:2O:83:ALA:HA	2.19	0.43
21:2Z:93:ASP:OD1	21:2Z:93:ASP:N	2.52	0.43
40:2i:55:ALA:HB1	40:2i:58:HIS:HB2	2.01	0.43
1:1A:242:G:C8	30:18:5:LYS:HG2	2.53	0.43
1:1A:580:C:H2'	1:1A:581:C:C6	2.54	0.43
1:1A:603:A:N1	1:1A:625:G:O2'	2.46	0.43
1:1A:1903:G:OP1	3:1D:241:PRO:HB2	2.19	0.43
1:1A:2114:A:H1'	1:1A:2168:G:H5'	2.00	0.43
1:1A:2864:G:OP1	15:1T:119:LYS:HD2	2.19	0.43
2:1B:31:C:N4	14:1S:32:LEU:HD22	2.34	0.43
3:1D:232:PRO:HB3	3:1D:244:ARG:CZ	2.48	0.43
3:1D:260:ARG:NH1	3:1D:267:SER:OG	2.50	0.43
11:1P:101:VAL:HG22	11:1P:106:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:56:GLY:O	15:1T:59:THR:HG23	2.18	0.43
20:1Y:38:ILE:HD11	20:1Y:66:PRO:HG3	2.01	0.43
29:17:21:ARG:HD3	60:17:206:HOH:O	2.18	0.43
32:1a:584:G:H5'	48:1q:91:ARG:NH2	2.33	0.43
32:1a:1203:C:H2'	32:1a:1204:A:H8	1.83	0.43
41:1j:19:SER:O	41:1j:23:ILE:HG12	2.19	0.43
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.54	0.43
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.53	0.43
1:2A:272(J):C:H2'	1:2A:274:G:H8	1.83	0.43
1:2A:455:C:N3	1:2A:472:A:H2'	2.34	0.43
1:2A:625:G:O6	11:2P:107:LYS:NZ	2.50	0.43
1:2A:861:A:H2'	1:2A:862:G:O4'	2.18	0.43
1:2A:1056:G:H21	1:2A:1103:A:H62	1.67	0.43
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.53	0.43
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.54	0.43
10:2O:104:ARG:NH2	15:2T:36:GLU:OE2	2.48	0.43
13:2R:100:LEU:HD11	13:2R:113:LEU:HD23	2.01	0.43
15:2T:51:ARG:O	15:2T:61:PHE:HA	2.18	0.43
17:2V:5:VAL:CG1	17:2V:57:VAL:HG21	2.49	0.43
21:2Z:108:PRO:HG3	21:2Z:141:VAL:HG23	2.01	0.43
24:22:38:GLN:O	24:22:41:ILE:HG12	2.18	0.43
32:2a:677:U:O2	32:2a:777:A:O2'	2.37	0.43
32:2a:1075:C:H5"	33:2b:179:LYS:HE2	2.01	0.43
32:2a:1401:G:C2	32:2a:1402:4OC:H1'	2.53	0.43
33:2b:8:LYS:H	33:2b:8:LYS:HG2	1.60	0.43
51:2t:39:LYS:HE3	51:2t:39:LYS:HB2	1.94	0.43
1:1A:118:A:C8	1:1A:119:A:C8	3.07	0.42
1:1A:1268:A:C2	1:1A:2013:A:C4	3.07	0.42
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.17	0.42
1:1A:1712:C:H2'	1:1A:1713:U:O4'	2.18	0.42
1:1A:2615:U:H2'	1:1A:2616:C:C6	2.54	0.42
1:1A:2815:C:O2'	27:15:43:HIS:ND1	2.52	0.42
5:1F:46:ARG:HH11	5:1F:46:ARG:HA	1.84	0.42
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.66	0.42
32:1a:398:C:H2'	32:1a:399:G:H8	1.84	0.42
32:1a:1183:A:O2'	32:1a:1184:G:OP1	2.34	0.42
32:1a:1293:G:H2'	32:1a:1294:G:C8	2.54	0.42
33:1b:218:ALA:O	33:1b:222:ILE:HG13	2.18	0.42
35:1d:32:ALA:HB3	59:1d:306:SF4:S2	2.59	0.42
36:1e:48:ALA:HB3	36:1e:54:ALA:HB2	2.01	0.42
37:1f:3:ARG:HD3	37:1f:64:GLN:HE21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1f:45:LEU:HD12	37:1f:59:TYR:HD1	1.83	0.42
51:1t:36:LEU:HD12	51:1t:62:LEU:HD12	2.01	0.42
1:2A:335:C:H4'	20:2Y:73:ARG:HD2	2.01	0.42
1:2A:774:A:H2'	1:2A:774:A:N3	2.34	0.42
1:2A:839:U:H1'	1:2A:1191:G:H1'	2.01	0.42
1:2A:1823:G:OP1	3:2D:54:ARG:NH1	2.52	0.42
1:2A:2267:A:H5"	1:2A:2268:A:C5'	2.46	0.42
4:2E:79:ARG:HD3	4:2E:79:ARG:HA	1.85	0.42
8:2I:9:LEU:O	8:2I:11:ASN:N	2.52	0.42
18:2W:5:ALA:HB3	18:2W:54:ALA:HB2	2.01	0.42
32:2a:266:G:O2'	32:2a:267:C:OP2	2.29	0.42
32:2a:993:G:O2'	32:2a:994:A:N7	2.51	0.42
32:2a:1158:C:N4	32:2a:1181:G:H1	2.16	0.42
32:2a:1181:G:O2'	32:2a:1182:G:N7	2.45	0.42
32:2a:1512:U:H2'	32:2a:1513:A:H8	1.83	0.42
33:2b:179:LYS:HA	39:2h:72:PRO:HG3	2.01	0.42
35:2d:121:VAL:O	35:2d:134:ASP:HA	2.19	0.42
53:2y:4:ASN:O	53:2y:38:HIS:HA	2.19	0.42
1:1A:652(F):G:N2	1:1A:652(T):C:O2	2.53	0.42
1:1A:1321:A:H2'	1:1A:1322:A:O4'	2.18	0.42
1:1A:2010:G:N7	60:1A:4478:HOH:O	2.37	0.42
1:1A:2127:G:H1	1:1A:2161:C:H42	1.67	0.42
1:1A:2330:G:H2'	1:1A:2331:G:O4'	2.19	0.42
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.54	0.42
3:1D:164:GLN:OE1	3:1D:176:ARG:NH2	2.47	0.42
21:1Z:7:ALA:HB2	21:1Z:59:LEU:HD22	2.01	0.42
22:10:66:VAL:O	22:10:81:VAL:HA	2.19	0.42
26:14:20:ASN:ND2	26:14:36:CYS:SG	2.81	0.42
32:1a:321:A:N7	32:1a:328:C:O2'	2.41	0.42
32:1a:347:G:C8	56:1a:3272:MPD:H51	2.54	0.42
32:1a:814:A:H2'	32:1a:816:A:H5"	2.01	0.42
32:1a:834:C:C2	32:1a:853:G:C2	3.07	0.42
35:1d:98:GLU:O	35:1d:103:ASN:ND2	2.49	0.42
39:1h:38:ILE:HD12	39:1h:111:ILE:HG23	2.01	0.42
44:1m:49:THR:HG22	44:1m:51:ALA:H	1.84	0.42
49:1r:58:LEU:HB3	49:1r:62:GLU:HB2	2.01	0.42
53:1y:87:LYS:O	53:1y:91:LYS:HB2	2.19	0.42
1:2A:806:C:O2	1:2A:2444:G:O2'	2.34	0.42
1:2A:1102:C:H2'	1:2A:1103:A:C8	2.51	0.42
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	2.01	0.42
4:2E:11:MET:CG	4:2E:24:THR:HG23	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:15:PHE:HA	4:2E:19:ARG:O	2.19	0.42
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.51	0.42
6:2G:121:ASN:HD21	6:2G:123:ASN:HB2	1.85	0.42
7:2H:53:GLU:CA	7:2H:65:HIS:HE2	2.32	0.42
8:2I:9:LEU:HD23	8:2I:9:LEU:HA	1.87	0.42
18:2W:11:ARG:HD2	18:2W:11:ARG:HA	1.65	0.42
26:24:13:ARG:HH22	26:24:23:GLU:HG2	1.83	0.42
32:2a:149:A:H2'	32:2a:150:C:C6	2.54	0.42
32:2a:1030(A):G:H1'	32:2a:1030(C):G:N7	2.34	0.42
33:2b:163:PHE:HA	33:2b:185:ILE:O	2.19	0.42
40:2i:9:ARG:HB3	40:2i:104:ARG:HH21	1.84	0.42
42:2k:86:GLY:N	42:2k:112:THR:HG23	2.23	0.42
45:2n:9:LYS:HA	45:2n:12:ARG:HD3	2.01	0.42
53:2y:13:THR:C	53:2y:15:ALA:H	2.26	0.42
1:1A:271(L):U:H4'	8:1I:50:ARG:HH12	1.84	0.42
1:1A:862:G:H2'	1:1A:863:A:O4'	2.19	0.42
1:1A:868:U:C4	1:1A:869:G:N7	2.87	0.42
1:1A:1138:G:C2	9:1N:106:MET:HE2	2.54	0.42
1:1A:1912:A:O2'	32:1a:1494:G:O2'	2.35	0.42
4:1E:143:ASN:HD22	4:1E:147:PRO:HD3	1.84	0.42
5:1F:51:THR:HB	5:1F:88:VAL:HG11	2.00	0.42
32:1a:91:C:H2'	32:1a:92:C:H6	1.83	0.42
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.17	0.42
32:1a:1060:C:H5	34:1c:2:GLY:HA3	1.83	0.42
32:1a:1137:C:H4'	32:1a:1138:G:C2	2.54	0.42
32:1a:1153:C:OP1	41:1j:13:HIS:HE1	2.02	0.42
33:1b:118:LEU:HD23	33:1b:118:LEU:HA	1.90	0.42
35:1d:4:TYR:O	35:1d:6:GLY:N	2.52	0.42
35:1d:194:LEU:HD22	35:1d:194:LEU:HA	1.87	0.42
39:1h:87:SER:HA	39:1h:93:VAL:HG23	2.00	0.42
41:1j:8:LEU:HD23	41:1j:96:ILE:HG23	2.01	0.42
41:1j:34:VAL:HG12	41:1j:74:ILE:HA	2.01	0.42
1:2A:1184:G:C6	1:2A:1185:C:C4	3.06	0.42
1:2A:1843:C:H5'	3:2D:253:GLN:NE2	2.34	0.42
1:2A:2228:G:OP1	3:2D:261:LYS:HE2	2.19	0.42
4:2E:103:ASP:N	60:2E:401:HOH:O	2.13	0.42
6:2G:175:LEU:C	6:2G:177:GLY:H	2.27	0.42
7:2H:26:VAL:HG12	7:2H:79:VAL:HG21	2.02	0.42
10:2O:47:ILE:HG13	10:2O:47:ILE:H	1.71	0.42
11:2P:28:GLY:O	11:2P:30:THR:N	2.52	0.42
14:2S:25:ARG:HD3	14:2S:42:ASP:OD2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2Y:82:PRO:O	20:2Y:101:LYS:NZ	2.52	0.42
20:2Y:102:CYS:SG	20:2Y:104:GLY:N	2.76	0.42
21:2Z:5:LEU:HD22	21:2Z:47:VAL:HG21	2.01	0.42
32:2a:401:C:H2'	32:2a:402:G:H8	1.84	0.42
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.54	0.42
32:2a:1316:G:N2	32:2a:1318:A:H3'	2.34	0.42
32:2a:1338:G:H2'	32:2a:1339:A:C8	2.55	0.42
34:2c:79:ARG:O	34:2c:82:GLU:HB2	2.18	0.42
40:2i:12:GLU:O	40:2i:68:GLY:N	2.52	0.42
43:2l:113:ARG:NH2	60:2l:301:HOH:O	2.52	0.42
1:1A:1095:A:C6	1:1A:1096:A:C6	3.08	0.42
1:1A:1142(A):A:C4	1:1A:1144:G:N7	2.87	0.42
1:1A:1668:A:H4'	1:1A:1669:A:O5'	2.18	0.42
1:1A:1799:G:O2'	3:1D:181:GLU:OE2	2.29	0.42
1:1A:2536:G:C6	1:1A:2537:U:C4	3.07	0.42
2:1B:57:A:H1'	6:1G:29:TRP:HB2	2.02	0.42
7:1H:41:MET:HE1	7:1H:54:ARG:HB3	2.01	0.42
15:1T:96:ARG:HH11	15:1T:96:ARG:HB2	1.85	0.42
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.19	0.42
32:1a:20:U:H2'	32:1a:21:G:O4'	2.19	0.42
32:1a:200:G:H1	32:1a:217:C:N4	2.15	0.42
32:1a:1073:U:H2'	32:1a:1074:G:H8	1.84	0.42
32:1a:1309:G:OP1	44:1m:88:ARG:NH2	2.49	0.42
34:1c:180:ALA:HB1	34:1c:203:PHE:CE1	2.54	0.42
45:1n:7:ILE:HG13	45:1n:8:GLU:N	2.32	0.42
47:1p:58:TYR:O	47:1p:61:SER:OG	2.24	0.42
53:1y:6:THR:OG1	53:1y:38:HIS:HE1	2.01	0.42
1:2A:218:A:C2	1:2A:235:U:H4'	2.55	0.42
1:2A:403:U:H3'	60:2A:4806:HOH:O	2.19	0.42
1:2A:995:C:P	16:2U:53:ARG:HH21	2.42	0.42
1:2A:1589:C:H2'	1:2A:1590:U:C6	2.54	0.42
3:2D:274:ARG:O	3:2D:275:LYS:HG2	2.19	0.42
9:2N:23:LEU:HA	9:2N:60:ILE:HD11	2.01	0.42
15:2T:109:GLU:HG2	15:2T:112:ARG:NH2	2.30	0.42
24:22:29:LYS:HG2	24:22:57:ILE:HD13	2.00	0.42
32:2a:481:G:O2'	32:2a:483:C:N4	2.43	0.42
32:2a:600:C:OP1	39:2h:97:VAL:HG23	2.19	0.42
32:2a:913:A:H4'	32:2a:914:A:O5'	2.19	0.42
32:2a:1002:G:C2	32:2a:1003:G:C8	3.07	0.42
32:2a:1005:A:H1'	32:2a:1025:U:N3	2.35	0.42
32:2a:1129:C:N4	32:2a:1143:G:H1	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1151:A:O2'	32:2a:1152:A:O5'	2.36	0.42
33:2b:62:ALA:HB2	33:2b:222:ILE:HG22	2.00	0.42
36:2e:129:ILE:H	36:2e:129:ILE:HG13	1.67	0.42
1:1A:434:U:OP2	60:1A:4250:HOH:O	2.22	0.42
1:1A:1231:G:H2'	1:1A:1232:G:H8	1.82	0.42
1:1A:1721:G:H8	1:1A:1741:A:H62	1.67	0.42
1:1A:2142:C:N3	1:1A:2149:G:O6	2.52	0.42
1:1A:2438:U:O2'	1:1A:2440:C:OP1	2.32	0.42
1:1A:2820:A:O2'	1:1A:2821:A:OP1	2.37	0.42
2:1B:90:A:C5	2:1B:91:C:H1'	2.54	0.42
5:1F:183:VAL:HG13	60:1F:449:HOH:O	2.19	0.42
6:1G:125:PHE:HB3	6:1G:166:ASP:CG	2.45	0.42
20:1Y:28:LYS:HB3	20:1Y:28:LYS:HE2	1.78	0.42
21:1Z:40:ASP:HB3	21:1Z:43:GLU:HB2	2.02	0.42
22:10:23:VAL:HG22	22:10:38:VAL:HG22	2.00	0.42
22:10:70:GLN:OE1	22:10:80:HIS:NE2	2.50	0.42
32:1a:312:C:H2'	32:1a:313:A:C8	2.54	0.42
32:1a:1162:C:H42	32:1a:1174:G:H1	1.68	0.42
32:1a:1165:C:H2'	32:1a:1166:G:O4'	2.19	0.42
32:1a:1314:C:H2'	32:1a:1315:U:H6	1.85	0.42
32:1a:1505:G:H4'	32:1a:1506:U:H5"	2.01	0.42
38:1g:106:GLN:O	38:1g:110:GLN:HG2	2.19	0.42
42:1k:124:LYS:HE2	42:1k:125:PHE:CE2	2.55	0.42
50:1s:69:HIS:HB3	50:1s:73:GLU:CD	2.45	0.42
1:2A:83:G:OP1	20:2Y:95:LYS:NZ	2.51	0.42
1:2A:107:C:H2'	1:2A:108:U:C6	2.54	0.42
1:2A:1614:A:N6	18:2W:92:ARG:O	2.44	0.42
1:2A:1877:A:C5	1:2A:1878:G:H1'	2.54	0.42
1:2A:2097:C:H2'	1:2A:2098:U:C6	2.55	0.42
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.55	0.42
2:2B:7:G:H21	14:2S:38:GLN:CD	2.27	0.42
11:2P:121:LYS:HG2	11:2P:122:PRO:HD2	2.02	0.42
32:2a:189(L):G:H2'	32:2a:190:U:H6	1.84	0.42
32:2a:473:G:C2	32:2a:474:G:C4	3.08	0.42
32:2a:604:G:H2'	32:2a:605:U:O4'	2.19	0.42
32:2a:946:A:H2'	32:2a:947:G:C8	2.55	0.42
33:2b:18:GLY:HA3	33:2b:41:ILE:HA	2.00	0.42
33:2b:136:VAL:O	33:2b:139:LYS:HB3	2.20	0.42
34:2c:37:GLN:HE22	45:2n:52:GLN:HB3	1.84	0.42
38:2g:111:ARG:NH1	38:2g:113:GLU:OE2	2.52	0.42
43:2l:60:LEU:HA	43:2l:60:LEU:HD12	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1094:U:O2'	1:1A:1096:A:N7	2.43	0.42
1:1A:1266:G:H3'	60:1A:4566:HOH:O	2.19	0.42
1:1A:2240:C:OP1	60:1A:4247:HOH:O	2.21	0.42
1:1A:2505:G:O6	1:1A:2576:G:H2'	2.20	0.42
7:1H:7:LEU:HA	7:1H:8:PRO:HD3	1.94	0.42
9:1N:48:MET:HE3	9:1N:48:MET:HB2	1.91	0.42
12:1Q:7:MET:HE3	12:1Q:7:MET:HB2	1.57	0.42
24:12:67:LYS:HA	24:12:67:LYS:HD3	1.85	0.42
26:14:61:ARG:HH21	50:1s:42:PRO:CD	2.33	0.42
32:1a:19:C:H2'	32:1a:20:U:C6	2.55	0.42
32:1a:696:A:N1	32:1a:797:C:O2'	2.42	0.42
32:1a:1291:G:OP1	38:1g:41:ARG:NH2	2.52	0.42
32:1a:1479:C:H2'	32:1a:1480:G:H8	1.85	0.42
33:1b:84:GLU:O	33:1b:219:VAL:HG21	2.19	0.42
34:1c:25:GLY:O	34:1c:27:LYS:N	2.52	0.42
35:1d:79:PHE:CE1	35:1d:204:ILE:HD13	2.54	0.42
43:1l:59:ARG:HA	43:1l:65:GLU:HA	2.02	0.42
44:1m:108:ARG:HD3	44:1m:108:ARG:HA	1.71	0.42
47:1p:19:ILE:HG23	47:1p:37:GLY:C	2.44	0.42
1:2A:299:A:N1	1:2A:322:A:O2'	2.41	0.42
1:2A:2104:G:O6	1:2A:2185:C:C2	2.72	0.42
1:2A:2130:U:H2'	1:2A:2158:A:N6	2.30	0.42
2:2B:66:A:H61	2:2B:108:U:H3'	1.84	0.42
5:2F:130:ALA:H	5:2F:142:TRP:CD1	2.38	0.42
5:2F:136:THR:O	5:2F:140:LEU:HD22	2.20	0.42
9:2N:75:TYR:CE2	9:2N:77:GLY:HA2	2.55	0.42
12:2Q:8:LYS:HG3	21:2Z:197:ILE:HD12	2.01	0.42
14:2S:84:GLN:HA	14:2S:111:GLU:HB2	2.02	0.42
32:2a:137:C:H2'	32:2a:138:G:C8	2.54	0.42
32:2a:1340:A:OP1	53:2y:57:PRO:HB3	2.19	0.42
32:2a:1508:G:H2'	32:2a:1509:C:O4'	2.20	0.42
33:2b:28:PHE:CD1	33:2b:194:PRO:HG3	2.55	0.42
34:2c:6:HIS:HD2	34:2c:7:PRO:HD2	1.85	0.42
39:2h:6:ILE:HD11	39:2h:31:PHE:HD2	1.83	0.42
41:2j:32:ALA:HB1	41:2j:33:GLN:HA	2.02	0.42
47:2p:8:ARG:HB3	47:2p:28:ARG:NH1	2.34	0.42
1:1A:459:U:H5"	29:17:40:TRP:CD2	2.54	0.42
1:1A:972:G:OP2	1:1A:973:A:O2'	2.35	0.42
1:1A:1549:C:H2'	1:1A:1550:C:C6	2.54	0.42
1:1A:1721:G:H1'	1:1A:1741:A:N6	2.35	0.42
1:1A:1920:OMC:O2'	32:1a:1496:C:H4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2732:G:H3'	1:1A:2733:A:O4'	2.19	0.42
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.20	0.42
12:1Q:54:MET:HG3	12:1Q:121:ALA:HB2	2.02	0.42
19:1X:43:VAL:HG21	19:1X:81:VAL:HG11	2.00	0.42
23:11:3:LYS:HA	23:11:3:LYS:HD2	1.87	0.42
32:1a:295:C:H2'	32:1a:296:U:O4'	2.20	0.42
32:1a:642:A:H2'	32:1a:643:C:C6	2.54	0.42
48:1q:53:LEU:HD23	48:1q:82:MET:HE1	2.01	0.42
1:2A:885:C:H1'	1:2A:892:G:H22	1.85	0.42
1:2A:968:G:H2'	1:2A:969:U:C6	2.55	0.42
1:2A:1186:G:C2	1:2A:1187:G:H1'	2.54	0.42
1:2A:2051:A:OP2	1:2A:2051:A:H8	2.03	0.42
1:2A:2162:G:H4'	1:2A:2172:U:O2'	2.20	0.42
1:2A:2287:A:O2'	1:2A:2288:A:H5"	2.20	0.42
1:2A:2472:G:N2	1:2A:2477:C:OP1	2.51	0.42
1:2A:2584:U:H5"	1:2A:2602:A:H2	1.84	0.42
4:2E:7:VAL:HG13	4:2E:27:LEU:HB3	2.02	0.42
6:2G:76:SER:HA	6:2G:83:ARG:HA	2.01	0.42
26:24:45:GLY:C	26:24:47:GLN:H	2.28	0.42
27:25:20:ARG:HG2	27:25:23:HIS:ND1	2.35	0.42
32:2a:108:G:N1	51:2t:15:ARG:HG2	2.34	0.42
32:2a:187:C:H2'	32:2a:188:C:H6	1.85	0.42
32:2a:503:C:OP2	43:2l:116:SER:HB3	2.20	0.42
32:2a:547:A:H4'	32:2a:548:G:O5'	2.20	0.42
32:2a:1016:A:H2'	32:2a:1017:G:O4'	2.20	0.42
33:2b:24:TRP:CZ3	33:2b:26:PRO:HA	2.55	0.42
34:2c:123:GLN:HB3	34:2c:128:PHE:HB2	2.02	0.42
34:2c:177:THR:HG22	34:2c:180:ALA:H	1.85	0.42
1:1A:787:U:H5"	1:1A:788:A:H5'	2.02	0.42
1:1A:1048:A:N1	1:1A:1112:G:O2'	2.49	0.42
1:1A:1098:A:H2'	1:1A:1099:G:O4'	2.20	0.42
1:1A:1153:C:H2'	1:1A:1154:G:O4'	2.19	0.42
1:1A:1210:A:H5"	1:1A:1212:G:O4'	2.19	0.42
1:1A:1568:G:N7	60:1A:4491:HOH:O	2.37	0.42
3:1D:43:ARG:HA	3:1D:48:ARG:O	2.19	0.42
6:1G:97:ASP:O	6:1G:101:ILE:HG13	2.19	0.42
10:1O:70:LYS:HE2	10:1O:70:LYS:HB3	1.83	0.42
26:14:55:ARG:H	26:14:56:VAL:HA	1.85	0.42
32:1a:1025:U:H3'	32:1a:1025:U:H6	1.84	0.42
32:1a:1176:A:H2'	32:1a:1177:G:C8	2.54	0.42
32:1a:1358:U:OP1	45:1n:35:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:69:LEU:HD13	33:1b:91:PRO:HB2	2.01	0.42
35:1d:57:ARG:NE	35:1d:205:GLU:HB3	2.35	0.42
47:1p:26:ARG:NH1	47:1p:31:LYS:HB3	2.34	0.42
49:1r:35:ARG:O	49:1r:37:VAL:N	2.53	0.42
1:2A:286:C:H2'	1:2A:287:C:C6	2.55	0.42
1:2A:827:U:O2'	1:2A:2068:U:C2	2.62	0.42
1:2A:2165:G:H2'	1:2A:2166:G:C8	2.55	0.42
1:2A:2611:U:H6	1:2A:2611:U:H5'	1.84	0.42
5:2F:167:ALA:HA	5:2F:170:LEU:HD22	2.01	0.42
6:2G:117:PHE:CZ	6:2G:179:PRO:HG2	2.55	0.42
7:2H:55:PRO:HG2	7:2H:61:HIS:CE1	2.55	0.42
12:2Q:7:MET:O	21:2Z:196:VAL:HA	2.20	0.42
20:2Y:90:LEU:HB3	20:2Y:92:ASN:H	1.84	0.42
32:2a:659:U:OP1	46:2o:9:GLN:NE2	2.53	0.42
32:2a:1009:G:H2'	32:2a:1009:G:N3	2.35	0.42
48:2q:96:GLU:C	48:2q:98:LEU:H	2.28	0.42
1:1A:197:A:N6	1:1A:2430:A:O2'	2.53	0.42
1:1A:609:A:H2'	1:1A:610:G:O4'	2.20	0.42
1:1A:1257:C:H4'	5:1F:83:PHE:CD1	2.55	0.42
1:1A:2012:G:H4'	18:1W:96:ILE:HD13	2.01	0.42
1:1A:2207:G:O2'	1:1A:2208:A:OP1	2.35	0.42
1:1A:2563:U:H4'	10:1O:28:SER:HA	2.02	0.42
1:1A:2722:G:H2'	1:1A:2723:C:C6	2.55	0.42
1:1A:2791:C:H2'	1:1A:2792:G:H8	1.84	0.42
2:1B:42:C:O2	6:1G:93:THR:N	2.46	0.42
5:1F:7:TYR:O	5:1F:21:ALA:HA	2.19	0.42
9:1N:10:GLU:OE1	9:1N:11:PRO:HD2	2.19	0.42
27:15:47:PRO:O	27:15:60:VAL:HG21	2.20	0.42
32:1a:1024:G:H2'	32:1a:1024:G:N3	2.35	0.42
35:1d:156:GLU:O	35:1d:159:ARG:HG2	2.19	0.42
36:1e:33:VAL:HG13	36:1e:112:LEU:HD12	2.01	0.42
39:1h:20:TYR:HA	39:1h:65:TYR:CE1	2.55	0.42
39:1h:77:GLU:OE2	39:1h:81:HIS:NE2	2.52	0.42
46:1o:78:TYR:CZ	46:1o:82:ILE:HD13	2.55	0.42
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.85	0.42
1:2A:510:C:H2'	1:2A:511:U:O4'	2.19	0.42
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.55	0.42
1:2A:1525:G:C2	1:2A:1526:G:C4	3.07	0.42
1:2A:1665:A:H2'	1:2A:1666:G:O4'	2.20	0.42
1:2A:2043:C:OP1	1:2A:2777:G:O2'	2.34	0.42
1:2A:2168:G:H2'	1:2A:2170:A:OP2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.55	0.42
1:2A:2407:G:OP1	60:2A:3954:HOH:O	2.21	0.42
4:2E:54:GLN:HB2	4:2E:76:ARG:HG3	2.02	0.42
21:2Z:54:HIS:CG	21:2Z:101:PRO:HG3	2.55	0.42
21:2Z:82:ARG:HE	21:2Z:82:ARG:HB3	1.69	0.42
32:2a:300:A:H2'	32:2a:564:C:H42	1.85	0.42
32:2a:401:C:H2'	32:2a:402:G:C8	2.54	0.42
32:2a:1151:A:H5"	41:2j:41:PRO:HA	2.02	0.42
40:2i:85:LEU:HB3	40:2i:92:TYR:CD2	2.51	0.42
1:1A:1093:G:O2'	1:1A:1098:A:N6	2.53	0.42
1:1A:2345:G:N3	1:1A:2381:C:H2'	2.34	0.42
1:1A:2750:A:OP2	7:1H:62:LYS:NZ	2.46	0.42
1:1A:2876:G:H4'	15:1T:2:ASN:ND2	2.35	0.42
4:1E:35:GLN:HB3	4:1E:48:GLN:NE2	2.32	0.42
4:1E:61:ARG:N	4:1E:62:PRO:HD2	2.35	0.42
4:1E:103:ASP:OD2	4:1E:168:MET:HE3	2.19	0.42
6:1G:62:LEU:HD22	26:14:28:LYS:NZ	2.35	0.42
8:1I:132:PRO:HD2	8:1I:136:VAL:O	2.20	0.42
32:1a:123:C:OP1	32:1a:312:C:H5'	2.20	0.42
32:1a:184:G:H2'	32:1a:185:A:C8	2.54	0.42
32:1a:198:G:C6	32:1a:220:G:C2	3.07	0.42
32:1a:235:C:H5'	48:1q:70:ARG:HG3	2.02	0.42
32:1a:575:G:O2'	32:1a:821:G:H5'	2.20	0.42
32:1a:685:G:N1	32:1a:704:A:OP2	2.40	0.42
32:1a:973:G:H3'	32:1a:974:A:H5"	2.00	0.42
32:1a:1071:C:H2'	32:1a:1072:G:H8	1.83	0.42
32:1a:1154:G:C4	32:1a:1155:G:C8	3.08	0.42
32:1a:1327:C:H2'	32:1a:1328:C:C6	2.55	0.42
33:1b:87:ARG:HB2	33:1b:219:VAL:HG11	2.02	0.42
34:1c:56:ASP:O	34:1c:66:VAL:HA	2.20	0.42
35:1d:12:CYS:O	35:1d:16:GLY:N	2.49	0.42
1:2A:57:C:H2'	1:2A:58:G:O4'	2.19	0.42
1:2A:296:C:H2'	1:2A:297:C:C6	2.55	0.42
1:2A:1789:A:OP1	3:2D:222:ARG:HG3	2.20	0.42
1:2A:1810:A:H2'	1:2A:1811:G:O4'	2.20	0.42
1:2A:2040:C:H2'	1:2A:2041:U:O4'	2.20	0.42
1:2A:2621:A:H5"	60:2A:4228:HOH:O	2.20	0.42
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.31	0.42
1:2A:2647:U:H2'	1:2A:2648:C:H6	1.85	0.42
2:2B:32:C:H2'	2:2B:33:G:C8	2.54	0.42
2:2B:42:C:N4	6:2G:91:ARG:HH12	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2N:30:ILE:HG22	9:2N:34:LEU:HD22	2.02	0.42
11:2P:75:ILE:H	11:2P:75:ILE:HG12	1.58	0.42
11:2P:92:GLU:OE2	11:2P:121:LYS:NZ	2.43	0.42
13:2R:82:GLU:O	13:2R:85:PRO:HD2	2.19	0.42
18:2W:19:LEU:HD12	18:2W:19:LEU:HA	1.86	0.42
20:2Y:43:ASN:CG	20:2Y:65:ALA:HB3	2.45	0.42
20:2Y:67:LEU:HA	20:2Y:67:LEU:HD23	1.83	0.42
32:2a:232:G:H1'	32:2a:262:A:N1	2.35	0.42
32:2a:743:U:H2'	32:2a:744:C:C6	2.54	0.42
32:2a:772:U:H2'	32:2a:773:G:O4'	2.20	0.42
32:2a:1000:U:H3	32:2a:1041:A:H61	1.66	0.42
32:2a:1206:G:C6	32:2a:1207:2MG:C6	3.08	0.42
33:2b:45:GLN:HG3	33:2b:46:LYS:N	2.33	0.42
53:2y:20:VAL:HG21	53:2y:41:LEU:HD21	2.01	0.42
1:1A:35:G:H2'	1:1A:36:G:O4'	2.20	0.41
1:1A:719:C:H2'	1:1A:720:C:C6	2.55	0.41
1:1A:1800:C:H4'	60:1A:5619:HOH:O	2.19	0.41
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.55	0.41
1:1A:2748:A:H5'	7:1H:4:ILE:HD12	2.01	0.41
3:1D:13:ARG:HA	3:1D:13:ARG:HD2	1.83	0.41
4:1E:173:VAL:CG2	4:1E:185:LYS:HB2	2.50	0.41
10:1O:108:GLU:H	10:1O:108:GLU:HG3	1.40	0.41
21:1Z:35:ARG:HD2	21:1Z:35:ARG:HA	1.85	0.41
25:13:55:ARG:HD3	60:13:217:HOH:O	2.18	0.41
32:1a:67:C:H2'	32:1a:68:G:H8	1.82	0.41
32:1a:437:U:C5'	35:1d:155:LEU:HD11	2.50	0.41
32:1a:634:C:H2'	32:1a:635:G:H8	1.85	0.41
47:1p:42:ARG:HB3	47:1p:44:THR:HG23	2.01	0.41
48:1q:45:HIS:O	48:1q:73:VAL:HG23	2.19	0.41
1:2A:336:C:OP1	20:2Y:84:ARG:HG2	2.20	0.41
1:2A:581:C:H2'	1:2A:582:G:C8	2.55	0.41
1:2A:1027:A:N6	1:2A:1126:A:C4	2.88	0.41
1:2A:1287:A:C8	13:2R:104:ARG:HD3	2.54	0.41
1:2A:1297:C:OP1	1:2A:2710:C:H4'	2.20	0.41
1:2A:1529:G:C5	1:2A:1530:C:C4	3.07	0.41
1:2A:2056:G:N2	27:25:5:PRO:HA	2.35	0.41
1:2A:2820:A:O2'	4:2E:191:PRO:HG3	2.20	0.41
6:2G:108:ASN:HA	26:24:37:SER:HB3	2.02	0.41
7:2H:35:VAL:HA	7:2H:36:PRO:HD2	1.94	0.41
10:2O:68:GLU:HB3	10:2O:78:ARG:HD3	2.02	0.41
10:2O:97:ARG:HE	10:2O:97:ARG:HB2	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:29:LYS:HG2	11:2P:30:THR:HG23	2.02	0.41
18:2W:11:ARG:NH1	18:2W:99:ARG:O	2.53	0.41
21:2Z:23:LYS:HD3	21:2Z:40:ASP:HA	2.02	0.41
21:2Z:98:MET:HE2	21:2Z:98:MET:HB2	1.94	0.41
22:20:9:SER:OG	22:20:10:THR:N	2.53	0.41
22:20:36:ILE:HD13	22:20:60:PHE:HB3	2.02	0.41
32:2a:417:C:N3	32:2a:426:G:N2	2.68	0.41
32:2a:572:A:OP2	60:2a:3226:HOH:O	2.20	0.41
32:2a:952:U:H4'	32:2a:964:A:N1	2.35	0.41
32:2a:1363(A):A:H1'	32:2a:1365:G:N7	2.35	0.41
32:2a:1391:U:H2'	32:2a:1392:G:H8	1.84	0.41
33:2b:82:ARG:HG3	33:2b:92:TYR:CE2	2.55	0.41
40:2i:32:ASP:N	40:2i:35:GLU:OE1	2.46	0.41
50:2s:36:ARG:HB3	50:2s:72:GLY:CA	2.50	0.41
53:2y:3:MET:HB3	53:2y:37:PRO:HD2	2.01	0.41
1:1A:271(H):G:O2'	1:1A:271(I):G:H8	2.04	0.41
1:1A:784:A:OP2	60:1A:4255:HOH:O	2.22	0.41
1:1A:1236:G:N7	60:1A:4495:HOH:O	2.37	0.41
1:1A:1529:G:H1	1:1A:1540:U:H3	1.67	0.41
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.54	0.41
1:1A:1914:C:H2'	1:1A:1915:5MU:O2	2.20	0.41
4:1E:98:PRO:HG3	4:1E:175:VAL:HG12	2.02	0.41
11:1P:15:ARG:HD3	11:1P:15:ARG:HA	1.77	0.41
32:1a:456:C:H2'	32:1a:457:C:H6	1.85	0.41
32:1a:964:A:N3	32:1a:969:A:O2'	2.49	0.41
32:1a:965:A:H8	53:1y:8:LYS:HZ2	1.67	0.41
32:1a:982:U:H5"	45:1n:6:LEU:HD21	2.01	0.41
32:1a:1089:G:C6	32:1a:1090:U:C4	3.08	0.41
32:1a:1106:G:H5"	34:1c:172:ARG:HG3	2.02	0.41
33:1b:15:VAL:HG12	33:1b:16:HIS:HD2	1.84	0.41
34:1c:71:ALA:HB2	34:1c:115:LEU:HD21	2.02	0.41
35:1d:163:GLU:O	35:1d:166:LYS:HG2	2.20	0.41
44:1m:23:TYR:CE2	44:1m:71:ARG:HG3	2.54	0.41
44:1m:59:TYR:CE1	44:1m:63:THR:HG21	2.55	0.41
47:1p:43:LYS:HG2	47:1p:48:TRP:CE3	2.55	0.41
1:2A:195:A:H5"	1:2A:196:A:O5'	2.20	0.41
1:2A:271(Q):G:H2'	1:2A:271(R):G:C8	2.55	0.41
1:2A:856:C:O2'	1:2A:857:C:OP1	2.31	0.41
1:2A:1523:U:H2'	1:2A:1524:G:H8	1.85	0.41
1:2A:2439:A:N1	60:2A:4136:HOH:O	2.37	0.41
5:2F:17:ARG:O	5:2F:17:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.45	0.41
7:2H:7:LEU:HB3	7:2H:69:ARG:HE	1.85	0.41
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.59	0.41
8:2I:9:LEU:HD13	8:2I:12:LEU:HD12	2.02	0.41
20:2Y:83:THR:HG21	20:2Y:99:CYS:HB2	2.02	0.41
32:2a:683:G:C6	32:2a:684:A:C6	3.08	0.41
32:2a:939:G:C6	32:2a:940:C:C4	3.08	0.41
32:2a:1401:G:O6	32:2a:1504:G:N2	2.54	0.41
35:2d:13:ARG:HB3	35:2d:38:TYR:O	2.19	0.41
36:2e:91:LEU:HD13	36:2e:91:LEU:HA	1.90	0.41
36:2e:112:LEU:HD23	36:2e:112:LEU:HA	1.83	0.41
40:2i:4:TYR:CE1	40:2i:88:TYR:HA	2.55	0.41
40:2i:65:VAL:C	40:2i:66:ARG:HG2	2.44	0.41
1:1A:536:A:H2'	1:1A:537:C:C6	2.55	0.41
1:1A:864:G:O2'	1:1A:865:C:H5'	2.20	0.41
1:1A:1187:G:H5"	17:1V:81:TYR:CE1	2.55	0.41
1:1A:1300:U:H4'	1:1A:1301:A:H5"	2.01	0.41
1:1A:1847:A:H5'	60:1A:6980:HOH:O	2.20	0.41
1:1A:2632:A:O2'	1:1A:2811:G:O2'	2.29	0.41
3:1D:245:PRO:HA	3:1D:246:PRO:HD3	1.92	0.41
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	2.02	0.41
14:1S:26:LEU:HD13	14:1S:87:PHE:HD1	1.85	0.41
32:1a:41:G:H2'	32:1a:42:G:H8	1.84	0.41
32:1a:437:U:H5"	35:1d:155:LEU:HD11	2.02	0.41
32:1a:619:U:O2	35:1d:133:VAL:HA	2.19	0.41
32:1a:1005:A:N3	32:1a:1036:G:N2	2.61	0.41
32:1a:1479:C:H2'	32:1a:1480:G:C8	2.55	0.41
34:1c:5:ILE:HG13	34:1c:6:HIS:N	2.35	0.41
53:1y:3:MET:HB3	53:1y:3:MET:HE2	1.64	0.41
1:2A:153:C:OP1	23:21:92:LYS:HD3	2.21	0.41
1:2A:328:U:H4'	20:2Y:68:HIS:ND1	2.35	0.41
1:2A:922:U:H2'	1:2A:923:C:H6	1.82	0.41
1:2A:1588:C:H2'	1:2A:1589:C:C6	2.55	0.41
1:2A:1647:G:H3'	1:2A:1647:G:OP2	2.20	0.41
1:2A:1655:A:N6	1:2A:2005:A:O2'	2.53	0.41
1:2A:2712:U:H1'	1:2A:2712(A):A:C8	2.55	0.41
3:2D:71:ASP:HB3	3:2D:103:ARG:NH2	2.35	0.41
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.19	0.41
9:2N:108:PRO:O	9:2N:113:GLY:HA3	2.19	0.41
20:2Y:73:ARG:HG2	20:2Y:73:ARG:HH11	1.86	0.41
21:2Z:8:TYR:HB2	21:2Z:38:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1082:G:H2'	32:2a:1083:U:O4'	2.19	0.41
32:2a:1327:C:H2'	32:2a:1328:C:C6	2.54	0.41
32:2a:1504:G:OP1	32:2a:1507:A:H4'	2.20	0.41
38:2g:18:TYR:HD1	38:2g:59:LEU:HD22	1.85	0.41
38:2g:76:ARG:HB3	38:2g:156:TRP:CH2	2.55	0.41
46:2o:24:SER:O	46:2o:28:GLN:HG3	2.20	0.41
48:2q:62:SER:CB	48:2q:72:ARG:HH11	2.31	0.41
50:2s:18:LYS:H	50:2s:18:LYS:HG2	1.57	0.41
1:1A:1000:A:H62	1:1A:1154:G:H2'	1.85	0.41
1:1A:1567:A:OP2	3:1D:84:TYR:OH	2.30	0.41
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.35	0.41
1:1A:2347:C:H2'	1:1A:2348:U:H6	1.85	0.41
1:1A:2474:C:HO2'	1:1A:2475:C:P	2.42	0.41
13:1R:118:GLU:OXT	60:1R:302:HOH:O	2.22	0.41
32:1a:375:U:OP1	47:1p:69:THR:HG21	2.20	0.41
32:1a:838:G:H1	32:1a:848:C:H42	1.68	0.41
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.55	0.41
35:1d:170:VAL:HG12	35:1d:171:GLY:H	1.85	0.41
46:1o:22:THR:HG1	46:1o:23:GLY:H	1.67	0.41
50:1s:48:THR:HG22	50:1s:61:TYR:HD1	1.86	0.41
53:1y:87:LYS:HD3	53:1y:91:LYS:HD2	2.01	0.41
1:2A:631:A:H1'	11:2P:66:GLY:HA2	2.03	0.41
1:2A:1140:C:OP1	9:2N:23:LEU:HB3	2.20	0.41
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.20	0.41
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.53	0.41
1:2A:2136:C:H2'	1:2A:2137:C:C5	2.55	0.41
1:2A:2360:A:C2	1:2A:2361:A:H1'	2.55	0.41
1:2A:2484:G:H1'	12:2Q:124:LYS:HD2	2.01	0.41
1:2A:2557:G:H2'	1:2A:2558:C:C6	2.55	0.41
2:2B:42:C:C4	2:2B:43:C:C4	3.08	0.41
5:2F:187:VAL:HG12	11:2P:3:LEU:HD12	2.02	0.41
15:2T:28:VAL:HG13	15:2T:86:ILE:HG23	2.03	0.41
21:2Z:144:LEU:HD11	21:2Z:150:LEU:HD22	2.03	0.41
32:2a:625:G:H4'	47:2p:16:HIS:CD2	2.55	0.41
32:2a:643:C:H5'	39:2h:31:PHE:CE1	2.56	0.41
32:2a:659:U:H2'	32:2a:660:G:H8	1.85	0.41
32:2a:668:G:O2'	46:2o:46:HIS:HB3	2.19	0.41
32:2a:1158:C:H42	32:2a:1181:G:H1	1.67	0.41
33:2b:16:HIS:CD2	33:2b:210:SER:HB3	2.55	0.41
33:2b:178:ARG:NH1	39:2h:68:ARG:HH22	2.18	0.41
34:2c:182:ILE:HG23	34:2c:203:PHE:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:89:GLY:O	44:2m:93:ARG:HG3	2.20	0.41
1:1A:407:G:H2'	1:1A:408:G:C8	2.55	0.41
1:1A:1156:A:H5"	60:1A:5720:HOH:O	2.21	0.41
1:1A:1288:U:C2	1:1A:1327:C:O2	2.74	0.41
1:1A:2100:G:C6	1:1A:2190:G:C6	3.08	0.41
1:1A:2246:G:H2'	1:1A:2247:A:C8	2.55	0.41
1:1A:2335:A:C8	1:1A:2337:G:C5	3.08	0.41
1:1A:2626:C:H5'	60:1A:4378:HOH:O	2.20	0.41
4:1E:143:ASN:HD22	4:1E:147:PRO:CD	2.34	0.41
6:1G:2:PRO:HB3	6:1G:8:LYS:HZ3	1.86	0.41
9:1N:67:LEU:HB2	60:1N:323:HOH:O	2.19	0.41
22:10:43:THR:HG23	22:10:43:THR:O	2.21	0.41
36:1e:87:SER:OG	36:1e:125:SER:O	2.39	0.41
43:1l:83:VAL:HG13	43:1l:100:ILE:HG23	2.03	0.41
46:1o:5:LYS:O	46:1o:9:GLN:HG2	2.20	0.41
1:2A:25:U:H2'	1:2A:26:G:O4'	2.21	0.41
1:2A:830:G:H4'	1:2A:831:G:OP2	2.19	0.41
1:2A:990:A:N6	1:2A:1186:G:H1'	2.35	0.41
1:2A:1598:C:H2'	1:2A:1599:C:H6	1.85	0.41
1:2A:2402:C:H1'	1:2A:2403:C:H5	1.86	0.41
1:2A:2784:C:H4'	4:2E:41:LYS:O	2.20	0.41
2:2B:51:G:OP2	14:2S:61:ASN:HA	2.20	0.41
3:2D:80:ALA:HB3	3:2D:94:LEU:HB3	2.02	0.41
5:2F:31:HIS:HB2	11:2P:9:ASN:OD1	2.20	0.41
10:2O:87:ILE:HD12	10:2O:91:LEU:HA	2.02	0.41
16:2U:83:LEU:HD12	16:2U:88:ILE:HD12	2.02	0.41
20:2Y:20:TYR:CZ	20:2Y:43:ASN:HA	2.56	0.41
21:2Z:11:GLU:O	21:2Z:36:LYS:NZ	2.52	0.41
33:2b:15:VAL:HG12	33:2b:209:ARG:HD2	2.02	0.41
33:2b:45:GLN:HA	33:2b:48:MET:HE3	2.02	0.41
34:2c:8:ILE:HG12	34:2c:184:TYR:HB3	2.02	0.41
37:2f:61:LEU:HB3	37:2f:63:TYR:CE2	2.55	0.41
43:2l:46:LYS:HE2	43:2l:92:0TD:H4	2.01	0.41
49:2r:47:THR:HG23	49:2r:49:LYS:HG3	2.02	0.41
1:1A:116:C:OP2	60:1A:4253:HOH:O	2.22	0.41
1:1A:295:G:N7	60:1A:4492:HOH:O	2.37	0.41
1:1A:897:C:H2'	1:1A:898:C:H6	1.85	0.41
1:1A:1298:C:N4	1:1A:1299:G:C6	2.88	0.41
1:1A:1668:A:O2'	1:1A:1674:G:N7	2.51	0.41
1:1A:1897:G:H2'	1:1A:1898:U:O4'	2.21	0.41
1:1A:2836:U:H2'	1:1A:2837:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:44:LEU:HD12	8:1I:44:LEU:HA	1.87	0.41
20:1Y:6:HIS:H	20:1Y:6:HIS:HD2	1.66	0.41
21:1Z:157:LEU:HA	21:1Z:158:PRO:HD2	1.90	0.41
28:16:38:LYS:HE3	28:16:38:LYS:HB3	1.90	0.41
32:1a:925:G:C2	32:1a:927:G:C8	3.09	0.41
32:1a:1068:G:N2	32:1a:1191:A:N3	2.58	0.41
32:1a:1279:A:H5"	32:1a:1280:A:OP1	2.21	0.41
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	2.03	0.41
43:1l:33:ARG:HB3	43:1l:85:ILE:HD11	2.03	0.41
48:1q:58:GLU:O	48:1q:74:LEU:N	2.51	0.41
1:2A:154:G:H2'	1:2A:154(A):C:O4'	2.20	0.41
1:2A:658:C:H2'	1:2A:659:C:C6	2.56	0.41
1:2A:956:G:H2'	1:2A:957:A:H2'	2.02	0.41
1:2A:1000:A:C6	1:2A:1155:A:C8	3.08	0.41
1:2A:1022:G:C5	1:2A:1140:C:C4	3.09	0.41
1:2A:1364:G:P	23:21:3:LYS:HG3	2.61	0.41
1:2A:1589:C:H2'	1:2A:1590:U:H6	1.85	0.41
1:2A:2100:G:H2'	1:2A:2101:G:O4'	2.21	0.41
1:2A:2680:C:H1'	4:2E:187:ALA:HB1	2.03	0.41
3:2D:4:LYS:HB3	3:2D:4:LYS:HE2	1.76	0.41
4:2E:181:LEU:HA	4:2E:181:LEU:HD12	1.85	0.41
6:2G:142:PRO:HG2	6:2G:143:GLU:CD	2.45	0.41
10:2O:36:GLY:HA3	10:2O:109:LYS:HD2	2.01	0.41
14:2S:66:ALA:O	14:2S:69:VAL:HG12	2.20	0.41
16:2U:47:TYR:HA	16:2U:50:ARG:NH2	2.35	0.41
21:2Z:8:TYR:HB2	21:2Z:38:TYR:CZ	2.56	0.41
32:2a:424:G:O5'	32:2a:424:G:H8	2.04	0.41
32:2a:1068:G:H8	32:2a:1068:G:OP2	2.03	0.41
32:2a:1316:G:H4'	45:2n:18:VAL:CG1	2.51	0.41
38:2g:101:LEU:O	38:2g:105:VAL:HG23	2.21	0.41
39:2h:49:GLU:HG2	39:2h:62:TYR:HE2	1.84	0.41
40:2i:96:LEU:HD22	40:2i:101:PHE:HB2	2.02	0.41
44:2m:81:LEU:HD21	44:2m:88:ARG:NH2	2.35	0.41
1:1A:740:U:H2'	1:1A:741:G:C8	2.55	0.41
1:1A:783:A:O2'	1:1A:785:G:OP1	2.34	0.41
6:1G:11:TYR:CZ	6:1G:16:ARG:HD3	2.55	0.41
6:1G:67:LYS:H	26:14:6:HIS:CE1	2.38	0.41
7:1H:3:ARG:HG2	7:1H:6:ARG:CZ	2.51	0.41
7:1H:124:GLU:HG3	7:1H:132:ARG:HB3	2.01	0.41
20:1Y:86:ARG:HB2	20:1Y:98:VAL:HG23	2.03	0.41
20:1Y:92:ASN:H	20:1Y:92:ASN:ND2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:15:16:ARG:HG3	27:15:17:ASP:N	2.36	0.41
32:1a:62:U:H1'	32:1a:379:C:H1'	2.03	0.41
32:1a:236:G:H5"	48:1q:42:TYR:OH	2.20	0.41
32:1a:408:A:OP1	35:1d:113:SER:OG	2.36	0.41
32:1a:461:A:O2'	32:1a:470:C:H5'	2.21	0.41
32:1a:559:A:H4'	32:1a:560:U:H5"	2.01	0.41
32:1a:998:G:H2'	32:1a:999:C:C6	2.54	0.41
32:1a:1203:C:H2'	32:1a:1204:A:C8	2.56	0.41
32:1a:1318:A:H5"	50:1s:3:ARG:NH1	2.36	0.41
33:1b:217:ARG:HA	33:1b:217:ARG:HD3	1.89	0.41
39:1h:94:TYR:HE1	39:1h:132:GLU:HB2	1.85	0.41
1:2A:25:U:C4	1:2A:26:G:C6	3.08	0.41
1:2A:83:G:H1	1:2A:102:G:HO2'	1.65	0.41
1:2A:524:U:H2'	1:2A:525:U:C6	2.56	0.41
1:2A:1002:G:H2'	1:2A:1003:G:O4'	2.21	0.41
1:2A:1263:U:C4	1:2A:1264:G:C6	3.09	0.41
1:2A:2472:G:N1	1:2A:2477:C:OP1	2.44	0.41
1:2A:2508:G:C2	1:2A:2582:G:C6	3.09	0.41
1:2A:2886:G:H2'	1:2A:2887:U:H6	1.85	0.41
60:2A:4216:HOH:O	5:2F:74:ARG:HD2	2.20	0.41
2:2B:17:C:H2'	2:2B:18:G:O4'	2.20	0.41
12:2Q:16:ARG:HG3	12:2Q:17:LEU:H	1.85	0.41
16:2U:92:ARG:HA	16:2U:95:LEU:HB2	2.02	0.41
32:2a:130:A:N3	32:2a:263:A:O2'	2.45	0.41
32:2a:337:C:H2'	32:2a:338:A:C8	2.54	0.41
32:2a:401:C:H1'	32:2a:622:A:H1'	2.02	0.41
32:2a:536:C:H2'	32:2a:537:G:H8	1.83	0.41
32:2a:1159:U:O4'	32:2a:1182:G:N2	2.54	0.41
34:2c:131:ARG:NH2	36:2e:50:GLU:HG3	2.35	0.41
39:2h:12:ARG:HD3	39:2h:26:VAL:HG12	2.02	0.41
43:2l:53:ARG:NH2	43:2l:92:0TD:OD1	2.32	0.41
44:2m:106:ASN:OD1	44:2m:106:ASN:N	2.53	0.41
1:1A:118:A:H3'	1:1A:119:A:C5'	2.50	0.41
1:1A:375:C:H2'	1:1A:376:C:C6	2.56	0.41
1:1A:964:C:O2'	1:1A:2273:A:N3	2.41	0.41
1:1A:994:C:O2'	1:1A:996:A:OP1	2.30	0.41
1:1A:1412:A:H2'	1:1A:1413:G:C8	2.56	0.41
1:1A:2492:U:O2'	1:1A:2493:U:H5'	2.20	0.41
1:1A:2547:U:O2	10:1O:23:ARG:NH2	2.50	0.41
3:1D:147:LEU:N	60:1D:420:HOH:O	2.46	0.41
4:1E:28:ALA:HB3	4:1E:93:VAL:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:101:LEU:HD23	5:1F:106:ARG:HG2	2.03	0.41
8:1I:5:LEU:HD21	8:1I:12:LEU:HD23	2.02	0.41
10:1O:88:ASN:C	10:1O:90:GLN:H	2.28	0.41
13:1R:8:ARG:NE	13:1R:43:GLU:OE2	2.51	0.41
15:1T:37:GLY:HA2	15:1T:38:ASN:HA	1.60	0.41
26:14:58:ARG:NH1	50:1s:68:GLY:HA3	2.36	0.41
29:17:24:THR:HG23	29:17:27:GLY:H	1.86	0.41
32:1a:142:G:H2'	32:1a:143:A:C8	2.52	0.41
32:1a:526:C:OP2	43:1l:91:LYS:HE3	2.20	0.41
32:1a:562:C:H1'	43:1l:15:ARG:HD2	2.02	0.41
32:1a:922:G:H1'	36:1e:19:MET:HB3	2.02	0.41
32:1a:924:C:H2'	32:1a:925:G:C8	2.56	0.41
32:1a:1466:C:H2'	32:1a:1467:G:O4'	2.21	0.41
33:1b:70:PHE:O	33:1b:92:TYR:HA	2.20	0.41
33:1b:121:LEU:HD12	33:1b:126:GLU:HB3	2.01	0.41
35:1d:121:VAL:HA	35:1d:126:ILE:HG13	2.02	0.41
38:1g:8:GLU:OE1	38:1g:8:GLU:N	2.53	0.41
40:1i:45:ALA:O	40:1i:78:LYS:HG3	2.20	0.41
43:1l:92:0TD:O	43:1l:94:PRO:HD3	2.20	0.41
51:1t:56:MET:HE3	51:1t:85:MET:HG2	2.03	0.41
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.37	0.41
1:2A:824:A:H2'	1:2A:825:C:O4'	2.21	0.41
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.56	0.41
1:2A:2108:C:O2	1:2A:2182:G:N2	2.53	0.41
1:2A:2184:G:H2'	1:2A:2185:C:O4'	2.20	0.41
1:2A:2640:G:H5"	9:2N:74:ARG:NH2	2.35	0.41
1:2A:2749:A:OP1	7:2H:3:ARG:NH1	2.53	0.41
2:2B:90:A:C5	2:2B:91:C:H1'	2.55	0.41
4:2E:13:ARG:HA	4:2E:21:VAL:O	2.20	0.41
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	2.03	0.41
14:2S:34:HIS:HB2	14:2S:36:TYR:HE1	1.86	0.41
20:2Y:40:GLU:O	20:2Y:42:VAL:HG23	2.19	0.41
21:2Z:7:ALA:O	21:2Z:62:PRO:HD3	2.21	0.41
23:21:11:ARG:HD2	60:21:212:HOH:O	2.19	0.41
32:2a:5:U:O2	32:2a:6:G:N1	2.54	0.41
32:2a:8:A:N6	35:2d:209:ARG:HB2	2.36	0.41
32:2a:385:C:H2'	32:2a:386:C:C6	2.55	0.41
32:2a:458:C:H2'	32:2a:460:G:O4'	2.21	0.41
32:2a:707:C:OP1	42:2k:85:ARG:NH1	2.53	0.41
32:2a:1125:U:O2'	32:2a:1126:U:H2'	2.19	0.41
32:2a:1515:C:H2'	32:2a:1516:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2f:97:PHE:O	49:2r:31:LEU:HD12	2.21	0.41
41:2j:38:ILE:O	41:2j:38:ILE:HG13	2.19	0.41
44:2m:49:THR:O	44:2m:53:VAL:N	2.51	0.41
48:2q:56:VAL:O	48:2q:77:VAL:HB	2.20	0.41
53:2y:59:GLY:HA3	53:2y:88:LEU:HD13	2.03	0.41
1:1A:340:A:H2'	1:1A:341:G:O4'	2.21	0.41
1:1A:636:G:OP1	11:1P:132:LYS:HE2	2.21	0.41
1:1A:818:G:H4'	1:1A:838:C:O3'	2.21	0.41
1:1A:1041:C:H5'	1:1A:1042:G:OP2	2.20	0.41
1:1A:1759:A:H5'	60:1A:5466:HOH:O	2.21	0.41
1:1A:2319:G:H22	14:1S:3:ARG:HA	1.86	0.41
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.45	0.41
1:1A:2771:C:H2'	1:1A:2772:C:C6	2.56	0.41
1:1A:2802:G:N2	1:1A:2803:C:C2	2.89	0.41
60:1A:4538:HOH:O	9:1N:73:THR:HG21	2.21	0.41
2:1B:9:G:C6	2:1B:10:C:C4	3.09	0.41
2:1B:24:G:N7	2:1B:56:G:H2'	2.36	0.41
5:1F:144:LYS:HB2	5:1F:144:LYS:HE3	1.86	0.41
7:1H:72:ILE:O	7:1H:76:VAL:HG23	2.21	0.41
7:1H:124:GLU:OE2	7:1H:132:ARG:HD2	2.20	0.41
7:1H:152:ARG:HD3	7:1H:152:ARG:HA	1.71	0.41
8:1I:6:LEU:HD23	8:1I:6:LEU:HA	1.81	0.41
9:1N:107:LEU:HD23	9:1N:107:LEU:HA	1.95	0.41
10:1O:63:VAL:HG11	10:1O:85:VAL:HG23	2.01	0.41
13:1R:38:VAL:HG22	13:1R:112:ALA:HB2	2.03	0.41
13:1R:70:LEU:C	13:1R:72:ASP:H	2.28	0.41
26:14:53:GLU:O	26:14:56:VAL:HG12	2.21	0.41
32:1a:28:G:H2'	32:1a:29:G:O4'	2.21	0.41
32:1a:559:A:P	36:1e:126:ARG:HH22	2.44	0.41
32:1a:606:G:N2	32:1a:631:G:N7	2.69	0.41
32:1a:645:C:H2'	32:1a:646:U:C6	2.56	0.41
32:1a:782:A:O3'	32:1a:1515:C:H4'	2.20	0.41
32:1a:1187:G:H5'	40:1i:113:LYS:HE3	2.03	0.41
32:1a:1362:C:H2'	32:1a:1363:C:H5"	2.03	0.41
32:1a:1434:A:H2'	32:1a:1435:G:O4'	2.21	0.41
33:1b:28:PHE:CD1	33:1b:190:THR:HA	2.56	0.41
33:1b:211:ILE:O	33:1b:215:LEU:HB2	2.21	0.41
33:1b:212:GLN:NE2	33:1b:216:SER:HB3	2.36	0.41
35:1d:14:ARG:HA	35:1d:14:ARG:HD3	1.96	0.41
35:1d:101:LEU:HD23	35:1d:121:VAL:HG13	2.03	0.41
36:1e:152:ARG:HA	39:1h:64:LYS:NZ	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:41:VAL:C	40:1i:43:ALA:H	2.29	0.41
42:1k:73:MET:HG2	42:1k:103:LEU:HD21	2.02	0.41
45:1n:32:SER:O	45:1n:40:CYS:HA	2.21	0.41
47:1p:13:HIS:C	47:1p:15:PRO:HD3	2.45	0.41
53:1y:66:LYS:HB3	53:1y:66:LYS:HE2	1.82	0.41
1:2A:27:G:N2	1:2A:512:G:H1'	2.36	0.41
1:2A:96:G:H4'	24:22:48:HIS:NE2	2.35	0.41
1:2A:864:G:C6	1:2A:865:C:N4	2.89	0.41
1:2A:942:G:O2'	1:2A:1189:A:N3	2.52	0.41
1:2A:1057:A:H4'	1:2A:1058:G:OP1	2.21	0.41
1:2A:1073:A:H8	1:2A:1073:A:H5'	1.86	0.41
1:2A:1075:C:H4'	12:2Q:59:ARG:NH1	2.36	0.41
1:2A:1408:C:H2'	1:2A:1409:C:H6	1.86	0.41
1:2A:1707:G:C5	1:2A:1756:G:C6	3.09	0.41
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.20	0.41
1:2A:2059:A:O2'	5:2F:69:HIS:HD2	2.04	0.41
1:2A:2536:G:O6	60:2A:3946:HOH:O	2.20	0.41
1:2A:2722:G:H5'	13:2R:4:LEU:HD12	2.02	0.41
1:2A:2821:A:C2	1:2A:2822:G:C4	3.09	0.41
3:2D:69:ARG:HD2	60:2D:436:HOH:O	2.21	0.41
5:2F:170:LEU:HG	5:2F:172:TRP:NE1	2.36	0.41
6:2G:75:LYS:HE2	6:2G:77:ILE:HG13	2.02	0.41
7:2H:137:ASP:O	7:2H:141:VAL:HG23	2.20	0.41
9:2N:138:LEU:HD23	9:2N:138:LEU:HA	1.85	0.41
12:2Q:118:LEU:HB2	12:2Q:131:ILE:HD13	2.02	0.41
14:2S:83:LYS:HB3	14:2S:111:GLU:HG3	2.02	0.41
20:2Y:56:PRO:C	20:2Y:58:GLY:H	2.29	0.41
21:2Z:61:LEU:HD12	21:2Z:61:LEU:HA	1.85	0.41
26:24:61:ARG:O	26:24:61:ARG:NH1	2.53	0.41
32:2a:104:G:C2	32:2a:105:G:C8	3.09	0.41
32:2a:256:U:H2'	32:2a:257:G:H8	1.84	0.41
32:2a:325:A:H2'	32:2a:326:G:O4'	2.21	0.41
32:2a:335:C:H2'	32:2a:336:C:C6	2.56	0.41
32:2a:405:U:O4	35:2d:2:GLY:N	2.54	0.41
32:2a:600:C:H2'	32:2a:601:C:C6	2.56	0.41
32:2a:1123:A:H4'	41:2j:37:PRO:HD2	2.03	0.41
32:2a:1259:C:N4	32:2a:1260:C:O2	2.54	0.41
32:2a:1371:G:OP1	40:2i:12:GLU:HB2	2.21	0.41
32:2a:1414:U:H2'	32:2a:1415:G:H8	1.85	0.41
33:2b:48:MET:HE3	33:2b:48:MET:HB2	1.96	0.41
34:2c:36:ASP:OD1	34:2c:57:ILE:HG21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:4:TYR:N	40:2i:19:LEU:O	2.53	0.41
40:2i:5:TYR:HA	40:2i:17:VAL:O	2.21	0.41
40:2i:23:ASN:CG	40:2i:25:LYS:HD3	2.46	0.41
42:2k:18:ARG:O	42:2k:32:ILE:HA	2.21	0.41
44:2m:67:GLU:HB3	44:2m:68:GLY:H	1.69	0.41
45:2n:32:SER:O	45:2n:40:CYS:HA	2.20	0.41
46:2o:16:ALA:HB1	46:2o:21:ASP:CB	2.41	0.41
51:2t:33:ILE:CD1	51:2t:62:LEU:HB3	2.50	0.41
1:1A:244:A:H2'	1:1A:245:G:O4'	2.21	0.41
1:1A:518:G:H4'	18:1W:18:ARG:NH1	2.36	0.41
1:1A:868:U:O2'	12:1Q:8:LYS:HE3	2.20	0.41
1:1A:2193:G:H2'	1:1A:2194:G:C8	2.55	0.41
1:1A:2680:C:H5'	4:1E:189:PRO:HA	2.03	0.41
9:1N:72:TYR:N	9:1N:85:ILE:O	2.49	0.41
15:1T:108:ARG:HA	15:1T:111:ARG:NH1	2.36	0.41
26:14:15:ILE:HD12	26:14:21:VAL:HG22	2.02	0.41
32:1a:126:G:OP1	32:1a:605:U:O2'	2.26	0.41
32:1a:328:C:OP1	60:1a:3337:HOH:O	2.22	0.41
32:1a:374:A:C6	32:1a:375:U:C4	3.09	0.41
32:1a:560:U:H4'	32:1a:561:U:O5'	2.21	0.41
32:1a:747:C:H3'	32:1a:748:C:C6	2.55	0.41
32:1a:945:G:C6	32:1a:1337:G:C5	3.09	0.41
35:1d:61:LYS:HA	35:1d:203:VAL:HG22	2.03	0.41
40:1i:18:PHE:HD2	40:1i:62:TYR:HD2	1.69	0.41
40:1i:77:ILE:O	40:1i:81:ILE:HG23	2.21	0.41
1:2A:660:G:C6	1:2A:661:C:C4	3.09	0.41
1:2A:1057:A:N6	1:2A:1086:A:C2	2.89	0.41
1:2A:1815:A:OP1	60:2A:3965:HOH:O	2.22	0.41
1:2A:2238:G:N3	1:2A:2238:G:H2'	2.36	0.41
1:2A:2821:A:H2'	1:2A:2822:G:C8	2.56	0.41
2:2B:40:U:H1'	2:2B:45:A:H61	1.86	0.41
6:2G:33:ARG:O	6:2G:161:THR:HG23	2.21	0.41
11:2P:63:PRO:HB2	30:28:30:ARG:HH21	1.86	0.41
18:2W:10:VAL:HG12	18:2W:12:ILE:HG22	2.03	0.41
18:2W:34:ASN:HA	18:2W:37:ARG:NH1	2.36	0.41
23:21:54:ALA:HB1	23:21:83:GLU:HG3	2.03	0.41
32:2a:46:G:O2'	32:2a:365:U:H1'	2.21	0.41
32:2a:542:G:OP1	35:2d:10:ARG:NH1	2.46	0.41
32:2a:1010:G:H2'	32:2a:1011:G:C8	2.56	0.41
32:2a:1226:C:H41	44:2m:104:ARG:HD2	1.83	0.41
36:2e:118:ILE:HD12	36:2e:118:ILE:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2f:96:PRO:HB3	49:2r:30:ASP:CG	2.46	0.41
39:2h:38:ILE:HD12	39:2h:111:ILE:HG23	2.03	0.41
41:2j:46:ARG:HG2	41:2j:64:GLU:HB3	2.02	0.41
43:2l:33:ARG:HG2	43:2l:60:LEU:HG	2.01	0.41
45:2n:9:LYS:HA	45:2n:12:ARG:HB3	2.03	0.41
46:2o:80:ALA:O	46:2o:83:GLU:HG2	2.21	0.41
51:2t:47:GLY:HA3	51:2t:92:LEU:HD21	2.03	0.41
1:1A:679:C:H2'	1:1A:680:G:C8	2.56	0.40
1:1A:1155:A:O2'	1:1A:1156:A:H2'	2.21	0.40
1:1A:1368:G:C2	1:1A:1369:G:C8	3.09	0.40
1:1A:1754:C:H2'	1:1A:1755:A:O4'	2.21	0.40
1:1A:2619:C:H4'	4:1E:151:TYR:O	2.22	0.40
4:1E:1:MET:O	4:1E:84:PHE:HB2	2.21	0.40
5:1F:150:GLY:HA2	5:1F:172:TRP:CE3	2.55	0.40
5:1F:178:PRO:HB2	5:1F:201:VAL:CG2	2.52	0.40
8:1I:77:LEU:HD12	8:1I:77:LEU:HA	1.88	0.40
10:1O:70:LYS:O	60:1O:303:HOH:O	2.22	0.40
12:1Q:108:GLY:HA3	21:1Z:116:VAL:HG13	2.03	0.40
17:1V:21:ARG:HD3	17:1V:91:TYR:CD1	2.56	0.40
21:1Z:28:MET:O	21:1Z:34:ASN:HA	2.21	0.40
23:11:95:LEU:HA	23:11:95:LEU:HD12	1.84	0.40
32:1a:1218:C:OP2	45:1n:9:LYS:NZ	2.50	0.40
32:1a:1457:G:OP1	51:1t:39:LYS:NZ	2.53	0.40
32:1a:1511:G:H2'	32:1a:1512:U:O4'	2.21	0.40
40:1i:29:ASN:ND2	40:1i:65:VAL:O	2.52	0.40
43:1l:54:LYS:HD2	43:1l:54:LYS:N	2.36	0.40
1:2A:312:G:H4'	1:2A:331:A:C2	2.56	0.40
1:2A:686:G:N2	1:2A:788:A:H61	2.20	0.40
1:2A:749:C:H4'	1:2A:1271:G:N3	2.35	0.40
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.55	0.40
1:2A:1318:C:N4	60:2A:4346:HOH:O	2.53	0.40
1:2A:1592:C:H2'	1:2A:1593:G:H8	1.85	0.40
1:2A:2010:G:H5"	18:2W:42:ARG:HB2	2.02	0.40
1:2A:2298:A:H2'	1:2A:2299:G:O4'	2.20	0.40
1:2A:2557:G:H2'	1:2A:2558:C:H6	1.86	0.40
2:2B:50:G:H5"	2:2B:51:G:OP2	2.20	0.40
56:2B:221:MPD:H4	56:2B:221:MPD:H12	1.76	0.40
4:2E:101:ARG:HD2	4:2E:169:ASN:ND2	2.36	0.40
7:2H:3:ARG:NH2	7:2H:65:HIS:HB3	2.36	0.40
13:2R:85:PRO:C	13:2R:87:TYR:H	2.27	0.40
16:2U:11:ARG:O	16:2U:15:LYS:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2U:59:ARG:O	16:2U:63:VAL:HG23	2.22	0.40
17:2V:14:VAL:HA	17:2V:18:LEU:HD13	2.03	0.40
26:24:57:GLU:HA	26:24:58:ARG:HA	1.68	0.40
32:2a:781:A:H5'	32:2a:782:A:OP2	2.21	0.40
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.21	0.40
32:2a:1324:A:C4'	32:2a:1362:C:H4'	2.51	0.40
32:2a:1443:G:H22	32:2a:1460:A:H1'	1.85	0.40
35:2d:76:ARG:HD3	35:2d:207:TYR:CZ	2.56	0.40
36:2e:36:ASP:OD1	36:2e:38:GLN:N	2.54	0.40
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.55	0.40
44:2m:111:LYS:HB2	44:2m:111:LYS:HE3	1.84	0.40
1:1A:7:G:H4'	9:1N:13:TRP:CH2	2.56	0.40
1:1A:385:C:O2	11:1P:71:VAL:HG21	2.22	0.40
1:1A:764:A:H5'	3:1D:210:GLY:HA2	2.03	0.40
1:1A:1141:U:OP2	9:1N:63:THR:OG1	2.32	0.40
1:1A:1357:U:H2'	1:1A:1358:G:O4'	2.21	0.40
1:1A:2023:G:H4'	1:1A:2617:C:O3'	2.21	0.40
1:1A:2291:U:OP1	1:1A:2380:C:O2'	2.36	0.40
1:1A:2601:C:O2'	1:1A:2602:A:O4'	2.30	0.40
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.55	0.40
2:1B:74:U:H2'	2:1B:75:G:O4'	2.21	0.40
23:11:52:ARG:HE	23:11:52:ARG:HB3	1.61	0.40
24:12:53:LEU:O	24:12:56:GLN:HB2	2.21	0.40
26:14:40:HIS:HB3	26:14:43:TYR:CD2	2.43	0.40
32:1a:1073:U:O2'	33:1b:104:ASN:OD1	2.39	0.40
32:1a:1269:A:H2	32:1a:1312:G:N3	2.19	0.40
43:1l:109:GLY:HA3	43:1l:121:GLY:O	2.21	0.40
45:1n:15:LYS:HD2	45:1n:16:PHE:CE2	2.56	0.40
53:1y:55:ASN:HA	53:1y:60:VAL:HA	2.03	0.40
1:2A:271(W):G:O6	1:2A:271(X):G:N1	2.54	0.40
1:2A:911:A:H2'	12:2Q:9:TYR:OH	2.21	0.40
1:2A:1055:G:H1	1:2A:1104:C:H42	1.69	0.40
1:2A:1166:C:H2'	1:2A:1167:U:C6	2.56	0.40
1:2A:1517:G:C6	1:2A:1518:U:C4	3.09	0.40
1:2A:1556:C:H2'	1:2A:1557:C:H6	1.87	0.40
1:2A:1971:A:OP2	3:2D:242:ARG:NH1	2.47	0.40
1:2A:2251:OMG:HM23	1:2A:2251:OMG:H1'	1.74	0.40
2:2B:21:G:C2	2:2B:63:G:C2	3.09	0.40
5:2F:107:LYS:HE3	5:2F:107:LYS:HB2	1.79	0.40
7:2H:171:LEU:H	7:2H:171:LEU:HG	1.78	0.40
12:2Q:41:TRP:HB3	12:2Q:94:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:2V:76:LYS:HD2	17:2V:81:TYR:CD2	2.56	0.40
32:2a:586:C:O2'	32:2a:878:G:H4'	2.21	0.40
32:2a:600:C:H2'	32:2a:601:C:H6	1.86	0.40
32:2a:938:A:N6	32:2a:939:G:C6	2.89	0.40
32:2a:1151:A:C5'	41:2j:41:PRO:HA	2.51	0.40
32:2a:1278:U:C5'	32:2a:1279:A:H5'	2.37	0.40
39:2h:112:LEU:HD11	39:2h:124:ALA:HB2	2.03	0.40
40:2i:30:GLY:O	40:2i:31:GLN:HG3	2.21	0.40
40:2i:110:GLU:OE2	40:2i:113:LYS:NZ	2.54	0.40
43:2l:84:LEU:HB2	43:2l:105:TYR:CE2	2.56	0.40
48:2q:81:ARG:HB3	48:2q:84:LEU:HD12	2.02	0.40
51:2t:43:LEU:O	51:2t:47:GLY:HA2	2.20	0.40
51:2t:57:ARG:NH1	51:2t:101:GLY:O	2.50	0.40
1:1A:65:C:H2'	1:1A:66:C:C6	2.57	0.40
1:1A:118:A:H3'	1:1A:119:A:H5"	2.03	0.40
1:1A:226:G:H21	1:1A:228:A:H62	1.68	0.40
1:1A:903:C:H2'	1:1A:904:C:C6	2.57	0.40
1:1A:1054:A:H5'	1:1A:1055:G:OP2	2.21	0.40
1:1A:1380:G:C2	1:1A:1381:G:C8	3.09	0.40
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.20	0.40
1:1A:1857:G:C6	1:1A:1858:G:C6	3.10	0.40
1:1A:2773:C:H2'	1:1A:2774:C:H6	1.86	0.40
7:1H:3:ARG:HH21	7:1H:65:HIS:HB3	1.86	0.40
9:1N:42:TRP:CH2	9:1N:44:PRO:HB3	2.56	0.40
11:1P:107:LYS:HB2	11:1P:110:TYR:HD2	1.86	0.40
11:1P:147:LEU:HD23	11:1P:147:LEU:HA	1.77	0.40
17:1V:40:LEU:CB	17:1V:46:VAL:HG13	2.47	0.40
21:1Z:98:MET:O	21:1Z:125:LEU:HD12	2.22	0.40
32:1a:12:U:H4'	32:1a:526:C:O2'	2.21	0.40
32:1a:258:G:H2'	32:1a:259:G:H8	1.86	0.40
32:1a:398:C:H2'	32:1a:399:G:C8	2.56	0.40
32:1a:1494:G:H2'	32:1a:1495:U:C6	2.56	0.40
33:1b:15:VAL:HG22	33:1b:209:ARG:O	2.21	0.40
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.89	0.40
33:1b:51:LEU:HD23	33:1b:201:ILE:HD12	2.02	0.40
33:1b:178:ARG:HG3	39:1h:71:GLY:O	2.21	0.40
37:1f:9:VAL:HB	37:1f:87:ARG:HB2	2.03	0.40
1:2A:1062:G:N3	1:2A:1063:G:C8	2.90	0.40
1:2A:2883:A:OP1	27:25:52:TYR:OH	2.32	0.40
8:2I:43:ASN:HD22	8:2I:43:ASN:HA	1.61	0.40
13:2R:70:LEU:C	13:2R:72:ASP:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2W:18:ARG:HG2	18:2W:76:VAL:HB	2.03	0.40
23:21:53:VAL:HG22	23:21:74:VAL:HG13	2.03	0.40
32:2a:139:G:H2'	32:2a:139:G:N3	2.36	0.40
32:2a:476:G:C2	32:2a:477:A:C5	3.10	0.40
32:2a:953:G:H1	32:2a:1228:C:H42	1.69	0.40
33:2b:61:LEU:O	33:2b:61:LEU:HD12	2.20	0.40
38:2g:26:PHE:CE1	38:2g:105:VAL:HG22	2.56	0.40
38:2g:76:ARG:HB3	38:2g:156:TRP:HH2	1.86	0.40
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.19	0.40
1:1A:945:A:C4	1:1A:2448:A:C2	3.09	0.40
1:1A:1680:U:O2'	1:1A:1763:G:N7	2.54	0.40
1:1A:1792:G:H5'	3:1D:205:VAL:HG13	2.03	0.40
1:1A:2432:A:OP1	60:1A:4254:HOH:O	2.22	0.40
1:1A:2469:A:H5'	1:1A:2470:G:OP2	2.20	0.40
1:1A:2691:C:OP2	60:1A:4258:HOH:O	2.22	0.40
2:1B:12:C:O2'	2:1B:13:A:OP2	2.34	0.40
3:1D:146:GLU:HG2	3:1D:152:GLY:C	2.47	0.40
4:1E:168:MET:HE2	4:1E:168:MET:HB3	1.87	0.40
5:1F:7:TYR:CD2	5:1F:24:LEU:HB2	2.56	0.40
7:1H:41:MET:HB3	7:1H:41:MET:HE3	1.79	0.40
12:1Q:137:TYR:HD1	21:1Z:74:VAL:HG11	1.87	0.40
20:1Y:99:CYS:CB	20:1Y:106:LEU:HD21	2.50	0.40
21:1Z:75:ASN:HA	60:1Z:407:HOH:O	2.21	0.40
28:16:47:THR:HB	28:16:49:HIS:HE1	1.87	0.40
32:1a:187:C:H2'	32:1a:188:C:C6	2.57	0.40
32:1a:321:A:C2	32:1a:333:G:C2	3.09	0.40
32:1a:433:C:H2'	32:1a:434:U:C6	2.56	0.40
32:1a:936:C:H1'	32:1a:1382:C:H42	1.87	0.40
32:1a:1132:C:H2'	32:1a:1133:G:C8	2.56	0.40
32:1a:1183:A:H3'	32:1a:1184:G:C5'	2.51	0.40
32:1a:1206:G:C6	32:1a:1207:2MG:C5	3.09	0.40
32:1a:1513:A:H2'	32:1a:1514:C:C6	2.56	0.40
35:1d:36:ARG:HD2	35:1d:38:TYR:OH	2.20	0.40
41:1j:33:GLN:O	41:1j:75:ILE:N	2.54	0.40
42:1k:38:ASN:HA	42:1k:39:PRO:HD3	1.89	0.40
44:1m:51:ALA:O	44:1m:54:VAL:HG22	2.22	0.40
46:1o:56:LEU:O	46:1o:60:VAL:HG23	2.20	0.40
1:2A:484:C:H2'	1:2A:485:C:H6	1.87	0.40
1:2A:856:C:O4'	22:20:27:GLU:HB3	2.21	0.40
1:2A:1511:C:H2'	1:2A:1512:U:O4'	2.22	0.40
2:2B:33:G:O2'	2:2B:34:U:H5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:23:VAL:HA	4:2E:184:VAL:O	2.21	0.40
7:2H:59:ARG:HA	7:2H:59:ARG:HD2	1.77	0.40
9:2N:73:THR:HA	9:2N:83:LYS:O	2.20	0.40
12:2Q:31:ASP:OD2	12:2Q:107:ALA:HA	2.22	0.40
21:2Z:150:LEU:HD12	21:2Z:150:LEU:HA	1.89	0.40
22:20:50:ASN:HB3	22:20:63:VAL:HG22	2.03	0.40
22:20:52:GLY:O	22:20:59:LEU:HA	2.21	0.40
26:24:44:THR:C	26:24:46:GLN:H	2.29	0.40
32:2a:19:C:H2'	32:2a:20:U:H6	1.87	0.40
32:2a:229:U:H2'	32:2a:230:G:C8	2.56	0.40
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.36	0.40
32:2a:793:U:O2	32:2a:1516:G:H4'	2.21	0.40
32:2a:921:U:H2'	32:2a:922:G:O4'	2.22	0.40
32:2a:1002:G:C4	32:2a:1003:G:C8	3.04	0.40
33:2b:178:ARG:HH12	39:2h:68:ARG:NH2	2.19	0.40
36:2e:79:GLU:HA	36:2e:91:LEU:O	2.21	0.40
40:2i:108:VAL:HG12	40:2i:109:VAL:H	1.87	0.40
42:2k:99:GLN:C	42:2k:101:SER:H	2.30	0.40
44:2m:108:ARG:NE	44:2m:114:ARG:HG3	2.37	0.40
1:1A:1121:C:H2'	1:1A:1122:G:O4'	2.21	0.40
1:1A:1439:A:H2'	1:1A:1440:G:O4'	2.21	0.40
1:1A:1810:A:H2'	1:1A:1811:G:O4'	2.21	0.40
1:1A:2294:C:H2'	1:1A:2295:C:C6	2.56	0.40
2:1B:41:U:H5	6:1G:70:VAL:N	2.19	0.40
14:1S:64:GLU:O	14:1S:68:GLN:NE2	2.55	0.40
17:1V:28:GLU:HG3	17:1V:29:PRO:HD2	2.04	0.40
20:1Y:29:GLU:HG2	60:1Y:307:HOH:O	2.21	0.40
31:19:27:CYS:HB3	31:19:32:HIS:HB2	2.03	0.40
32:1a:321:A:H2'	32:1a:322:C:C6	2.57	0.40
32:1a:629:G:H2'	32:1a:630:G:O4'	2.22	0.40
32:1a:1131:G:H2'	32:1a:1132:C:H6	1.86	0.40
32:1a:1286:A:H2	52:1u:18:TYR:HH	1.65	0.40
33:1b:174:VAL:HG11	33:1b:196:LEU:HG	2.03	0.40
34:1c:148:GLY:HA3	34:1c:172:ARG:O	2.22	0.40
35:1d:119:GLN:O	35:1d:123:HIS:ND1	2.54	0.40
39:1h:14:ARG:O	39:1h:18:ARG:HG2	2.22	0.40
41:1j:8:LEU:HB3	41:1j:16:LEU:HD11	2.02	0.40
50:1s:37:ARG:H	50:1s:37:ARG:HG3	1.48	0.40
51:1t:18:GLN:O	51:1t:22:ARG:HG3	2.22	0.40
1:2A:257:A:H2'	1:2A:258:G:O4'	2.21	0.40
1:2A:1038:C:H42	1:2A:1117:G:H1	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1233:C:N4	60:2A:4239:HOH:O	2.54	0.40
1:2A:1381:G:O2'	60:2A:3967:HOH:O	2.22	0.40
1:2A:1633:G:OP2	60:2A:3966:HOH:O	2.22	0.40
1:2A:1709:U:H2'	1:2A:1710:C:H6	1.87	0.40
1:2A:2331:G:O2'	1:2A:2336:A:N1	2.47	0.40
1:2A:2721:A:H1'	1:2A:2873:A:O2'	2.21	0.40
3:2D:222:ARG:NH2	60:2D:416:HOH:O	2.54	0.40
4:2E:144:ARG:HB3	4:2E:145:LYS:H	1.54	0.40
10:2O:122:LEU:HD13	15:2T:72:VAL:HG11	2.04	0.40
21:2Z:48:PHE:O	21:2Z:52:SER:N	2.54	0.40
26:24:62:ARG:O	26:24:63:TYR:C	2.65	0.40
30:28:63:PRO:HG2	30:28:64:TYR:CE2	2.57	0.40
32:2a:35:G:C5	32:2a:36:C:C4	3.09	0.40
32:2a:251:G:H4'	32:2a:252:U:O5'	2.22	0.40
32:2a:277:C:P	48:2q:68:ARG:HH12	2.44	0.40
32:2a:922:G:H2'	32:2a:923:A:C8	2.57	0.40
32:2a:1120:G:C6	32:2a:1121:U:C4	3.10	0.40
38:2g:69:VAL:HG11	38:2g:104:LEU:HD22	2.03	0.40
40:2i:111:ARG:HD2	45:2n:61:TRP:CD1	2.57	0.40
48:2q:31:LEU:HD23	48:2q:32:TYR:CZ	2.57	0.40
50:2s:66:MET:H	50:2s:66:MET:HG2	1.50	0.40
51:2t:57:ARG:HH22	51:2t:100:ILE:CD1	2.32	0.40
53:2y:41:LEU:HD12	53:2y:50:ALA:HB1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	256 (94%)	17 (6%)	0	100	100
3	2D	273/276 (99%)	256 (94%)	17 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	1E	202/206 (98%)	186 (92%)	15 (7%)	1 (0%)	24 54
4	2E	202/206 (98%)	187 (93%)	14 (7%)	1 (0%)	24 54
5	1F	201/210 (96%)	191 (95%)	8 (4%)	2 (1%)	12 39
5	2F	201/210 (96%)	190 (94%)	9 (4%)	2 (1%)	12 39
6	1G	179/182 (98%)	159 (89%)	16 (9%)	4 (2%)	5 20
6	2G	179/182 (98%)	158 (88%)	18 (10%)	3 (2%)	7 26
7	1H	172/180 (96%)	159 (92%)	11 (6%)	2 (1%)	10 34
7	2H	171/180 (95%)	151 (88%)	18 (10%)	2 (1%)	10 34
8	1I	145/148 (98%)	128 (88%)	15 (10%)	2 (1%)	9 30
8	2I	144/148 (97%)	124 (86%)	17 (12%)	3 (2%)	5 21
9	1N	138/140 (99%)	129 (94%)	9 (6%)	0	100 100
9	2N	138/140 (99%)	126 (91%)	11 (8%)	1 (1%)	18 48
10	1O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16 44
10	2O	120/122 (98%)	111 (92%)	9 (8%)	0	100 100
11	1P	147/150 (98%)	139 (95%)	8 (5%)	0	100 100
11	2P	147/150 (98%)	138 (94%)	7 (5%)	2 (1%)	9 30
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100 100
12	2Q	139/141 (99%)	129 (93%)	10 (7%)	0	100 100
13	1R	116/118 (98%)	108 (93%)	7 (6%)	1 (1%)	14 41
13	2R	116/118 (98%)	107 (92%)	9 (8%)	0	100 100
14	1S	108/112 (96%)	99 (92%)	6 (6%)	3 (3%)	4 15
14	2S	108/112 (96%)	98 (91%)	7 (6%)	3 (3%)	4 15
15	1T	129/146 (88%)	120 (93%)	7 (5%)	2 (2%)	7 27
15	2T	129/146 (88%)	119 (92%)	9 (7%)	1 (1%)	16 44
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100 100
16	2U	114/118 (97%)	110 (96%)	4 (4%)	0	100 100
17	1V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12 39
17	2V	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	6 22
18	1W	110/113 (97%)	110 (100%)	0	0	100 100
18	2W	110/113 (97%)	107 (97%)	2 (2%)	1 (1%)	14 41
19	1X	93/96 (97%)	93 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	2X	93/96 (97%)	84 (90%)	8 (9%)	1 (1%)	11 36
20	1Y	105/110 (96%)	94 (90%)	11 (10%)	0	100 100
20	2Y	105/110 (96%)	96 (91%)	9 (9%)	0	100 100
21	1Z	201/206 (98%)	187 (93%)	14 (7%)	0	100 100
21	2Z	199/206 (97%)	173 (87%)	25 (13%)	1 (0%)	24 54
22	10	75/85 (88%)	69 (92%)	6 (8%)	0	100 100
22	20	75/85 (88%)	67 (89%)	8 (11%)	0	100 100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11 36
23	21	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11 36
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100 100
24	22	68/72 (94%)	64 (94%)	4 (6%)	0	100 100
25	13	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
25	23	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
26	14	67/71 (94%)	48 (72%)	13 (19%)	6 (9%)	0 1
26	24	67/71 (94%)	49 (73%)	13 (19%)	5 (8%)	1 2
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100 100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100 100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100 100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100 100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100 100
30	28	62/65 (95%)	57 (92%)	5 (8%)	0	100 100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
33	1b	229/256 (90%)	189 (82%)	30 (13%)	10 (4%)	2 8
33	2b	229/256 (90%)	200 (87%)	20 (9%)	9 (4%)	2 10
34	1c	204/239 (85%)	175 (86%)	27 (13%)	2 (1%)	12 39
34	2c	204/239 (85%)	179 (88%)	22 (11%)	3 (2%)	8 28
35	1d	206/209 (99%)	180 (87%)	22 (11%)	4 (2%)	6 23
35	2d	206/209 (99%)	186 (90%)	17 (8%)	3 (2%)	8 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
36	1e	146/162 (90%)	133 (91%)	12 (8%)	1 (1%)	18 48
36	2e	146/162 (90%)	131 (90%)	13 (9%)	2 (1%)	9 30
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100 100
37	2f	98/101 (97%)	89 (91%)	9 (9%)	0	100 100
38	1g	153/156 (98%)	145 (95%)	7 (5%)	1 (1%)	18 48
38	2g	153/156 (98%)	135 (88%)	17 (11%)	1 (1%)	18 48
39	1h	135/138 (98%)	124 (92%)	11 (8%)	0	100 100
39	2h	135/138 (98%)	123 (91%)	12 (9%)	0	100 100
40	1i	125/128 (98%)	102 (82%)	22 (18%)	1 (1%)	16 44
40	2i	124/128 (97%)	102 (82%)	18 (14%)	4 (3%)	3 13
41	1j	95/105 (90%)	78 (82%)	9 (10%)	8 (8%)	0 1
41	2j	94/105 (90%)	81 (86%)	12 (13%)	1 (1%)	11 36
42	1k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	14 41
42	2k	112/129 (87%)	102 (91%)	10 (9%)	0	100 100
43	1l	119/132 (90%)	107 (90%)	12 (10%)	0	100 100
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100 100
44	1m	114/126 (90%)	100 (88%)	11 (10%)	3 (3%)	4 17
44	2m	112/126 (89%)	100 (89%)	11 (10%)	1 (1%)	14 41
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100 100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100 100
46	1o	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	10 34
46	2o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	10 34
47	1p	80/88 (91%)	61 (76%)	18 (22%)	1 (1%)	9 32
47	2p	80/88 (91%)	73 (91%)	6 (8%)	1 (1%)	9 32
48	1q	97/105 (92%)	87 (90%)	10 (10%)	0	100 100
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100 100
49	1r	66/88 (75%)	58 (88%)	5 (8%)	3 (4%)	2 8
49	2r	66/88 (75%)	62 (94%)	4 (6%)	0	100 100
50	1s	81/93 (87%)	70 (86%)	10 (12%)	1 (1%)	10 34
50	2s	81/93 (87%)	68 (84%)	12 (15%)	1 (1%)	10 34
51	1t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	5 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
51	2t	96/106 (91%)	87 (91%)	7 (7%)	2 (2%)	5 21
52	1u	21/27 (78%)	20 (95%)	0	1 (5%)	2 7
52	2u	21/27 (78%)	16 (76%)	3 (14%)	2 (10%)	0 1
53	1y	95/113 (84%)	92 (97%)	3 (3%)	0	100 100
53	2y	94/113 (83%)	84 (89%)	9 (10%)	1 (1%)	11 36
All	All	11629/12354 (94%)	10577 (91%)	925 (8%)	127 (1%)	11 36

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	47	LYS
7	1H	126	PRO
8	1I	11	ASN
26	14	49	PHE
33	1b	8	LYS
33	1b	9	GLU
35	1d	5	ILE
35	1d	164	ALA
41	1j	82	ILE
51	1t	95	ALA
4	2E	51	PHE
5	2F	130	ALA
8	2I	10	GLU
8	2I	85	GLU
26	24	45	GLY
26	24	62	ARG
33	2b	9	GLU
33	2b	17	PHE
33	2b	20	GLU
40	2i	44	VAL
40	2i	54	ASP
40	2i	55	ALA
44	2m	67	GLU
53	2y	45	PRO
6	1G	124	SER
7	1H	159	GLU
15	1T	127	ALA
15	1T	128	GLU
17	1V	79	VAL

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Mol	Chain	Res	Type
26	14	47	GLN
26	14	61	ARG
33	1b	17	PHE
40	1i	54	ASP
41	1j	55	LYS
41	1j	79	ARG
42	1k	105	VAL
44	1m	3	ARG
44	1m	67	GLU
46	1o	23	GLY
49	1r	36	ASN
6	2G	81	LYS
6	2G	96	ARG
8	2I	39	ALA
11	2P	29	LYS
15	2T	127	ALA
17	2V	79	VAL
19	2X	94	GLY
33	2b	16	HIS
35	2d	5	ILE
35	2d	171	GLY
41	2j	79	ARG
52	2u	7	ARG
4	1E	52	LEU
5	1F	160	ASN
8	1I	117	GLU
14	1S	94	TYR
26	14	44	THR
33	1b	21	ARG
33	1b	127	ILE
34	1c	26	LYS
35	1d	3	ARG
36	1e	77	PRO
49	1r	25	THR
50	1s	24	ALA
52	1u	7	ARG
7	2H	119	GLU
7	2H	126	PRO
14	2S	93	LYS
17	2V	100	ARG
23	21	3	LYS
26	24	39	CYS

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Mol	Chain	Res	Type
26	24	49	PHE
33	2b	8	LYS
33	2b	124	SER
35	2d	20	TYR
38	2g	7	ALA
6	1G	43	LEU
14	1S	59	LYS
23	11	3	LYS
33	1b	20	GLU
33	1b	95	GLN
33	1b	124	SER
33	1b	125	PRO
38	1g	35	LYS
41	1j	31	GLY
41	1j	77	PRO
41	1j	78	ASN
49	1r	54	ARG
51	1t	100	ILE
14	2S	31	SER
26	24	55	ARG
33	2b	125	PRO
34	2c	160	ALA
6	1G	44	GLY
13	1R	71	GLN
14	1S	57	LYS
26	14	65	ASP
33	1b	22	LYS
41	1j	75	ILE
44	1m	11	ARG
47	1p	48	TRP
5	2F	21	ALA
6	2G	43	LEU
18	2W	71	VAL
33	2b	232	PRO
34	2c	47	LEU
34	2c	204	LEU
36	2e	150	ARG
47	2p	61	SER
50	2s	69	HIS
10	1O	5	GLN
26	14	55	ARG
9	2N	119	ARG

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Mol	Chain	Res	Type
33	2b	10	LEU
36	2e	11	ILE
40	2i	121	ARG
46	2o	88	ARG
51	2t	100	ILE
52	2u	23	PRO
34	1c	174	PRO
14	2S	35	ILE
35	1d	142	PRO
41	1j	39	PRO
51	2t	102	GLY
21	2Z	68	PRO
11	2P	93	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1D	214/218 (98%)	198 (92%)	16 (8%)	12 37
3	2D	215/218 (99%)	196 (91%)	19 (9%)	9 29
4	1E	164/166 (99%)	141 (86%)	23 (14%)	3 11
4	2E	164/166 (99%)	142 (87%)	22 (13%)	4 12
5	1F	160/166 (96%)	139 (87%)	21 (13%)	4 13
5	2F	159/166 (96%)	133 (84%)	26 (16%)	2 8
6	1G	144/156 (92%)	123 (85%)	21 (15%)	3 10
6	2G	142/156 (91%)	117 (82%)	25 (18%)	2 6
7	1H	144/148 (97%)	133 (92%)	11 (8%)	12 36
7	2H	143/148 (97%)	120 (84%)	23 (16%)	2 8
8	1I	111/124 (90%)	88 (79%)	23 (21%)	1 4
8	2I	108/124 (87%)	92 (85%)	16 (15%)	3 10
9	1N	119/119 (100%)	107 (90%)	12 (10%)	7 24
9	2N	118/119 (99%)	101 (86%)	17 (14%)	3 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	1O	100/100 (100%)	91 (91%)	9 (9%)	9 28
10	2O	100/100 (100%)	91 (91%)	9 (9%)	9 28
11	1P	115/116 (99%)	104 (90%)	11 (10%)	8 26
11	2P	115/116 (99%)	101 (88%)	14 (12%)	5 16
12	1Q	111/111 (100%)	100 (90%)	11 (10%)	7 24
12	2Q	111/111 (100%)	100 (90%)	11 (10%)	7 24
13	1R	101/101 (100%)	86 (85%)	15 (15%)	3 10
13	2R	101/101 (100%)	89 (88%)	12 (12%)	5 16
14	1S	87/88 (99%)	76 (87%)	11 (13%)	4 14
14	2S	85/88 (97%)	71 (84%)	14 (16%)	2 8
15	1T	115/127 (91%)	106 (92%)	9 (8%)	11 35
15	2T	113/127 (89%)	101 (89%)	12 (11%)	6 22
16	1U	93/94 (99%)	85 (91%)	8 (9%)	10 30
16	2U	93/94 (99%)	83 (89%)	10 (11%)	6 21
17	1V	81/82 (99%)	70 (86%)	11 (14%)	3 12
17	2V	80/82 (98%)	67 (84%)	13 (16%)	2 8
18	1W	90/92 (98%)	78 (87%)	12 (13%)	4 12
18	2W	90/92 (98%)	79 (88%)	11 (12%)	5 16
19	1X	77/78 (99%)	68 (88%)	9 (12%)	5 17
19	2X	77/78 (99%)	71 (92%)	6 (8%)	11 35
20	1Y	86/91 (94%)	77 (90%)	9 (10%)	6 22
20	2Y	86/91 (94%)	71 (83%)	15 (17%)	2 7
21	1Z	169/179 (94%)	145 (86%)	24 (14%)	3 11
21	2Z	165/179 (92%)	144 (87%)	21 (13%)	4 14
22	10	61/67 (91%)	55 (90%)	6 (10%)	7 25
22	20	61/67 (91%)	56 (92%)	5 (8%)	10 32
23	11	79/83 (95%)	72 (91%)	7 (9%)	9 28
23	21	81/83 (98%)	69 (85%)	12 (15%)	3 10
24	12	65/67 (97%)	60 (92%)	5 (8%)	12 35
24	22	66/67 (98%)	53 (80%)	13 (20%)	1 5
25	13	51/52 (98%)	47 (92%)	4 (8%)	11 35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
25	23	50/52 (96%)	44 (88%)	6 (12%)	5 16
26	14	58/63 (92%)	51 (88%)	7 (12%)	5 16
26	24	54/63 (86%)	47 (87%)	7 (13%)	4 13
27	15	51/52 (98%)	44 (86%)	7 (14%)	3 12
27	25	50/52 (96%)	45 (90%)	5 (10%)	7 24
28	16	51/52 (98%)	46 (90%)	5 (10%)	7 25
28	26	50/52 (96%)	46 (92%)	4 (8%)	11 34
29	17	41/42 (98%)	38 (93%)	3 (7%)	13 38
29	27	41/42 (98%)	36 (88%)	5 (12%)	5 16
30	18	54/55 (98%)	50 (93%)	4 (7%)	13 38
30	28	54/55 (98%)	47 (87%)	7 (13%)	4 13
31	19	34/34 (100%)	32 (94%)	2 (6%)	18 48
31	29	34/34 (100%)	31 (91%)	3 (9%)	9 29
33	1b	191/220 (87%)	159 (83%)	32 (17%)	2 7
33	2b	187/220 (85%)	165 (88%)	22 (12%)	5 17
34	1c	144/188 (77%)	131 (91%)	13 (9%)	9 28
34	2c	140/188 (74%)	126 (90%)	14 (10%)	7 24
35	1d	171/181 (94%)	151 (88%)	20 (12%)	5 17
35	2d	172/181 (95%)	147 (86%)	25 (14%)	3 10
36	1e	114/123 (93%)	100 (88%)	14 (12%)	4 15
36	2e	114/123 (93%)	104 (91%)	10 (9%)	9 29
37	1f	85/90 (94%)	76 (89%)	9 (11%)	6 22
37	2f	85/90 (94%)	75 (88%)	10 (12%)	5 17
38	1g	120/127 (94%)	109 (91%)	11 (9%)	8 27
38	2g	119/127 (94%)	108 (91%)	11 (9%)	8 27
39	1h	116/119 (98%)	99 (85%)	17 (15%)	3 10
39	2h	114/119 (96%)	101 (89%)	13 (11%)	5 18
40	1i	91/99 (92%)	75 (82%)	16 (18%)	2 6
40	2i	88/99 (89%)	71 (81%)	17 (19%)	1 5
41	1j	68/92 (74%)	62 (91%)	6 (9%)	9 29
41	2j	68/92 (74%)	55 (81%)	13 (19%)	1 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
42	1k	83/99 (84%)	71 (86%)	12 (14%)	3 10
42	2k	83/99 (84%)	72 (87%)	11 (13%)	4 12
43	1l	96/108 (89%)	86 (90%)	10 (10%)	7 23
43	2l	96/108 (89%)	81 (84%)	15 (16%)	2 9
44	1m	90/101 (89%)	77 (86%)	13 (14%)	3 11
44	2m	87/101 (86%)	69 (79%)	18 (21%)	1 4
45	1n	49/50 (98%)	41 (84%)	8 (16%)	2 8
45	2n	49/50 (98%)	43 (88%)	6 (12%)	5 16
46	1o	78/80 (98%)	73 (94%)	5 (6%)	16 44
46	2o	78/80 (98%)	70 (90%)	8 (10%)	7 23
47	1p	69/74 (93%)	58 (84%)	11 (16%)	2 8
47	2p	68/74 (92%)	59 (87%)	9 (13%)	4 13
48	1q	94/97 (97%)	87 (93%)	7 (7%)	13 38
48	2q	94/97 (97%)	84 (89%)	10 (11%)	6 22
49	1r	59/77 (77%)	54 (92%)	5 (8%)	10 31
49	2r	59/77 (77%)	50 (85%)	9 (15%)	3 9
50	1s	68/80 (85%)	61 (90%)	7 (10%)	7 23
50	2s	67/80 (84%)	58 (87%)	9 (13%)	4 12
51	1t	71/82 (87%)	63 (89%)	8 (11%)	5 19
51	2t	70/82 (85%)	61 (87%)	9 (13%)	4 13
52	1u	18/22 (82%)	15 (83%)	3 (17%)	2 7
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19 50
53	1y	82/98 (84%)	77 (94%)	5 (6%)	17 46
53	2y	79/98 (81%)	66 (84%)	13 (16%)	2 8
All	All	9524/10260 (93%)	8360 (88%)	1164 (12%)	5 16

All (1164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	13	ARG
3	1D	20	ASP
3	1D	27	THR
3	1D	61	LEU
3	1D	69	ARG

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Mol	Chain	Res	Type
3	1D	94	LEU
3	1D	111	LEU
3	1D	127	VAL
3	1D	138	VAL
3	1D	141	VAL
3	1D	173	VAL
3	1D	193	VAL
3	1D	204	ILE
3	1D	211	ARG
3	1D	221	VAL
3	1D	229	VAL
4	1E	1	MET
4	1E	7	VAL
4	1E	9	VAL
4	1E	12	THR
4	1E	33	VAL
4	1E	34	VAL
4	1E	42	ASP
4	1E	47	VAL
4	1E	49	LEU
4	1E	59	VAL
4	1E	73	GLU
4	1E	75	VAL
4	1E	77	ILE
4	1E	78	LEU
4	1E	94	GLU
4	1E	116	VAL
4	1E	119	ARG
4	1E	144	ARG
4	1E	154	LYS
4	1E	170	LEU
4	1E	178	GLU
4	1E	181	LEU
4	1E	184	VAL
5	1F	12	LEU
5	1F	18	ARG
5	1F	24	LEU
5	1F	27	GLU
5	1F	38	ARG
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG

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Mol	Chain	Res	Type
5	1F	88	VAL
5	1F	108	LYS
5	1F	110	LEU
5	1F	125	LEU
5	1F	132	VAL
5	1F	162	LEU
5	1F	170	LEU
5	1F	175	THR
5	1F	176	LEU
5	1F	183	VAL
5	1F	192	LEU
5	1F	197	ASP
5	1F	203	GLN
6	1G	5	VAL
6	1G	7	LEU
6	1G	31	VAL
6	1G	43	LEU
6	1G	52	ILE
6	1G	70	VAL
6	1G	79	ASN
6	1G	81	LYS
6	1G	111	LEU
6	1G	126	ASP
6	1G	132	ASN
6	1G	135	LEU
6	1G	139	LEU
6	1G	140	ILE
6	1G	148	MET
6	1G	159	VAL
6	1G	165	THR
6	1G	167	GLU
6	1G	170	ARG
6	1G	175	LEU
6	1G	181	ARG
7	1H	15	VAL
7	1H	24	VAL
7	1H	45	VAL
7	1H	49	VAL
7	1H	71	LEU
7	1H	85	LYS
7	1H	98	LEU
7	1H	105	LEU

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Mol	Chain	Res	Type
7	1H	129	THR
7	1H	141	VAL
7	1H	153	LYS
8	1I	5	LEU
8	1I	9	LEU
8	1I	15	VAL
8	1I	19	VAL
8	1I	35	LEU
8	1I	38	LEU
8	1I	40	THR
8	1I	41	GLU
8	1I	42	SER
8	1I	44	LEU
8	1I	47	LEU
8	1I	50	ARG
8	1I	76	THR
8	1I	78	THR
8	1I	85	GLU
8	1I	87	LYS
8	1I	92	VAL
8	1I	101	LEU
8	1I	109	ILE
8	1I	117	GLU
8	1I	127	VAL
8	1I	140	LEU
8	1I	144	VAL
9	1N	33	LEU
9	1N	34	LEU
9	1N	39	ARG
9	1N	46	VAL
9	1N	48	MET
9	1N	59	LYS
9	1N	62	VAL
9	1N	67	LEU
9	1N	87	LEU
9	1N	97	ARG
9	1N	99	LEU
9	1N	133	GLN
10	1O	10	VAL
10	1O	20	MET
10	1O	21	CYS
10	1O	24	VAL

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Mol	Chain	Res	Type
10	1O	58	VAL
10	1O	82	ASN
10	1O	98	VAL
10	1O	108	GLU
10	1O	121	VAL
11	1P	3	LEU
11	1P	56	SER
11	1P	59	LEU
11	1P	65	ARG
11	1P	70	GLN
11	1P	83	VAL
11	1P	95	VAL
11	1P	96	THR
11	1P	112	LEU
11	1P	125	VAL
11	1P	126	VAL
12	1Q	1	MET
12	1Q	6	ARG
12	1Q	7	MET
12	1Q	8	LYS
12	1Q	55	VAL
12	1Q	75	THR
12	1Q	81	VAL
12	1Q	89	ASN
12	1Q	101	ARG
12	1Q	109	VAL
12	1Q	110	THR
13	1R	29	LEU
13	1R	36	THR
13	1R	37	THR
13	1R	40	LYS
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	75	LEU
13	1R	96	ARG
13	1R	100	LEU
13	1R	104	ARG
13	1R	111	LEU
13	1R	114	VAL
13	1R	117	VAL

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Mol	Chain	Res	Type
14	1S	10	ARG
14	1S	14	VAL
14	1S	26	LEU
14	1S	36	TYR
14	1S	43	GLU
14	1S	46	VAL
14	1S	59	LYS
14	1S	68	GLN
14	1S	85	VAL
14	1S	107	GLU
14	1S	110	LEU
15	1T	13	ARG
15	1T	28	VAL
15	1T	33	LYS
15	1T	34	VAL
15	1T	49	VAL
15	1T	59	THR
15	1T	78	LEU
15	1T	89	VAL
15	1T	124	ASP
16	1U	8	VAL
16	1U	20	LEU
16	1U	31	SER
16	1U	34	LYS
16	1U	59	ARG
16	1U	74	LEU
16	1U	95	LEU
16	1U	104	GLN
17	1V	35	LEU
17	1V	38	LEU
17	1V	46	VAL
17	1V	52	VAL
17	1V	57	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	73	SER
17	1V	79	VAL
17	1V	92	THR
18	1W	1	MET
18	1W	6	ILE
18	1W	11	ARG

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Mol	Chain	Res	Type
18	1W	17	VAL
18	1W	19	LEU
18	1W	20	VAL
18	1W	35	ILE
18	1W	67	ASP
18	1W	85	VAL
18	1W	95	ILE
18	1W	96	ILE
18	1W	107	LEU
19	1X	15	GLU
19	1X	23	GLU
19	1X	35	THR
19	1X	38	GLU
19	1X	52	VAL
19	1X	59	VAL
19	1X	60	ARG
19	1X	66	LEU
19	1X	92	LEU
20	1Y	7	VAL
20	1Y	11	ASP
20	1Y	31	LEU
20	1Y	43	ASN
20	1Y	47	LYS
20	1Y	72	VAL
20	1Y	85	VAL
20	1Y	90	LEU
20	1Y	99	CYS
21	1Z	18	LEU
21	1Z	31	ARG
21	1Z	33	LEU
21	1Z	37	VAL
21	1Z	41	LEU
21	1Z	52	SER
21	1Z	61	LEU
21	1Z	73	GLN
21	1Z	76	LEU
21	1Z	91	LEU
21	1Z	94	GLU
21	1Z	119	GLU
21	1Z	122	ARG
21	1Z	126	VAL
21	1Z	150	LEU

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Mol	Chain	Res	Type
21	1Z	154	ASP
21	1Z	161	VAL
21	1Z	163	LEU
21	1Z	171	ILE
21	1Z	180	VAL
21	1Z	182	LYS
21	1Z	191	VAL
21	1Z	197	ILE
21	1Z	203	GLU
22	10	14	ARG
22	10	32	ARG
22	10	39	ARG
22	10	59	LEU
22	10	66	VAL
22	10	68	GLU
23	11	11	ARG
23	11	21	ARG
23	11	46	LEU
23	11	50	ARG
23	11	51	VAL
23	11	81	LYS
23	11	95	LEU
24	12	4	SER
24	12	32	LEU
24	12	53	LEU
24	12	64	LEU
24	12	70	GLN
25	13	6	VAL
25	13	8	LEU
25	13	54	VAL
25	13	56	VAL
26	14	1	MET
26	14	5	ILE
26	14	28	LYS
26	14	50	VAL
26	14	52	THR
26	14	61	ARG
26	14	69	LYS
27	15	6	VAL
27	15	16	ARG
27	15	26	THR
27	15	29	THR

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Mol	Chain	Res	Type
27	15	48	GLU
27	15	57	VAL
27	15	58	LEU
28	16	14	THR
28	16	24	GLU
28	16	27	LYS
28	16	48	VAL
28	16	52	VAL
29	17	1	MET
29	17	41	ARG
29	17	43	THR
30	18	11	LYS
30	18	14	VAL
30	18	29	LYS
30	18	32	LEU
31	19	4	ARG
31	19	17	ILE
33	1b	7	VAL
33	1b	8	LYS
33	1b	12	GLU
33	1b	15	VAL
33	1b	35	GLU
33	1b	43	ASP
33	1b	67	THR
33	1b	68	ILE
33	1b	71	VAL
33	1b	80	ILE
33	1b	82	ARG
33	1b	93	VAL
33	1b	96	ARG
33	1b	108	ILE
33	1b	117	GLU
33	1b	124	SER
33	1b	144	ARG
33	1b	158	LEU
33	1b	164	VAL
33	1b	169	LYS
33	1b	178	ARG
33	1b	185	ILE
33	1b	187	LEU
33	1b	195	ASP
33	1b	208	ILE

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Mol	Chain	Res	Type
33	1b	209	ARG
33	1b	212	GLN
33	1b	215	LEU
33	1b	221	LEU
33	1b	226	ARG
33	1b	229	VAL
33	1b	231	GLU
34	1c	26	LYS
34	1c	38	ARG
34	1c	52	LEU
34	1c	58	GLU
34	1c	64	VAL
34	1c	77	ILE
34	1c	89	GLU
34	1c	98	ASN
34	1c	103	VAL
34	1c	104	GLN
34	1c	190	ARG
34	1c	192	THR
34	1c	207	VAL
35	1d	5	ILE
35	1d	58	LEU
35	1d	80	GLU
35	1d	104	VAL
35	1d	108	LEU
35	1d	126	ILE
35	1d	127	THR
35	1d	135	LEU
35	1d	137	SER
35	1d	150	GLU
35	1d	155	LEU
35	1d	158	ILE
35	1d	159	ARG
35	1d	162	LEU
35	1d	182	LYS
35	1d	188	LEU
35	1d	190	ASP
35	1d	194	LEU
35	1d	196	LEU
35	1d	208	SER
36	1e	12	LEU
36	1e	19	MET

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Mol	Chain	Res	Type
36	1e	31	LEU
36	1e	41	VAL
36	1e	67	VAL
36	1e	76	ILE
36	1e	79	GLU
36	1e	80	ILE
36	1e	82	VAL
36	1e	91	LEU
36	1e	107	ARG
36	1e	120	THR
36	1e	126	ARG
36	1e	147	ASP
37	1f	17	SER
37	1f	25	ILE
37	1f	40	VAL
37	1f	65	VAL
37	1f	69	GLU
37	1f	72	VAL
37	1f	73	ASN
37	1f	81	ILE
37	1f	98	LEU
38	1g	12	LEU
38	1g	15	ASP
38	1g	27	ILE
38	1g	32	ARG
38	1g	41	ARG
38	1g	52	GLU
38	1g	110	GLN
38	1g	113	GLU
38	1g	135	VAL
38	1g	138	LYS
38	1g	144	MET
39	1h	3	THR
39	1h	19	VAL
39	1h	24	THR
39	1h	25	ASP
39	1h	26	VAL
39	1h	39	LEU
39	1h	52	ASP
39	1h	53	VAL
39	1h	54	ASP
39	1h	56	LYS

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Mol	Chain	Res	Type
39	1h	63	LEU
39	1h	69	ARG
39	1h	95	VAL
39	1h	115	SER
39	1h	120	THR
39	1h	133	LEU
39	1h	137	VAL
40	1i	2	GLU
40	1i	27	THR
40	1i	47	LEU
40	1i	48	GLU
40	1i	53	VAL
40	1i	60	ASP
40	1i	65	VAL
40	1i	66	ARG
40	1i	81	ILE
40	1i	83	ARG
40	1i	103	THR
40	1i	107	ARG
40	1i	108	VAL
40	1i	109	VAL
40	1i	111	ARG
40	1i	125	TYR
41	1j	49	VAL
41	1j	65	LEU
41	1j	84	GLN
41	1j	92	THR
41	1j	96	ILE
41	1j	100	THR
42	1k	31	THR
42	1k	33	THR
42	1k	40	ILE
42	1k	70	LYS
42	1k	80	VAL
42	1k	81	ASP
42	1k	87	THR
42	1k	92	GLU
42	1k	95	ILE
42	1k	108	ILE
42	1k	109	VAL
42	1k	112	THR
43	1l	6	THR

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Mol	Chain	Res	Type
43	1l	18	VAL
43	1l	27	LEU
43	1l	36	VAL
43	1l	39	VAL
43	1l	60	LEU
43	1l	67	THR
43	1l	85	ILE
43	1l	113	ARG
43	1l	118	SER
44	1m	12	ASN
44	1m	15	VAL
44	1m	16	ASP
44	1m	17	VAL
44	1m	19	LEU
44	1m	54	VAL
44	1m	55	ARG
44	1m	56	LEU
44	1m	70	LEU
44	1m	103	THR
44	1m	105	THR
44	1m	116	THR
44	1m	117	VAL
45	1n	3	ARG
45	1n	8	GLU
45	1n	13	THR
45	1n	17	LYS
45	1n	18	VAL
45	1n	22	THR
45	1n	33	VAL
45	1n	35	ARG
46	1o	5	LYS
46	1o	22	THR
46	1o	39	LEU
46	1o	66	LEU
46	1o	87	ILE
47	1p	1	MET
47	1p	2	VAL
47	1p	8	ARG
47	1p	19	ILE
47	1p	20	VAL
47	1p	27	LYS
47	1p	29	ASP

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Mol	Chain	Res	Type
47	1p	42	ARG
47	1p	60	LEU
47	1p	62	VAL
47	1p	67	THR
48	1q	16	GLN
48	1q	31	LEU
48	1q	39	SER
48	1q	50	LYS
48	1q	60	ILE
48	1q	85	VAL
48	1q	88	TYR
49	1r	37	VAL
49	1r	65	ILE
49	1r	76	LEU
49	1r	84	LYS
49	1r	86	VAL
50	1s	28	LYS
50	1s	31	ILE
50	1s	37	ARG
50	1s	41	VAL
50	1s	48	THR
50	1s	79	THR
50	1s	83	HIS
51	1t	8	ARG
51	1t	10	LEU
51	1t	11	SER
51	1t	37	SER
51	1t	62	LEU
51	1t	64	ASP
51	1t	84	LEU
51	1t	100	ILE
52	1u	6	ARG
52	1u	15	ARG
52	1u	17	THR
53	1y	3	MET
53	1y	41	LEU
53	1y	44	GLU
53	1y	60	VAL
53	1y	76	GLU
3	2D	3	VAL
3	2D	4	LYS
3	2D	71	ASP

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Mol	Chain	Res	Type
3	2D	94	LEU
3	2D	103	ARG
3	2D	111	LEU
3	2D	113	VAL
3	2D	117	VAL
3	2D	136	ILE
3	2D	138	VAL
3	2D	141	VAL
3	2D	155	LEU
3	2D	183	ARG
3	2D	193	VAL
3	2D	211	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
4	2E	9	VAL
4	2E	12	THR
4	2E	21	VAL
4	2E	24	THR
4	2E	33	VAL
4	2E	34	VAL
4	2E	38	THR
4	2E	40	GLU
4	2E	52	LEU
4	2E	75	VAL
4	2E	77	ILE
4	2E	87	GLU
4	2E	93	VAL
4	2E	116	VAL
4	2E	118	LYS
4	2E	144	ARG
4	2E	167	VAL
4	2E	170	LEU
4	2E	175	VAL
4	2E	181	LEU
4	2E	184	VAL
4	2E	188	VAL
5	2F	17	ARG
5	2F	20	LEU
5	2F	24	LEU
5	2F	27	GLU

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Mol	Chain	Res	Type
5	2F	33	LEU
5	2F	38	ARG
5	2F	53	THR
5	2F	57	VAL
5	2F	70	THR
5	2F	74	ARG
5	2F	78	ILE
5	2F	88	VAL
5	2F	105	VAL
5	2F	132	VAL
5	2F	140	LEU
5	2F	144	LYS
5	2F	153	SER
5	2F	170	LEU
5	2F	175	THR
5	2F	183	VAL
5	2F	192	LEU
5	2F	194	MET
5	2F	195	ASP
5	2F	197	ASP
5	2F	200	GLU
5	2F	201	VAL
6	2G	3	LEU
6	2G	5	VAL
6	2G	28	VAL
6	2G	31	VAL
6	2G	40	ASN
6	2G	49	ASP
6	2G	63	ILE
6	2G	70	VAL
6	2G	77	ILE
6	2G	88	ILE
6	2G	92	VAL
6	2G	98	ARG
6	2G	106	LEU
6	2G	115	ARG
6	2G	126	ASP
6	2G	133	LEU
6	2G	138	GLN
6	2G	139	LEU
6	2G	145	THR
6	2G	149	VAL

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Mol	Chain	Res	Type
6	2G	152	LEU
6	2G	159	VAL
6	2G	165	THR
6	2G	172	LEU
6	2G	181	ARG
7	2H	6	ARG
7	2H	7	LEU
7	2H	16	SER
7	2H	23	ARG
7	2H	27	LYS
7	2H	33	LEU
7	2H	37	VAL
7	2H	40	GLU
7	2H	47	GLU
7	2H	65	HIS
7	2H	68	THR
7	2H	71	LEU
7	2H	81	GLU
7	2H	88	LEU
7	2H	105	LEU
7	2H	114	VAL
7	2H	121	ILE
7	2H	122	THR
7	2H	134	SER
7	2H	136	ILE
7	2H	139	GLN
7	2H	171	LEU
7	2H	175	LYS
8	2I	5	LEU
8	2I	37	VAL
8	2I	38	LEU
8	2I	44	LEU
8	2I	47	LEU
8	2I	54	GLN
8	2I	57	ARG
8	2I	58	LEU
8	2I	68	LEU
8	2I	75	LEU
8	2I	76	THR
8	2I	77	LEU
8	2I	86	THR
8	2I	92	VAL

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Mol	Chain	Res	Type
8	2I	101	LEU
8	2I	116	LEU
9	2N	8	GLN
9	2N	22	THR
9	2N	28	THR
9	2N	33	LEU
9	2N	34	LEU
9	2N	48	MET
9	2N	55	VAL
9	2N	58	ASP
9	2N	60	ILE
9	2N	62	VAL
9	2N	65	LYS
9	2N	68	GLU
9	2N	73	THR
9	2N	87	LEU
9	2N	99	LEU
9	2N	119	ARG
9	2N	140	VAL
10	2O	10	VAL
10	2O	18	LYS
10	2O	19	ILE
10	2O	23	ARG
10	2O	24	VAL
10	2O	28	SER
10	2O	42	SER
10	2O	86	ILE
10	2O	98	VAL
11	2P	16	ARG
11	2P	42	SER
11	2P	56	SER
11	2P	59	LEU
11	2P	65	ARG
11	2P	71	VAL
11	2P	75	ILE
11	2P	83	VAL
11	2P	95	VAL
11	2P	96	THR
11	2P	101	VAL
11	2P	133	SER
11	2P	147	LEU
11	2P	148	LEU

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Mol	Chain	Res	Type
12	2Q	3	MET
12	2Q	6	ARG
12	2Q	8	LYS
12	2Q	16	ARG
12	2Q	21	THR
12	2Q	55	VAL
12	2Q	106	VAL
12	2Q	109	VAL
12	2Q	110	THR
12	2Q	133	ARG
12	2Q	138	ASP
13	2R	18	LEU
13	2R	24	GLN
13	2R	44	LEU
13	2R	54	LEU
13	2R	65	LEU
13	2R	67	LEU
13	2R	74	LYS
13	2R	79	LEU
13	2R	100	LEU
13	2R	102	GLU
13	2R	111	LEU
13	2R	118	GLU
14	2S	3	ARG
14	2S	19	LYS
14	2S	30	ARG
14	2S	36	TYR
14	2S	40	ILE
14	2S	48	LEU
14	2S	50	SER
14	2S	52	SER
14	2S	53	SER
14	2S	56	LEU
14	2S	64	GLU
14	2S	75	GLU
14	2S	93	LYS
14	2S	107	GLU
15	2T	16	ARG
15	2T	23	ARG
15	2T	27	THR
15	2T	28	VAL
15	2T	42	ILE

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Mol	Chain	Res	Type
15	2T	49	VAL
15	2T	65	LYS
15	2T	80	SER
15	2T	89	VAL
15	2T	95	ARG
15	2T	96	ARG
15	2T	107	ASP
16	2U	6	THR
16	2U	8	VAL
16	2U	17	ILE
16	2U	20	LEU
16	2U	31	SER
16	2U	36	ARG
16	2U	50	ARG
16	2U	74	LEU
16	2U	83	LEU
16	2U	95	LEU
17	2V	5	VAL
17	2V	21	ARG
17	2V	25	LEU
17	2V	32	THR
17	2V	46	VAL
17	2V	47	VAL
17	2V	51	VAL
17	2V	57	VAL
17	2V	72	VAL
17	2V	79	VAL
17	2V	82	ARG
17	2V	95	LEU
17	2V	100	ARG
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	19	LEU
18	2W	21	VAL
18	2W	23	LEU
18	2W	71	VAL
18	2W	100	THR
18	2W	101	SER
18	2W	103	ILE
18	2W	107	LEU
19	2X	8	ILE

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Mol	Chain	Res	Type
19	2X	38	GLU
19	2X	57	LEU
19	2X	59	VAL
19	2X	81	VAL
19	2X	83	VAL
20	2Y	3	VAL
20	2Y	9	LYS
20	2Y	13	VAL
20	2Y	14	LEU
20	2Y	19	LYS
20	2Y	38	ILE
20	2Y	44	ILE
20	2Y	55	TYR
20	2Y	57	GLN
20	2Y	64	GLU
20	2Y	72	VAL
20	2Y	85	VAL
20	2Y	88	LYS
20	2Y	92	ASN
20	2Y	99	CYS
21	2Z	18	LEU
21	2Z	31	ARG
21	2Z	42	VAL
21	2Z	61	LEU
21	2Z	76	LEU
21	2Z	80	ARG
21	2Z	86	VAL
21	2Z	91	LEU
21	2Z	94	GLU
21	2Z	96	VAL
21	2Z	107	THR
21	2Z	119	GLU
21	2Z	121	HIS
21	2Z	136	PHE
21	2Z	141	VAL
21	2Z	146	ILE
21	2Z	150	LEU
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	175	VAL
21	2Z	197	ILE
22	20	9	SER

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Mol	Chain	Res	Type
22	20	21	LEU
22	20	30	VAL
22	20	39	ARG
22	20	66	VAL
23	21	4	VAL
23	21	11	ARG
23	21	21	ARG
23	21	27	GLU
23	21	30	VAL
23	21	51	VAL
23	21	75	GLU
23	21	80	LEU
23	21	82	LEU
23	21	85	LEU
23	21	95	LEU
23	21	97	LEU
24	22	3	LEU
24	22	16	LEU
24	22	25	VAL
24	22	30	ARG
24	22	32	LEU
24	22	40	SER
24	22	41	ILE
24	22	51	ARG
24	22	53	LEU
24	22	59	ARG
24	22	60	LEU
24	22	63	VAL
24	22	70	GLN
25	23	23	LEU
25	23	31	LEU
25	23	52	HIS
25	23	53	LEU
25	23	54	VAL
25	23	59	VAL
26	24	1	MET
26	24	21	VAL
26	24	34	GLU
26	24	49	PHE
26	24	50	VAL
26	24	53	GLU
26	24	61	ARG

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Mol	Chain	Res	Type
27	25	6	VAL
27	25	29	THR
27	25	30	LEU
27	25	55	ARG
27	25	56	LYS
28	26	19	ARG
28	26	29	ASN
28	26	34	LEU
28	26	48	VAL
29	27	1	MET
29	27	4	THR
29	27	29	LYS
29	27	43	THR
29	27	46	VAL
30	28	14	VAL
30	28	15	LYS
30	28	32	LEU
30	28	46	ARG
30	28	58	ILE
30	28	59	LYS
30	28	62	LEU
31	29	7	VAL
31	29	12	ASP
31	29	17	ILE
33	2b	7	VAL
33	2b	10	LEU
33	2b	17	PHE
33	2b	45	GLN
33	2b	52	GLU
33	2b	61	LEU
33	2b	68	ILE
33	2b	80	ILE
33	2b	81	VAL
33	2b	90	MET
33	2b	93	VAL
33	2b	94	ASN
33	2b	96	ARG
33	2b	97	TRP
33	2b	157	ARG
33	2b	164	VAL
33	2b	168	THR
33	2b	175	ARG

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Mol	Chain	Res	Type
33	2b	189	ASP
33	2b	222	ILE
33	2b	224	GLN
33	2b	230	VAL
34	2c	15	THR
34	2c	16	ARG
34	2c	28	GLN
34	2c	32	LEU
34	2c	35	GLU
34	2c	52	LEU
34	2c	68	VAL
34	2c	77	ILE
34	2c	115	LEU
34	2c	131	ARG
34	2c	152	ILE
34	2c	161	GLU
34	2c	166	GLU
34	2c	179	ARG
35	2d	3	ARG
35	2d	5	ILE
35	2d	8	VAL
35	2d	13	ARG
35	2d	34	GLU
35	2d	35	ARG
35	2d	38	TYR
35	2d	49	ARG
35	2d	53	ASP
35	2d	58	LEU
35	2d	76	ARG
35	2d	99	SER
35	2d	105	VAL
35	2d	106	TYR
35	2d	135	LEU
35	2d	140	VAL
35	2d	141	ARG
35	2d	155	LEU
35	2d	157	LEU
35	2d	158	ILE
35	2d	175	SER
35	2d	184	LYS
35	2d	188	LEU
35	2d	190	ASP

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Mol	Chain	Res	Type
35	2d	194	LEU
36	2e	31	LEU
36	2e	41	VAL
36	2e	69	VAL
36	2e	72	GLN
36	2e	75	THR
36	2e	81	GLU
36	2e	90	VAL
36	2e	91	LEU
36	2e	120	THR
36	2e	148	VAL
37	2f	17	SER
37	2f	28	ARG
37	2f	46	ARG
37	2f	61	LEU
37	2f	63	TYR
37	2f	70	ASP
37	2f	75	LEU
37	2f	86	ARG
37	2f	94	GLN
37	2f	95	GLU
38	2g	9	VAL
38	2g	28	ASN
38	2g	41	ARG
38	2g	64	GLN
38	2g	75	VAL
38	2g	104	LEU
38	2g	105	VAL
38	2g	110	GLN
38	2g	111	ARG
38	2g	113	GLU
38	2g	115	ARG
39	2h	13	ILE
39	2h	25	ASP
39	2h	39	LEU
39	2h	52	ASP
39	2h	63	LEU
39	2h	77	GLU
39	2h	81	HIS
39	2h	97	VAL
39	2h	99	GLU
39	2h	100	ILE

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Mol	Chain	Res	Type
39	2h	104	ARG
39	2h	109	ILE
39	2h	112	LEU
40	2i	14	VAL
40	2i	17	VAL
40	2i	23	ASN
40	2i	26	VAL
40	2i	35	GLU
40	2i	53	VAL
40	2i	64	THR
40	2i	65	VAL
40	2i	71	SER
40	2i	81	ILE
40	2i	86	VAL
40	2i	87	GLN
40	2i	102	LEU
40	2i	104	ARG
40	2i	108	VAL
40	2i	111	ARG
40	2i	127	LYS
41	2j	6	ILE
41	2j	16	LEU
41	2j	34	VAL
41	2j	43	ARG
41	2j	47	PHE
41	2j	67	THR
41	2j	68	HIS
41	2j	69	ASN
41	2j	71	LEU
41	2j	72	VAL
41	2j	92	THR
41	2j	95	GLU
41	2j	98	ILE
42	2k	14	VAL
42	2k	33	THR
42	2k	47	VAL
42	2k	84	VAL
42	2k	87	THR
42	2k	99	GLN
42	2k	109	VAL
42	2k	112	THR
42	2k	114	VAL

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Mol	Chain	Res	Type
42	2k	116	HIS
42	2k	117	ASN
43	2l	6	THR
43	2l	18	VAL
43	2l	23	LYS
43	2l	27	LEU
43	2l	36	VAL
43	2l	38	THR
43	2l	39	VAL
43	2l	41	ARG
43	2l	47	LYS
43	2l	52	LEU
43	2l	60	LEU
43	2l	70	ILE
43	2l	81	SER
43	2l	97	ARG
43	2l	104	VAL
44	2m	8	GLU
44	2m	12	ASN
44	2m	19	LEU
44	2m	20	THR
44	2m	47	ASP
44	2m	49	THR
44	2m	52	GLU
44	2m	67	GLU
44	2m	70	LEU
44	2m	73	GLU
44	2m	80	ARG
44	2m	84	ILE
44	2m	90	LEU
44	2m	94	ARG
44	2m	98	VAL
44	2m	106	ASN
44	2m	109	THR
44	2m	116	THR
45	2n	8	GLU
45	2n	9	LYS
45	2n	13	THR
45	2n	15	LYS
45	2n	18	VAL
45	2n	33	VAL
46	2o	3	ILE

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Mol	Chain	Res	Type
46	2o	4	THR
46	2o	17	ARG
46	2o	22	THR
46	2o	35	ARG
46	2o	39	LEU
46	2o	64	ARG
46	2o	87	ILE
47	2p	1	MET
47	2p	2	VAL
47	2p	20	VAL
47	2p	42	ARG
47	2p	54	GLU
47	2p	60	LEU
47	2p	62	VAL
47	2p	69	THR
47	2p	72	ARG
48	2q	9	VAL
48	2q	34	LYS
48	2q	56	VAL
48	2q	63	ARG
48	2q	72	ARG
48	2q	74	LEU
48	2q	75	ARG
48	2q	84	LEU
48	2q	96	GLU
48	2q	97	SER
49	2r	25	THR
49	2r	26	LEU
49	2r	31	LEU
49	2r	35	ARG
49	2r	37	VAL
49	2r	66	LEU
49	2r	75	ILE
49	2r	76	LEU
49	2r	86	VAL
50	2s	5	LEU
50	2s	30	LEU
50	2s	35	SER
50	2s	41	VAL
50	2s	48	THR
50	2s	65	ASN
50	2s	66	MET

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Mol	Chain	Res	Type
50	2s	77	THR
50	2s	79	THR
51	2t	24	LEU
51	2t	38	LYS
51	2t	45	GLN
51	2t	55	ILE
51	2t	61	SER
51	2t	62	LEU
51	2t	72	LEU
51	2t	84	LEU
51	2t	100	ILE
52	2u	8	THR
53	2y	9	GLN
53	2y	11	GLU
53	2y	16	ILE
53	2y	20	VAL
53	2y	24	LEU
53	2y	39	ILE
53	2y	40	ILE
53	2y	41	LEU
53	2y	51	ASP
53	2y	54	ILE
53	2y	60	VAL
53	2y	62	VAL
53	2y	77	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	253	GLN
4	1E	48	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
6	1G	132	ASN
7	1H	158	HIS
8	1I	133	HIS
9	1N	38	HIS
9	1N	94	HIS
9	1N	133	GLN
12	1Q	12	GLN

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Mol	Chain	Res	Type
12	1Q	57	HIS
13	1R	13	HIS
13	1R	24	GLN
13	1R	31	HIS
13	1R	71	GLN
14	1S	68	GLN
15	1T	58	ASN
15	1T	104	ASN
16	1U	94	ASN
16	1U	117	GLN
18	1W	34	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
20	1Y	92	ASN
21	1Z	73	GLN
21	1Z	118	GLN
21	1Z	151	HIS
23	11	16	ASN
24	12	48	HIS
24	12	65	ASN
25	13	32	GLN
30	18	35	GLN
33	1b	19	HIS
33	1b	40	HIS
33	1b	78	GLN
33	1b	146	GLN
33	1b	212	GLN
34	1c	6	HIS
34	1c	37	GLN
35	1d	77	ASN
35	1d	119	GLN
35	1d	123	HIS
35	1d	161	ASN
36	1e	130	ASN
37	1f	7	ASN
37	1f	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	56	GLN
38	1g	64	GLN

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Mol	Chain	Res	Type
38	1g	68	ASN
38	1g	109	ASN
38	1g	110	GLN
40	1i	34	ASN
41	1j	13	HIS
41	1j	56	HIS
41	1j	84	GLN
42	1k	78	GLN
42	1k	93	GLN
46	1o	28	GLN
50	1s	14	HIS
50	1s	56	GLN
53	1y	38	HIS
53	1y	46	GLN
53	1y	79	ASN
3	2D	87	ASN
3	2D	126	GLN
3	2D	253	GLN
4	2E	169	ASN
4	2E	192	ASN
5	2F	69	HIS
5	2F	75	HIS
5	2F	203	GLN
6	2G	40	ASN
6	2G	123	ASN
6	2G	132	ASN
6	2G	138	GLN
8	2I	43	ASN
8	2I	104	GLN
8	2I	133	HIS
9	2N	94	HIS
10	2O	5	GLN
13	2R	13	HIS
13	2R	50	HIS
14	2S	84	GLN
15	2T	79	HIS
16	2U	66	ASN
17	2V	64	HIS
19	2X	31	HIS
20	2Y	6	HIS
21	2Z	121	HIS
21	2Z	151	HIS

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Mol	Chain	Res	Type
25	23	32	GLN
26	24	20	ASN
26	24	40	HIS
33	2b	37	ASN
33	2b	78	GLN
33	2b	135	GLN
33	2b	212	GLN
34	2c	37	GLN
34	2c	98	ASN
34	2c	181	ASN
35	2d	74	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	161	ASN
37	2f	64	GLN
37	2f	100	ASN
38	2g	11	GLN
38	2g	68	ASN
38	2g	86	GLN
38	2g	109	ASN
38	2g	148	ASN
40	2i	58	HIS
40	2i	87	GLN
42	2k	26	ASN
42	2k	93	GLN
42	2k	117	ASN
44	2m	62	ASN
46	2o	28	GLN
46	2o	46	HIS
47	2p	16	HIS
50	2s	47	HIS
50	2s	69	HIS
51	2t	45	GLN
53	2y	4	ASN
53	2y	89	GLN

5.3.3 RNA

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	447 (15%)	26 (0%)
1	2A	2858/2915 (98%)	519 (18%)	33 (1%)
2	1B	119/121 (98%)	12 (10%)	0
2	2B	119/121 (98%)	21 (17%)	0
32	1a	1497/1521 (98%)	257 (17%)	0
32	2a	1501/1521 (98%)	283 (18%)	0
All	All	8959/9114 (98%)	1539 (17%)	59 (0%)

All (1539) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	8	A
1	1A	10	G
1	1A	12	U
1	1A	14	A
1	1A	34	C
1	1A	45	C
1	1A	61	G
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	181	A
1	1A	182	A
1	1A	196	A
1	1A	197	A
1	1A	199	A
1	1A	204	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	265	A

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Mol	Chain	Res	Type
1	1A	271(I)	G
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(J)	C
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	428	A
1	1A	448	U
1	1A	451	C
1	1A	456	C
1	1A	479	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	518	G
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	574	C
1	1A	575	A
1	1A	588	U
1	1A	603	A

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Mol	Chain	Res	Type
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	616	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(T)	C
1	1A	652(U)	G
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	792	G
1	1A	802	A
1	1A	805	G
1	1A	811	U
1	1A	812	C
1	1A	827	U
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	880	G
1	1A	884	C
1	1A	886	C
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	892	G
1	1A	896	A
1	1A	897	C
1	1A	907	U
1	1A	910	A

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Mol	Chain	Res	Type
1	1A	932	G
1	1A	938	G
1	1A	945	A
1	1A	946	G
1	1A	958	U
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	990	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1026	U
1	1A	1033	U
1	1A	1041	C
1	1A	1042	G
1	1A	1043	C
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1053	C
1	1A	1054	A
1	1A	1055	G
1	1A	1060	U
1	1A	1061	U
1	1A	1062	G
1	1A	1063	G
1	1A	1065	U
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1078	U
1	1A	1079	C
1	1A	1083	U
1	1A	1085	A
1	1A	1087	G
1	1A	1088	A

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Mol	Chain	Res	Type
1	1A	1089	G
1	1A	1090	U
1	1A	1096	A
1	1A	1097	U
1	1A	1109	C
1	1A	1112	G
1	1A	1115	G
1	1A	1116	C
1	1A	1128	A
1	1A	1129	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1155	A
1	1A	1157	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1210	A
1	1A	1211	U
1	1A	1218	C
1	1A	1220	A
1	1A	1244	G
1	1A	1253	A
1	1A	1255	U
1	1A	1256	G
1	1A	1267	U
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1313	U
1	1A	1321	A
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A

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Mol	Chain	Res	Type
1	1A	1365	A
1	1A	1370	C
1	1A	1384	A
1	1A	1385	G
1	1A	1386	C
1	1A	1395	A
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1452	A
1	1A	1455	G
1	1A	1467	C
1	1A	1471	A
1	1A	1482	G
1	1A	1493	C
1	1A	1497	U
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1514	U
1	1A	1532	C
1	1A	1540	U
1	1A	1542	A
1	1A	1543	C
1	1A	1558	A
1	1A	1559	G
1	1A	1569	A
1	1A	1578	U
1	1A	1579	A
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1607	C
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1634	A

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Mol	Chain	Res	Type
1	1A	1648	C
1	1A	1654	A
1	1A	1664	A
1	1A	1674	G
1	1A	1675	C
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1713	U
1	1A	1721	G
1	1A	1722	A
1	1A	1739	U
1	1A	1740	G
1	1A	1756	G
1	1A	1763	G
1	1A	1764	G
1	1A	1769	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1786	A
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1812	A
1	1A	1816	G
1	1A	1828	G
1	1A	1839	G
1	1A	1847	A
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1896	G
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
1	1A	1914	C
1	1A	1919	A
1	1A	1929	G
1	1A	1930	G
1	1A	1931	U
1	1A	1938	A

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Mol	Chain	Res	Type
1	1A	1941	C
1	1A	1955	U
1	1A	1963	U
1	1A	1964	G
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1984	G
1	1A	1991	U
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2103	C
1	1A	2104	G
1	1A	2107	C
1	1A	2108	C
1	1A	2110	G
1	1A	2116	G
1	1A	2117	A
1	1A	2118	U
1	1A	2123	G
1	1A	2125	G
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U

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Mol	Chain	Res	Type
1	1A	2133	G
1	1A	2135	A
1	1A	2136	C
1	1A	2138	C
1	1A	2141	G
1	1A	2142	C
1	1A	2146	C
1	1A	2154	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2160	G
1	1A	2162	G
1	1A	2165	G
1	1A	2172	U
1	1A	2179	C
1	1A	2183	C
1	1A	2184	G
1	1A	2185	C
1	1A	2186	G
1	1A	2187	G
1	1A	2188	C
1	1A	2190	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2268	A
1	1A	2269	A
1	1A	2273	A
1	1A	2278	A
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G

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Mol	Chain	Res	Type
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2372	G
1	1A	2383	G
1	1A	2385	C
1	1A	2402	C
1	1A	2406	U
1	1A	2414	G
1	1A	2422	A
1	1A	2423	U
1	1A	2424	C
1	1A	2425	A
1	1A	2428	G
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2449	U
1	1A	2468	G
1	1A	2469	A
1	1A	2475	C
1	1A	2476	A
1	1A	2478	A
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U
1	1A	2507	C
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2602	A
1	1A	2603	G
1	1A	2609	U
1	1A	2611	U

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Mol	Chain	Res	Type
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2632	A
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2725	A
1	1A	2726	U
1	1A	2732	G
1	1A	2733	A
1	1A	2757	A
1	1A	2758	A
1	1A	2764	A
1	1A	2765	A
1	1A	2766	G
1	1A	2769	C
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2802	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2845	G
1	1A	2872	G
1	1A	2873	A
1	1A	2876	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
2	1B	2	C
2	1B	7	G
2	1B	13	A

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Mol	Chain	Res	Type
2	1B	32	C
2	1B	45	A
2	1B	53	A
2	1B	56	G
2	1B	73	A
2	1B	85	G
2	1B	88	C
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	33	A
32	1a	39	G
32	1a	48	C
32	1a	51	A
32	1a	55	A
32	1a	61	G
32	1a	73	G
32	1a	79	G
32	1a	96	U
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	139	G
32	1a	151	A
32	1a	159	G
32	1a	163	C
32	1a	166	G
32	1a	170	U
32	1a	173	U
32	1a	174	C
32	1a	181	G
32	1a	182	U
32	1a	189(F)	U
32	1a	195	A
32	1a	197	A
32	1a	201	C

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Mol	Chain	Res	Type
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	222	U
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	299	G
32	1a	321	A
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	382	A
32	1a	384	G
32	1a	388	G
32	1a	398	C
32	1a	406	G
32	1a	411	A
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	477	A
32	1a	480	U

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Mol	Chain	Res	Type
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	527	G7M
32	1a	532	A
32	1a	545	C
32	1a	547	A
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	581	G
32	1a	596	C
32	1a	618	C
32	1a	619	U
32	1a	627	G
32	1a	628	G
32	1a	630	G
32	1a	633	G
32	1a	650	G
32	1a	653	A
32	1a	660	G
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	702	A
32	1a	723	U
32	1a	731	G
32	1a	755	G
32	1a	759	A
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	817	C

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Mol	Chain	Res	Type
32	1a	828	A
32	1a	829	G
32	1a	838	G
32	1a	839	U
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	851	G
32	1a	875	C
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	928	G
32	1a	931	C
32	1a	934	C
32	1a	935	A
32	1a	946	A
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	998	G
32	1a	1000	U
32	1a	1001(A)	G
32	1a	1003	G
32	1a	1005	A
32	1a	1009	G
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C

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Mol	Chain	Res	Type
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1037	C
32	1a	1038	C
32	1a	1044	A
32	1a	1053	G
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1070	U
32	1a	1081	G
32	1a	1086	U
32	1a	1094	G
32	1a	1095	U
32	1a	1096	C
32	1a	1097	C
32	1a	1101	A
32	1a	1125	U
32	1a	1132	C
32	1a	1134	G
32	1a	1135	U
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1152	A
32	1a	1159	U
32	1a	1163	C
32	1a	1166	G
32	1a	1168	A
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1200	C
32	1a	1201	A
32	1a	1202	G
32	1a	1208	C

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Mol	Chain	Res	Type
32	1a	1212	U
32	1a	1213	A
32	1a	1220	G
32	1a	1224	G
32	1a	1227	A
32	1a	1238	A
32	1a	1240	U
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1262	C
32	1a	1270	C
32	1a	1272	G
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1312	G
32	1a	1320	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1368	G
32	1a	1370	G
32	1a	1377	A
32	1a	1378	C
32	1a	1397	C
32	1a	1399	C
32	1a	1419	G
32	1a	1441	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1452	C
32	1a	1457	G
32	1a	1491	G

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Mol	Chain	Res	Type
32	1a	1492	A
32	1a	1493	A
32	1a	1497	G
32	1a	1499	A
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1519	MA6
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
1	2A	10	G
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	36	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	78	A
1	2A	84	A
1	2A	90	U
1	2A	96	G
1	2A	102	G
1	2A	118	A
1	2A	120	U
1	2A	157	U
1	2A	173	G
1	2A	182	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	228	A

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Mol	Chain	Res	Type
1	2A	229	A
1	2A	230	U
1	2A	248	G
1	2A	249	C
1	2A	250	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	312	G
1	2A	317	G
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	353	G
1	2A	362	U
1	2A	363	G
1	2A	370	G
1	2A	386	G
1	2A	399	G
1	2A	405	U
1	2A	407	G
1	2A	411	G
1	2A	412	A
1	2A	415	A
1	2A	428	A
1	2A	435	C
1	2A	443	A
1	2A	444	C
1	2A	455	C
1	2A	457	A
1	2A	470	A
1	2A	480	A
1	2A	481	G
1	2A	505	A

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Mol	Chain	Res	Type
1	2A	509	C
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	556	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	619	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	653	A
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	793	A

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Mol	Chain	Res	Type
1	2A	802	A
1	2A	805	G
1	2A	812	C
1	2A	816	C
1	2A	827	U
1	2A	828	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	877	U
1	2A	880	G
1	2A	881	G
1	2A	883	G
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	896	A
1	2A	897	C
1	2A	906	G
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	936	C
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	980	A
1	2A	983	A
1	2A	996	A
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1021	A
1	2A	1022	G

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Mol	Chain	Res	Type
1	2A	1026	U
1	2A	1033	U
1	2A	1037	G
1	2A	1038	C
1	2A	1041	C
1	2A	1044	G
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1052	C
1	2A	1053	C
1	2A	1054	A
1	2A	1057	A
1	2A	1058	G
1	2A	1060	U
1	2A	1065	U
1	2A	1066	U
1	2A	1067	A
1	2A	1068	G
1	2A	1069	A
1	2A	1070	A
1	2A	1071	G
1	2A	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1077	A
1	2A	1078	U
1	2A	1079	C
1	2A	1082	U
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1088	A
1	2A	1090	U
1	2A	1091	G
1	2A	1092	C
1	2A	1093	G
1	2A	1094	U
1	2A	1096	A
1	2A	1097	U
1	2A	1098	A

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Mol	Chain	Res	Type
1	2A	1109	C
1	2A	1111	A
1	2A	1112	G
1	2A	1128	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1141	U
1	2A	1156	A
1	2A	1171	G
1	2A	1204	A
1	2A	1206	G
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1236	G
1	2A	1244	G
1	2A	1253	A
1	2A	1256	G
1	2A	1262	A
1	2A	1264	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1284	A
1	2A	1300	U
1	2A	1301	A
1	2A	1306	C
1	2A	1313	U
1	2A	1314	C
1	2A	1319	G
1	2A	1321	A
1	2A	1329	U
1	2A	1342	A
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1380	G
1	2A	1384	A

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Mol	Chain	Res	Type
1	2A	1385	G
1	2A	1386	C
1	2A	1395	A
1	2A	1396	U
1	2A	1416	G
1	2A	1417	C
1	2A	1419	A
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
1	2A	1465	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1530	C
1	2A	1531	C
1	2A	1537	G
1	2A	1542	A
1	2A	1543	C
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A

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Mol	Chain	Res	Type
1	2A	1640	C
1	2A	1647	G
1	2A	1648	C
1	2A	1664	A
1	2A	1667	G
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1750	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1861	G
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A

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Mol	Chain	Res	Type
1	2A	1955	U
1	2A	1963	U
1	2A	1964	G
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2030	A
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2063	C
1	2A	2069	G
1	2A	2093	G
1	2A	2096	U
1	2A	2097	C
1	2A	2101	G
1	2A	2103	C
1	2A	2104	G
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2110	G
1	2A	2112	G
1	2A	2114	A
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2119	A
1	2A	2121	G

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Mol	Chain	Res	Type
1	2A	2123	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2130	U
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2136	C
1	2A	2145	C
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G
1	2A	2150	U
1	2A	2151	G
1	2A	2159	G
1	2A	2161	C
1	2A	2162	G
1	2A	2163	C
1	2A	2164	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2172	U
1	2A	2173	A
1	2A	2180	U
1	2A	2183	C
1	2A	2186	G
1	2A	2189	U
1	2A	2192	G
1	2A	2196	C
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2235	G
1	2A	2238	G
1	2A	2239	G
1	2A	2243	U

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Mol	Chain	Res	Type
1	2A	2252	G
1	2A	2267	A
1	2A	2268	A
1	2A	2269	A
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2305	A
1	2A	2308	G
1	2A	2311	A
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2343	C
1	2A	2347	C
1	2A	2350	C
1	2A	2352	A
1	2A	2383	G
1	2A	2385	C
1	2A	2391	G
1	2A	2396	G
1	2A	2403	C
1	2A	2406	U
1	2A	2410	G
1	2A	2413	G
1	2A	2414	G
1	2A	2422	A
1	2A	2423	U
1	2A	2425	A
1	2A	2428	G
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A

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Mol	Chain	Res	Type
1	2A	2441	C
1	2A	2448	A
1	2A	2459	A
1	2A	2469	A
1	2A	2470	G
1	2A	2474	C
1	2A	2475	C
1	2A	2476	A
1	2A	2478	A
1	2A	2486	G
1	2A	2490	G
1	2A	2497	A
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2529	G
1	2A	2549	G
1	2A	2554	U
1	2A	2564	A
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2577	A
1	2A	2582	G
1	2A	2585	U
1	2A	2586	C
1	2A	2602	A
1	2A	2603	G
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2629	A
1	2A	2630	G
1	2A	2645	G
1	2A	2654	A
1	2A	2663	G
1	2A	2669	G
1	2A	2689	U
1	2A	2690	C

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Mol	Chain	Res	Type
1	2A	2691	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2757	A
1	2A	2758	A
1	2A	2759	G
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2793	G
1	2A	2811	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2823	A
1	2A	2833	G
1	2A	2835	A
1	2A	2839	G
1	2A	2849	U
1	2A	2872	G
1	2A	2875	C
1	2A	2880	C
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	3	C
2	2B	8	U
2	2B	9	G
2	2B	13	A
2	2B	19	G
2	2B	30	C
2	2B	31	C
2	2B	32	C
2	2B	45	A
2	2B	50	G
2	2B	51	G
2	2B	70	C

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Mol	Chain	Res	Type
2	2B	73	A
2	2B	74	U
2	2B	84	C
2	2B	106	G
2	2B	109	C
2	2B	110	G
2	2B	116	G
2	2B	120	A
32	2a	5	U
32	2a	6	G
32	2a	7	G
32	2a	9	G
32	2a	32	A
32	2a	39	G
32	2a	44	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	52	G
32	2a	65	U
32	2a	66	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	120	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	139	G
32	2a	151	A
32	2a	156	G
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	189(H)	G
32	2a	195	A
32	2a	197	A

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Mol	Chain	Res	Type
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	220	G
32	2a	240	C
32	2a	243	A
32	2a	247	G
32	2a	251	G
32	2a	257	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	298	A
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	350	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	382	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	404	U
32	2a	406	G
32	2a	409	G
32	2a	412	A
32	2a	413	G
32	2a	423	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	451	A
32	2a	452	A
32	2a	458	C
32	2a	461	A
32	2a	470	C

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Mol	Chain	Res	Type
32	2a	471	G
32	2a	482	A
32	2a	484	G
32	2a	485	G
32	2a	487	A
32	2a	496	A
32	2a	498	U
32	2a	500	G
32	2a	505	G
32	2a	508	C
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	524	G
32	2a	528	C
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	550	G
32	2a	553	A
32	2a	559	A
32	2a	561	U
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	607	A
32	2a	630	G
32	2a	632	A
32	2a	639	G
32	2a	649	G
32	2a	650	G
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	702	A
32	2a	721	G

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Mol	Chain	Res	Type
32	2a	723	U
32	2a	731	G
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	770	C
32	2a	773	G
32	2a	777	A
32	2a	787	A
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	827	U
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	848	C
32	2a	853	G
32	2a	855	G
32	2a	859	A
32	2a	871	U
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	960	U
32	2a	961	U
32	2a	966	M2G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	978	A

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Mol	Chain	Res	Type
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	999	C
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1017	G
32	2a	1020	U
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1030(C)	G
32	2a	1030(D)	A
32	2a	1031	G
32	2a	1035	A
32	2a	1038	C
32	2a	1041	A
32	2a	1043	C
32	2a	1053	G
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1085	U
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1111	A
32	2a	1112	C
32	2a	1113	C
32	2a	1117	G
32	2a	1122	U

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Mol	Chain	Res	Type
32	2a	1125	U
32	2a	1127	G
32	2a	1128	C
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1154	G
32	2a	1157	A
32	2a	1159	U
32	2a	1162	C
32	2a	1169	A
32	2a	1175	G
32	2a	1176	A
32	2a	1183	A
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1211	U
32	2a	1212	U
32	2a	1224	G
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1250	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1261	A
32	2a	1262	C
32	2a	1270	C
32	2a	1275	A
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A

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Mol	Chain	Res	Type
32	2a	1281	U
32	2a	1282	C
32	2a	1286	A
32	2a	1287	A
32	2a	1300	G
32	2a	1305	G
32	2a	1317	C
32	2a	1322	C
32	2a	1323	G
32	2a	1340	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1365	G
32	2a	1368	G
32	2a	1370	G
32	2a	1379	G
32	2a	1399	C
32	2a	1402	4OC
32	2a	1404	5MC
32	2a	1413	A
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1487	G
32	2a	1492	A
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1532	U

All (59) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	34	C
1	1A	196	A
1	1A	266	G
1	1A	278	A
1	1A	827	U
1	1A	839	U
1	1A	888	C
1	1A	895	U
1	1A	1047	G
1	1A	1065	U
1	1A	1067	A
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1211	U
1	1A	1420	U
1	1A	1442	G
1	1A	1653	G
1	1A	2126	A
1	1A	2288	A
1	1A	2422	A
1	1A	2430	A
1	1A	2474	C
1	1A	2602	A
1	1A	2689	U
1	1A	2756	U
1	2A	9	U
1	2A	195	A
1	2A	196	A
1	2A	249	C
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	503	A
1	2A	764	A
1	2A	827	U
1	2A	840	C
1	2A	856	C
1	2A	1053	C
1	2A	1057	A
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A

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Mol	Chain	Res	Type
1	2A	1145	C
1	2A	1210	A
1	2A	1379	A
1	2A	1395	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1992	G
1	2A	2126	A
1	2A	2171	A
1	2A	2172	U
1	2A	2321	G
1	2A	2601	C
1	2A	2602	A
1	2A	2689	U
1	2A	2756	U

5.4 Non-standard residues in protein, DNA, RNA chains (i)

48 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	M2G	1a	966	32	24,27,28	1.28	3 (12%)	33,40,43	1.81	6 (18%)
43	0TD	1l	92	43	8,9,10	4.84	2 (25%)	6,11,13	6.10	2 (33%)
32	G7M	1a	527	54,32	23,26,27	1.54	4 (17%)	34,39,42	1.68	5 (14%)
1	OMU	2A	2552	54,1	19,22,23	1.21	3 (15%)	25,31,34	1.79	5 (20%)
32	UR3	2a	1498	32	19,22,23	0.94	1 (5%)	26,32,35	1.84	3 (11%)
1	5MU	1A	1939	1	19,22,23	1.37	4 (21%)	27,32,35	2.05	6 (22%)
32	5MC	1a	1407	32	19,22,23	1.72	3 (15%)	26,32,35	1.15	3 (11%)
32	5MC	2a	967	32	19,22,23	1.77	3 (15%)	26,32,35	1.12	2 (7%)
1	OMG	1A	2251	54,1	23,26,27	1.27	3 (13%)	32,38,41	2.03	5 (15%)
1	5MU	2A	1939	54,1	19,22,23	1.45	5 (26%)	27,32,35	2.19	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	1A	2605	1	18,21,22	1.37	2 (11%)	21,30,33	1.93	4 (19%)
32	M2G	2a	966	32	24,27,28	1.28	4 (16%)	33,40,43	1.79	6 (18%)
32	2MG	2a	1207	32	23,26,27	1.28	4 (17%)	33,38,41	2.10	5 (15%)
1	PSU	1A	1911	1	18,21,22	1.37	3 (16%)	21,30,33	2.12	5 (23%)
1	2MA	2A	2503	54,1	22,25,26	1.48	5 (22%)	32,37,40	2.34	8 (25%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	1.99	5 (23%)
32	G7M	2a	527	54,32	23,26,27	1.52	3 (13%)	34,39,42	1.67	5 (14%)
1	5MC	1A	1942	1	19,22,23	1.50	3 (15%)	26,32,35	1.20	3 (11%)
32	5MC	1a	967	32	19,22,23	1.58	3 (15%)	26,32,35	1.11	3 (11%)
32	MA6	1a	1518	32	23,26,27	0.39	0	33,38,41	2.00	10 (30%)
1	5MU	1A	1915	1	19,22,23	1.46	5 (26%)	27,32,35	2.34	9 (33%)
1	OMC	1A	1920	1	19,22,23	0.83	0	25,31,34	0.96	1 (4%)
1	OMG	2A	2251	54,1	23,26,27	1.22	2 (8%)	32,38,41	2.04	6 (18%)
32	UR3	1a	1498	32	19,22,23	1.03	2 (10%)	26,32,35	1.70	5 (19%)
32	2MG	1a	1207	54,32	23,26,27	1.26	4 (17%)	33,38,41	2.32	8 (24%)
32	5MC	2a	1400	32	19,22,23	1.65	3 (15%)	26,32,35	1.20	4 (15%)
32	5MC	2a	1407	32	19,22,23	1.75	3 (15%)	26,32,35	1.25	3 (11%)
32	MA6	2a	1519	32	23,26,27	0.44	0	33,38,41	2.14	10 (30%)
1	PSU	1A	1917	1	18,21,22	1.38	2 (11%)	21,30,33	2.02	4 (19%)
1	5MU	2A	1915	1	19,22,23	1.48	4 (21%)	27,32,35	2.20	10 (37%)
1	OMC	2A	1920	1	19,22,23	0.80	0	25,31,34	0.96	1 (4%)
1	PSU	2A	2605	1	18,21,22	1.35	2 (11%)	21,30,33	1.98	4 (19%)
32	4OC	2a	1402	32	20,23,24	0.76	0	25,32,35	0.98	1 (4%)
1	PSU	2A	1917	1	18,21,22	1.41	3 (16%)	21,30,33	1.98	4 (19%)
1	5MC	2A	1942	1	19,22,23	1.65	3 (15%)	26,32,35	1.05	2 (7%)
1	OMU	1A	2552	54,1	19,22,23	1.26	3 (15%)	25,31,34	1.79	4 (16%)
32	PSU	1a	516	54,32	18,21,22	1.41	2 (11%)	21,30,33	1.92	4 (19%)
1	PSU	2A	1911	1	18,21,22	1.31	2 (11%)	21,30,33	1.99	5 (23%)
32	5MC	2a	1404	32	19,22,23	1.69	3 (15%)	26,32,35	1.21	3 (11%)
1	2MA	1A	2503	54,1	22,25,26	1.46	4 (18%)	32,37,40	2.29	6 (18%)
32	5MC	1a	1400	32	19,22,23	1.62	3 (15%)	26,32,35	1.22	3 (11%)
32	5MC	1a	1404	32	19,22,23	1.66	3 (15%)	26,32,35	1.14	3 (11%)
32	MA6	1a	1519	32	23,26,27	0.43	0	33,38,41	1.94	9 (27%)
43	0TD	2l	92	43	8,9,10	4.34	1 (12%)	6,11,13	2.04	3 (50%)
32	MA6	2a	1518	32	23,26,27	0.43	0	33,38,41	2.03	9 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5MC	2A	1962	54,1	19,22,23	1.51	3 (15%)	26,32,35	1.14	2 (7%)
1	5MC	1A	1962	54,1	19,22,23	1.43	3 (15%)	26,32,35	1.19	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.77	0	25,32,35	0.92	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
43	0TD	1l	92	43	-	2/7/12/14	-
32	G7M	1a	527	54,32	-	3/7/25/26	0/3/3/3
1	OMU	2A	2552	54,1	-	0/9/27/28	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	54,1	-	1/9/27/28	0/3/3/3
1	5MU	2A	1939	54,1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	2MG	2a	1207	32	-	2/9/27/28	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	54,1	-	3/7/25/26	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	54,32	-	2/7/25/26	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	OMG	2A	2251	54,1	-	2/9/27/28	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	54,32	-	0/9/27/28	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	1/11/29/30	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	54,1	-	0/9/27/28	0/2/2/2
32	PSU	1a	516	54,32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
1	2MA	1A	2503	54,1	-	2/7/25/26	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
43	0TD	2l	92	43	-	2/7/12/14	-
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
1	5MC	2A	1962	54,1	-	2/7/25/26	0/2/2/2
1	5MC	1A	1962	54,1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	3/9/29/30	0/2/2/2

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.74	1.69	1.82
43	2l	92	0TD	CB-SB	-11.93	1.70	1.82
32	2a	967	5MC	C5-C4	6.63	1.49	1.44
32	2a	1407	5MC	C5-C4	6.38	1.49	1.44
32	1a	1407	5MC	C5-C4	6.31	1.48	1.44
32	2a	1404	5MC	C5-C4	6.20	1.48	1.44
32	1a	1404	5MC	C5-C4	6.18	1.48	1.44
32	2a	1400	5MC	C5-C4	6.04	1.48	1.44
1	2A	1942	5MC	C5-C4	5.97	1.48	1.44
32	1a	1400	5MC	C5-C4	5.70	1.48	1.44
32	1a	967	5MC	C5-C4	5.65	1.48	1.44
1	2A	1962	5MC	C5-C4	5.26	1.48	1.44
1	1A	1942	5MC	C5-C4	5.14	1.48	1.44
32	1a	527	G7M	C5-N7	-4.71	1.33	1.39
1	1A	1962	5MC	C5-C4	4.64	1.47	1.44
32	2a	527	G7M	C5-N7	-4.57	1.33	1.39
1	2A	2503	2MA	C5-C4	4.38	1.46	1.39
1	1A	2503	2MA	C5-C4	4.22	1.46	1.39
43	1l	92	0TD	CB-CA	-3.94	1.53	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	516	PSU	C6-C5	3.73	1.39	1.35
1	2A	1917	PSU	C6-C5	3.70	1.39	1.35
32	2a	516	PSU	C6-C5	3.48	1.39	1.35
1	2A	2605	PSU	C6-C5	3.46	1.39	1.35
1	1A	2605	PSU	C6-C5	3.40	1.39	1.35
32	2a	1207	2MG	C5-C4	3.39	1.48	1.38
1	1A	1911	PSU	C6-C5	3.37	1.39	1.35
32	1a	527	G7M	C5-C4	3.35	1.46	1.38
32	1a	966	M2G	C5-C4	3.34	1.47	1.38
32	2a	527	G7M	C5-C4	3.33	1.46	1.38
1	1A	1917	PSU	C6-C5	3.27	1.38	1.35
1	2A	1915	5MU	C2-N1	3.22	1.43	1.38
1	2A	2251	OMG	C5-C4	3.16	1.47	1.38
32	2a	966	M2G	C5-C4	3.14	1.47	1.38
32	1a	1207	2MG	C5-C4	3.13	1.47	1.38
1	2A	1911	PSU	C6-C5	3.09	1.38	1.35
1	1A	2251	OMG	C5-C4	3.08	1.47	1.38
1	1A	1915	5MU	C2-N1	3.01	1.43	1.38
1	1A	2503	2MA	C5-N7	-3.00	1.33	1.39
1	1A	2251	OMG	C6-N1	-2.97	1.33	1.38
32	2a	1407	5MC	C6-C5	2.90	1.39	1.34
32	1a	1400	5MC	C6-C5	2.88	1.39	1.34
1	2A	2552	OMU	C4-N3	-2.88	1.33	1.38
32	2a	966	M2G	C2-N2	2.88	1.40	1.35
32	2a	1404	5MC	C6-C5	2.87	1.39	1.34
1	1A	1962	5MC	C6-C5	2.79	1.39	1.34
1	2A	1942	5MC	C6-C5	2.77	1.39	1.34
1	1A	1917	PSU	C4-N3	-2.76	1.33	1.38
1	1A	2552	OMU	C2-N3	-2.76	1.33	1.38
32	1a	967	5MC	C6-C5	2.75	1.39	1.34
32	1a	1407	5MC	C6-C5	2.74	1.39	1.34
1	1A	1915	5MU	C4-N3	-2.72	1.33	1.38
1	2A	1915	5MU	C6-C5	2.72	1.39	1.34
1	2A	1939	5MU	C6-N1	-2.71	1.33	1.38
1	2A	1911	PSU	C4-N3	-2.70	1.33	1.38
1	1A	1942	5MC	C6-C5	2.70	1.39	1.34
1	2A	2251	OMG	C6-N1	-2.69	1.33	1.38
32	2a	967	5MC	C6-C5	2.69	1.39	1.34
32	1a	966	M2G	C2-N2	2.67	1.40	1.35
1	2A	1962	5MC	C6-C5	2.67	1.39	1.34
1	1A	2552	OMU	C4-N3	-2.67	1.34	1.38
1	2A	1939	5MU	C6-C5	2.64	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1915	5MU	C6-C5	2.63	1.38	1.34
32	2a	527	G7M	C6-N1	-2.61	1.34	1.38
1	1A	1939	5MU	C6-N1	-2.58	1.33	1.38
1	2A	1915	5MU	C4-C5	2.57	1.49	1.44
1	1A	1911	PSU	C4-N3	-2.56	1.34	1.38
1	2A	1939	5MU	C4-N3	-2.55	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.53	1.34	1.38
1	2A	2503	2MA	C8-N7	2.52	1.36	1.31
1	2A	2605	PSU	C4-N3	-2.51	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.50	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.49	1.34	1.38
1	2A	1939	5MU	C4-C5	2.47	1.48	1.44
32	2a	1400	5MC	C6-C5	2.47	1.38	1.34
32	2a	516	PSU	C4-N3	-2.47	1.34	1.38
32	1a	516	PSU	C4-N3	-2.46	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.46	1.34	1.38
1	2A	2503	2MA	C5-C6	2.45	1.47	1.41
1	1A	1939	5MU	C4-N3	-2.44	1.34	1.38
1	2A	2503	2MA	C5-N7	-2.44	1.34	1.39
32	1a	1404	5MC	C6-N1	-2.43	1.33	1.38
1	1A	1939	5MU	C6-C5	2.43	1.38	1.34
1	2A	1939	5MU	C2-N3	-2.42	1.33	1.38
32	1a	1400	5MC	C6-N1	-2.39	1.33	1.38
32	1a	1498	UR3	C2-N1	2.39	1.41	1.38
1	1A	2503	2MA	C8-N7	2.37	1.36	1.31
32	2a	1400	5MC	C6-N1	-2.36	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.35	1.34	1.38
32	1a	966	M2G	C6-N1	-2.34	1.34	1.38
32	1a	527	G7M	C6-N1	-2.34	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.32	1.34	1.38
1	1A	1915	5MU	C4-C5	2.32	1.48	1.44
1	1A	2552	OMU	C5-C4	-2.31	1.38	1.43
1	2A	2552	OMU	C2-N3	-2.30	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.28	1.34	1.38
1	1A	2605	PSU	C4-N3	-2.25	1.34	1.38
32	1a	1404	5MC	C6-C5	2.24	1.38	1.34
32	2a	966	M2G	C6-N1	-2.22	1.34	1.38
32	2a	1207	2MG	C2-N3	2.22	1.36	1.32
32	2a	967	5MC	C6-N1	-2.22	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.21	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.20	1.34	1.38
1	1A	2503	2MA	C5-C6	2.19	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2251	OMG	C5-N7	-2.16	1.34	1.39
1	1A	1915	5MU	C2-N3	-2.16	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.13	1.34	1.38
32	1a	1207	2MG	C5-N7	-2.11	1.34	1.39
1	2A	2503	2MA	C4-N9	-2.10	1.33	1.37
32	1a	967	5MC	C6-N1	-2.09	1.34	1.38
32	1a	1207	2MG	C2-N3	2.08	1.35	1.32
1	2A	2552	OMU	C5-C4	-2.08	1.39	1.43
1	1A	1939	5MU	C4-C5	2.07	1.48	1.44
32	1a	1407	5MC	C6-N1	-2.06	1.34	1.38
1	2A	1917	PSU	C4-C5	2.06	1.50	1.44
32	1a	527	G7M	C5-C6	2.05	1.48	1.43
32	2a	1498	UR3	C6-C5	2.03	1.39	1.35
32	2a	1207	2MG	C5-N7	-2.03	1.35	1.39
32	1a	1498	UR3	C6-C5	2.02	1.39	1.35
1	1A	1911	PSU	C2-N3	-2.01	1.34	1.37
32	2a	966	M2G	C4-N9	-2.00	1.33	1.38

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	-14.60	76.11	102.36
1	1A	2503	2MA	C5-C4-N3	-8.40	118.33	127.18
1	2A	2503	2MA	C5-C4-N3	-8.31	118.42	127.18
32	2a	1498	UR3	C4-N3-C2	-7.53	118.52	124.58
32	1a	1207	2MG	C2-N3-C4	7.26	121.09	112.00
32	2a	1207	2MG	C2-N3-C4	6.83	120.54	112.00
1	1A	1911	PSU	N1-C2-N3	6.65	122.18	115.17
32	1a	1498	UR3	C4-N3-C2	-6.64	119.24	124.58
1	2A	2251	OMG	C5-C4-N3	-6.51	118.03	128.39
1	1A	2251	OMG	C5-C4-N3	-6.50	118.04	128.39
1	2A	2503	2MA	N3-C4-N9	6.45	135.17	126.99
1	1A	1917	PSU	N1-C2-N3	6.38	121.89	115.17
1	1A	2503	2MA	N3-C4-N9	6.30	134.99	126.99
32	2a	1207	2MG	C5-C4-N3	-6.23	118.48	128.39
32	1a	1207	2MG	C5-C4-N3	-6.21	118.50	128.39
1	2A	2605	PSU	N1-C2-N3	6.03	121.53	115.17
32	2a	516	PSU	N1-C2-N3	6.01	121.51	115.17
1	2A	1911	PSU	N1-C2-N3	5.99	121.49	115.17
32	1a	966	M2G	C5-C4-N3	-5.93	118.96	128.39
1	2A	1917	PSU	N1-C2-N3	5.85	121.34	115.17
32	1a	516	PSU	N1-C2-N3	5.82	121.31	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	966	M2G	C5-C4-N3	-5.70	119.32	128.39
1	2A	1939	5MU	N3-C2-N1	5.56	122.13	114.89
1	2A	1939	5MU	C4-N3-C2	-5.37	120.30	127.34
32	2a	527	G7M	N9-C4-N3	5.34	136.63	125.95
1	1A	2605	PSU	N1-C2-N3	5.32	120.78	115.17
32	1a	527	G7M	C5-C4-N3	-5.31	118.11	128.15
32	1a	527	G7M	N9-C4-N3	5.28	136.50	125.95
1	2A	2251	OMG	C2-N3-C4	5.15	121.17	112.30
1	1A	2251	OMG	C2-N3-C4	5.12	121.13	112.30
32	2a	527	G7M	C5-C4-N3	-5.12	118.47	128.15
32	2a	1519	MA6	N1-C2-N3	-5.09	120.87	128.58
32	1a	1518	MA6	N1-C2-N3	-5.08	120.90	128.58
1	1A	1915	5MU	N3-C2-N1	5.04	121.45	114.89
32	2a	1519	MA6	C5-C4-N3	-4.94	119.92	126.72
1	1A	1939	5MU	C4-N3-C2	-4.92	120.89	127.34
32	2a	1518	MA6	N1-C2-N3	-4.90	121.16	128.58
32	1a	1519	MA6	C5-C4-N3	-4.84	120.05	126.72
1	1A	1915	5MU	C4-N3-C2	-4.78	121.07	127.34
1	2A	2552	OMU	C4-N3-C2	-4.76	120.70	126.61
1	2A	1915	5MU	N3-C2-N1	4.75	121.07	114.89
1	1A	2251	OMG	N9-C4-N3	4.73	135.40	125.95
1	2A	2251	OMG	N9-C4-N3	4.71	135.37	125.95
1	1A	2552	OMU	C4-N3-C2	-4.67	120.82	126.61
32	1a	527	G7M	C2-N3-C4	4.64	120.29	112.30
1	1A	1915	5MU	C5-C4-N3	4.49	119.23	115.32
1	1A	1915	5MU	C1'-N1-C2	4.49	125.66	117.59
1	2A	1915	5MU	C4-N3-C2	-4.47	121.48	127.34
1	1A	1939	5MU	N3-C2-N1	4.45	120.69	114.89
32	2a	966	M2G	C2-N3-C4	4.44	120.72	112.51
32	2a	1207	2MG	N9-C4-N3	4.43	134.81	125.95
32	1a	966	M2G	N9-C4-N3	4.42	134.79	125.95
32	2a	527	G7M	C2-N3-C4	4.39	119.86	112.30
1	1A	1939	5MU	O4-C4-C5	-4.37	119.92	124.92
1	2A	1915	5MU	C1'-N1-C2	4.36	125.42	117.59
32	2a	1518	MA6	C5-C4-N3	-4.36	120.72	126.72
1	2A	1911	PSU	C4-N3-C2	-4.29	120.46	126.37
32	1a	966	M2G	C2-N3-C4	4.25	120.37	112.51
32	1a	1519	MA6	N1-C2-N3	-4.25	122.15	128.58
1	2A	2552	OMU	N3-C2-N1	4.24	120.41	114.89
1	1A	1911	PSU	C4-N3-C2	-4.24	120.54	126.37
32	1a	1518	MA6	C2-N1-C6	4.22	122.15	111.83
1	1A	2552	OMU	C5-C4-N3	4.15	120.62	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1917	PSU	C4-N3-C2	-4.13	120.69	126.37
32	1a	1207	2MG	N9-C4-N3	4.10	134.16	125.95
1	2A	1939	5MU	O4-C4-C5	-4.09	120.24	124.92
1	1A	1939	5MU	C5-C6-N1	-4.05	118.92	123.31
32	2a	516	PSU	C4-N3-C2	-4.04	120.81	126.37
32	2a	966	M2G	N9-C4-N3	4.03	134.00	125.95
1	2A	2605	PSU	C4-N3-C2	-4.02	120.84	126.37
32	2a	1519	MA6	C4-C5-N7	-4.01	106.00	110.58
32	2a	1518	MA6	C2-N1-C6	4.00	121.61	111.83
32	1a	1518	MA6	C5-C4-N3	-3.99	121.22	126.72
1	1A	2552	OMU	N3-C2-N1	3.99	120.08	114.89
32	2a	1519	MA6	C2-N1-C6	3.99	121.57	111.83
1	2A	1917	PSU	C4-N3-C2	-3.94	120.94	126.37
1	1A	2605	PSU	O2-C2-N1	-3.93	118.74	122.79
1	1A	1942	5MC	C5-C6-N1	-3.90	119.08	123.31
1	2A	1939	5MU	C5-C6-N1	-3.88	119.10	123.31
1	1A	1939	5MU	C5-C4-N3	3.87	118.68	115.32
32	1a	1400	5MC	C5-C6-N1	-3.83	119.15	123.31
32	2a	1518	MA6	C5-N7-C8	3.83	109.46	103.45
1	2A	1915	5MU	C5-C4-N3	3.82	118.65	115.32
1	1A	1915	5MU	O4-C4-C5	-3.82	120.55	124.92
32	2a	1519	MA6	C5-N7-C8	3.82	109.45	103.45
1	1A	1915	5MU	C1'-N1-C6	-3.81	114.87	121.15
1	2A	1915	5MU	C1'-N1-C6	-3.76	114.96	121.15
1	2A	1939	5MU	C5-C4-N3	3.76	118.59	115.32
1	1A	1911	PSU	O2-C2-N1	-3.75	118.93	122.79
32	2a	1518	MA6	C4-C5-N7	-3.74	106.31	110.58
1	2A	2552	OMU	C5-C4-N3	3.72	120.01	114.80
32	1a	1404	5MC	C5-C6-N1	-3.71	119.28	123.31
32	2a	1519	MA6	C2-N3-C4	3.70	120.87	111.83
32	2a	1400	5MC	C5-C6-N1	-3.69	119.30	123.31
32	1a	1519	MA6	C2-N1-C6	3.69	120.85	111.83
1	1A	2605	PSU	C4-N3-C2	-3.64	121.35	126.37
32	2a	967	5MC	C5-C6-N1	-3.62	119.39	123.31
32	1a	516	PSU	C4-N3-C2	-3.61	121.40	126.37
1	2A	1962	5MC	C5-C6-N1	-3.61	119.39	123.31
32	1a	1518	MA6	C5-N7-C8	3.58	109.08	103.45
32	2a	1498	UR3	C5-C4-N3	3.55	119.71	115.04
32	1a	1207	2MG	C6-C5-N7	3.54	136.73	130.29
32	1a	1518	MA6	N9-C8-N7	-3.50	108.97	113.94
32	1a	1519	MA6	C4-C5-N7	-3.44	106.65	110.58
1	2A	2503	2MA	C4-C5-N7	-3.43	106.66	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1518	MA6	C2-N3-C4	3.41	120.17	111.83
32	2a	1518	MA6	N9-C8-N7	-3.40	109.11	113.94
32	2a	1407	5MC	C5-C6-N1	-3.40	119.62	123.31
32	1a	516	PSU	O2-C2-N1	-3.40	119.28	122.79
1	1A	2503	2MA	N6-C6-N1	3.37	121.58	117.03
1	1A	1917	PSU	O2-C2-N1	-3.37	119.31	122.79
32	2a	966	M2G	C6-C5-N7	3.36	136.41	130.29
32	1a	1519	MA6	C2-N3-C4	3.30	119.88	111.83
1	2A	1939	5MU	O2-C2-N1	-3.29	118.51	122.80
1	2A	2251	OMG	C6-C5-N7	3.29	136.28	130.29
32	2a	1404	5MC	C5-C6-N1	-3.29	119.74	123.31
32	1a	1518	MA6	C2-N3-C4	3.28	119.83	111.83
32	2a	1519	MA6	N9-C8-N7	-3.26	109.31	113.94
32	1a	1519	MA6	C5-N7-C8	3.24	108.55	103.45
1	2A	2503	2MA	N6-C6-N1	3.21	121.36	117.03
1	1A	2503	2MA	C4-C5-N7	-3.19	106.93	110.58
32	1a	1518	MA6	C4-C5-N7	-3.18	106.94	110.58
1	2A	1911	PSU	O2-C2-N1	-3.18	119.51	122.79
1	2A	2605	PSU	O2-C2-N1	-3.18	119.51	122.79
1	1A	1962	5MC	C5-C6-N1	-3.17	119.87	123.31
32	1a	967	5MC	C5-C6-N1	-3.15	119.89	123.31
43	2l	92	0TD	OD2-CG-CB	3.13	119.90	113.15
1	2A	1917	PSU	O2-C2-N1	-3.12	119.57	122.79
1	1A	2552	OMU	O4-C4-C5	-3.11	119.80	125.16
1	1A	2251	OMG	C6-C5-N7	3.10	135.94	130.29
32	2a	1207	2MG	C6-C5-N7	3.08	135.89	130.29
32	1a	966	M2G	C6-C5-N7	3.06	135.87	130.29
1	2A	1942	5MC	C5-C6-N1	-3.05	120.00	123.31
1	2A	2552	OMU	O2-C2-N1	-3.04	118.83	122.80
32	1a	1519	MA6	C4-C5-C6	3.04	119.06	115.91
1	2A	1915	5MU	O4-C4-C5	-3.04	121.44	124.92
1	1A	1962	5MC	C5-C4-N3	-3.02	118.66	121.75
32	2a	1404	5MC	C5-C4-N3	-3.01	118.67	121.75
32	1a	1207	2MG	C4-C5-N7	-2.99	105.93	110.67
32	1a	1498	UR3	C5-C4-N3	2.95	118.93	115.04
32	2a	1407	5MC	C5-C4-N3	-2.95	118.73	121.75
32	2a	516	PSU	O2-C2-N1	-2.95	119.75	122.79
32	1a	1407	5MC	C5-C4-N3	-2.91	118.77	121.75
1	2A	2503	2MA	C4-N9-C8	2.88	108.77	105.74
32	1a	1519	MA6	N3-C4-N9	2.85	132.01	127.17
32	2a	1519	MA6	N3-C4-N9	2.83	131.98	127.17
32	1a	1400	5MC	C5-C4-N3	-2.81	118.87	121.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1942	5MC	C5-C4-N3	-2.80	118.88	121.75
43	2l	92	0TD	CSB-SB-CB	-2.80	97.34	102.36
1	2A	2251	OMG	C4-C5-N7	-2.79	106.25	110.67
32	1a	1518	MA6	N3-C4-N9	2.78	131.89	127.17
1	2A	1917	PSU	C6-C5-C4	-2.77	116.30	118.17
1	1A	1915	5MU	O2-C2-N3	-2.72	116.47	121.49
1	1A	2251	OMG	C4-C5-N7	-2.71	106.38	110.67
32	1a	1407	5MC	C5-C6-N1	-2.68	120.40	123.31
32	2a	1407	5MC	O2-C2-N3	-2.68	118.11	122.33
32	2a	1518	MA6	N3-C4-N9	2.67	131.71	127.17
32	2a	1207	2MG	C4-C5-N7	-2.66	106.45	110.67
1	1A	1939	5MU	O2-C2-N1	-2.63	119.37	122.80
32	1a	1207	2MG	N1-C2-N2	2.62	119.24	116.56
32	2a	1519	MA6	C4-C5-C6	2.62	118.62	115.91
1	2A	1962	5MC	C5-C4-N3	-2.60	119.09	121.75
1	2A	1915	5MU	C5M-C5-C4	2.59	121.54	118.78
32	2a	1400	5MC	C5-C4-N3	-2.55	119.14	121.75
32	1a	1519	MA6	N9-C8-N7	-2.55	110.31	113.94
1	2A	2503	2MA	C5-N7-C8	2.54	107.45	103.45
32	1a	1407	5MC	O2-C2-N3	-2.54	118.33	122.33
1	2A	1915	5MU	O2-C2-N3	-2.51	116.86	121.49
32	2a	966	M2G	C4-C5-N7	-2.51	106.70	110.67
1	2A	2552	OMU	O4-C4-C5	-2.49	120.88	125.16
1	1A	1915	5MU	C5M-C5-C4	2.47	121.42	118.78
32	1a	1404	5MC	C5-C4-N3	-2.46	119.23	121.75
1	2A	2503	2MA	C2-N1-C6	2.46	121.88	118.10
32	2a	1402	4OC	C6-C5-C4	2.46	119.96	117.00
1	2A	1915	5MU	C5-C6-N1	-2.46	120.64	123.31
1	1A	1911	PSU	C5-C6-N1	-2.43	118.77	122.14
32	1a	967	5MC	C5-C4-N3	-2.42	119.27	121.75
32	2a	516	PSU	O4'-C1'-C2'	2.42	108.50	105.15
1	1A	1915	5MU	C5-C6-N1	-2.41	120.69	123.31
1	1A	2503	2MA	C5-N7-C8	2.39	107.20	103.45
1	1A	1920	OMC	O2-C2-N3	-2.38	118.58	122.33
1	1A	2503	2MA	C2-N1-C6	2.38	121.75	118.10
43	1l	92	0TD	OD2-CG-CB	2.37	118.26	113.15
32	1a	1400	5MC	O2-C2-N3	-2.36	118.61	122.33
1	1A	1917	PSU	C5-C6-N1	-2.36	118.87	122.14
32	2a	527	G7M	O6-C6-C5	-2.34	122.78	128.01
32	1a	966	M2G	C4-C5-N7	-2.34	106.96	110.67
43	2l	92	0TD	OD1-CG-CB	-2.34	117.55	122.44
32	2a	1498	UR3	C3U-N3-C4	2.30	121.05	117.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	967	5MC	C5-C4-N3	-2.29	119.40	121.75
32	1a	516	PSU	O4'-C1'-C2'	2.29	108.31	105.15
32	1a	1518	MA6	C4-N9-C8	2.28	108.13	105.74
1	2A	2503	2MA	N9-C8-N7	-2.27	110.72	113.94
32	1a	1402	4OC	C6-C5-C4	2.27	119.73	117.00
32	2a	1404	5MC	O2-C2-N3	-2.27	118.76	122.33
1	1A	2605	PSU	O4-C4-C5	-2.25	118.41	124.01
32	1a	1207	2MG	O3'-C3'-C2'	2.24	119.00	111.82
32	1a	1404	5MC	CM5-C5-C6	-2.24	119.82	122.85
1	2A	1920	OMC	O2-C2-N3	-2.22	118.82	122.33
32	2a	1518	MA6	C4-C5-C6	2.22	118.21	115.91
32	1a	1498	UR3	C3U-N3-C4	2.22	120.95	117.87
1	1A	1942	5MC	C5-C4-N3	-2.22	119.48	121.75
32	1a	966	M2G	O6-C6-C5	-2.21	120.69	126.53
32	1a	527	G7M	O6-C6-C5	-2.20	123.09	128.01
32	1a	967	5MC	O2-C2-N3	-2.20	118.86	122.33
32	2a	1400	5MC	CM5-C5-C6	-2.20	119.88	122.85
32	2a	966	M2G	O6-C6-C5	-2.19	120.76	126.53
1	2A	1915	5MU	C5M-C5-C6	-2.16	119.92	122.85
1	2A	2605	PSU	C5-C6-N1	-2.13	119.18	122.14
32	2a	516	PSU	C5-C6-N1	-2.13	119.18	122.14
32	2a	527	G7M	C5-C6-N1	2.12	116.21	111.84
32	1a	1207	2MG	N2-C2-N3	-2.10	117.83	120.51
1	1A	1942	5MC	O2-C2-N3	-2.10	119.02	122.33
32	2a	1519	MA6	C5-C4-N9	2.10	108.10	105.81
1	2A	1911	PSU	C5-C6-N1	-2.08	119.26	122.14
32	1a	527	G7M	C5-C6-N1	2.07	116.12	111.84
32	1a	1498	UR3	C6-N1-C2	-2.05	120.12	121.80
1	1A	1911	PSU	O4'-C1'-C2'	2.03	107.96	105.15
32	1a	1518	MA6	C4-C5-C6	2.03	118.01	115.91
1	2A	2251	OMG	C5-C6-N1	2.02	118.40	113.25
32	1a	1498	UR3	O2-C2-N3	-2.01	118.55	121.33
1	2A	1911	PSU	O4'-C1'-C2'	2.01	107.93	105.15
32	2a	1400	5MC	O2-C2-N3	-2.00	119.18	122.33

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
32	1a	1519	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
32	2a	1207	2MG	N1-C2-N2-CM2
32	2a	1207	2MG	N3-C2-N2-CM2
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1404	5MC	O4'-C4'-C5'-O5'
32	1a	527	G7M	O4'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	1404	5MC	C3'-C4'-C5'-O5'
1	2A	2503	2MA	C3'-C4'-C5'-O5'
1	2A	2251	OMG	C1'-C2'-O2'-CM2
32	2a	527	G7M	O4'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
43	1l	92	0TD	SB-CB-CG-OD1
43	2l	92	0TD	SB-CB-CG-OD1
1	1A	2503	2MA	C4'-C5'-O5'-P
32	1a	527	G7M	C4'-C5'-O5'-P
1	2A	2503	2MA	C4'-C5'-O5'-P
1	1A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C2'-O2'-CM2
1	2A	2251	OMG	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
1	1A	2251	OMG	C4'-C5'-O5'-P
43	1l	92	0TD	CG-CB-SB-CSB
32	1a	1402	4OC	C3'-C4'-C5'-O5'
1	2A	1962	5MC	C2'-C1'-N1-C6
1	1A	1920	OMC	C2'-C1'-N1-C2
1	2A	1962	5MC	O4'-C1'-N1-C6
32	1a	1519	MA6	C4'-C5'-O5'-P
1	2A	1920	OMC	C2'-C1'-N1-C2

There are no ring outliers.

27 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	966	M2G	2	0
43	1l	92	0TD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1498	UR3	2	0
1	1A	1939	5MU	2	0
1	1A	2251	OMG	1	0
1	2A	1939	5MU	1	0
1	1A	2605	PSU	1	0
32	2a	966	M2G	1	0
32	2a	1207	2MG	1	0
1	2A	2503	2MA	1	0
1	1A	1942	5MC	1	0
32	1a	1518	MA6	2	0
1	1A	1915	5MU	1	0
1	1A	1920	OMC	2	0
1	2A	2251	OMG	1	0
32	1a	1498	UR3	1	0
32	1a	1207	2MG	1	0
32	2a	1400	5MC	2	0
32	2a	1519	MA6	1	0
1	2A	1915	5MU	1	0
1	2A	1920	OMC	1	0
32	2a	1402	4OC	2	0
1	2A	1917	PSU	1	0
32	1a	1519	MA6	3	0
43	2l	92	0TD	2	0
32	2a	1518	MA6	1	0
32	1a	1402	4OC	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2505 ligands modelled in this entry, 2492 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
56	MPD	2A	3735	-	7,7,7	0.31	0	9,10,10	0.27	0
56	MPD	1a	3271	-	7,7,7	0.34	0	9,10,10	0.32	0
56	MPD	1a	3272	-	7,7,7	0.33	0	9,10,10	0.50	0
56	MPD	2B	221	-	7,7,7	0.32	0	9,10,10	0.30	0
59	SF4	1d	306	35	0,12,12	-	-	-		
55	A1CRE	1A	4012	-	43,45,45	2.53	11 (25%)	57,68,68	2.16	18 (31%)
57	ARG	1B	231	54	10,11,11	0.78	1 (10%)	9,13,13	1.04	1 (11%)
56	MPD	18	105	-	7,7,7	0.32	0	9,10,10	0.43	0
56	MPD	1A	4013	-	7,7,7	0.32	0	9,10,10	0.19	0
59	SF4	2d	501	35	0,12,12	-	-	-		
56	MPD	2A	3734	-	7,7,7	0.33	0	9,10,10	0.30	0
57	ARG	1F	317	-	10,11,11	0.80	1 (10%)	9,13,13	0.99	1 (11%)
55	A1CRE	2A	3733	-	43,45,45	2.50	13 (30%)	57,68,68	2.26	18 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	MPD	2A	3735	-	-	4/5/5/5	-
56	MPD	1a	3271	-	-	0/5/5/5	-
56	MPD	1a	3272	-	-	4/5/5/5	-
56	MPD	2B	221	-	-	1/5/5/5	-
59	SF4	1d	306	35	-	-	0/6/5/5
55	A1CRE	1A	4012	-	-	9/17/79/79	0/5/5/5
57	ARG	1B	231	54	-	1/11/11/11	-
56	MPD	18	105	-	-	4/5/5/5	-
56	MPD	1A	4013	-	-	2/5/5/5	-
59	SF4	2d	501	35	-	-	0/6/5/5
56	MPD	2A	3734	-	-	1/5/5/5	-
57	ARG	1F	317	-	-	5/11/11/11	-
55	A1CRE	2A	3733	-	-	4/17/79/79	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1A	4012	A1CRE	CAT-CAQ	-9.09	1.36	1.51
55	1A	4012	A1CRE	CAA-CAQ	-8.58	1.40	1.53
55	2A	3733	A1CRE	CAA-CAQ	-8.27	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2A	3733	A1CRE	CAT-CAQ	-7.73	1.38	1.51
55	1A	4012	A1CRE	CBI-CBJ	-4.91	1.39	1.50
55	2A	3733	A1CRE	CBI-CBJ	-4.85	1.39	1.50
55	2A	3733	A1CRE	OAU-CAC	-3.68	1.40	1.46
55	2A	3733	A1CRE	CAS-CAD	-3.56	1.47	1.54
55	1A	4012	A1CRE	OAU-CAC	-3.49	1.40	1.46
55	2A	3733	A1CRE	CAB-CAC	-3.39	1.53	1.56
55	2A	3733	A1CRE	CAB-CAG	-3.32	1.51	1.56
55	2A	3733	A1CRE	CAH-CAI	-3.22	1.52	1.56
55	1A	4012	A1CRE	CAB-CAG	-3.15	1.51	1.56
55	1A	4012	A1CRE	CAS-CAD	-3.14	1.48	1.54
55	1A	4012	A1CRE	CAF-CAG	-2.93	1.49	1.53
55	2A	3733	A1CRE	CBF-CBE	-2.93	1.31	1.36
55	1A	4012	A1CRE	CAH-CAI	-2.82	1.53	1.56
55	2A	3733	A1CRE	CAF-CAG	-2.79	1.49	1.53
55	1A	4012	A1CRE	CBE-NBD	-2.77	1.31	1.36
55	1A	4012	A1CRE	CBF-CBE	-2.73	1.32	1.36
55	2A	3733	A1CRE	CAK-CAC	-2.54	1.50	1.53
55	2A	3733	A1CRE	CBE-NBD	-2.54	1.31	1.36
55	1A	4012	A1CRE	CAD-CAH	-2.36	1.53	1.56
57	1B	231	ARG	OXT-C	-2.24	1.23	1.30
57	1F	317	ARG	OXT-C	-2.20	1.23	1.30
55	2A	3733	A1CRE	CAS-CAT	-2.14	1.47	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1A	4012	A1CRE	CAK-CAC-CAB	-7.75	107.96	116.28
55	2A	3733	A1CRE	CAK-CAC-CAB	-7.53	108.20	116.28
55	2A	3733	A1CRE	CAZ-CAB-CAC	-5.08	103.63	108.81
55	1A	4012	A1CRE	CAF-CAG-CAB	-4.66	106.37	111.57
55	2A	3733	A1CRE	CAT-CAQ-CAA	4.41	113.22	108.53
55	2A	3733	A1CRE	CAF-CAG-CAB	-4.27	106.81	111.57
55	1A	4012	A1CRE	CAE-CAD-CAA	4.21	114.11	106.82
55	1A	4012	A1CRE	CAZ-CAB-CAC	-3.96	104.76	108.81
55	1A	4012	A1CRE	CAE-CAF-CAG	-3.85	107.41	112.38
55	2A	3733	A1CRE	CAE-CAD-CAA	3.79	113.39	106.82
55	1A	4012	A1CRE	CAD-CAA-CAB	-3.76	112.86	117.94
55	1A	4012	A1CRE	OAU-CAC-CAB	3.74	112.15	106.32
55	2A	3733	A1CRE	CAE-CAF-CAG	-3.65	107.67	112.38
55	2A	3733	A1CRE	CAD-CAA-CAB	-3.65	113.02	117.94
55	1A	4012	A1CRE	CBI-OBH-CBG	-3.50	108.36	112.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1A	4012	A1CRE	CAC-OAU-CAV	-3.40	111.84	118.03
55	2A	3733	A1CRE	CAC-OAU-CAV	-3.38	111.88	118.03
55	2A	3733	A1CRE	OAR-CAQ-CAT	-3.24	120.88	125.52
55	2A	3733	A1CRE	CBG-CBE-CBF	-3.23	124.65	130.22
55	2A	3733	A1CRE	CAT-CAS-CAD	-3.19	101.63	105.63
55	2A	3733	A1CRE	CAL-CAH-CAI	-3.16	109.65	112.20
57	1B	231	ARG	OXT-C-O	-2.99	117.29	124.08
55	2A	3733	A1CRE	OAU-CAC-CAB	2.81	110.69	106.32
57	1F	317	ARG	OXT-C-O	-2.80	117.73	124.08
55	1A	4012	A1CRE	CAL-CAH-CAI	-2.66	110.06	112.20
55	1A	4012	A1CRE	OAR-CAQ-CAT	-2.65	121.74	125.52
55	2A	3733	A1CRE	CBE-NBD-NBC	-2.61	106.19	109.01
55	2A	3733	A1CRE	CAS-CAD-CAH	-2.49	107.66	110.55
55	1A	4012	A1CRE	CAG-CAB-CAC	2.45	113.79	112.13
55	1A	4012	A1CRE	CBF-NBB-NBC	-2.44	108.38	110.75
55	1A	4012	A1CRE	CAS-CAD-CAH	-2.41	107.76	110.55
55	1A	4012	A1CRE	CAL-CAH-CAD	-2.29	108.27	111.23
55	2A	3733	A1CRE	CAL-CAH-CAD	-2.23	108.35	111.23
55	2A	3733	A1CRE	CBF-CBE-NBD	2.22	110.82	108.12
55	1A	4012	A1CRE	CBG-CBE-CBF	-2.19	126.44	130.22
55	2A	3733	A1CRE	CBA-NBB-NBC	2.15	125.09	120.78
55	1A	4012	A1CRE	CBE-NBD-NBC	-2.11	106.73	109.01
55	1A	4012	A1CRE	OAM-CAI-CAH	-2.09	108.17	110.91

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	1A	4012	A1CRE	CAI-CAJ-CAN-CBA
55	1A	4012	A1CRE	CAK-CAJ-CAN-CBA
55	2A	3733	A1CRE	CAK-CAJ-CAN-CBA
55	2A	3733	A1CRE	CAJ-CAN-CBA-NBB
56	1a	3272	MPD	C2-C3-C4-O4
56	1a	3272	MPD	C2-C3-C4-C5
56	2A	3735	MPD	C2-C3-C4-O4
56	2A	3735	MPD	C2-C3-C4-C5
57	1F	317	ARG	C-CA-CB-CG
55	2A	3733	A1CRE	CBE-CBG-OBH-CBI
57	1B	231	ARG	NE-CD-CG-CB
57	1F	317	ARG	CA-CB-CG-CD
56	1A	4013	MPD	O2-C2-C3-C4
56	18	105	MPD	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
56	1a	3272	MPD	C1-C2-C3-C4
56	2A	3735	MPD	C1-C2-C3-C4
57	1F	317	ARG	N-CA-CB-CG
55	1A	4012	A1CRE	OAU-CAV-CAW-OAY
57	1F	317	ARG	O-C-CA-N
55	1A	4012	A1CRE	CBJ-CBI-OBH-CBG
55	1A	4012	A1CRE	CAW-CAV-OAU-CAC
57	1F	317	ARG	OXT-C-CA-N
55	1A	4012	A1CRE	CAJ-CAN-CBA-NBB
55	2A	3733	A1CRE	OAX-CAV-OAU-CAC
56	18	105	MPD	O2-C2-C3-C4
55	1A	4012	A1CRE	OAX-CAV-OAU-CAC
56	1A	4013	MPD	C2-C3-C4-O4
56	18	105	MPD	C2-C3-C4-O4
56	2A	3734	MPD	C2-C3-C4-O4
56	2B	221	MPD	C2-C3-C4-O4
56	18	105	MPD	CM-C2-C3-C4
56	1a	3272	MPD	CM-C2-C3-C4
56	2A	3735	MPD	CM-C2-C3-C4
55	1A	4012	A1CRE	CAN-CBA-NBB-CBF
55	1A	4012	A1CRE	CAN-CBA-NBB-NBC

There are no ring outliers.

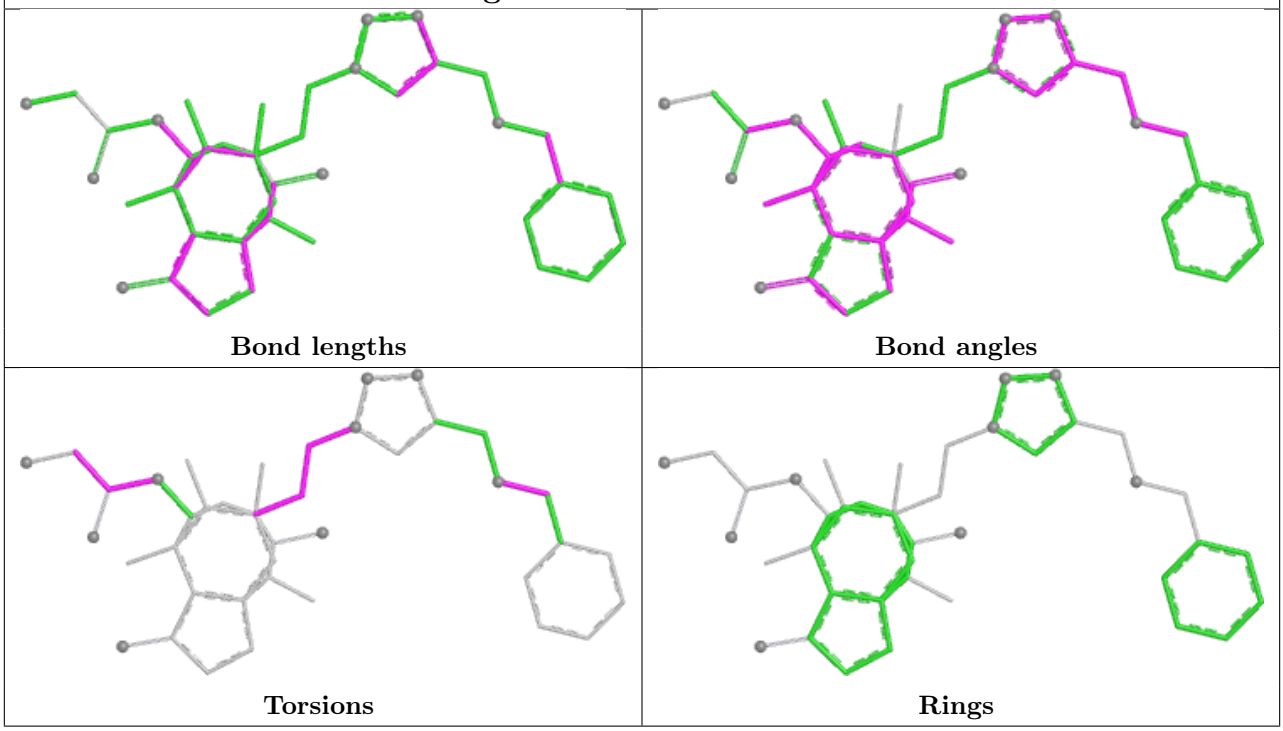
8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	1a	3271	MPD	1	0
56	1a	3272	MPD	1	0
56	2B	221	MPD	1	0
59	1d	306	SF4	1	0
57	1B	231	ARG	2	0
56	18	105	MPD	1	0
56	1A	4013	MPD	1	0
57	1F	317	ARG	2	0

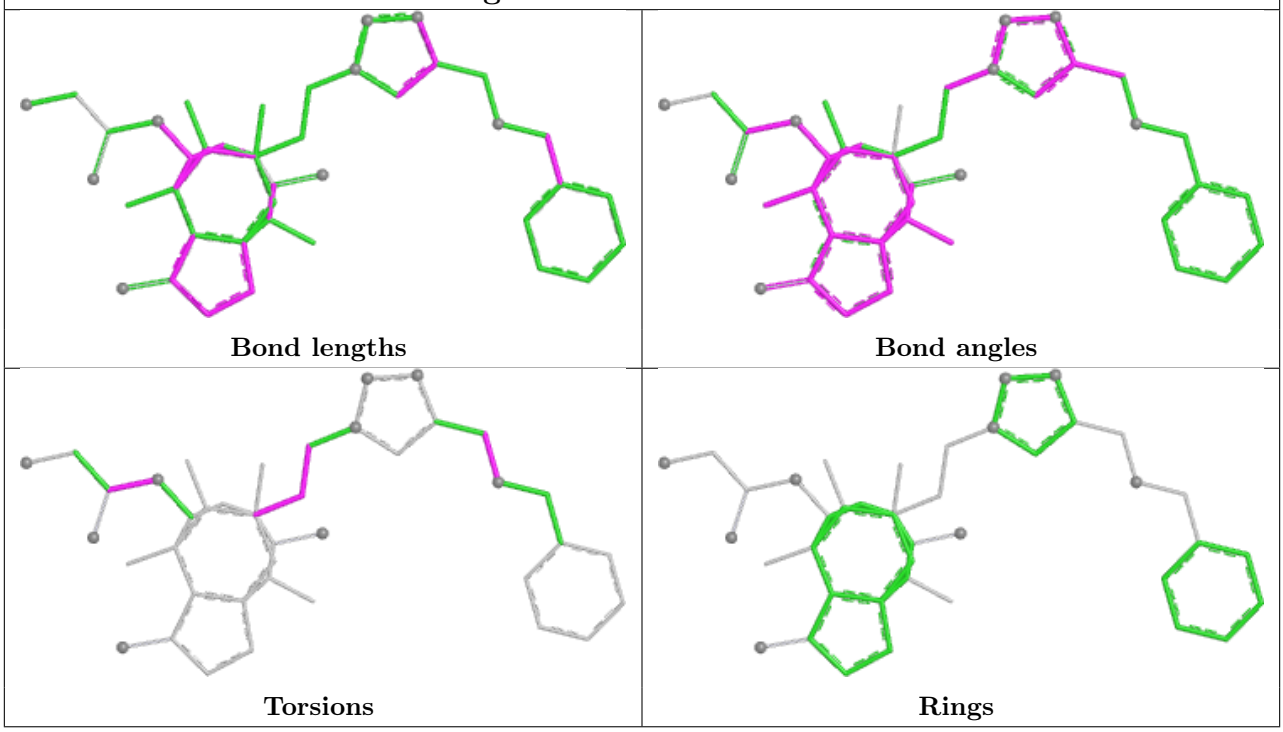
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand A1CRE 1A 4012



Ligand A1CRE 2A 3733



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1A	2861/2915 (98%)	-0.24	149 (5%) 33 26	14, 32, 95, 109	0
1	2A	2856/2915 (97%)	0.23	178 (6%) 26 21	28, 51, 97, 114	0
2	1B	120/121 (99%)	-0.09	1 (0%) 82 77	26, 49, 65, 83	0
2	2B	120/121 (99%)	0.97	11 (9%) 14 12	54, 76, 85, 91	0
3	1D	275/276 (99%)	-0.09	5 (1%) 67 59	18, 32, 47, 66	0
3	2D	275/276 (99%)	0.30	7 (2%) 58 48	27, 45, 60, 78	0
4	1E	204/206 (99%)	-0.07	1 (0%) 87 83	16, 36, 55, 79	0
4	2E	204/206 (99%)	0.46	5 (2%) 58 48	28, 51, 68, 78	0
5	1F	203/210 (96%)	-0.03	1 (0%) 87 83	15, 36, 65, 88	0
5	2F	203/210 (96%)	0.56	7 (3%) 48 39	33, 58, 75, 88	0
6	1G	181/182 (99%)	0.84	14 (7%) 19 16	42, 61, 79, 88	0
6	2G	181/182 (99%)	1.60	55 (30%) 1 1	68, 79, 90, 94	0
7	1H	174/180 (96%)	0.33	4 (2%) 61 52	33, 49, 62, 70	0
7	2H	173/180 (96%)	1.21	26 (15%) 5 4	62, 78, 87, 94	0
8	1I	147/148 (99%)	0.87	13 (8%) 15 13	39, 66, 76, 81	0
8	2I	146/148 (98%)	1.07	14 (9%) 13 11	47, 72, 84, 90	0
9	1N	140/140 (100%)	0.01	1 (0%) 84 79	22, 34, 58, 74	0
9	2N	140/140 (100%)	0.55	4 (2%) 53 45	39, 57, 73, 76	0
10	1O	122/122 (100%)	-0.04	1 (0%) 82 77	25, 34, 52, 58	0
10	2O	122/122 (100%)	0.54	7 (5%) 29 23	39, 50, 62, 71	0
11	1P	149/150 (99%)	0.08	5 (3%) 48 39	17, 40, 59, 72	0
11	2P	149/150 (99%)	0.51	3 (2%) 65 56	33, 61, 77, 83	0
12	1Q	141/141 (100%)	0.06	3 (2%) 63 54	22, 37, 51, 65	0
12	2Q	141/141 (100%)	0.73	8 (5%) 29 23	41, 56, 68, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.17	0 100 100	20, 32, 44, 53	0
13	2R	118/118 (100%)	0.21	1 (0%) 82 77	35, 47, 59, 70	0
14	1S	110/112 (98%)	0.34	1 (0%) 81 75	37, 50, 61, 70	0
14	2S	110/112 (98%)	1.29	15 (13%) 7 5	61, 70, 78, 84	0
15	1T	131/146 (89%)	0.16	4 (3%) 51 42	31, 41, 68, 80	0
15	2T	131/146 (89%)	0.39	5 (3%) 44 36	44, 53, 71, 78	0
16	1U	116/118 (98%)	-0.19	2 (1%) 69 61	18, 26, 47, 65	0
16	2U	116/118 (98%)	0.53	5 (4%) 40 31	33, 55, 70, 73	0
17	1V	101/101 (100%)	-0.14	1 (0%) 79 73	20, 38, 53, 65	0
17	2V	101/101 (100%)	0.77	4 (3%) 42 34	33, 63, 73, 83	0
18	1W	112/113 (99%)	-0.19	1 (0%) 81 75	18, 26, 47, 75	0
18	2W	112/113 (99%)	0.11	1 (0%) 81 75	30, 43, 59, 77	0
19	1X	95/96 (98%)	-0.07	1 (1%) 78 71	24, 34, 56, 71	0
19	2X	95/96 (98%)	0.62	3 (3%) 50 41	40, 53, 72, 80	0
20	1Y	107/110 (97%)	0.41	2 (1%) 66 58	31, 47, 64, 74	0
20	2Y	107/110 (97%)	1.29	22 (20%) 2 2	54, 67, 81, 90	0
21	1Z	203/206 (98%)	0.65	10 (4%) 35 27	34, 56, 75, 83	0
21	2Z	201/206 (97%)	1.26	34 (16%) 4 3	57, 73, 84, 90	0
22	10	77/85 (90%)	0.18	2 (2%) 57 48	24, 33, 50, 62	0
22	20	77/85 (90%)	0.84	5 (6%) 25 20	44, 55, 68, 75	0
23	11	97/98 (98%)	0.48	4 (4%) 41 33	23, 38, 63, 70	0
23	21	97/98 (98%)	0.55	4 (4%) 41 33	34, 50, 71, 75	0
24	12	70/72 (97%)	0.16	1 (1%) 73 65	29, 43, 54, 76	0
24	22	70/72 (97%)	1.13	11 (15%) 5 4	53, 65, 74, 75	0
25	13	59/60 (98%)	0.21	1 (1%) 69 61	23, 34, 57, 75	0
25	23	59/60 (98%)	0.55	1 (1%) 69 61	46, 55, 75, 80	0
26	14	69/71 (97%)	1.25	11 (15%) 5 4	61, 80, 91, 103	0
26	24	69/71 (97%)	2.10	36 (52%) 0 0	77, 88, 97, 102	0
27	15	59/60 (98%)	0.08	2 (3%) 48 39	17, 32, 63, 67	0
27	25	59/60 (98%)	0.52	1 (1%) 69 61	30, 51, 74, 80	0
28	16	53/54 (98%)	-0.06	0 100 100	28, 37, 50, 60	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.56	4 (7%) 20 16	44, 54, 63, 71	0
29	17	48/49 (97%)	-0.23	3 (6%) 26 20	15, 22, 58, 64	0
29	27	48/49 (97%)	0.49	4 (8%) 17 14	29, 38, 63, 65	0
30	18	64/65 (98%)	-0.05	1 (1%) 70 62	21, 29, 37, 47	0
30	28	64/65 (98%)	0.66	6 (9%) 14 12	40, 47, 58, 63	0
31	19	37/37 (100%)	-0.24	0 100 100	29, 38, 54, 66	0
31	29	37/37 (100%)	0.72	0 100 100	51, 62, 72, 79	0
32	1a	1488/1521 (97%)	0.67	86 (5%) 29 22	29, 70, 96, 117	0
32	2a	1492/1521 (98%)	0.75	120 (8%) 18 15	39, 72, 96, 111	0
33	1b	231/256 (90%)	1.48	53 (22%) 2 2	64, 78, 89, 97	0
33	2b	231/256 (90%)	1.49	54 (23%) 2 2	69, 81, 90, 96	0
34	1c	206/239 (86%)	1.35	34 (16%) 4 3	62, 77, 85, 88	0
34	2c	206/239 (86%)	1.79	68 (33%) 1 1	68, 82, 88, 99	0
35	1d	208/209 (99%)	1.64	61 (29%) 1 1	55, 71, 80, 85	0
35	2d	208/209 (99%)	1.29	37 (17%) 4 3	57, 69, 79, 86	0
36	1e	148/162 (91%)	0.76	8 (5%) 31 24	41, 63, 72, 79	0
36	2e	148/162 (91%)	1.16	15 (10%) 12 10	52, 68, 79, 91	0
37	1f	100/101 (99%)	0.93	11 (11%) 10 9	55, 68, 75, 81	0
37	2f	100/101 (99%)	1.12	15 (15%) 5 4	54, 68, 78, 82	0
38	1g	155/156 (99%)	0.91	12 (7%) 19 16	62, 72, 81, 93	0
38	2g	155/156 (99%)	1.06	20 (12%) 7 6	65, 77, 84, 89	0
39	1h	137/138 (99%)	0.80	3 (2%) 62 53	52, 65, 72, 78	0
39	2h	137/138 (99%)	0.96	9 (6%) 24 19	60, 70, 76, 82	0
40	1i	127/128 (99%)	1.83	43 (33%) 1 1	67, 80, 88, 90	0
40	2i	126/128 (98%)	2.14	68 (53%) 0 0	68, 84, 89, 93	0
41	1j	97/105 (92%)	1.98	41 (42%) 0 0	66, 82, 89, 95	0
41	2j	96/105 (91%)	2.10	51 (53%) 0 0	74, 85, 92, 94	0
42	1k	114/129 (88%)	0.92	12 (10%) 11 10	39, 60, 74, 79	0
42	2k	114/129 (88%)	0.99	9 (7%) 18 15	57, 68, 78, 82	0
43	1l	121/132 (91%)	0.69	3 (2%) 58 48	46, 57, 68, 74	0
43	2l	121/132 (91%)	0.95	8 (6%) 24 19	51, 63, 71, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	116/126 (92%)	1.34	21 (18%) 3 3	62, 76, 83, 86	0
44	2m	114/126 (90%)	1.66	38 (33%) 1 1	71, 82, 87, 89	0
45	1n	60/61 (98%)	1.72	22 (36%) 1 0	62, 75, 82, 85	0
45	2n	60/61 (98%)	2.32	30 (50%) 0 0	75, 83, 88, 90	0
46	1o	88/89 (98%)	0.80	8 (9%) 15 12	47, 63, 74, 80	0
46	2o	88/89 (98%)	0.66	3 (3%) 48 39	57, 68, 78, 82	0
47	1p	82/88 (93%)	1.22	12 (14%) 6 4	58, 71, 81, 87	0
47	2p	82/88 (93%)	1.06	10 (12%) 8 7	55, 64, 74, 79	0
48	1q	99/105 (94%)	0.82	5 (5%) 33 26	48, 63, 73, 78	0
48	2q	99/105 (94%)	0.77	5 (5%) 33 26	51, 63, 74, 78	0
49	1r	68/88 (77%)	1.14	8 (11%) 9 7	54, 66, 78, 82	0
49	2r	68/88 (77%)	0.93	5 (7%) 20 17	59, 68, 79, 81	0
50	1s	83/93 (89%)	1.73	27 (32%) 1 1	69, 79, 86, 90	0
50	2s	83/93 (89%)	2.11	37 (44%) 0 0	72, 86, 93, 97	0
51	1t	96/106 (90%)	1.23	22 (22%) 2 2	57, 70, 77, 83	0
51	2t	98/106 (92%)	0.81	8 (8%) 17 14	56, 65, 76, 83	0
52	1u	23/27 (85%)	1.85	9 (39%) 1 0	66, 72, 78, 81	0
52	2u	23/27 (85%)	2.11	13 (56%) 0 0	72, 81, 85, 88	0
53	1y	97/113 (85%)	0.79	4 (4%) 41 33	50, 64, 74, 78	0
53	2y	96/113 (84%)	1.88	37 (38%) 1 0	68, 81, 88, 92	0
All	All	20766/21468 (96%)	0.57	1897 (9%) 15 12	14, 60, 89, 117	0

All (1897) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	11	2	SER	12.1
1	2A	2119	A	8.9
1	1A	1087	G	8.6
45	2n	2	ALA	8.4
1	1A	1091	G	8.4
35	1d	4	TYR	8.1
1	2A	2173	A	7.8
7	1H	2	SER	7.6
44	2m	102	ARG	7.2
1	1A	2174	C	7.2

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Mol	Chain	Res	Type	RSRZ
1	1A	2173	A	7.1
1	1A	1076	C	7.1
1	1A	1092	C	7.1
1	2A	2125	G	7.0
1	2A	2118	U	6.9
23	21	2	SER	6.8
1	2A	2169	A	6.7
1	1A	2172	U	6.6
1	1A	1089	G	6.6
1	2A	2162	G	6.6
1	1A	1072	C	6.6
1	2A	2174	C	6.5
1	1A	1103	A	6.5
1	2A	2168	G	6.4
1	2A	2107	C	6.4
35	2d	4	TYR	6.4
1	1A	2176	A	6.4
1	1A	1093	G	6.4
1	2A	2123	G	6.4
1	1A	1064	C	6.3
1	1A	2117	A	6.3
1	2A	2147	G	6.2
1	2A	2172	U	6.2
1	2A	2170	A	6.1
53	2y	98	ALA	6.0
1	2A	2176	A	5.9
1	1A	2123	G	5.9
1	2A	2110	G	5.9
1	1A	1088	A	5.9
1	2A	2120	G	5.8
1	1A	1086	A	5.8
1	1A	1104	C	5.8
44	1m	2	ALA	5.8
1	1A	2108	C	5.7
50	2s	11	VAL	5.7
1	2A	2124	G	5.6
32	2a	1094	G	5.6
32	2a	1001(A)	G	5.5
1	1A	2116	G	5.5
1	1A	1071	G	5.5
1	2A	2166	G	5.5
45	1n	2	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
1	2A	1075	C	5.4
32	2a	1030(B)	C	5.4
35	1d	115	ARG	5.4
1	2A	1083	U	5.4
1	1A	1081	U	5.4
1	1A	2161	C	5.3
1	2A	2175	C	5.3
26	24	49	PHE	5.3
1	2A	1089	G	5.3
20	2Y	1	MET	5.3
1	2A	1076	C	5.2
33	1b	213	LEU	5.2
1	2A	2171	A	5.2
36	2e	20	GLN	5.2
40	2i	126	SER	5.2
1	1A	2109	U	5.2
1	1A	1102	C	5.2
26	24	45	GLY	5.1
1	1A	2175	C	5.1
12	2Q	22	LYS	5.1
1	2A	2148	G	5.1
1	1A	1066	U	5.1
12	2Q	59	ARG	5.1
1	2A	1536	C	5.1
1	2A	2130	U	5.1
28	26	20	ASN	5.0
53	1y	98	ALA	5.0
11	1P	15	ARG	5.0
50	2s	12	ASP	5.0
51	1t	103	GLY	5.0
32	2a	1039	C	4.9
1	1A	1063	G	4.9
50	1s	84	GLY	4.9
32	2a	1036	G	4.9
44	2m	106	ASN	4.9
38	2g	32	ARG	4.9
15	1T	131	ALA	4.9
53	2y	38	HIS	4.9
41	2j	55	LYS	4.9
1	2A	2131	G	4.8
21	2Z	72	ARG	4.8
50	2s	79	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	2A	1046	A	4.8
32	1a	630	G	4.8
1	2A	2126	A	4.8
1	2A	2129	C	4.8
1	2A	2165	G	4.8
32	1a	1036	G	4.8
40	1i	15	ALA	4.8
40	2i	102	LEU	4.7
1	2A	2802	G	4.7
45	2n	32	SER	4.7
1	1A	1085	A	4.7
40	1i	66	ARG	4.7
6	2G	28	VAL	4.7
44	2m	103	THR	4.7
32	2a	1003	G	4.7
32	1a	1001	A	4.7
1	1A	1083	U	4.6
1	2A	2112	G	4.6
1	2A	1088	A	4.6
1	2A	1171	G	4.6
1	2A	2127	G	4.6
41	1j	44	VAL	4.6
26	14	59	PHE	4.6
40	2i	7	THR	4.6
1	2A	2179	C	4.6
32	2a	1030(A)	G	4.6
40	1i	106	ALA	4.5
44	1m	100	GLY	4.5
1	2A	2111	C	4.5
32	2a	1037	C	4.5
32	2a	1068	G	4.5
51	2t	6	PRO	4.5
1	1A	1090	U	4.5
1	1A	2119	A	4.5
1	2A	2106	G	4.4
1	1A	1057	A	4.4
32	2a	1027	C	4.4
1	2A	2121	G	4.4
44	2m	5	ALA	4.4
1	1A	1067	A	4.4
1	2A	2167	U	4.4
35	1d	5	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
20	1Y	1	MET	4.4
1	2A	1070	A	4.4
1	2A	1178	C	4.4
1	1A	2120	G	4.3
1	1A	2125	G	4.3
32	1a	174	C	4.3
34	2c	163	ALA	4.3
26	24	57	GLU	4.3
40	1i	102	LEU	4.3
52	2u	9	ARG	4.3
1	1A	2147	G	4.3
1	1A	2148	G	4.3
1	1A	2171	A	4.3
49	1r	76	LEU	4.3
1	2A	2602	A	4.3
32	2a	1224	G	4.3
14	2S	34	HIS	4.3
1	2A	652(B)	A	4.2
1	2A	1071	G	4.2
1	2A	2136	C	4.2
35	2d	5	ILE	4.2
40	2i	66	ARG	4.2
1	1A	2177	C	4.2
38	2g	33	ASP	4.2
1	1A	2150	U	4.2
33	1b	237	ALA	4.2
35	1d	21	LEU	4.2
1	2A	2146	C	4.2
32	1a	1026	G	4.2
50	2s	33	THR	4.2
1	1A	2129	C	4.1
1	1A	2110	G	4.1
1	2A	1091	G	4.1
32	2a	1002	G	4.1
23	21	26	ARG	4.1
40	1i	109	VAL	4.1
41	2j	44	VAL	4.1
41	1j	38	ILE	4.1
1	1A	1074	G	4.1
1	1A	2124	G	4.1
33	2b	237	ALA	4.1
40	2i	106	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
6	2G	35	GLU	4.1
3	2D	276	LYS	4.1
41	2j	65	LEU	4.1
37	1f	6	VAL	4.1
6	2G	2	PRO	4.1
41	1j	76	ASN	4.1
34	1c	2	GLY	4.1
1	1A	2149	G	4.1
1	2A	2117	A	4.1
41	2j	40	LEU	4.1
34	2c	8	ILE	4.1
35	1d	6	GLY	4.1
1	2A	1087	G	4.1
53	2y	42	SER	4.0
1	1A	2107	C	4.0
1	2A	2177	C	4.0
51	1t	18	GLN	4.0
6	1G	139	LEU	4.0
1	2A	2133	G	4.0
53	2y	62	VAL	4.0
37	2f	89	MET	4.0
41	1j	32	ALA	4.0
35	1d	3	ARG	4.0
24	22	1	MET	4.0
16	2U	7	GLY	4.0
33	1b	227	GLY	4.0
34	2c	158	GLY	4.0
34	2c	159	GLY	4.0
40	1i	128	ARG	3.9
1	1A	1080	C	3.9
26	14	57	GLU	3.9
45	1n	4	LYS	3.9
6	2G	76	SER	3.9
44	1m	117	VAL	3.9
1	1A	1062	G	3.9
23	11	26	ARG	3.9
43	1l	89	ARG	3.9
35	1d	171	GLY	3.9
50	1s	16	LEU	3.9
1	1A	1077	A	3.9
1	2A	2138	C	3.9
6	2G	53	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
41	1j	40	LEU	3.9
33	1b	95	GLN	3.9
8	2I	86	THR	3.9
26	14	50	VAL	3.8
45	2n	18	VAL	3.8
42	2k	117	ASN	3.8
40	2i	15	ALA	3.8
32	1a	1001(A)	G	3.8
35	1d	11	LEU	3.8
40	1i	56	LEU	3.8
51	2t	103	GLY	3.8
1	2A	2108	C	3.8
50	2s	9	VAL	3.8
52	2u	6	ARG	3.8
40	2i	127	LYS	3.8
14	2S	32	LEU	3.8
1	2A	2161	C	3.8
32	1a	221	C	3.8
32	2a	1116	C	3.8
32	1a	1035	A	3.8
53	1y	2	THR	3.8
45	1n	3	ARG	3.8
1	1A	2168	G	3.8
1	2A	1059	G	3.8
1	2A	1074	G	3.8
1	2A	2151	G	3.8
1	2A	2122	U	3.8
26	24	63	TYR	3.8
1	1A	1084	A	3.8
1	2A	1067	A	3.8
20	2Y	73	ARG	3.7
34	1c	179	ARG	3.7
34	2c	190	ARG	3.7
26	24	22	ILE	3.7
47	1p	68	ASP	3.7
33	2b	97	TRP	3.7
1	1A	2127	G	3.7
1	1A	2160	G	3.7
1	2A	2135	A	3.7
33	2b	12	GLU	3.7
41	1j	42	THR	3.7
6	2G	88	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
41	2j	37	PRO	3.7
33	2b	121	LEU	3.7
40	2i	5	TYR	3.7
32	1a	1003	G	3.7
40	1i	121	ARG	3.7
1	1A	1073	A	3.7
1	1A	2169	A	3.7
33	1b	133	LYS	3.7
44	1m	102	ARG	3.7
33	2b	22	LYS	3.7
44	1m	116	THR	3.7
34	2c	66	VAL	3.7
1	1A	2166	G	3.7
1	2A	1062	G	3.7
1	2A	2894	G	3.7
32	1a	1139	G	3.7
45	2n	30	ALA	3.7
35	1d	10	ARG	3.7
45	2n	3	ARG	3.7
1	2A	2139	C	3.6
34	2c	2	GLY	3.6
41	1j	4	ILE	3.6
1	2A	2109	U	3.6
53	1y	9	GLN	3.6
36	2e	21	ALA	3.6
32	1a	1037	C	3.6
50	1s	13	ASP	3.6
26	24	52	THR	3.6
1	2A	1081	U	3.6
50	2s	50	ALA	3.6
35	1d	118	ARG	3.6
1	2A	2164	C	3.6
32	1a	1030(B)	C	3.6
40	2i	2	GLU	3.6
41	2j	49	VAL	3.6
53	2y	60	VAL	3.6
42	2k	119	CYS	3.6
49	1r	20	ALA	3.6
53	2y	50	ALA	3.6
41	2j	46	ARG	3.6
40	2i	125	TYR	3.6
1	2A	1095	A	3.6

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Mol	Chain	Res	Type	RSRZ
32	2a	1035	A	3.6
24	22	9	GLN	3.5
26	24	35	VAL	3.5
17	2V	91	TYR	3.5
1	2A	1096	A	3.5
6	2G	41	GLN	3.5
6	1G	44	GLY	3.5
1	1A	2121	G	3.5
50	1s	79	THR	3.5
1	2A	2140	C	3.5
32	2a	1001	A	3.5
1	1A	2167	U	3.5
41	1j	10	GLY	3.5
38	2g	80	VAL	3.5
19	1X	95	LEU	3.5
35	2d	39	PRO	3.5
33	2b	236	TYR	3.5
34	1c	193	TYR	3.5
1	1A	2115	G	3.5
1	2A	2128	C	3.5
35	1d	170	VAL	3.5
1	2A	2132	U	3.5
40	2i	110	GLU	3.5
1	2A	2149	G	3.4
24	22	19	VAL	3.4
53	2y	43	LYS	3.4
1	1A	1079	C	3.4
1	2A	2113	U	3.4
35	2d	73	ARG	3.4
40	2i	105	ASP	3.4
6	2G	146	TYR	3.4
20	2Y	55	TYR	3.4
45	2n	34	TYR	3.4
6	2G	44	GLY	3.4
44	1m	24	GLY	3.4
47	1p	12	LYS	3.4
33	1b	15	VAL	3.4
53	2y	41	LEU	3.4
41	2j	79	ARG	3.4
32	2a	1093	A	3.4
32	1a	1027	C	3.4
15	1T	130	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
40	1i	103	THR	3.4
53	2y	9	GLN	3.4
40	1i	30	GLY	3.4
45	2n	25	VAL	3.4
52	2u	11	GLY	3.4
41	1j	39	PRO	3.4
1	1A	1105	U	3.4
1	1A	2162	G	3.4
1	2A	1057	A	3.4
1	2A	1085	A	3.4
32	1a	1034	G	3.4
32	2a	1026	G	3.4
35	1d	195	ALA	3.4
42	1k	60	ALA	3.4
5	2F	175	THR	3.4
1	1A	2128	C	3.4
1	2A	2803	C	3.4
33	1b	154	LEU	3.4
39	2h	112	LEU	3.4
7	2H	82	GLY	3.4
50	2s	84	GLY	3.4
45	2n	49	HIS	3.4
8	2I	89	TYR	3.4
14	2S	58	LEU	3.3
32	2a	1067	A	3.4
20	2Y	58	GLY	3.3
35	2d	2	GLY	3.3
30	28	29	LYS	3.3
1	1A	2118	U	3.3
41	1j	33	GLN	3.3
53	2y	53	THR	3.3
8	1I	89	TYR	3.3
33	1b	148	TYR	3.3
36	2e	133	TYR	3.3
18	1W	112	GLY	3.3
6	1G	35	GLU	3.3
1	1A	1075	C	3.3
1	2A	1104	C	3.3
1	1A	11	G	3.3
1	2A	2159	G	3.3
32	2a	1034	G	3.3
21	2Z	1	MET	3.3

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Mol	Chain	Res	Type	RSRZ
34	2c	188	LEU	3.3
35	1d	162	LEU	3.3
1	1A	1082	U	3.3
1	2A	2180	U	3.3
2	2B	1	U	3.3
16	2U	8	VAL	3.3
32	2a	1040	U	3.3
8	2I	84	GLY	3.3
43	2l	87	GLY	3.3
50	2s	53	ASN	3.3
1	2A	1084	A	3.3
7	2H	136	ILE	3.3
32	1a	1129	C	3.3
33	1b	127	ILE	3.3
53	2y	40	ILE	3.3
1	2A	2115	G	3.3
1	2A	2160	G	3.3
32	1a	1002	G	3.3
35	1d	194	LEU	3.3
48	1q	98	LEU	3.3
40	2i	64	THR	3.3
33	2b	38	GLY	3.3
44	2m	6	GLY	3.3
40	2i	11	LYS	3.3
50	2s	55	LYS	3.3
33	1b	207	ALA	3.3
34	2c	189	ALA	3.3
1	2A	652(T)	C	3.3
1	2A	1072	C	3.3
7	2H	6	ARG	3.3
32	1a	1038	C	3.3
41	1j	66	ARG	3.3
33	1b	67	THR	3.3
21	1Z	200	GLY	3.3
41	2j	52	GLY	3.3
24	22	52	ASP	3.2
41	1j	78	ASN	3.2
33	2b	201	ILE	3.2
6	2G	50	ALA	3.2
29	27	45	ALA	3.2
32	1a	162	A	3.2
1	1A	1065	U	3.2

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Mol	Chain	Res	Type	RSRZ
1	1A	2112	G	3.2
7	2H	118	PRO	3.2
8	2I	74	ASN	3.2
21	1Z	1	MET	3.2
32	1a	1030(A)	G	3.2
32	2a	1108	G	3.2
33	1b	125	PRO	3.2
41	1j	69	ASN	3.2
6	1G	88	ILE	3.2
35	1d	188	LEU	3.2
50	2s	14	HIS	3.2
39	2h	3	THR	3.2
6	2G	142	PRO	3.2
21	2Z	87	ASP	3.2
40	2i	91	ASP	3.2
3	1D	2	ALA	3.2
45	2n	6	LEU	3.2
1	1A	10	G	3.2
7	2H	45	VAL	3.2
34	2c	153	VAL	3.2
44	1m	27	LYS	3.2
26	14	52	THR	3.2
33	1b	222	ILE	3.2
35	2d	7	PRO	3.2
49	1r	34	TYR	3.2
51	1t	64	ASP	3.2
35	2d	122	ARG	3.2
40	2i	99	LEU	3.2
1	2A	362	U	3.2
2	1B	1	U	3.2
40	2i	43	ALA	3.2
47	1p	13	HIS	3.2
3	2D	38	LYS	3.2
29	27	48	LYS	3.2
37	2f	90	VAL	3.2
26	24	47	GLN	3.2
32	1a	102	G	3.2
32	2a	630	G	3.2
40	1i	7	THR	3.2
1	2A	2114	A	3.1
19	2X	68	ARG	3.1
20	2Y	52	SER	3.1

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Mol	Chain	Res	Type	RSRZ
50	1s	38	SER	3.1
50	2s	30	LEU	3.1
36	1e	45	PHE	3.1
32	2a	1149	C	3.1
38	2g	21	VAL	3.1
40	2i	86	VAL	3.1
44	2m	60	VAL	3.1
45	2n	33	VAL	3.1
1	1A	2165	G	3.1
1	2A	1058	G	3.1
1	2A	1533	G	3.1
1	2A	2116	G	3.1
32	1a	1143	G	3.1
32	2a	1017	G	3.1
50	2s	34	TRP	3.1
6	1G	146	TYR	3.1
26	24	67	TYR	3.1
34	2c	187	ALA	3.1
35	1d	137	SER	3.1
51	1t	68	LYS	3.1
1	1A	548	A	3.1
1	1A	2170	A	3.1
1	2A	1073	A	3.1
40	1i	18	PHE	3.1
20	2Y	57	GLN	3.1
35	1d	2	GLY	3.1
40	2i	39	GLY	3.1
6	2G	45	GLU	3.1
41	2j	39	PRO	3.1
50	2s	15	LEU	3.1
34	1c	26	LYS	3.1
53	2y	8	LYS	3.1
33	1b	120	ALA	3.1
1	1A	2151	G	3.1
6	2G	149	VAL	3.1
32	1a	198	G	3.1
32	1a	1224	G	3.1
32	2a	1117	G	3.1
40	1i	105	ASP	3.1
40	2i	108	VAL	3.1
32	1a	1447	A	3.1
32	2a	1219	U	3.1

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Mol	Chain	Res	Type	RSRZ
35	1d	42	GLN	3.1
7	2H	4	ILE	3.1
41	1j	6	ILE	3.1
41	1j	74	ILE	3.1
1	2A	2137	C	3.1
1	2A	2178	C	3.1
1	2A	2896	C	3.1
29	17	47	ARG	3.1
34	2c	79	ARG	3.1
28	26	21	TYR	3.1
33	2b	136	VAL	3.1
34	2c	128	PHE	3.1
40	2i	18	PHE	3.1
33	2b	72	GLY	3.1
1	1A	2122	U	3.1
38	2g	42	ILE	3.1
39	2h	35	ILE	3.1
45	2n	7	ILE	3.1
20	2Y	54	LYS	3.1
33	1b	232	PRO	3.1
50	2s	48	THR	3.1
21	2Z	192	ALA	3.0
32	1a	1030	C	3.1
21	2Z	191	VAL	3.0
40	1i	86	VAL	3.0
50	2s	10	PHE	3.0
50	2s	52	TYR	3.0
4	2E	1	MET	3.0
15	1T	38	ASN	3.0
35	2d	23	GLY	3.0
40	2i	6	GLY	3.0
53	2y	46	GLN	3.0
33	2b	127	ILE	3.0
35	1d	135	LEU	3.0
41	1j	8	LEU	3.0
1	1A	12	U	3.0
1	2A	1060	U	3.0
1	2A	614(B)	G	3.0
32	1a	1030(C)	G	3.0
34	2c	137	ALA	3.0
34	1c	128	PHE	3.0
38	2g	9	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
40	1i	17	VAL	3.0
32	2a	1325	C	3.0
33	1b	66	GLY	3.0
10	2O	66	LYS	3.0
20	2Y	4	LYS	3.0
38	2g	4	ARG	3.0
25	13	2	PRO	3.0
33	2b	232	PRO	3.0
41	2j	41	PRO	3.0
32	2a	1235	U	3.0
41	2j	42	THR	3.0
1	2A	229	A	3.0
53	1y	97	ALA	3.0
12	2Q	1	MET	3.0
40	1i	58	HIS	3.0
44	2m	54	VAL	3.0
1	1A	2133	G	3.0
1	2A	2104	G	3.0
32	1a	104	G	3.0
32	1a	220	G	3.0
32	2a	1032	G	3.0
1	1A	2140	C	3.0
33	2b	214	ILE	3.0
41	1j	5	ARG	3.0
42	2k	123	LYS	3.0
34	2c	3	ASN	3.0
34	2c	170	GLN	3.0
52	1u	24	ARG	3.0
53	2y	79	ASN	3.0
35	2d	21	LEU	3.0
50	2s	16	LEU	3.0
10	1O	108	GLU	3.0
1	2A	2150	U	3.0
21	2Z	184	ALA	3.0
29	27	46	VAL	3.0
40	1i	53	VAL	3.0
1	2A	653	A	3.0
6	2G	118	ARG	3.0
36	2e	64	ARG	3.0
40	2i	9	ARG	3.0
46	1o	88	ARG	3.0
26	14	54	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
33	1b	221	LEU	3.0
35	1d	124	GLY	3.0
50	2s	71	LEU	3.0
1	2A	10	G	3.0
1	1A	1532	C	3.0
6	2G	87	PRO	3.0
32	2a	1038	C	3.0
34	2c	168	ALA	3.0
41	2j	87	THR	3.0
41	2j	47	PHE	3.0
32	1a	1000	U	3.0
12	2Q	5	ARG	2.9
20	2Y	2	ARG	2.9
22	20	74	ARG	2.9
35	1d	76	ARG	2.9
1	1A	1095	A	2.9
1	1A	2126	A	2.9
33	1b	236	TYR	2.9
37	1f	94	GLN	2.9
35	1d	102	ASP	2.9
37	2f	17	SER	2.9
1	1A	1058	G	2.9
6	2G	155	MET	2.9
32	2a	1021	G	2.9
32	1a	1029	C	2.9
44	1m	98	VAL	2.9
45	1n	16	PHE	2.9
1	2A	12	U	2.9
7	2H	59	ARG	2.9
34	2c	156	ARG	2.9
6	1G	52	ILE	2.9
34	2c	118	GLN	2.9
52	1u	18	TYR	2.9
34	1c	73	PRO	2.9
6	2G	48	GLU	2.9
34	2c	105	GLU	2.9
35	1d	145	GLU	2.9
34	2c	56	ASP	2.9
6	1G	50	ALA	2.9
37	2f	88	VAL	2.9
6	2G	47	LYS	2.9
1	1A	2138	C	2.9

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Mol	Chain	Res	Type	RSRZ
32	1a	163	C	2.9
35	2d	3	ARG	2.9
35	2d	118	ARG	2.9
45	2n	12	ARG	2.9
51	1t	8	ARG	2.9
1	2A	1093	G	2.9
1	2A	2893	G	2.9
32	1a	1023	G	2.9
6	2G	39	ILE	2.9
44	2m	19	LEU	2.9
34	1c	13	GLY	2.9
40	2i	8	GLY	2.9
47	1p	41	PRO	2.9
32	2a	1004	A	2.9
4	1E	204	ALA	2.9
34	2c	207	VAL	2.9
37	2f	6	VAL	2.9
43	2l	32	PHE	2.9
24	22	51	ARG	2.9
6	1G	157	ILE	2.9
47	2p	19	ILE	2.9
53	2y	39	ILE	2.9
34	2c	52	LEU	2.9
41	1j	65	LEU	2.9
1	1A	1509	C	2.9
1	1A	2130	U	2.9
44	1m	85	GLY	2.9
44	2m	24	GLY	2.9
1	2A	2141	G	2.9
1	2A	2153	G	2.9
1	2A	2154	G	2.9
32	1a	1031	G	2.9
32	2a	1202	G	2.9
26	14	32	TYR	2.9
37	2f	4	TYR	2.9
38	2g	85	TYR	2.9
45	2n	21	TYR	2.9
41	2j	83	GLU	2.9
45	2n	8	GLU	2.9
21	2Z	201	LYS	2.9
8	2I	146	ALA	2.9
33	2b	165	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
41	2j	63	PHE	2.9
1	1A	2629	A	2.9
6	2G	83	ARG	2.9
22	10	55	ARG	2.9
40	2i	120	ARG	2.9
44	2m	99	ARG	2.9
44	2m	116	THR	2.9
50	1s	33	THR	2.9
40	2i	40	LEU	2.9
35	1d	7	PRO	2.8
46	1o	62	GLN	2.8
1	1A	2178	C	2.8
1	2A	1080	C	2.8
21	2Z	29	TYR	2.8
32	1a	1039	C	2.8
33	2b	126	GLU	2.8
1	1A	2153	G	2.8
29	17	46	VAL	2.8
38	1g	87	VAL	2.8
40	2i	109	VAL	2.8
47	2p	68	ASP	2.8
51	2t	11	SER	2.8
33	1b	39	ILE	2.8
34	1c	204	LEU	2.8
37	1f	19	LEU	2.8
37	2f	43	LEU	2.8
50	1s	72	GLY	2.8
3	2D	150	LYS	2.8
41	2j	7	LYS	2.8
3	2D	28	GLU	2.8
8	1I	85	GLU	2.8
33	2b	129	GLU	2.8
47	1p	17	TYR	2.8
14	2S	12	PHE	2.8
32	2a	1320	C	2.8
35	2d	115	ARG	2.8
40	2i	94	ALA	2.8
51	1t	97	ALA	2.8
6	2G	27	ASN	2.8
12	2Q	2	LEU	2.8
41	2j	85	LEU	2.8
45	1n	7	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
46	1o	57	LEU	2.8
35	2d	137	SER	2.8
1	2A	545	G	2.8
1	2A	652(U)	G	2.8
1	2A	2152	G	2.8
1	2A	654	A	2.8
40	1i	6	GLY	2.8
41	1j	93	GLY	2.8
8	1I	147	GLN	2.8
41	2j	91	PRO	2.8
50	2s	2	PRO	2.8
50	2s	76	PRO	2.8
35	2d	34	GLU	2.8
33	2b	137	ARG	2.8
41	1j	43	ARG	2.8
32	1a	1049	U	2.8
32	2a	1020	U	2.8
50	1s	9	VAL	2.8
34	2c	129	ALA	2.8
35	2d	195	ALA	2.8
26	24	15	ILE	2.8
40	2i	50	LEU	2.8
1	1A	2142	C	2.8
41	2j	10	GLY	2.8
35	2d	172	PRO	2.8
44	2m	113	PRO	2.8
11	1P	70	GLN	2.8
12	1Q	141	GLN	2.8
32	2a	949	A	2.8
37	1f	87	ARG	2.8
40	2i	10	ARG	2.8
45	2n	31	ARG	2.8
34	2c	195	VAL	2.8
33	2b	92	TYR	2.8
22	10	84	LEU	2.8
33	1b	187	LEU	2.8
47	2p	13	HIS	2.8
41	2j	69	ASN	2.8
6	2G	147	ASP	2.8
9	2N	43	THR	2.8
26	14	69	LYS	2.8
51	1t	14	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
52	1u	17	THR	2.8
1	2A	1049	C	2.8
32	1a	219	C	2.8
32	2a	1066	C	2.8
40	1i	126	SER	2.8
41	2j	19	SER	2.8
3	1D	234	GLY	2.8
6	2G	89	GLY	2.8
8	1I	90	GLY	2.8
33	2b	99	GLY	2.8
35	1d	69	GLY	2.8
35	2d	37	PRO	2.8
40	2i	21	PRO	2.8
8	1I	41	GLU	2.7
35	1d	122	ARG	2.7
21	2Z	27	VAL	2.7
21	2Z	56	VAL	2.7
41	1j	72	VAL	2.7
1	1A	275	G	2.7
1	1A	2157	G	2.7
1	1A	2602	A	2.7
1	2A	171	G	2.7
1	2A	1056	G	2.7
32	2a	1092	A	2.7
40	2i	52	ALA	2.7
14	2S	54	LEU	2.7
26	24	32	TYR	2.7
34	1c	87	LEU	2.7
1	1A	271(K)	U	2.7
33	2b	133	LYS	2.7
51	2t	9	ASN	2.7
37	2f	55	ASP	2.7
41	2j	100	THR	2.7
52	2u	8	THR	2.7
34	2c	114	PRO	2.7
35	1d	37	PRO	2.7
45	2n	14	PRO	2.7
1	2A	34	C	2.7
24	12	70	GLN	2.7
40	1i	120	ARG	2.7
27	15	59	GLU	2.7
8	2I	92	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
33	2b	7	VAL	2.7
40	1i	65	VAL	2.7
15	2T	130	ALA	2.7
41	2j	32	ALA	2.7
45	2n	61	TRP	2.7
33	2b	19	HIS	2.7
34	1c	6	HIS	2.7
44	1m	87	TYR	2.7
1	1A	529	A	2.7
32	1a	1286	A	2.7
32	2a	1005	A	2.7
45	2n	15	LYS	2.7
51	1t	74	LYS	2.7
1	1A	2181	G	2.7
1	1A	2894	G	2.7
1	2A	2181	G	2.7
32	1a	993	G	2.7
32	2a	1033	G	2.7
20	1Y	92	ASN	2.7
26	24	44	THR	2.7
33	2b	67	THR	2.7
34	1c	177	THR	2.7
51	2t	69	GLY	2.7
41	2j	53	PRO	2.7
6	1G	76	SER	2.7
44	2m	104	ARG	2.7
45	2n	29	ARG	2.7
50	1s	37	ARG	2.7
50	2s	4	SER	2.7
50	2s	29	ARG	2.7
26	24	30	GLU	2.7
20	2Y	45	VAL	2.7
26	24	21	VAL	2.7
1	1A	2164	C	2.7
24	22	58	ALA	2.7
26	24	14	ILE	2.7
32	2a	1018	C	2.7
32	2a	1029	C	2.7
38	1g	7	ALA	2.7
41	1j	71	LEU	2.7
44	1m	51	ALA	2.7
52	2u	13	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
20	2Y	5	MET	2.7
1	1A	1177	A	2.7
1	1A	1078	U	2.7
1	2A	1082	U	2.7
37	2f	7	ASN	2.7
53	2y	4	ASN	2.7
21	2Z	103	ARG	2.7
34	2c	80	GLY	2.7
52	1u	6	ARG	2.7
1	2A	11	G	2.7
26	24	46	GLN	2.7
32	1a	78	G	2.7
32	1a	1131	G	2.7
32	2a	1010	G	2.7
37	1f	17	SER	2.7
47	1p	82	GLN	2.7
7	2H	11	VAL	2.7
21	2Z	42	VAL	2.7
49	1r	60	ALA	2.7
1	1A	154(A)	C	2.7
32	1a	1019	C	2.7
32	2a	1128	C	2.7
41	2j	31	GLY	2.7
50	2s	63	THR	2.7
32	2a	1236	A	2.7
23	11	47	GLN	2.7
34	2c	64	VAL	2.7
48	2q	98	LEU	2.7
26	24	59	PHE	2.6
51	1t	66	ALA	2.6
1	1A	2141	G	2.6
1	2A	361	G	2.6
32	1a	1033	G	2.6
33	1b	48	MET	2.6
35	1d	173	TRP	2.6
26	14	63	TYR	2.6
37	1f	50	TYR	2.6
32	1a	1028	C	2.6
34	1c	174	PRO	2.6
44	2m	100	GLY	2.6
35	1d	154	ASN	2.6
1	1A	1101	U	2.6

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Mol	Chain	Res	Type	RSRZ
21	2Z	125	LEU	2.6
34	2c	162	GLN	2.6
35	1d	108	LEU	2.6
36	2e	12	LEU	2.6
41	1j	34	VAL	2.6
41	2j	8	LEU	2.6
45	2n	17	LYS	2.6
47	2p	12	LYS	2.6
50	2s	41	VAL	2.6
1	2A	1077	A	2.6
34	2c	182	ILE	2.6
40	2i	59	PHE	2.6
41	1j	30	SER	2.6
1	1A	1176	G	2.6
32	2a	1220	G	2.6
33	1b	131	PRO	2.6
1	2A	1064	C	2.6
1	2A	2163	C	2.6
8	1I	141	LYS	2.6
15	2T	55	ASN	2.6
23	21	92	LYS	2.6
29	17	48	LYS	2.6
32	2a	1129	C	2.6
32	2a	1223	C	2.6
35	1d	169	LYS	2.6
44	2m	115	LYS	2.6
33	2b	61	LEU	2.6
33	2b	86	GLU	2.6
41	2j	34	VAL	2.6
8	2I	79	ILE	2.6
1	1A	1097	U	2.6
32	2a	1065	U	2.6
40	1i	75	ASP	2.6
51	2t	97	ALA	2.6
26	24	66	SER	2.6
32	2a	1111	A	2.6
33	2b	40	HIS	2.6
41	1j	68	HIS	2.6
35	2d	159	ARG	2.6
38	2g	79	ARG	2.6
52	2u	24	ARG	2.6
28	26	42	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
8	1I	84	GLY	2.6
20	2Y	53	PRO	2.6
26	24	54	GLY	2.6
22	20	84	LEU	2.6
6	2G	52	ILE	2.6
32	2a	1030(C)	G	2.6
32	2a	1222	G	2.6
33	2b	44	LEU	2.6
34	2c	191	THR	2.6
40	1i	19	LEU	2.6
40	2i	96	LEU	2.6
33	1b	223	ILE	2.6
34	2c	124	ILE	2.6
42	1k	40	ILE	2.6
35	1d	62	GLN	2.6
44	2m	58	GLU	2.6
53	2y	44	GLU	2.6
44	2m	51	ALA	2.6
45	2n	36	PHE	2.6
1	1A	2136	C	2.6
32	2a	1109	C	2.6
32	1a	1025	U	2.6
32	2a	1257	U	2.6
15	2T	125	ARG	2.6
20	2Y	50	ARG	2.6
50	2s	3	ARG	2.6
51	1t	79	ARG	2.6
52	1u	15	ARG	2.6
52	2u	15	ARG	2.6
32	2a	1286	A	2.6
33	2b	234	PRO	2.6
40	2i	114	TYR	2.6
50	2s	28	LYS	2.6
40	2i	115	GLY	2.6
14	2S	46	VAL	2.6
20	2Y	44	ILE	2.6
34	2c	116	VAL	2.6
35	2d	170	VAL	2.6
37	2f	9	VAL	2.6
40	2i	14	VAL	2.6
6	1G	48	GLU	2.6
35	1d	150	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
45	1n	52	GLN	2.6
34	1c	50	ALA	2.6
34	1c	187	ALA	2.6
41	2j	78	ASN	2.6
45	1n	30	ALA	2.6
26	24	51	ASP	2.6
35	1d	134	ASP	2.6
6	1G	136	ARG	2.5
29	27	47	ARG	2.5
32	1a	173	U	2.5
32	2a	950	U	2.5
40	2i	58	HIS	2.5
1	1A	1584	C	2.5
1	1A	2139	C	2.5
1	2A	1092	C	2.5
32	1a	103	C	2.5
32	2a	1054	C	2.5
21	2Z	127	LYS	2.5
1	2A	1086	A	2.5
1	2A	2134	A	2.5
1	2A	2801(A)	A	2.5
32	1a	1030(D)	A	2.5
5	2F	170	LEU	2.5
17	1V	101	GLY	2.5
40	1i	49	PRO	2.5
35	2d	157	LEU	2.5
43	2l	88	GLY	2.5
43	2l	95	GLY	2.5
45	1n	6	LEU	2.5
45	2n	28	GLY	2.5
35	2d	207	TYR	2.5
6	2G	140	ILE	2.5
7	2H	41	MET	2.5
36	2e	129	ILE	2.5
49	1r	86	VAL	2.5
50	2s	67	VAL	2.5
41	1j	64	GLU	2.5
41	1j	92	THR	2.5
20	2Y	89	PHE	2.5
40	2i	46	ALA	2.5
53	2y	63	ALA	2.5
34	2c	108	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
38	1g	84	ASN	2.5
33	1b	217	ARG	2.5
41	2j	70	ARG	2.5
50	1s	36	ARG	2.5
51	1t	15	ARG	2.5
3	1D	275	LYS	2.5
32	1a	65	U	2.5
50	2s	35	SER	2.5
1	1A	271(M)	G	2.5
1	1A	2131	G	2.5
1	1A	2159	G	2.5
1	2A	652(C)	G	2.5
1	2A	2155	G	2.5
1	2A	2190	G	2.5
1	2A	2319	G	2.5
2	2B	103	G	2.5
1	1A	645	C	2.5
33	2b	154	LEU	2.5
34	1c	52	LEU	2.5
39	2h	67	PRO	2.5
45	1n	55	GLY	2.5
51	1t	69	GLY	2.5
53	2y	27	LEU	2.5
21	1Z	98	MET	2.5
35	1d	165	MET	2.5
34	1c	86	VAL	2.5
50	1s	40	ILE	2.5
44	2m	87	TYR	2.5
48	2q	95	TYR	2.5
32	2a	1256	A	2.5
8	1I	10	GLU	2.5
36	2e	86	ALA	2.5
40	2i	76	ALA	2.5
51	1t	67	ALA	2.5
14	1S	13	ARG	2.5
33	1b	96	ARG	2.5
35	1d	132	ARG	2.5
38	2g	5	ARG	2.5
40	1i	117	HIS	2.5
33	1b	156	LYS	2.5
41	1j	7	LYS	2.5
41	2j	80	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	2A	1090	U	2.5
47	2p	11	SER	2.5
48	2q	97	SER	2.5
53	2y	7	SER	2.5
34	2c	109	PRO	2.5
41	1j	41	PRO	2.5
4	2E	88	GLY	2.5
6	2G	85	GLY	2.5
8	2I	71	ILE	2.5
20	2Y	61	ILE	2.5
26	24	17	GLY	2.5
35	2d	6	GLY	2.5
40	1i	39	GLY	2.5
41	2j	50	ILE	2.5
46	1o	87	ILE	2.5
6	2G	109	VAL	2.5
21	1Z	86	VAL	2.5
21	2Z	105	VAL	2.5
33	1b	229	VAL	2.5
34	2c	138	VAL	2.5
1	1A	1049	C	2.5
32	1a	63	C	2.5
32	1a	1024	G	2.5
32	2a	1042	G	2.5
34	1c	184	TYR	2.5
34	2c	48	TYR	2.5
33	1b	12	GLU	2.5
33	1b	212	GLN	2.5
34	1c	113	ALA	2.5
44	2m	43	THR	2.5
44	2m	105	THR	2.5
1	2A	2158	A	2.5
32	2a	1183	A	2.5
32	2a	1280	A	2.5
32	2a	1324	A	2.5
35	1d	66	ARG	2.5
45	1n	23	ARG	2.5
45	2n	41	ARG	2.5
23	21	78	LYS	2.5
38	2g	28	ASN	2.5
50	2s	70	LYS	2.5
21	2Z	121	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
41	2j	62	HIS	2.5
6	2G	62	LEU	2.5
33	2b	142	LEU	2.5
39	1h	112	LEU	2.5
21	2Z	166	SER	2.5
52	2u	23	PRO	2.5
1	2A	2144	U	2.5
7	2H	9	ILE	2.5
32	2a	1126	U	2.5
33	1b	228	GLY	2.5
34	1c	9	GLY	2.5
50	2s	8	GLY	2.5
34	2c	75	VAL	2.5
40	1i	14	VAL	2.5
42	1k	14	VAL	2.5
44	2m	53	VAL	2.5
50	1s	19	VAL	2.5
53	2y	49	VAL	2.5
45	1n	8	GLU	2.5
33	1b	123	ALA	2.5
40	1i	104	ARG	2.5
40	2i	83	ARG	2.5
1	1A	2163	C	2.5
1	2A	1043	C	2.5
14	2S	33	LYS	2.5
32	1a	1254	C	2.5
32	2a	980	C	2.5
50	1s	77	THR	2.5
34	2c	72	LYS	2.5
43	2l	46	LYS	2.5
1	1A	1068	G	2.5
32	1a	1021	G	2.5
32	2a	993	G	2.5
32	2a	1024	G	2.5
32	2a	1304	G	2.5
1	1A	2801(A)	A	2.5
32	1a	161	A	2.5
32	1a	1183	A	2.5
32	1a	1256	A	2.5
32	2a	975	A	2.5
32	2a	994	A	2.5
33	1b	40	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
35	1d	123	HIS	2.5
7	2H	114	VAL	2.4
34	2c	103	VAL	2.4
42	2k	14	VAL	2.4
45	2n	55	GLY	2.4
35	1d	152	SER	2.4
49	1r	59	SER	2.4
1	1A	2113	U	2.4
1	1A	2132	U	2.4
14	2S	17	ARG	2.4
35	1d	156	GLU	2.4
40	2i	42	ARG	2.4
45	1n	57	ARG	2.4
49	2r	72	ARG	2.4
3	2D	272	ALA	2.4
6	2G	8	LYS	2.4
34	2c	104	GLN	2.4
34	2c	160	ALA	2.4
35	1d	38	TYR	2.4
49	2r	20	ALA	2.4
41	1j	67	THR	2.4
1	1A	2143	C	2.4
1	2A	2142	C	2.4
9	2N	45	ASN	2.4
38	2g	84	ASN	2.4
21	2Z	41	LEU	2.4
1	1A	1106	G	2.4
12	2Q	25	ASP	2.4
41	2j	74	ILE	2.4
42	2k	36	ASP	2.4
6	2G	160	VAL	2.4
34	1c	55	VAL	2.4
42	1k	52	GLY	2.4
14	2S	3	ARG	2.4
33	2b	96	ARG	2.4
35	1d	65	ARG	2.4
44	2m	88	ARG	2.4
45	1n	29	ARG	2.4
15	2T	22	PHE	2.4
34	2c	19	GLU	2.4
35	1d	110	PHE	2.4
37	1f	92	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
48	2q	100	LYS	2.4
37	2f	63	TYR	2.4
45	1n	34	TYR	2.4
47	2p	82	GLN	2.4
45	2n	22	THR	2.4
33	2b	98	LEU	2.4
26	24	20	ASN	2.4
50	1s	53	ASN	2.4
37	1f	52	ILE	2.4
1	1A	886	C	2.4
32	2a	1030	C	2.4
40	2i	98	PRO	2.4
45	2n	40	CYS	2.4
12	1Q	25	ASP	2.4
34	2c	197	GLY	2.4
20	2Y	87	LYS	2.4
33	2b	132	LYS	2.4
38	1g	4	ARG	2.4
6	2G	102	PHE	2.4
12	2Q	104	PHE	2.4
32	2a	1023	G	2.4
32	2a	1131	G	2.4
41	2j	59	SER	2.4
53	2y	11	GLU	2.4
34	2c	117	ALA	2.4
41	2j	27	ALA	2.4
42	1k	42	TRP	2.4
50	1s	75	ALA	2.4
39	1h	70	GLN	2.4
50	2s	56	GLN	2.4
32	1a	1278	U	2.4
26	24	43	TYR	2.4
47	2p	39	TYR	2.4
21	2Z	170	THR	2.4
19	2X	95	LEU	2.4
37	1f	21	LEU	2.4
38	1g	12	LEU	2.4
38	2g	38	LEU	2.4
33	1b	42	ILE	2.4
33	2b	41	ILE	2.4
33	2b	200	ILE	2.4
40	1i	21	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
16	1U	7	GLY	2.4
26	24	64	GLY	2.4
35	2d	171	GLY	2.4
43	2l	18	VAL	2.4
44	2m	68	GLY	2.4
46	2o	86	GLY	2.4
50	2s	26	GLY	2.4
14	2S	13	ARG	2.4
38	1g	33	ASP	2.4
51	1t	80	ARG	2.4
1	1A	1100	C	2.4
1	1A	2111	C	2.4
32	1a	1452	C	2.4
1	2A	6	A	2.4
32	1a	171	A	2.4
32	2a	983	A	2.4
40	2i	101	PHE	2.4
45	1n	36	PHE	2.4
16	2U	96	ALA	2.4
33	2b	123	ALA	2.4
34	2c	121	ALA	2.4
36	1e	21	ALA	2.4
38	2g	83	ALA	2.4
5	2F	8	GLN	2.4
1	1A	1537	G	2.4
1	2A	2631	G	2.4
32	2a	65	U	2.4
32	2a	1373	G	2.4
42	2k	31	THR	2.4
44	2m	21	TYR	2.4
53	2y	13	THR	2.4
14	2S	110	LEU	2.4
35	2d	176	LEU	2.4
36	2e	31	LEU	2.4
38	2g	99	LEU	2.4
33	1b	200	ILE	2.4
51	1t	100	ILE	2.4
7	2H	44	VAL	2.3
20	2Y	101	LYS	2.3
26	24	56	VAL	2.3
26	24	58	ARG	2.3
35	2d	69	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
39	2h	131	GLY	2.3
40	2i	24	GLY	2.3
41	2j	93	GLY	2.3
43	1l	19	ARG	2.3
44	2m	114	ARG	2.3
26	24	65	ASP	2.3
35	2d	134	ASP	2.3
50	1s	12	ASP	2.3
53	2y	51	ASP	2.3
5	2F	167	ALA	2.3
38	2g	150	ALA	2.3
53	2y	68	GLU	2.3
1	2A	2789	C	2.3
1	2A	2804	C	2.3
32	2a	1096	C	2.3
32	2a	1326	C	2.3
32	2a	1363	C	2.3
40	2i	124	GLN	2.3
1	1A	1070	A	2.3
1	1A	2134	A	2.3
32	1a	152	A	2.3
48	2q	99	SER	2.3
3	2D	97	TYR	2.3
6	2G	131	TYR	2.3
41	2j	13	HIS	2.3
44	2m	96	LEU	2.3
51	1t	62	LEU	2.3
6	2G	63	ILE	2.3
33	1b	201	ILE	2.3
41	1j	96	ILE	2.3
26	24	28	LYS	2.3
40	1i	127	LYS	2.3
40	2i	95	LYS	2.3
7	2H	69	ARG	2.3
32	2a	1221	G	2.3
33	1b	7	VAL	2.3
35	1d	168	ARG	2.3
38	1g	32	ARG	2.3
40	2i	107	ARG	2.3
40	2i	121	ARG	2.3
11	2P	91	PHE	2.3
21	2Z	89	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
3	2D	99	ASP	2.3
16	2U	89	GLU	2.3
40	2i	12	GLU	2.3
10	2O	5	GLN	2.3
6	2G	34	LEU	2.3
6	2G	139	LEU	2.3
34	1c	188	LEU	2.3
39	2h	119	LEU	2.3
49	1r	58	LEU	2.3
50	1s	35	SER	2.3
1	1A	2179	C	2.3
1	2A	893	C	2.3
34	2c	69	HIS	2.3
1	1A	887	A	2.3
1	1A	2114	A	2.3
1	2A	1098	A	2.3
32	1a	983	A	2.3
36	2e	60	TYR	2.3
40	1i	88	TYR	2.3
44	1m	9	ILE	2.3
13	2R	105	ARG	2.3
21	1Z	72	ARG	2.3
35	1d	40	PRO	2.3
38	1g	5	ARG	2.3
41	2j	43	ARG	2.3
52	2u	7	ARG	2.3
53	2y	14	PRO	2.3
8	2I	3	VAL	2.3
4	2E	148	GLY	2.3
38	2g	26	PHE	2.3
47	1p	80	PHE	2.3
1	1A	171	G	2.3
1	1A	2893	G	2.3
2	2B	54	G	2.3
7	2H	58	GLU	2.3
32	2a	1022	G	2.3
45	2n	46	GLU	2.3
52	2u	5	ASP	2.3
6	2G	3	LEU	2.3
40	1i	85	LEU	2.3
49	2r	76	LEU	2.3
53	2y	81	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
16	2U	85	LYS	2.3
34	2c	14	ILE	2.3
50	1s	14	HIS	2.3
41	1j	59	SER	2.3
9	2N	73	THR	2.3
14	2S	47	THR	2.3
11	2P	65	ARG	2.3
33	2b	31	TYR	2.3
40	2i	62	TYR	2.3
41	1j	70	ARG	2.3
7	2H	21	PRO	2.3
1	1A	6	A	2.3
1	1A	1046	A	2.3
10	2O	52	VAL	2.3
35	1d	140	VAL	2.3
36	1e	67	VAL	2.3
40	2i	41	VAL	2.3
41	1j	77	PRO	2.3
32	1a	1493	A	2.3
32	2a	1045	C	2.3
32	2a	1097	C	2.3
32	2a	1218	C	2.3
32	2a	84	U	2.3
32	2a	1025	U	2.3
32	2a	1150	U	2.3
11	1P	93	GLY	2.3
42	1k	45	GLY	2.3
46	2o	61	GLY	2.3
3	1D	225	ALA	2.3
6	2G	137	GLU	2.3
8	1I	46	ALA	2.3
8	2I	55	ALA	2.3
21	2Z	193	GLU	2.3
33	2b	134	GLU	2.3
35	2d	32	ALA	2.3
35	2d	192	GLU	2.3
38	1g	89	MET	2.3
41	1j	97	GLU	2.3
53	2y	21	ALA	2.3
34	2c	12	LEU	2.3
39	2h	70	GLN	2.3
40	1i	40	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
24	22	8	LYS	2.3
34	1c	135	LYS	2.3
1	1A	2156	G	2.3
32	1a	199	G	2.3
32	1a	200	G	2.3
32	1a	1017	G	2.3
32	1a	1032	G	2.3
32	2a	1013	G	2.3
41	2j	68	HIS	2.3
43	2l	100	ILE	2.3
52	1u	13	ILE	2.3
5	1F	15	SER	2.3
26	24	13	ARG	2.3
26	24	55	ARG	2.3
33	1b	97	TRP	2.3
39	1h	115	SER	2.3
40	1i	83	ARG	2.3
44	1m	88	ARG	2.3
44	2m	3	ARG	2.3
48	1q	63	ARG	2.3
52	1u	7	ARG	2.3
33	1b	33	TYR	2.3
33	2b	148	TYR	2.3
38	2g	154	TYR	2.3
42	1k	75	TYR	2.3
26	14	56	VAL	2.3
33	1b	219	VAL	2.3
7	1H	66	GLY	2.3
15	1T	37	GLY	2.3
35	1d	90	GLY	2.3
32	1a	1125	U	2.3
1	1A	2794	C	2.2
1	2A	652(V)	C	2.2
1	2A	655	A	2.2
32	2a	999	C	2.2
32	2a	1030(D)	A	2.2
32	2a	1041	A	2.2
32	2a	1110	A	2.2
32	2a	1531	A	2.2
33	2b	70	PHE	2.2
35	1d	185	PHE	2.2
50	1s	10	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
30	28	25	MET	2.2
35	2d	165	MET	2.2
5	2F	169	ASN	2.2
11	1P	149	GLU	2.2
12	1Q	140	ALA	2.2
21	2Z	97	GLU	2.2
30	18	33	ASN	2.2
41	2j	61	GLU	2.2
45	1n	5	ALA	2.2
8	2I	131	LYS	2.2
34	2c	107	GLN	2.2
34	1c	17	ASP	2.2
26	24	31	ILE	2.2
9	2N	115	ARG	2.2
19	2X	60	ARG	2.2
35	2d	107	ARG	2.2
50	1s	78	ARG	2.2
52	1u	9	ARG	2.2
52	2u	10	ARG	2.2
53	2y	67	HIS	2.2
6	2G	64	THR	2.2
38	1g	156	TRP	2.2
6	2G	78	SER	2.2
7	2H	79	VAL	2.2
34	2c	20	SER	2.2
40	2i	28	VAL	2.2
44	2m	17	VAL	2.2
45	1n	56	VAL	2.2
1	1A	2207	G	2.2
1	2A	859	G	2.2
2	2B	51	G	2.2
32	1a	105	G	2.2
42	2k	118	GLY	2.2
21	2Z	88	PHE	2.2
53	2y	48	PHE	2.2
1	2A	2895	U	2.2
32	1a	1040	U	2.2
6	1G	46	ALA	2.2
10	2O	33	ALA	2.2
15	2T	131	ALA	2.2
21	1Z	203	GLU	2.2
33	1b	186	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
33	1b	158	LEU	2.2
33	1b	231	GLU	2.2
36	1e	94	ALA	2.2
32	2a	977	A	2.2
32	2a	1019	C	2.2
32	2a	1237	C	2.2
32	2a	1268	A	2.2
35	1d	174	LEU	2.2
40	2i	19	LEU	2.2
44	2m	27	LYS	2.2
30	28	41	ILE	2.2
34	2c	152	ILE	2.2
7	1H	3	ARG	2.2
34	2c	16	ARG	2.2
46	2o	68	ARG	2.2
51	1t	25	ARG	2.2
7	2H	169	VAL	2.2
39	2h	53	VAL	2.2
45	1n	33	VAL	2.2
50	1s	11	VAL	2.2
52	2u	14	TRP	2.2
53	2y	45	PRO	2.2
21	2Z	99	TYR	2.2
34	2c	29	TYR	2.2
40	2i	92	TYR	2.2
20	2Y	93	GLY	2.2
40	2i	37	PHE	2.2
21	2Z	46	LYS	2.2
1	2A	1044	G	2.2
1	2A	2182	G	2.2
1	2A	2318	G	2.2
6	2G	60	LEU	2.2
6	2G	152	LEU	2.2
34	1c	24	ALA	2.2
35	2d	18	LYS	2.2
39	2h	110	ALA	2.2
40	1i	45	ALA	2.2
44	2m	13	LYS	2.2
47	1p	7	ALA	2.2
50	2s	75	ALA	2.2
53	2y	24	LEU	2.2
53	2y	26	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
32	1a	64	G	2.2
32	2a	963	G	2.2
32	2a	1031	G	2.2
1	2A	1066	U	2.2
1	2A	2585	U	2.2
2	2B	55	U	2.2
32	1a	1281	U	2.2
14	2S	61	ASN	2.2
35	2d	154	ASN	2.2
21	1Z	73	GLN	2.2
26	14	47	GLN	2.2
34	1c	77	ILE	2.2
35	2d	158	ILE	2.2
36	2e	109	ILE	2.2
41	2j	5	ARG	2.2
46	1o	3	ILE	2.2
46	1o	54	ARG	2.2
1	1A	2158	A	2.2
32	2a	197	A	2.2
32	1a	1018	C	2.2
32	2a	1006	C	2.2
6	2G	38	VAL	2.2
14	2S	69	VAL	2.2
33	1b	93	VAL	2.2
35	1d	112	VAL	2.2
26	24	27	THR	2.2
33	2b	190	THR	2.2
47	2p	44	THR	2.2
52	1u	8	THR	2.2
34	2c	155	GLY	2.2
41	2j	36	GLY	2.2
48	1q	66	SER	2.2
50	1s	82	GLY	2.2
6	2G	75	LYS	2.2
33	2b	152	PHE	2.2
6	2G	135	LEU	2.2
7	2H	71	LEU	2.2
33	1b	98	LEU	2.2
34	1c	12	LEU	2.2
37	2f	48	LEU	2.2
40	2i	56	LEU	2.2
44	1m	19	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
45	2n	44	LEU	2.2
10	2O	45	GLU	2.2
17	2V	55	ALA	2.2
21	2Z	113	ALA	2.2
40	2i	61	ALA	2.2
33	2b	208	ILE	2.2
34	1c	124	ILE	2.2
35	1d	153	ARG	2.2
36	1e	118	ILE	2.2
41	1j	75	ILE	2.2
43	2l	89	ARG	2.2
45	2n	57	ARG	2.2
50	2s	31	ILE	2.2
1	1A	2180	U	2.2
51	1t	17	ARG	2.2
1	2A	281	G	2.2
1	2A	1099	G	2.2
1	2A	2101	G	2.2
1	2A	2833	G	2.2
1	1A	2135	A	2.2
2	2B	52	A	2.2
21	2Z	95	PRO	2.2
32	2a	1269	A	2.2
33	1b	165	VAL	2.2
40	2i	53	VAL	2.2
1	1A	2146	C	2.2
1	2A	154(A)	C	2.2
1	2A	1079	C	2.2
32	2a	1359	C	2.2
6	2G	145	THR	2.2
8	1I	108	THR	2.2
41	1j	86	MET	2.2
6	2G	29	TRP	2.2
8	2I	45	LYS	2.2
22	20	8	GLY	2.2
26	24	19	GLY	2.2
34	2c	9	GLY	2.2
40	2i	80	GLY	2.2
44	2m	95	GLY	2.2
33	1b	122	PHE	2.2
33	2b	17	PHE	2.2
46	1o	69	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
37	2f	21	LEU	2.2
50	1s	5	LEU	2.2
6	2G	46	ALA	2.2
9	1N	47	ALA	2.2
34	1c	206	GLU	2.2
5	2F	205	ARG	2.1
33	2b	211	ILE	2.1
38	2g	120	ILE	2.1
40	1i	9	ARG	2.1
41	1j	98	ILE	2.1
50	2s	49	ILE	2.1
40	2i	38	GLN	2.1
44	2m	101	GLN	2.1
7	2H	49	VAL	2.1
8	2I	137	PRO	2.1
20	2Y	56	PRO	2.1
21	2Z	159	PRO	2.1
21	2Z	175	VAL	2.1
50	1s	58	VAL	2.1
6	2G	182	LYS	2.1
24	22	49	LYS	2.1
2	2B	102	A	2.1
32	2a	1011	G	2.1
40	2i	103	THR	2.1
41	2j	14	LYS	2.1
47	2p	31	LYS	2.1
49	2r	71	LYS	2.1
51	1t	21	LYS	2.1
33	2b	163	PHE	2.1
47	2p	48	TRP	2.1
1	2A	271(B)	C	2.1
1	2A	1041	C	2.1
2	2B	109	C	2.1
5	2F	12	LEU	2.1
33	1b	115	LEU	2.1
33	2b	187	LEU	2.1
35	1d	186	LEU	2.1
45	1n	47	LEU	2.1
10	2O	7	TYR	2.1
35	1d	68	TYR	2.1
33	2b	207	ALA	2.1
35	1d	48	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
42	1k	15	ALA	2.1
45	2n	20	ALA	2.1
6	2G	101	ILE	2.1
20	2Y	38	ILE	2.1
33	1b	211	ILE	2.1
34	2c	57	ILE	2.1
30	28	35	GLN	2.1
7	1H	158	HIS	2.1
7	2H	29	PRO	2.1
26	24	41	PRO	2.1
33	2b	15	VAL	2.1
35	1d	172	PRO	2.1
40	2i	49	PRO	2.1
44	1m	113	PRO	2.1
45	1n	25	VAL	2.1
53	2y	70	MET	2.1
36	2e	121	LYS	2.1
51	2t	74	LYS	2.1
6	2G	116	ASP	2.1
7	2H	57	ASP	2.1
6	2G	177	GLY	2.1
17	2V	67	GLY	2.1
27	15	54	GLY	2.1
33	2b	14	GLY	2.1
34	1c	194	GLY	2.1
40	1i	100	GLY	2.1
45	1n	51	GLY	2.1
6	2G	90	LEU	2.1
6	2G	107	LEU	2.1
21	2Z	136	PHE	2.1
33	1b	145	LEU	2.1
41	2j	54	PHE	2.1
50	1s	15	LEU	2.1
3	1D	263	ARG	2.1
14	2S	51	ALA	2.1
17	2V	21	ARG	2.1
26	24	68	ARG	2.1
34	2c	23	TYR	2.1
35	1d	131	ARG	2.1
42	1k	64	ALA	2.1
53	2y	96	ARG	2.1
53	2y	97	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	1A	271(H)	G	2.1
1	1A	1047	G	2.1
1	1A	2802	G	2.1
1	2A	1068	G	2.1
8	1I	71	ILE	2.1
8	1I	99	GLU	2.1
8	2I	88	ILE	2.1
32	1a	1144	G	2.1
32	2a	198	G	2.1
32	2a	1255	G	2.1
38	1g	57	GLU	2.1
41	2j	35	SER	2.1
44	2m	4	ILE	2.1
50	1s	31	ILE	2.1
50	2s	40	ILE	2.1
1	1A	889	C	2.1
32	1a	218	C	2.1
32	1a	488	C	2.1
32	2a	1214	C	2.1
16	1U	117	GLN	2.1
6	1G	47	LYS	2.1
8	1I	127	VAL	2.1
24	22	65	ASN	2.1
33	1b	90	MET	2.1
34	2c	97	LYS	2.1
34	2c	150	LYS	2.1
35	2d	17	VAL	2.1
35	1d	29	PRO	2.1
40	1i	78	LYS	2.1
44	1m	54	VAL	2.1
48	1q	73	VAL	2.1
1	2A	1078	U	2.1
1	2A	1113	U	2.1
32	1a	190	U	2.1
32	1a	992	U	2.1
11	2P	93	GLY	2.1
18	2W	112	GLY	2.1
30	28	38	GLY	2.1
34	1c	62	ASP	2.1
34	2c	101	LEU	2.1
40	2i	47	LEU	2.1
44	2m	70	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
12	2Q	29	PHE	2.1
21	2Z	69	THR	2.1
26	14	49	PHE	2.1
36	1e	116	THR	2.1
37	2f	60	PHE	2.1
42	1k	125	PHE	2.1
44	2m	64	TRP	2.1
33	1b	13	ALA	2.1
34	1c	71	ALA	2.1
35	1d	164	ALA	2.1
41	1j	50	ILE	2.1
49	2r	60	ALA	2.1
28	26	39	TYR	2.1
33	2b	141	GLU	2.1
36	2e	61	TYR	2.1
40	1i	35	GLU	2.1
41	1j	83	GLU	2.1
44	2m	23	TYR	2.1
1	1A	899	A	2.1
1	2A	1913	A	2.1
35	1d	175	SER	2.1
43	1l	116	SER	2.1
1	1A	2155	G	2.1
1	2A	352	G	2.1
1	2A	1509	C	2.1
1	2A	1537	G	2.1
1	2A	1543	C	2.1
1	2A	2105	C	2.1
32	2a	409	G	2.1
32	2a	1114	C	2.1
32	2a	1124	G	2.1
37	1f	90	VAL	2.1
42	2k	47	VAL	2.1
44	2m	65	LYS	2.1
50	1s	18	LYS	2.1
36	2e	130	ASN	2.1
41	2j	76	ASN	2.1
51	1t	75	ASN	2.1
7	2H	7	LEU	2.1
24	22	60	LEU	2.1
47	1p	49	LEU	2.1
2	2B	104	U	2.1

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Mol	Chain	Res	Type	RSRZ
32	2a	1281	U	2.1
34	1c	10	PHE	2.1
52	2u	2	GLY	2.1
4	2E	58	ARG	2.1
22	20	55	ARG	2.1
35	2d	47	ARG	2.1
36	1e	64	ARG	2.1
36	2e	27	ARG	2.1
40	1i	54	ASP	2.1
44	1m	105	THR	2.1
41	2j	18	ALA	2.1
42	1k	29	ILE	2.1
44	1m	25	ILE	2.1
44	1m	84	ILE	2.1
51	1t	49	ALA	2.1
21	1Z	190	GLU	2.1
40	1i	2	GLU	2.1
40	2i	88	TYR	2.1
33	1b	22	LYS	2.0
33	2b	48	MET	2.0
41	2j	57	LYS	2.0
44	1m	115	LYS	2.0
51	1t	73	HIS	2.0
27	25	60	VAL	2.0
32	1a	344	A	2.0
32	1a	1157	A	2.0
32	2a	1014	A	2.0
32	2a	1130	A	2.0
37	2f	40	VAL	2.0
40	2i	17	VAL	2.0
47	1p	2	VAL	2.0
25	23	2	PRO	2.0
1	1A	2137	C	2.0
1	2A	1118	C	2.0
32	1a	1043	C	2.0
32	2a	1327	C	2.0
33	1b	149	LEU	2.0
35	1d	157	LEU	2.0
35	2d	11	LEU	2.0
1	2A	1740	G	2.0
1	2A	2805	G	2.0
2	2B	23	G	2.0

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Mol	Chain	Res	Type	RSRZ
22	20	76	GLY	2.0
23	11	28	GLY	2.0
26	24	61	ARG	2.0
30	28	28	GLY	2.0
32	1a	79	G	2.0
32	1a	191	G	2.0
32	1a	380	G	2.0
32	2a	973	G	2.0
32	2a	1312	G	2.0
34	1c	21	ARG	2.0
38	2g	76	ARG	2.0
47	1p	75	ARG	2.0
50	2s	78	ARG	2.0
32	1a	1135	U	2.0
32	2a	1095	U	2.0
41	2j	38	ILE	2.0
49	1r	75	ILE	2.0
7	2H	20	ALA	2.0
38	1g	83	ALA	2.0
40	2i	122	ALA	2.0
21	2Z	2	GLU	2.0
34	2c	89	GLU	2.0
6	1G	182	LYS	2.0
21	2Z	78	LYS	2.0
34	2c	45	LYS	2.0
46	1o	5	LYS	2.0
47	1p	38	TYR	2.0
48	1q	100	LYS	2.0
4	2E	54	GLN	2.0
7	2H	43	VAL	2.0
24	22	6	VAL	2.0
34	2c	136	GLN	2.0
37	1f	37	VAL	2.0
41	1j	24	VAL	2.0
42	2k	22	HIS	2.0
1	2A	1103	A	2.0
21	2Z	76	LEU	2.0
32	1a	197	A	2.0
32	2a	1225	A	2.0
32	2a	1279	A	2.0
33	2b	215	LEU	2.0
41	2j	71	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
45	1n	39	LEU	2.0
6	2G	95	ARG	2.0
40	1i	42	ARG	2.0
44	2m	29	ARG	2.0
7	2H	120	GLY	2.0
20	2Y	60	PHE	2.0
33	2b	55	PHE	2.0
36	2e	84	PHE	2.0
2	2B	62	C	2.0
32	2a	979	C	2.0
53	2y	54	ILE	2.0
21	1Z	109	ALA	2.0
34	2c	95	THR	2.0
1	2A	2897	U	2.0
1	1A	2152	G	2.0
1	1A	2631	G	2.0
1	2A	7	G	2.0
1	2A	2100	G	2.0
1	2A	2792	G	2.0
10	2O	108	GLU	2.0
11	1P	74	GLU	2.0
21	1Z	185	GLU	2.0
32	1a	306	G	2.0
32	1a	1138	G	2.0
32	2a	1053	G	2.0
34	2c	4	LYS	2.0
34	2c	135	LYS	2.0
35	1d	166	LYS	2.0
40	1i	113	LYS	2.0
40	2i	116	LYS	2.0
51	2t	7	LYS	2.0
34	1c	48	TYR	2.0
42	1k	25	TYR	2.0
44	1m	21	TYR	2.0
6	2G	159	VAL	2.0
7	2H	15	VAL	2.0
34	2c	68	VAL	2.0
35	2d	121	VAL	2.0
36	1e	115	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MU	2A	1915	21/22	0.79	0.14	78,83,92,101	0
32	2MG	2a	1207	24/25	0.81	0.16	82,87,93,96	0
1	5MU	1A	1915	21/22	0.84	0.14	66,78,92,99	0
32	2MG	1a	1207	24/25	0.86	0.14	74,80,84,89	0
32	5MC	2a	967	21/22	0.87	0.13	73,77,87,91	0
32	PSU	2a	516	20/21	0.88	0.11	76,81,88,98	0
1	PSU	2A	1917	20/21	0.89	0.11	70,73,87,91	0
1	PSU	2A	1911	20/21	0.90	0.12	61,68,75,78	0
43	0TD	1l	92	10/11	0.90	0.15	53,59,63,75	0
32	M2G	2a	966	25/26	0.91	0.12	69,74,83,92	0
32	M2G	1a	966	25/26	0.91	0.13	54,61,70,76	0
32	G7M	2a	527	24/25	0.91	0.13	60,65,68,71	0
43	0TD	2l	92	10/11	0.91	0.13	65,68,73,79	0
32	5MC	1a	967	21/22	0.92	0.12	58,63,75,81	0
32	PSU	1a	516	20/21	0.92	0.11	60,70,76,82	0
32	5MC	2a	1400	21/22	0.92	0.14	57,71,76,79	0
1	PSU	1A	1917	20/21	0.92	0.10	57,68,77,78	0
32	4OC	2a	1402	22/23	0.93	0.12	55,62,64,73	0
1	PSU	1A	1911	20/21	0.93	0.11	43,62,65,66	0
32	5MC	1a	1400	21/22	0.94	0.12	37,55,59,61	0
32	5MC	2a	1407	21/22	0.94	0.10	55,63,67,67	0
32	UR3	2a	1498	21/22	0.94	0.12	49,56,61,68	0
32	5MC	1a	1407	21/22	0.94	0.10	45,53,59,61	0
32	UR3	1a	1498	21/22	0.95	0.12	39,46,51,60	0
32	MA6	1a	1519	24/25	0.95	0.11	37,44,53,56	0
32	4OC	1a	1402	22/23	0.95	0.12	45,52,60,64	0
1	OMC	2A	1920	21/22	0.95	0.11	59,62,66,70	0
32	MA6	2a	1518	24/25	0.95	0.10	56,63,66,69	0
32	MA6	2a	1519	24/25	0.95	0.12	53,60,66,70	0
1	5MC	2A	1942	21/22	0.95	0.11	43,50,54,55	0
32	5MC	2a	1404	21/22	0.96	0.10	44,56,60,66	0
32	G7M	1a	527	24/25	0.96	0.09	47,55,61,65	0
1	OMG	2A	2251	24/25	0.96	0.08	32,37,43,50	0
1	2MA	2A	2503	23/24	0.96	0.09	27,30,38,40	0
1	5MC	1A	1942	21/22	0.96	0.11	22,33,37,37	0
32	MA6	1a	1518	24/25	0.96	0.10	39,44,49,57	0
1	5MU	2A	1939	21/22	0.97	0.09	33,39,44,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	OMG	1A	2251	24/25	0.97	0.08	15,22,25,27	0
1	5MC	2A	1962	21/22	0.97	0.07	40,42,49,59	0
1	5MU	1A	1939	21/22	0.97	0.08	19,24,28,30	0
32	5MC	1a	1404	21/22	0.97	0.09	41,44,48,54	0
1	OMC	1A	1920	21/22	0.97	0.09	39,54,61,62	0
1	PSU	1A	2605	20/21	0.98	0.07	23,24,30,30	0
1	5MC	1A	1962	21/22	0.98	0.07	30,34,37,44	0
1	2MA	1A	2503	23/24	0.98	0.06	13,18,21,22	0
1	OMU	2A	2552	21/22	0.98	0.07	30,36,42,44	0
1	PSU	2A	2605	20/21	0.98	0.07	32,37,41,45	0
1	OMU	1A	2552	21/22	0.98	0.07	21,23,29,35	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3119	1/1	0.43	0.20	85,85,85,85	0
54	MG	2A	3118	1/1	0.51	0.33	80,80,80,80	0
54	MG	1a	3233	1/1	0.53	0.26	78,78,78,78	0
54	MG	2A	3452	1/1	0.54	0.32	78,78,78,78	0
54	MG	1T	203	1/1	0.56	0.15	77,77,77,77	0
54	MG	2a	3151	1/1	0.56	0.20	74,74,74,74	0
54	MG	2A	3409	1/1	0.57	0.19	77,77,77,77	0
54	MG	1A	3902	1/1	0.58	0.21	35,35,35,35	0
54	MG	1Z	301	1/1	0.59	0.23	63,63,63,63	0
54	MG	1t	202	1/1	0.60	0.17	80,80,80,80	0
54	MG	2A	3199	1/1	0.62	0.20	58,58,58,58	0
54	MG	2a	3066	1/1	0.64	0.12	74,74,74,74	0
54	MG	2A	3518	1/1	0.65	0.20	75,75,75,75	0
54	MG	2A	3593	1/1	0.66	0.26	88,88,88,88	0
54	MG	1y	201	1/1	0.66	0.26	76,76,76,76	0
54	MG	1B	202	1/1	0.66	0.20	55,55,55,55	0
54	MG	2a	3126	1/1	0.67	0.19	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3704	1/1	0.68	0.18	73,73,73,73	0
54	MG	2A	3453	1/1	0.68	0.27	67,67,67,67	0
54	MG	1A	3853	1/1	0.68	0.18	79,79,79,79	0
54	MG	2A	3112	1/1	0.68	0.21	61,61,61,61	0
54	MG	1a	3161	1/1	0.69	0.24	69,69,69,69	0
54	MG	1a	3089	1/1	0.70	0.33	71,71,71,71	0
54	MG	2A	3462	1/1	0.70	0.20	65,65,65,65	0
54	MG	2A	3510	1/1	0.70	0.19	81,81,81,81	0
54	MG	1B	227	1/1	0.71	0.18	64,64,64,64	0
54	MG	1A	3283	1/1	0.71	0.17	78,78,78,78	0
54	MG	2A	3732	1/1	0.71	0.22	76,76,76,76	0
54	MG	2a	3063	1/1	0.71	0.17	80,80,80,80	0
54	MG	1a	3190	1/1	0.71	0.22	69,69,69,69	0
54	MG	1A	3939	1/1	0.71	0.14	70,70,70,70	0
54	MG	1A	3221	1/1	0.71	0.17	70,70,70,70	0
54	MG	2A	3229	1/1	0.72	0.19	68,68,68,68	0
54	MG	2A	3523	1/1	0.72	0.22	59,59,59,59	0
54	MG	2A	3277	1/1	0.72	0.23	78,78,78,78	0
54	MG	1A	3198	1/1	0.72	0.20	58,58,58,58	0
54	MG	2A	3078	1/1	0.72	0.12	74,74,74,74	0
54	MG	2a	3004	1/1	0.72	0.22	69,69,69,69	0
54	MG	2a	3047	1/1	0.72	0.16	75,75,75,75	0
54	MG	1a	3065	1/1	0.72	0.28	74,74,74,74	0
54	MG	2A	3460	1/1	0.72	0.19	65,65,65,65	0
54	MG	1G	202	1/1	0.72	0.17	54,54,54,54	0
54	MG	1A	3767	1/1	0.72	0.27	74,74,74,74	0
54	MG	2A	3496	1/1	0.73	0.16	58,58,58,58	0
54	MG	2A	3345	1/1	0.73	0.16	57,57,57,57	0
54	MG	1A	4005	1/1	0.73	0.12	49,49,49,49	0
54	MG	1A	3769	1/1	0.73	0.20	59,59,59,59	0
54	MG	2a	3033	1/1	0.73	0.16	69,69,69,69	0
54	MG	1a	3098	1/1	0.74	0.17	57,57,57,57	0
54	MG	2A	3706	1/1	0.74	0.48	55,55,55,55	0
54	MG	1B	228	1/1	0.74	0.13	57,57,57,57	0
54	MG	1A	3996	1/1	0.74	0.52	43,43,43,43	0
54	MG	1A	3671	1/1	0.74	0.18	58,58,58,58	0
54	MG	1A	3558	1/1	0.75	0.20	68,68,68,68	0
54	MG	2A	3157	1/1	0.75	0.12	58,58,58,58	0
54	MG	1d	302	1/1	0.75	0.24	68,68,68,68	0
54	MG	2a	3024	1/1	0.75	0.23	70,70,70,70	0
54	MG	1e	201	1/1	0.75	0.27	53,53,53,53	0
54	MG	1a	3097	1/1	0.75	0.35	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3316	1/1	0.75	0.14	56,56,56,56	0
54	MG	1a	3164	1/1	0.75	0.19	53,53,53,53	0
54	MG	1a	3076	1/1	0.75	0.23	80,80,80,80	0
54	MG	1a	3198	1/1	0.75	0.14	72,72,72,72	0
54	MG	1a	3068	1/1	0.76	0.34	67,67,67,67	0
54	MG	1f	202	1/1	0.76	0.22	73,73,73,73	0
54	MG	2a	3034	1/1	0.76	0.14	69,69,69,69	0
54	MG	1a	3197	1/1	0.76	0.14	78,78,78,78	0
54	MG	1A	3677	1/1	0.76	0.15	71,71,71,71	0
54	MG	1A	3664	1/1	0.76	0.17	69,69,69,69	0
54	MG	2A	3110	1/1	0.76	0.16	88,88,88,88	0
54	MG	1A	3176	1/1	0.76	0.17	52,52,52,52	0
54	MG	2a	3107	1/1	0.77	0.15	66,66,66,66	0
54	MG	1A	3946	1/1	0.77	0.30	84,84,84,84	0
54	MG	1a	3013	1/1	0.77	0.17	74,74,74,74	0
54	MG	2A	3724	1/1	0.78	0.17	60,60,60,60	0
54	MG	1A	3856	1/1	0.78	0.46	35,35,35,35	0
54	MG	2A	3475	1/1	0.78	0.11	71,71,71,71	0
54	MG	1A	3275	1/1	0.78	0.24	52,52,52,52	0
54	MG	1a	3085	1/1	0.78	0.18	67,67,67,67	0
54	MG	1f	201	1/1	0.78	0.15	55,55,55,55	0
54	MG	2A	3450	1/1	0.78	0.14	53,53,53,53	0
54	MG	2A	3533	1/1	0.78	0.18	63,63,63,63	0
54	MG	1A	3920	1/1	0.78	0.11	49,49,49,49	0
54	MG	2A	3673	1/1	0.78	0.16	64,64,64,64	0
54	MG	1a	3213	1/1	0.78	0.12	57,57,57,57	0
54	MG	1a	3215	1/1	0.78	0.25	65,65,65,65	0
54	MG	2a	3171	1/1	0.78	0.14	68,68,68,68	0
54	MG	2A	3164	1/1	0.79	0.14	69,69,69,69	0
54	MG	2A	3612	1/1	0.79	0.14	40,40,40,40	0
54	MG	2A	3653	1/1	0.79	0.21	95,95,95,95	0
54	MG	2A	3084	1/1	0.79	0.19	68,68,68,68	0
54	MG	2A	3702	1/1	0.79	0.16	54,54,54,54	0
54	MG	1a	3152	1/1	0.79	0.25	55,55,55,55	0
54	MG	2a	3068	1/1	0.79	0.23	69,69,69,69	0
54	MG	1d	305	1/1	0.79	0.13	78,78,78,78	0
54	MG	2a	3125	1/1	0.79	0.17	52,52,52,52	0
54	MG	1A	3871	1/1	0.79	0.17	51,51,51,51	0
54	MG	1A	3439	1/1	0.79	0.15	61,61,61,61	0
54	MG	2A	3570	1/1	0.79	0.20	73,73,73,73	0
56	MPD	1a	3271	8/8	0.79	0.28	68,72,77,78	0
54	MG	2A	3077	1/1	0.80	0.28	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3189	1/1	0.80	0.13	57,57,57,57	0
54	MG	2A	3708	1/1	0.80	0.15	59,59,59,59	0
54	MG	1A	3507	1/1	0.80	0.13	42,42,42,42	0
54	MG	1a	3049	1/1	0.80	0.14	49,49,49,49	0
54	MG	1a	3058	1/1	0.80	0.19	69,69,69,69	0
54	MG	1a	3251	1/1	0.80	0.15	55,55,55,55	0
54	MG	2A	3481	1/1	0.80	0.13	60,60,60,60	0
54	MG	1a	3263	1/1	0.80	0.17	63,63,63,63	0
54	MG	2a	3046	1/1	0.80	0.25	76,76,76,76	0
54	MG	1a	3146	1/1	0.80	0.15	50,50,50,50	0
54	MG	2A	3195	1/1	0.80	0.18	67,67,67,67	0
54	MG	1A	3805	1/1	0.80	0.14	57,57,57,57	0
54	MG	1A	3813	1/1	0.80	0.19	34,34,34,34	0
54	MG	2a	3074	1/1	0.80	0.14	58,58,58,58	0
54	MG	2a	3093	1/1	0.80	0.26	70,70,70,70	0
54	MG	1A	3272	1/1	0.80	0.27	48,48,48,48	0
54	MG	2a	3124	1/1	0.80	0.21	58,58,58,58	0
54	MG	2A	3289	1/1	0.80	0.13	55,55,55,55	0
54	MG	1a	3177	1/1	0.80	0.11	77,77,77,77	0
54	MG	1a	3081	1/1	0.80	0.18	90,90,90,90	0
54	MG	2a	3152	1/1	0.80	0.27	98,98,98,98	0
54	MG	1A	3689	1/1	0.80	0.11	49,49,49,49	0
54	MG	2A	3443	1/1	0.80	0.29	78,78,78,78	0
54	MG	1A	3188	1/1	0.81	0.30	35,35,35,35	0
54	MG	18	104	1/1	0.81	0.16	54,54,54,54	0
54	MG	1B	207	1/1	0.81	0.14	54,54,54,54	0
54	MG	2G	201	1/1	0.81	0.14	81,81,81,81	0
54	MG	1a	3027	1/1	0.81	0.14	67,67,67,67	0
54	MG	2A	3201	1/1	0.81	0.21	61,61,61,61	0
54	MG	2A	3502	1/1	0.81	0.16	26,26,26,26	0
54	MG	1a	3048	1/1	0.81	0.12	60,60,60,60	0
54	MG	2A	3023	1/1	0.81	0.24	76,76,76,76	0
54	MG	1A	3949	1/1	0.81	0.22	73,73,73,73	0
54	MG	2a	3057	1/1	0.81	0.16	67,67,67,67	0
54	MG	1A	3979	1/1	0.81	0.10	83,83,83,83	0
54	MG	2A	3568	1/1	0.81	0.13	77,77,77,77	0
54	MG	1A	3772	1/1	0.81	0.14	49,49,49,49	0
54	MG	2A	3577	1/1	0.81	0.16	51,51,51,51	0
54	MG	2A	3092	1/1	0.81	0.36	71,71,71,71	0
54	MG	2A	3606	1/1	0.81	0.15	42,42,42,42	0
54	MG	2A	3432	1/1	0.81	0.11	57,57,57,57	0
54	MG	2A	3435	1/1	0.81	0.22	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3817	1/1	0.81	0.11	27,27,27,27	0
54	MG	2A	3689	1/1	0.81	0.24	65,65,65,65	0
54	MG	1T	205	1/1	0.81	0.16	48,48,48,48	0
54	MG	1a	3166	1/1	0.81	0.17	74,74,74,74	0
54	MG	2a	3181	1/1	0.81	0.17	58,58,58,58	0
54	MG	2a	3183	1/1	0.81	0.15	69,69,69,69	0
54	MG	2A	3121	1/1	0.81	0.13	42,42,42,42	0
56	MPD	1a	3272	8/8	0.81	0.23	59,70,79,81	0
54	MG	1a	3257	1/1	0.82	0.15	54,54,54,54	0
54	MG	2A	3355	1/1	0.82	0.17	63,63,63,63	0
54	MG	2A	3369	1/1	0.82	0.28	70,70,70,70	0
54	MG	1A	3257	1/1	0.82	0.10	42,42,42,42	0
54	MG	2A	3173	1/1	0.82	0.17	52,52,52,52	0
54	MG	1A	3367	1/1	0.82	0.20	43,43,43,43	0
54	MG	2a	3103	1/1	0.82	0.18	75,75,75,75	0
54	MG	2a	3105	1/1	0.82	0.11	61,61,61,61	0
54	MG	1A	3076	1/1	0.82	0.29	46,46,46,46	0
54	MG	2B	207	1/1	0.82	0.17	81,81,81,81	0
54	MG	2B	216	1/1	0.82	0.14	77,77,77,77	0
54	MG	2E	304	1/1	0.82	0.12	55,55,55,55	0
54	MG	18	102	1/1	0.82	0.47	42,42,42,42	0
54	MG	1B	208	1/1	0.82	0.12	44,44,44,44	0
54	MG	1A	3027	1/1	0.82	0.26	56,56,56,56	0
54	MG	2a	3177	1/1	0.82	0.12	60,60,60,60	0
54	MG	2A	3280	1/1	0.82	0.11	53,53,53,53	0
54	MG	1A	3683	1/1	0.82	0.25	43,43,43,43	0
54	MG	2A	3293	1/1	0.82	0.12	28,28,28,28	0
54	MG	1A	3811	1/1	0.82	0.22	48,48,48,48	0
54	MG	2A	3730	1/1	0.83	0.16	58,58,58,58	0
54	MG	2A	3136	1/1	0.83	0.23	58,58,58,58	0
54	MG	1a	3017	1/1	0.83	0.21	59,59,59,59	0
54	MG	1A	3271	1/1	0.83	0.33	47,47,47,47	0
54	MG	1a	3042	1/1	0.83	0.16	69,69,69,69	0
54	MG	1a	3269	1/1	0.83	0.09	55,55,55,55	0
54	MG	1A	3969	1/1	0.83	0.14	54,54,54,54	0
54	MG	1A	3655	1/1	0.83	0.16	53,53,53,53	0
54	MG	1A	3987	1/1	0.83	0.15	32,32,32,32	0
54	MG	2A	3239	1/1	0.83	0.18	62,62,62,62	0
54	MG	2a	3035	1/1	0.83	0.16	85,85,85,85	0
54	MG	2A	3514	1/1	0.83	0.18	77,77,77,77	0
54	MG	2A	3516	1/1	0.83	0.13	57,57,57,57	0
54	MG	2A	3248	1/1	0.83	0.15	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3059	1/1	0.83	0.18	65,65,65,65	0
54	MG	1a	3172	1/1	0.83	0.19	72,72,72,72	0
54	MG	1a	3173	1/1	0.83	0.15	62,62,62,62	0
54	MG	1A	3438	1/1	0.83	0.16	60,60,60,60	0
54	MG	2a	3086	1/1	0.83	0.12	50,50,50,50	0
54	MG	1A	4000	1/1	0.83	0.11	52,52,52,52	0
54	MG	1A	3089	1/1	0.83	0.17	61,61,61,61	0
54	MG	13	103	1/1	0.83	0.24	43,43,43,43	0
54	MG	2A	3368	1/1	0.83	0.18	64,64,64,64	0
54	MG	2A	3616	1/1	0.83	0.14	66,66,66,66	0
54	MG	1A	3845	1/1	0.83	0.14	31,31,31,31	0
54	MG	2A	3398	1/1	0.83	0.24	59,59,59,59	0
54	MG	2A	3680	1/1	0.83	0.17	78,78,78,78	0
54	MG	1B	206	1/1	0.83	0.28	56,56,56,56	0
54	MG	2A	3425	1/1	0.83	0.20	65,65,65,65	0
54	MG	1a	3227	1/1	0.83	0.12	79,79,79,79	0
54	MG	1a	3229	1/1	0.83	0.23	69,69,69,69	0
54	MG	1A	3365	1/1	0.83	0.14	38,38,38,38	0
54	MG	2A	3720	1/1	0.83	0.09	76,76,76,76	0
54	MG	1a	3250	1/1	0.83	0.19	72,72,72,72	0
56	MPD	2B	221	8/8	0.83	0.29	58,69,74,76	0
57	ARG	1F	317	12/12	0.83	0.17	44,58,74,78	0
54	MG	2B	212	1/1	0.84	0.12	49,49,49,49	0
54	MG	1A	3506	1/1	0.84	0.21	36,36,36,36	0
54	MG	1A	3259	1/1	0.84	0.22	42,42,42,42	0
54	MG	1a	3158	1/1	0.84	0.19	73,73,73,73	0
54	MG	2A	3233	1/1	0.84	0.16	53,53,53,53	0
54	MG	2a	3021	1/1	0.84	0.17	50,50,50,50	0
54	MG	1A	3678	1/1	0.84	0.15	52,52,52,52	0
54	MG	1a	3031	1/1	0.84	0.14	57,57,57,57	0
54	MG	2A	3251	1/1	0.84	0.16	45,45,45,45	0
54	MG	1A	3516	1/1	0.84	0.64	32,32,32,32	0
54	MG	1i	3100	1/1	0.84	0.15	69,69,69,69	0
54	MG	1B	217	1/1	0.84	0.25	64,64,64,64	0
54	MG	2a	3053	1/1	0.84	0.21	62,62,62,62	0
54	MG	1B	225	1/1	0.84	0.15	50,50,50,50	0
54	MG	2a	3059	1/1	0.84	0.14	69,69,69,69	0
54	MG	2a	3061	1/1	0.84	0.15	75,75,75,75	0
54	MG	2A	3562	1/1	0.84	0.15	50,50,50,50	0
54	MG	1A	3963	1/1	0.84	0.10	55,55,55,55	0
54	MG	2A	3051	1/1	0.84	0.13	43,43,43,43	0
54	MG	1a	3182	1/1	0.84	0.16	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3383	1/1	0.84	0.11	24,24,24,24	0
54	MG	1E	302	1/1	0.84	0.89	43,43,43,43	0
54	MG	2A	3376	1/1	0.84	0.15	52,52,52,52	0
54	MG	2a	3104	1/1	0.84	0.18	72,72,72,72	0
54	MG	1F	312	1/1	0.84	0.23	34,34,34,34	0
54	MG	1A	3972	1/1	0.84	0.42	54,54,54,54	0
54	MG	2A	3414	1/1	0.84	0.17	64,64,64,64	0
54	MG	1A	3729	1/1	0.84	0.20	56,56,56,56	0
54	MG	1A	3981	1/1	0.84	0.14	57,57,57,57	0
54	MG	2A	3433	1/1	0.84	0.18	59,59,59,59	0
54	MG	1A	3740	1/1	0.84	0.14	51,51,51,51	0
54	MG	2a	3161	1/1	0.84	0.14	66,66,66,66	0
54	MG	1A	3285	1/1	0.84	0.16	62,62,62,62	0
54	MG	1A	3199	1/1	0.84	0.15	46,46,46,46	0
54	MG	1a	3103	1/1	0.84	0.16	51,51,51,51	0
54	MG	1A	3770	1/1	0.84	0.27	62,62,62,62	0
54	MG	2j	201	1/1	0.84	0.10	75,75,75,75	0
54	MG	2t	201	1/1	0.84	0.16	56,56,56,56	0
54	MG	2y	201	1/1	0.84	0.20	93,93,93,93	0
54	MG	2A	3456	1/1	0.84	0.32	70,70,70,70	0
54	MG	2A	3457	1/1	0.84	0.20	62,62,62,62	0
56	MPD	2A	3734	8/8	0.84	0.26	36,44,51,51	0
54	MG	2B	201	1/1	0.84	0.15	73,73,73,73	0
54	MG	1a	3133	1/1	0.84	0.16	54,54,54,54	0
54	MG	2A	3241	1/1	0.85	0.21	59,59,59,59	0
54	MG	1a	3080	1/1	0.85	0.21	67,67,67,67	0
54	MG	1O	202	1/1	0.85	0.09	52,52,52,52	0
54	MG	2A	3266	1/1	0.85	0.18	68,68,68,68	0
54	MG	2A	3275	1/1	0.85	0.14	53,53,53,53	0
54	MG	1T	202	1/1	0.85	0.14	42,42,42,42	0
54	MG	1A	3411	1/1	0.85	0.12	65,65,65,65	0
54	MG	1a	3267	1/1	0.85	0.12	50,50,50,50	0
54	MG	2A	3290	1/1	0.85	0.15	45,45,45,45	0
54	MG	1A	3989	1/1	0.85	0.25	43,43,43,43	0
54	MG	1b	301	1/1	0.85	0.17	62,62,62,62	0
54	MG	1A	3418	1/1	0.85	0.14	25,25,25,25	0
54	MG	2B	206	1/1	0.85	0.19	57,57,57,57	0
54	MG	1d	304	1/1	0.85	0.11	91,91,91,91	0
54	MG	2B	208	1/1	0.85	0.15	72,72,72,72	0
54	MG	1A	3426	1/1	0.85	0.25	55,55,55,55	0
54	MG	2B	213	1/1	0.85	0.18	61,61,61,61	0
54	MG	1a	3117	1/1	0.85	0.11	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	15	106	1/1	0.85	0.11	55,55,55,55	0
54	MG	18	101	1/1	0.85	0.44	40,40,40,40	0
54	MG	2I	201	1/1	0.85	0.15	79,79,79,79	0
54	MG	2a	3002	1/1	0.85	0.28	59,59,59,59	0
54	MG	1g	202	1/1	0.85	0.09	53,53,53,53	0
54	MG	2a	3005	1/1	0.85	0.17	69,69,69,69	0
54	MG	2a	3011	1/1	0.85	0.09	54,54,54,54	0
54	MG	1g	203	1/1	0.85	0.23	68,68,68,68	0
54	MG	1A	4003	1/1	0.85	0.17	58,58,58,58	0
54	MG	1t	201	1/1	0.85	0.17	61,61,61,61	0
54	MG	1A	3877	1/1	0.85	0.12	55,55,55,55	0
54	MG	1a	3006	1/1	0.85	0.13	66,66,66,66	0
54	MG	2A	3006	1/1	0.85	0.18	62,62,62,62	0
54	MG	1A	3168	1/1	0.85	0.12	51,51,51,51	0
54	MG	2A	3042	1/1	0.85	0.27	55,55,55,55	0
54	MG	1A	3791	1/1	0.85	0.48	31,31,31,31	0
54	MG	2A	3071	1/1	0.85	0.15	59,59,59,59	0
54	MG	1A	3933	1/1	0.85	0.14	20,20,20,20	0
54	MG	2a	3062	1/1	0.85	0.24	68,68,68,68	0
54	MG	1a	3028	1/1	0.85	0.19	50,50,50,50	0
54	MG	1A	3797	1/1	0.85	0.17	59,59,59,59	0
54	MG	1a	3176	1/1	0.85	0.13	73,73,73,73	0
54	MG	1A	3700	1/1	0.85	0.35	34,34,34,34	0
54	MG	2a	3076	1/1	0.85	0.15	52,52,52,52	0
54	MG	1a	3043	1/1	0.85	0.15	48,48,48,48	0
54	MG	1A	3727	1/1	0.85	0.09	69,69,69,69	0
54	MG	1a	3196	1/1	0.85	0.13	57,57,57,57	0
54	MG	2A	3123	1/1	0.85	0.18	54,54,54,54	0
54	MG	2A	3515	1/1	0.85	0.36	69,69,69,69	0
54	MG	1A	3237	1/1	0.85	0.82	28,28,28,28	0
54	MG	2a	3116	1/1	0.85	0.17	62,62,62,62	0
54	MG	1A	3393	1/1	0.85	0.13	23,23,23,23	0
54	MG	1D	318	1/1	0.85	0.15	49,49,49,49	0
54	MG	1a	3061	1/1	0.85	0.21	65,65,65,65	0
54	MG	2A	3537	1/1	0.85	0.11	61,61,61,61	0
54	MG	2A	3544	1/1	0.85	0.23	83,83,83,83	0
54	MG	2a	3156	1/1	0.85	0.13	58,58,58,58	0
54	MG	2a	3158	1/1	0.85	0.11	80,80,80,80	0
54	MG	2a	3159	1/1	0.85	0.13	65,65,65,65	0
54	MG	2A	3183	1/1	0.85	0.17	64,64,64,64	0
54	MG	2A	3185	1/1	0.85	0.12	45,45,45,45	0
54	MG	2a	3175	1/1	0.85	0.16	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3838	1/1	0.85	0.18	64,64,64,64	0
54	MG	2A	3573	1/1	0.85	0.11	54,54,54,54	0
54	MG	1a	3228	1/1	0.85	0.12	67,67,67,67	0
54	MG	1A	3764	1/1	0.85	0.16	51,51,51,51	0
54	MG	2q	201	1/1	0.85	0.10	52,52,52,52	0
54	MG	2A	3604	1/1	0.85	0.11	38,38,38,38	0
54	MG	2A	3220	1/1	0.85	0.12	50,50,50,50	0
54	MG	2A	3610	1/1	0.85	0.24	92,92,92,92	0
54	MG	1A	3848	1/1	0.85	0.13	38,38,38,38	0
54	MG	1a	3239	1/1	0.85	0.09	56,56,56,56	0
56	MPD	2A	3735	8/8	0.85	0.22	58,65,69,71	0
54	MG	2A	3641	1/1	0.85	0.14	83,83,83,83	0
54	MG	1a	3248	1/1	0.85	0.19	73,73,73,73	0
54	MG	2P	203	1/1	0.86	0.15	61,61,61,61	0
54	MG	1a	3093	1/1	0.86	0.26	55,55,55,55	0
54	MG	2A	3511	1/1	0.86	0.16	46,46,46,46	0
54	MG	1a	3094	1/1	0.86	0.15	65,65,65,65	0
54	MG	2a	3006	1/1	0.86	0.12	64,64,64,64	0
54	MG	1A	3192	1/1	0.86	0.32	34,34,34,34	0
54	MG	2a	3017	1/1	0.86	0.21	68,68,68,68	0
54	MG	1y	205	1/1	0.86	0.12	66,66,66,66	0
54	MG	1a	3217	1/1	0.86	0.15	69,69,69,69	0
54	MG	2A	3017	1/1	0.86	0.42	53,53,53,53	0
54	MG	2A	3531	1/1	0.86	0.11	52,52,52,52	0
54	MG	1a	3226	1/1	0.86	0.10	63,63,63,63	0
54	MG	2A	3031	1/1	0.86	0.11	53,53,53,53	0
54	MG	1E	305	1/1	0.86	0.21	50,50,50,50	0
54	MG	2a	3051	1/1	0.86	0.25	54,54,54,54	0
54	MG	1A	3936	1/1	0.86	0.17	43,43,43,43	0
54	MG	1a	3104	1/1	0.86	0.25	57,57,57,57	0
54	MG	2A	3296	1/1	0.86	0.25	62,62,62,62	0
54	MG	1A	3300	1/1	0.86	0.14	70,70,70,70	0
54	MG	2A	3341	1/1	0.86	0.25	66,66,66,66	0
54	MG	1A	3941	1/1	0.86	0.12	67,67,67,67	0
54	MG	1a	3126	1/1	0.86	0.15	72,72,72,72	0
54	MG	2A	3605	1/1	0.86	0.11	65,65,65,65	0
54	MG	2a	3071	1/1	0.86	0.14	59,59,59,59	0
54	MG	1T	201	1/1	0.86	0.15	59,59,59,59	0
54	MG	2A	3099	1/1	0.86	0.28	59,59,59,59	0
54	MG	1A	3597	1/1	0.86	0.28	31,31,31,31	0
54	MG	2A	3382	1/1	0.86	0.15	59,59,59,59	0
54	MG	2a	3098	1/1	0.86	0.28	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3619	1/1	0.86	0.12	52,52,52,52	0
54	MG	1A	3603	1/1	0.86	0.21	58,58,58,58	0
54	MG	2A	3642	1/1	0.86	0.24	60,60,60,60	0
54	MG	2A	3648	1/1	0.86	0.18	73,73,73,73	0
54	MG	1A	3778	1/1	0.86	0.19	59,59,59,59	0
54	MG	2A	3412	1/1	0.86	0.23	63,63,63,63	0
54	MG	2A	3676	1/1	0.86	0.13	66,66,66,66	0
54	MG	1A	3628	1/1	0.86	0.15	58,58,58,58	0
54	MG	2a	3137	1/1	0.86	0.14	70,70,70,70	0
54	MG	2a	3149	1/1	0.86	0.19	64,64,64,64	0
54	MG	11	103	1/1	0.86	0.12	53,53,53,53	0
54	MG	2A	3431	1/1	0.86	0.13	53,53,53,53	0
54	MG	1A	3864	1/1	0.86	0.10	22,22,22,22	0
54	MG	1d	301	1/1	0.86	0.21	49,49,49,49	0
54	MG	1B	221	1/1	0.86	0.14	53,53,53,53	0
54	MG	1a	3073	1/1	0.86	0.21	47,47,47,47	0
54	MG	2A	3448	1/1	0.86	0.11	56,56,56,56	0
54	MG	2A	3449	1/1	0.86	0.13	71,71,71,71	0
54	MG	1a	3175	1/1	0.86	0.18	61,61,61,61	0
54	MG	1A	3629	1/1	0.86	0.16	48,48,48,48	0
54	MG	2B	203	1/1	0.86	0.23	79,79,79,79	0
54	MG	2a	3190	1/1	0.86	0.10	45,45,45,45	0
54	MG	2A	3190	1/1	0.86	0.22	56,56,56,56	0
54	MG	1A	3409	1/1	0.86	0.13	23,23,23,23	0
54	MG	1A	3267	1/1	0.86	0.08	52,52,52,52	0
54	MG	1B	230	1/1	0.86	0.14	61,61,61,61	0
54	MG	2A	3205	1/1	0.86	0.12	49,49,49,49	0
54	MG	2B	214	1/1	0.86	0.17	93,93,93,93	0
54	MG	2A	3216	1/1	0.86	0.17	59,59,59,59	0
54	MG	1a	3088	1/1	0.86	0.21	59,59,59,59	0
54	MG	1A	3025	1/1	0.86	0.56	46,46,46,46	0
54	MG	1p	101	1/1	0.86	0.10	50,50,50,50	0
54	MG	2A	3152	1/1	0.87	0.20	56,56,56,56	0
54	MG	1a	3019	1/1	0.87	0.10	44,44,44,44	0
54	MG	2A	3163	1/1	0.87	0.32	64,64,64,64	0
54	MG	1a	3022	1/1	0.87	0.14	53,53,53,53	0
54	MG	1a	3121	1/1	0.87	0.24	60,60,60,60	0
54	MG	2A	3175	1/1	0.87	0.12	69,69,69,69	0
54	MG	1A	3149	1/1	0.87	0.27	54,54,54,54	0
54	MG	2G	202	1/1	0.87	0.15	81,81,81,81	0
54	MG	1A	3156	1/1	0.87	0.36	37,37,37,37	0
54	MG	1a	3142	1/1	0.87	0.17	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	23	101	1/1	0.87	0.27	54,54,54,54	0
54	MG	2A	3194	1/1	0.87	0.14	52,52,52,52	0
54	MG	1D	314	1/1	0.87	0.12	28,28,28,28	0
54	MG	2A	3489	1/1	0.87	0.12	55,55,55,55	0
54	MG	2A	3494	1/1	0.87	0.14	72,72,72,72	0
54	MG	1a	3150	1/1	0.87	0.15	58,58,58,58	0
54	MG	2A	3497	1/1	0.87	0.37	48,48,48,48	0
54	MG	2A	3499	1/1	0.87	0.12	55,55,55,55	0
54	MG	1a	3038	1/1	0.87	0.17	59,59,59,59	0
54	MG	2a	3029	1/1	0.87	0.30	78,78,78,78	0
54	MG	2A	3504	1/1	0.87	0.14	57,57,57,57	0
54	MG	2A	3506	1/1	0.87	0.25	61,61,61,61	0
54	MG	1a	3040	1/1	0.87	0.19	61,61,61,61	0
54	MG	2A	3211	1/1	0.87	0.28	62,62,62,62	0
54	MG	2A	3512	1/1	0.87	0.14	68,68,68,68	0
54	MG	1A	3965	1/1	0.87	0.15	39,39,39,39	0
54	MG	1a	3163	1/1	0.87	0.13	70,70,70,70	0
54	MG	1A	3517	1/1	0.87	0.17	51,51,51,51	0
54	MG	1A	3555	1/1	0.87	0.29	34,34,34,34	0
54	MG	1A	3974	1/1	0.87	0.14	25,25,25,25	0
54	MG	1A	3055	1/1	0.87	0.09	41,41,41,41	0
54	MG	1A	3709	1/1	0.87	0.17	50,50,50,50	0
54	MG	2A	3249	1/1	0.87	0.10	64,64,64,64	0
54	MG	2A	3539	1/1	0.87	0.24	72,72,72,72	0
54	MG	2a	3069	1/1	0.87	0.24	58,58,58,58	0
54	MG	1A	3711	1/1	0.87	0.15	54,54,54,54	0
54	MG	2A	3262	1/1	0.87	0.20	70,70,70,70	0
54	MG	1a	3064	1/1	0.87	0.28	79,79,79,79	0
54	MG	1A	3712	1/1	0.87	0.12	30,30,30,30	0
54	MG	2a	3087	1/1	0.87	0.11	49,49,49,49	0
54	MG	2a	3092	1/1	0.87	0.10	57,57,57,57	0
54	MG	1a	3186	1/1	0.87	0.14	72,72,72,72	0
54	MG	1a	3067	1/1	0.87	0.16	61,61,61,61	0
54	MG	2A	3281	1/1	0.87	0.25	53,53,53,53	0
54	MG	1A	3282	1/1	0.87	0.20	63,63,63,63	0
54	MG	2A	3025	1/1	0.87	0.17	44,44,44,44	0
54	MG	1a	3072	1/1	0.87	0.25	54,54,54,54	0
54	MG	2a	3108	1/1	0.87	0.12	69,69,69,69	0
54	MG	2A	3036	1/1	0.87	0.14	71,71,71,71	0
54	MG	2a	3122	1/1	0.87	0.13	62,62,62,62	0
54	MG	1A	3057	1/1	0.87	0.12	53,53,53,53	0
54	MG	2A	3615	1/1	0.87	0.17	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3326	1/1	0.87	0.11	39,39,39,39	0
54	MG	2A	3327	1/1	0.87	0.14	53,53,53,53	0
54	MG	1a	3212	1/1	0.87	0.21	64,64,64,64	0
54	MG	2A	3053	1/1	0.87	0.10	57,57,57,57	0
54	MG	2A	3056	1/1	0.87	0.16	53,53,53,53	0
54	MG	1A	3100	1/1	0.87	0.15	49,49,49,49	0
54	MG	2A	3655	1/1	0.87	0.10	31,31,31,31	0
54	MG	2A	3662	1/1	0.87	0.16	73,73,73,73	0
54	MG	1A	3120	1/1	0.87	0.37	40,40,40,40	0
54	MG	2a	3167	1/1	0.87	0.12	48,48,48,48	0
54	MG	1A	3647	1/1	0.87	0.18	55,55,55,55	0
54	MG	1A	3908	1/1	0.87	0.11	38,38,38,38	0
54	MG	1A	3650	1/1	0.87	0.32	62,62,62,62	0
54	MG	2A	3696	1/1	0.87	0.14	68,68,68,68	0
54	MG	2A	3404	1/1	0.87	0.16	56,56,56,56	0
54	MG	2a	3189	1/1	0.87	0.12	58,58,58,58	0
54	MG	1A	3651	1/1	0.87	0.15	57,57,57,57	0
54	MG	2A	3410	1/1	0.87	0.15	58,58,58,58	0
54	MG	1A	3652	1/1	0.87	0.11	50,50,50,50	0
54	MG	2A	3413	1/1	0.87	0.13	50,50,50,50	0
54	MG	1a	3005	1/1	0.87	0.16	50,50,50,50	0
54	MG	1A	3266	1/1	0.87	0.15	53,53,53,53	0
54	MG	1A	3458	1/1	0.87	0.12	35,35,35,35	0
54	MG	1A	3139	1/1	0.87	0.20	34,34,34,34	0
54	MG	1a	3018	1/1	0.87	0.09	61,61,61,61	0
54	MG	2A	3137	1/1	0.87	0.21	45,45,45,45	0
54	MG	2A	3147	1/1	0.87	0.43	52,52,52,52	0
54	MG	2A	3509	1/1	0.88	0.14	50,50,50,50	0
54	MG	1a	3079	1/1	0.88	0.16	52,52,52,52	0
54	MG	28	102	1/1	0.88	0.14	54,54,54,54	0
54	MG	2A	3022	1/1	0.88	0.18	63,63,63,63	0
54	MG	2A	3261	1/1	0.88	0.14	58,58,58,58	0
54	MG	1A	3621	1/1	0.88	0.13	28,28,28,28	0
54	MG	2A	3024	1/1	0.88	0.15	52,52,52,52	0
54	MG	1A	3742	1/1	0.88	0.13	54,54,54,54	0
54	MG	2a	3014	1/1	0.88	0.16	61,61,61,61	0
54	MG	1A	3744	1/1	0.88	0.19	47,47,47,47	0
54	MG	1A	3827	1/1	0.88	0.13	59,59,59,59	0
54	MG	2A	3529	1/1	0.88	0.17	33,33,33,33	0
54	MG	1A	3750	1/1	0.88	0.12	57,57,57,57	0
54	MG	1a	3091	1/1	0.88	0.14	45,45,45,45	0
54	MG	1A	3954	1/1	0.88	0.13	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3055	1/1	0.88	0.15	55,55,55,55	0
54	MG	2A	3541	1/1	0.88	0.37	51,51,51,51	0
54	MG	1a	3219	1/1	0.88	0.32	67,67,67,67	0
54	MG	2A	3549	1/1	0.88	0.15	71,71,71,71	0
54	MG	2A	3308	1/1	0.88	0.10	40,40,40,40	0
54	MG	1A	3962	1/1	0.88	0.15	48,48,48,48	0
54	MG	1A	3841	1/1	0.88	0.13	63,63,63,63	0
54	MG	1D	307	1/1	0.88	0.17	50,50,50,50	0
54	MG	1A	3761	1/1	0.88	0.12	13,13,13,13	0
54	MG	1a	3021	1/1	0.88	0.20	68,68,68,68	0
54	MG	2A	3598	1/1	0.88	0.13	38,38,38,38	0
54	MG	1a	3235	1/1	0.88	0.14	69,69,69,69	0
54	MG	2A	3101	1/1	0.88	0.14	49,49,49,49	0
54	MG	1a	3108	1/1	0.88	0.17	58,58,58,58	0
54	MG	2A	3371	1/1	0.88	0.12	38,38,38,38	0
54	MG	2A	3111	1/1	0.88	0.13	65,65,65,65	0
54	MG	1a	3240	1/1	0.88	0.09	64,64,64,64	0
54	MG	1a	3241	1/1	0.88	0.16	67,67,67,67	0
54	MG	2A	3618	1/1	0.88	0.14	92,92,92,92	0
54	MG	1D	315	1/1	0.88	0.28	31,31,31,31	0
54	MG	2a	3094	1/1	0.88	0.13	68,68,68,68	0
54	MG	2A	3620	1/1	0.88	0.20	53,53,53,53	0
54	MG	2A	3622	1/1	0.88	0.32	64,64,64,64	0
54	MG	2A	3632	1/1	0.88	0.23	71,71,71,71	0
54	MG	1A	3310	1/1	0.88	0.20	42,42,42,42	0
54	MG	2A	3134	1/1	0.88	0.12	55,55,55,55	0
54	MG	1A	3397	1/1	0.88	0.21	58,58,58,58	0
54	MG	1A	3538	1/1	0.88	0.09	59,59,59,59	0
54	MG	2A	3140	1/1	0.88	0.12	54,54,54,54	0
54	MG	1A	3468	1/1	0.88	0.10	26,26,26,26	0
54	MG	1a	3138	1/1	0.88	0.10	56,56,56,56	0
54	MG	1A	3482	1/1	0.88	0.11	29,29,29,29	0
54	MG	2a	3131	1/1	0.88	0.17	68,68,68,68	0
54	MG	1N	201	1/1	0.88	0.18	49,49,49,49	0
54	MG	1a	3149	1/1	0.88	0.11	67,67,67,67	0
54	MG	1A	3562	1/1	0.88	0.12	64,64,64,64	0
54	MG	2A	3174	1/1	0.88	0.26	61,61,61,61	0
54	MG	1a	3045	1/1	0.88	0.09	65,65,65,65	0
54	MG	1a	3156	1/1	0.88	0.23	66,66,66,66	0
54	MG	1R	206	1/1	0.88	0.12	50,50,50,50	0
54	MG	1A	3899	1/1	0.88	0.40	37,37,37,37	0
54	MG	1A	3569	1/1	0.88	0.30	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3402	1/1	0.88	0.11	36,36,36,36	0
54	MG	1T	204	1/1	0.88	0.10	56,56,56,56	0
54	MG	1A	3096	1/1	0.88	0.32	43,43,43,43	0
54	MG	2A	3465	1/1	0.88	0.10	61,61,61,61	0
54	MG	1n	101	1/1	0.88	0.11	63,63,63,63	0
54	MG	2a	3185	1/1	0.88	0.12	86,86,86,86	0
54	MG	2a	3187	1/1	0.88	0.11	65,65,65,65	0
54	MG	1V	204	1/1	0.88	0.11	40,40,40,40	0
54	MG	1A	3922	1/1	0.88	0.20	42,42,42,42	0
54	MG	2A	3490	1/1	0.88	0.13	43,43,43,43	0
54	MG	10	103	1/1	0.88	0.11	35,35,35,35	0
54	MG	1A	3927	1/1	0.88	0.16	47,47,47,47	0
54	MG	1A	3806	1/1	0.88	0.12	21,21,21,21	0
54	MG	2D	307	1/1	0.88	0.12	35,35,35,35	0
54	MG	2A	3235	1/1	0.88	0.09	44,44,44,44	0
54	MG	2A	3002	1/1	0.88	0.15	54,54,54,54	0
54	MG	15	104	1/1	0.88	0.16	46,46,46,46	0
54	MG	2G	203	1/1	0.88	0.11	63,63,63,63	0
54	MG	2A	3010	1/1	0.88	0.17	64,64,64,64	0
54	MG	2A	3426	1/1	0.89	0.11	46,46,46,46	0
54	MG	2A	3115	1/1	0.89	0.18	59,59,59,59	0
54	MG	1A	3579	1/1	0.89	0.12	21,21,21,21	0
54	MG	1A	3725	1/1	0.89	0.11	39,39,39,39	0
54	MG	1a	3236	1/1	0.89	0.17	64,64,64,64	0
54	MG	2A	3440	1/1	0.89	0.10	46,46,46,46	0
54	MG	2A	3126	1/1	0.89	0.10	59,59,59,59	0
54	MG	2A	3447	1/1	0.89	0.10	38,38,38,38	0
54	MG	1A	3580	1/1	0.89	0.12	35,35,35,35	0
54	MG	1a	3101	1/1	0.89	0.13	67,67,67,67	0
54	MG	1B	209	1/1	0.89	0.19	52,52,52,52	0
54	MG	1a	3246	1/1	0.89	0.09	54,54,54,54	0
54	MG	1a	3010	1/1	0.89	0.15	58,58,58,58	0
54	MG	2E	301	1/1	0.89	0.13	47,47,47,47	0
54	MG	1a	3107	1/1	0.89	0.19	54,54,54,54	0
54	MG	1A	3132	1/1	0.89	0.09	35,35,35,35	0
54	MG	2A	3459	1/1	0.89	0.11	28,28,28,28	0
54	MG	1a	3252	1/1	0.89	0.13	62,62,62,62	0
54	MG	1B	218	1/1	0.89	0.12	57,57,57,57	0
54	MG	1A	3448	1/1	0.89	0.28	64,64,64,64	0
54	MG	2W	203	1/1	0.89	0.11	61,61,61,61	0
54	MG	2A	3474	1/1	0.89	0.10	46,46,46,46	0
54	MG	25	102	1/1	0.89	0.13	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3120	1/1	0.89	0.09	69,69,69,69	0
54	MG	1A	3604	1/1	0.89	0.16	52,52,52,52	0
54	MG	2A	3486	1/1	0.89	0.26	64,64,64,64	0
54	MG	2A	3488	1/1	0.89	0.16	53,53,53,53	0
54	MG	2A	3181	1/1	0.89	0.18	50,50,50,50	0
54	MG	2a	3009	1/1	0.89	0.17	56,56,56,56	0
54	MG	2A	3182	1/1	0.89	0.18	43,43,43,43	0
54	MG	2a	3012	1/1	0.89	0.13	68,68,68,68	0
54	MG	2A	3492	1/1	0.89	0.12	70,70,70,70	0
54	MG	1a	3125	1/1	0.89	0.10	62,62,62,62	0
54	MG	2A	3495	1/1	0.89	0.09	53,53,53,53	0
54	MG	1A	3208	1/1	0.89	0.45	38,38,38,38	0
54	MG	1A	3274	1/1	0.89	0.35	56,56,56,56	0
54	MG	2a	3030	1/1	0.89	0.22	53,53,53,53	0
54	MG	1a	3024	1/1	0.89	0.10	45,45,45,45	0
54	MG	1A	3138	1/1	0.89	0.07	22,22,22,22	0
54	MG	2A	3196	1/1	0.89	0.15	58,58,58,58	0
54	MG	2a	3037	1/1	0.89	0.09	61,61,61,61	0
54	MG	2a	3040	1/1	0.89	0.15	67,67,67,67	0
54	MG	1A	3631	1/1	0.89	0.29	33,33,33,33	0
54	MG	1A	3504	1/1	0.89	0.09	37,37,37,37	0
54	MG	1A	3279	1/1	0.89	0.27	58,58,58,58	0
54	MG	1g	201	1/1	0.89	0.12	52,52,52,52	0
54	MG	1A	3184	1/1	0.89	0.21	30,30,30,30	0
54	MG	1A	3115	1/1	0.89	0.14	50,50,50,50	0
54	MG	1h	201	1/1	0.89	0.09	46,46,46,46	0
54	MG	1a	3157	1/1	0.89	0.08	57,57,57,57	0
54	MG	1A	3142	1/1	0.89	0.15	55,55,55,55	0
54	MG	1A	3782	1/1	0.89	0.22	57,57,57,57	0
54	MG	1F	315	1/1	0.89	0.15	45,45,45,45	0
54	MG	2A	3245	1/1	0.89	0.15	55,55,55,55	0
54	MG	1A	3656	1/1	0.89	0.14	35,35,35,35	0
54	MG	1a	3054	1/1	0.89	0.29	50,50,50,50	0
54	MG	1a	3169	1/1	0.89	0.12	62,62,62,62	0
54	MG	2a	3077	1/1	0.89	0.13	54,54,54,54	0
54	MG	2a	3079	1/1	0.89	0.25	54,54,54,54	0
54	MG	2A	3260	1/1	0.89	0.33	59,59,59,59	0
54	MG	1a	3055	1/1	0.89	0.18	64,64,64,64	0
54	MG	1A	3661	1/1	0.89	0.11	53,53,53,53	0
54	MG	2A	3558	1/1	0.89	0.14	39,39,39,39	0
54	MG	2A	3263	1/1	0.89	0.13	50,50,50,50	0
54	MG	2A	3566	1/1	0.89	0.12	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3532	1/1	0.89	0.13	31,31,31,31	0
54	MG	1A	3536	1/1	0.89	0.12	29,29,29,29	0
54	MG	1A	3807	1/1	0.89	0.33	40,40,40,40	0
54	MG	1a	3180	1/1	0.89	0.12	57,57,57,57	0
54	MG	1A	3417	1/1	0.89	0.13	31,31,31,31	0
54	MG	2a	3113	1/1	0.89	0.15	61,61,61,61	0
54	MG	2A	3288	1/1	0.89	0.15	56,56,56,56	0
54	MG	2A	3600	1/1	0.89	0.12	36,36,36,36	0
54	MG	1A	3543	1/1	0.89	0.18	43,43,43,43	0
54	MG	1a	3188	1/1	0.89	0.12	64,64,64,64	0
54	MG	2A	3291	1/1	0.89	0.11	40,40,40,40	0
54	MG	1A	3980	1/1	0.89	0.13	56,56,56,56	0
54	MG	1a	3195	1/1	0.89	0.11	69,69,69,69	0
54	MG	2a	3148	1/1	0.89	0.16	79,79,79,79	0
54	MG	2A	3043	1/1	0.89	0.15	56,56,56,56	0
54	MG	2A	3044	1/1	0.89	0.13	58,58,58,58	0
54	MG	2A	3045	1/1	0.89	0.14	49,49,49,49	0
54	MG	1A	3110	1/1	0.89	0.21	35,35,35,35	0
54	MG	1A	3131	1/1	0.89	0.11	61,61,61,61	0
54	MG	2A	3054	1/1	0.89	0.30	65,65,65,65	0
54	MG	2A	3631	1/1	0.89	0.15	75,75,75,75	0
54	MG	1a	3074	1/1	0.89	0.11	52,52,52,52	0
54	MG	1a	3206	1/1	0.89	0.11	83,83,83,83	0
54	MG	1A	3696	1/1	0.89	0.49	27,27,27,27	0
54	MG	1A	3991	1/1	0.89	0.19	33,33,33,33	0
54	MG	10	105	1/1	0.89	0.12	35,35,35,35	0
54	MG	2A	3378	1/1	0.89	0.14	65,65,65,65	0
54	MG	2A	3083	1/1	0.89	0.18	49,49,49,49	0
54	MG	2A	3383	1/1	0.89	0.14	51,51,51,51	0
54	MG	1a	3216	1/1	0.89	0.20	73,73,73,73	0
54	MG	10	107	1/1	0.89	0.13	58,58,58,58	0
54	MG	2A	3687	1/1	0.89	0.22	63,63,63,63	0
54	MG	2A	3407	1/1	0.89	0.11	46,46,46,46	0
54	MG	1A	3697	1/1	0.89	0.22	56,56,56,56	0
54	MG	2A	3698	1/1	0.89	0.17	60,60,60,60	0
56	MPD	1A	4013	8/8	0.89	0.25	42,54,56,59	0
54	MG	1A	3699	1/1	0.89	0.21	78,78,78,78	0
54	MG	2A	3108	1/1	0.89	0.23	40,40,40,40	0
54	MG	1A	3437	1/1	0.89	0.24	57,57,57,57	0
54	MG	1A	3353	1/1	0.89	0.10	44,44,44,44	0
54	MG	2A	3716	1/1	0.89	0.21	53,53,53,53	0
54	MG	1A	3577	1/1	0.89	0.08	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3748	1/1	0.90	0.10	40,40,40,40	0
54	MG	1A	3865	1/1	0.90	0.13	82,82,82,82	0
54	MG	2a	3013	1/1	0.90	0.30	49,49,49,49	0
54	MG	1A	3302	1/1	0.90	0.10	76,76,76,76	0
54	MG	2a	3016	1/1	0.90	0.12	44,44,44,44	0
54	MG	1A	3127	1/1	0.90	0.14	44,44,44,44	0
54	MG	2a	3019	1/1	0.90	0.18	46,46,46,46	0
54	MG	2a	3020	1/1	0.90	0.09	47,47,47,47	0
54	MG	2A	3187	1/1	0.90	0.12	43,43,43,43	0
54	MG	1A	3890	1/1	0.90	0.11	29,29,29,29	0
54	MG	2A	3607	1/1	0.90	0.12	64,64,64,64	0
54	MG	2A	3191	1/1	0.90	0.15	49,49,49,49	0
54	MG	1A	3574	1/1	0.90	0.12	21,21,21,21	0
54	MG	1A	3488	1/1	0.90	0.09	60,60,60,60	0
54	MG	1A	3903	1/1	0.90	0.24	50,50,50,50	0
54	MG	1a	3008	1/1	0.90	0.28	66,66,66,66	0
54	MG	1A	3311	1/1	0.90	0.33	38,38,38,38	0
54	MG	1a	3012	1/1	0.90	0.09	24,24,24,24	0
54	MG	1a	3222	1/1	0.90	0.13	72,72,72,72	0
54	MG	1a	3224	1/1	0.90	0.13	53,53,53,53	0
54	MG	2a	3052	1/1	0.90	0.19	55,55,55,55	0
54	MG	1A	3910	1/1	0.90	0.24	45,45,45,45	0
54	MG	1A	3505	1/1	0.90	0.09	36,36,36,36	0
54	MG	1A	3584	1/1	0.90	0.10	40,40,40,40	0
54	MG	2A	3645	1/1	0.90	0.09	47,47,47,47	0
54	MG	1A	3351	1/1	0.90	0.11	52,52,52,52	0
54	MG	2A	3651	1/1	0.90	0.09	45,45,45,45	0
54	MG	1A	3244	1/1	0.90	0.17	45,45,45,45	0
54	MG	1A	3788	1/1	0.90	0.11	38,38,38,38	0
54	MG	1A	3062	1/1	0.90	0.08	30,30,30,30	0
54	MG	1A	3698	1/1	0.90	0.26	45,45,45,45	0
54	MG	2A	3059	1/1	0.90	0.11	54,54,54,54	0
54	MG	2A	3068	1/1	0.90	0.14	43,43,43,43	0
54	MG	1A	3802	1/1	0.90	0.18	32,32,32,32	0
54	MG	1A	3284	1/1	0.90	0.14	49,49,49,49	0
54	MG	1a	3037	1/1	0.90	0.28	55,55,55,55	0
54	MG	1F	304	1/1	0.90	0.45	42,42,42,42	0
54	MG	1a	3039	1/1	0.90	0.15	76,76,76,76	0
54	MG	1A	3531	1/1	0.90	0.11	32,32,32,32	0
54	MG	2A	3276	1/1	0.90	0.16	57,57,57,57	0
54	MG	1A	3705	1/1	0.90	0.14	22,22,22,22	0
54	MG	2A	3711	1/1	0.90	0.12	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1G	201	1/1	0.90	0.13	69,69,69,69	0
54	MG	1A	3809	1/1	0.90	0.09	19,19,19,19	0
54	MG	1a	3264	1/1	0.90	0.16	77,77,77,77	0
54	MG	2A	3726	1/1	0.90	0.17	64,64,64,64	0
54	MG	2A	3728	1/1	0.90	0.10	45,45,45,45	0
54	MG	1A	3708	1/1	0.90	0.12	28,28,28,28	0
54	MG	2a	3117	1/1	0.90	0.14	62,62,62,62	0
54	MG	2a	3120	1/1	0.90	0.12	57,57,57,57	0
54	MG	1A	3007	1/1	0.90	0.09	38,38,38,38	0
54	MG	1P	201	1/1	0.90	0.47	27,27,27,27	0
54	MG	2B	202	1/1	0.90	0.18	59,59,59,59	0
54	MG	1a	3162	1/1	0.90	0.18	64,64,64,64	0
54	MG	2B	205	1/1	0.90	0.12	49,49,49,49	0
54	MG	1P	204	1/1	0.90	0.37	35,35,35,35	0
54	MG	2A	3306	1/1	0.90	0.13	48,48,48,48	0
54	MG	1A	3296	1/1	0.90	0.18	52,52,52,52	0
54	MG	2B	210	1/1	0.90	0.13	61,61,61,61	0
54	MG	2A	3309	1/1	0.90	0.11	52,52,52,52	0
54	MG	2a	3153	1/1	0.90	0.11	88,88,88,88	0
54	MG	1A	3824	1/1	0.90	0.12	53,53,53,53	0
54	MG	2A	3131	1/1	0.90	0.12	54,54,54,54	0
54	MG	1a	3168	1/1	0.90	0.14	56,56,56,56	0
54	MG	2B	218	1/1	0.90	0.14	83,83,83,83	0
54	MG	2A	3334	1/1	0.90	0.09	40,40,40,40	0
54	MG	2A	3135	1/1	0.90	0.10	61,61,61,61	0
54	MG	1A	3632	1/1	0.90	0.15	44,44,44,44	0
54	MG	2A	3354	1/1	0.90	0.14	53,53,53,53	0
54	MG	1A	3830	1/1	0.90	0.08	30,30,30,30	0
54	MG	2A	3367	1/1	0.90	0.13	27,27,27,27	0
54	MG	1A	3222	1/1	0.90	0.14	44,44,44,44	0
54	MG	2A	3146	1/1	0.90	0.11	54,54,54,54	0
54	MG	2Q	204	1/1	0.90	0.17	69,69,69,69	0
54	MG	2T	203	1/1	0.90	0.12	58,58,58,58	0
54	MG	2U	201	1/1	0.90	0.38	67,67,67,67	0
54	MG	2k	201	1/1	0.90	0.12	64,64,64,64	0
54	MG	1A	3986	1/1	0.90	0.11	45,45,45,45	0
54	MG	1A	3648	1/1	0.90	0.15	27,27,27,27	0
54	MG	1A	3453	1/1	0.90	0.11	57,57,57,57	0
54	MG	1A	3549	1/1	0.90	0.25	52,52,52,52	0
54	MG	1A	3456	1/1	0.90	0.08	41,41,41,41	0
54	MG	2a	3003	1/1	0.90	0.17	57,57,57,57	0
54	MG	2A	3165	1/1	0.90	0.10	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3400	1/1	0.90	0.19	52,52,52,52	0
54	MG	1A	3862	1/1	0.90	0.11	48,48,48,48	0
54	MG	13	102	1/1	0.90	0.13	61,61,61,61	0
58	ZN	24	501	1/1	0.90	0.12	148,148,148,148	0
54	MG	2A	3129	1/1	0.91	0.24	62,62,62,62	0
54	MG	1A	3760	1/1	0.91	0.10	43,43,43,43	0
54	MG	1a	3220	1/1	0.91	0.09	72,72,72,72	0
54	MG	2B	211	1/1	0.91	0.13	58,58,58,58	0
54	MG	2A	3439	1/1	0.91	0.09	56,56,56,56	0
54	MG	1H	4102	1/1	0.91	0.09	60,60,60,60	0
54	MG	1A	3513	1/1	0.91	0.16	66,66,66,66	0
54	MG	1a	3069	1/1	0.91	0.12	55,55,55,55	0
54	MG	1A	3413	1/1	0.91	0.09	53,53,53,53	0
54	MG	2D	304	1/1	0.91	0.24	42,42,42,42	0
54	MG	1A	3935	1/1	0.91	0.27	35,35,35,35	0
54	MG	1A	3636	1/1	0.91	0.14	69,69,69,69	0
54	MG	2A	3149	1/1	0.91	0.11	41,41,41,41	0
54	MG	2F	301	1/1	0.91	0.16	38,38,38,38	0
54	MG	1a	3230	1/1	0.91	0.10	69,69,69,69	0
54	MG	1P	206	1/1	0.91	0.11	74,74,74,74	0
54	MG	1a	3234	1/1	0.91	0.08	67,67,67,67	0
54	MG	1A	3319	1/1	0.91	0.11	48,48,48,48	0
54	MG	1A	3527	1/1	0.91	0.11	43,43,43,43	0
54	MG	2Q	202	1/1	0.91	0.22	47,47,47,47	0
54	MG	1A	3942	1/1	0.91	0.08	46,46,46,46	0
54	MG	1A	3528	1/1	0.91	0.10	42,42,42,42	0
54	MG	1A	3777	1/1	0.91	0.11	47,47,47,47	0
54	MG	1A	3065	1/1	0.91	0.09	48,48,48,48	0
54	MG	1A	3425	1/1	0.91	0.12	46,46,46,46	0
54	MG	1a	3092	1/1	0.91	0.16	46,46,46,46	0
54	MG	1A	3039	1/1	0.91	0.14	53,53,53,53	0
54	MG	1A	3429	1/1	0.91	0.22	55,55,55,55	0
54	MG	2A	3188	1/1	0.91	0.14	61,61,61,61	0
54	MG	1A	3360	1/1	0.91	0.10	41,41,41,41	0
54	MG	1A	3800	1/1	0.91	0.15	64,64,64,64	0
54	MG	1A	3548	1/1	0.91	0.11	37,37,37,37	0
54	MG	1A	3364	1/1	0.91	0.16	45,45,45,45	0
54	MG	1a	3268	1/1	0.91	0.14	60,60,60,60	0
54	MG	2A	3498	1/1	0.91	0.09	55,55,55,55	0
54	MG	1A	3672	1/1	0.91	0.11	69,69,69,69	0
54	MG	1A	3002	1/1	0.91	0.11	46,46,46,46	0
54	MG	1A	3141	1/1	0.91	0.45	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3111	1/1	0.91	0.15	68,68,68,68	0
54	MG	1a	3114	1/1	0.91	0.16	68,68,68,68	0
54	MG	2A	3219	1/1	0.91	0.09	44,44,44,44	0
54	MG	1A	3681	1/1	0.91	0.12	51,51,51,51	0
54	MG	2A	3223	1/1	0.91	0.16	45,45,45,45	0
54	MG	2A	3225	1/1	0.91	0.31	40,40,40,40	0
54	MG	1A	3373	1/1	0.91	0.08	37,37,37,37	0
54	MG	2A	3230	1/1	0.91	0.14	61,61,61,61	0
54	MG	1A	3564	1/1	0.91	0.11	19,19,19,19	0
54	MG	19	102	1/1	0.91	0.10	54,54,54,54	0
54	MG	2a	3036	1/1	0.91	0.15	42,42,42,42	0
54	MG	1a	3001	1/1	0.91	0.15	68,68,68,68	0
54	MG	1A	3567	1/1	0.91	0.07	35,35,35,35	0
54	MG	2a	3045	1/1	0.91	0.09	50,50,50,50	0
54	MG	2A	3532	1/1	0.91	0.17	79,79,79,79	0
54	MG	1a	3132	1/1	0.91	0.09	72,72,72,72	0
54	MG	1A	3381	1/1	0.91	0.12	34,34,34,34	0
54	MG	1a	3135	1/1	0.91	0.13	54,54,54,54	0
54	MG	2A	3250	1/1	0.91	0.17	35,35,35,35	0
54	MG	1a	3007	1/1	0.91	0.10	58,58,58,58	0
54	MG	2a	3058	1/1	0.91	0.14	61,61,61,61	0
54	MG	2A	3252	1/1	0.91	0.10	40,40,40,40	0
54	MG	2A	3553	1/1	0.91	0.10	56,56,56,56	0
54	MG	1a	3140	1/1	0.91	0.16	72,72,72,72	0
54	MG	1a	3141	1/1	0.91	0.15	58,58,58,58	0
54	MG	2a	3065	1/1	0.91	0.13	62,62,62,62	0
54	MG	1A	3270	1/1	0.91	0.12	52,52,52,52	0
54	MG	1a	3144	1/1	0.91	0.23	61,61,61,61	0
54	MG	2A	3569	1/1	0.91	0.09	34,34,34,34	0
54	MG	1A	3293	1/1	0.91	0.13	57,57,57,57	0
54	MG	1a	3148	1/1	0.91	0.15	64,64,64,64	0
54	MG	2a	3075	1/1	0.91	0.10	59,59,59,59	0
54	MG	1A	3476	1/1	0.91	0.10	21,21,21,21	0
54	MG	1A	3842	1/1	0.91	0.12	30,30,30,30	0
54	MG	1a	3014	1/1	0.91	0.11	55,55,55,55	0
54	MG	1A	3701	1/1	0.91	0.16	44,44,44,44	0
54	MG	2A	3284	1/1	0.91	0.09	37,37,37,37	0
54	MG	1A	3847	1/1	0.91	0.08	31,31,31,31	0
54	MG	1A	3033	1/1	0.91	0.41	43,43,43,43	0
54	MG	1a	3159	1/1	0.91	0.12	50,50,50,50	0
54	MG	1A	3038	1/1	0.91	0.11	44,44,44,44	0
54	MG	1A	3592	1/1	0.91	0.13	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3614	1/1	0.91	0.09	46,46,46,46	0
54	MG	1a	3023	1/1	0.91	0.12	50,50,50,50	0
54	MG	1B	220	1/1	0.91	0.10	43,43,43,43	0
54	MG	2A	3617	1/1	0.91	0.19	62,62,62,62	0
54	MG	1A	3499	1/1	0.91	0.11	38,38,38,38	0
54	MG	1A	3601	1/1	0.91	0.16	56,56,56,56	0
54	MG	1A	3719	1/1	0.91	0.31	48,48,48,48	0
54	MG	2A	3322	1/1	0.91	0.14	56,56,56,56	0
54	MG	2A	3052	1/1	0.91	0.11	60,60,60,60	0
54	MG	1a	3034	1/1	0.91	0.31	69,69,69,69	0
54	MG	2A	3636	1/1	0.91	0.12	66,66,66,66	0
54	MG	2A	3330	1/1	0.91	0.15	63,63,63,63	0
54	MG	1a	3035	1/1	0.91	0.10	37,37,37,37	0
54	MG	1a	3036	1/1	0.91	0.10	53,53,53,53	0
54	MG	1A	3154	1/1	0.91	0.26	55,55,55,55	0
54	MG	2A	3350	1/1	0.91	0.13	60,60,60,60	0
54	MG	1A	3872	1/1	0.91	0.18	43,43,43,43	0
54	MG	1A	3403	1/1	0.91	0.17	39,39,39,39	0
54	MG	2A	3356	1/1	0.91	0.14	49,49,49,49	0
54	MG	1A	3887	1/1	0.91	0.10	14,14,14,14	0
54	MG	1a	3183	1/1	0.91	0.12	90,90,90,90	0
54	MG	2A	3678	1/1	0.91	0.12	58,58,58,58	0
54	MG	1A	3609	1/1	0.91	0.10	16,16,16,16	0
54	MG	1D	316	1/1	0.91	0.13	59,59,59,59	0
54	MG	1A	3613	1/1	0.91	0.17	52,52,52,52	0
54	MG	2a	3172	1/1	0.91	0.14	52,52,52,52	0
54	MG	1a	3192	1/1	0.91	0.16	72,72,72,72	0
54	MG	1A	3620	1/1	0.91	0.20	68,68,68,68	0
54	MG	1A	3250	1/1	0.91	0.28	46,46,46,46	0
54	MG	2A	3396	1/1	0.91	0.20	63,63,63,63	0
54	MG	2A	3397	1/1	0.91	0.11	58,58,58,58	0
54	MG	1E	307	1/1	0.91	0.07	43,43,43,43	0
54	MG	2A	3109	1/1	0.91	0.10	57,57,57,57	0
54	MG	2A	3406	1/1	0.91	0.09	67,67,67,67	0
54	MG	2a	3191	1/1	0.91	0.11	72,72,72,72	0
54	MG	1A	3278	1/1	0.91	0.13	35,35,35,35	0
54	MG	1a	3057	1/1	0.91	0.12	36,36,36,36	0
54	MG	1F	307	1/1	0.91	0.18	25,25,25,25	0
54	MG	2A	3727	1/1	0.91	0.15	52,52,52,52	0
54	MG	2A	3411	1/1	0.91	0.11	37,37,37,37	0
54	MG	2A	3113	1/1	0.91	0.08	35,35,35,35	0
54	MG	2A	3731	1/1	0.91	0.08	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3511	1/1	0.91	0.12	45,45,45,45	0
54	MG	1A	3912	1/1	0.91	0.13	54,54,54,54	0
54	MG	2A	3418	1/1	0.91	0.11	56,56,56,56	0
54	MG	1a	3063	1/1	0.91	0.11	66,66,66,66	0
54	MG	1A	3756	1/1	0.91	0.23	43,43,43,43	0
54	MG	1a	3218	1/1	0.91	0.08	62,62,62,62	0
54	MG	1A	3035	1/1	0.92	0.10	36,36,36,36	0
54	MG	1A	3851	1/1	0.92	0.07	33,33,33,33	0
54	MG	1a	3062	1/1	0.92	0.17	64,64,64,64	0
54	MG	1h	202	1/1	0.92	0.11	49,49,49,49	0
54	MG	1A	3160	1/1	0.92	0.16	43,43,43,43	0
54	MG	2A	3445	1/1	0.92	0.08	73,73,73,73	0
54	MG	2A	3446	1/1	0.92	0.10	56,56,56,56	0
54	MG	2A	3193	1/1	0.92	0.12	60,60,60,60	0
54	MG	1A	3572	1/1	0.92	0.10	43,43,43,43	0
54	MG	1n	102	1/1	0.92	0.16	58,58,58,58	0
54	MG	1A	3166	1/1	0.92	0.14	44,44,44,44	0
54	MG	2A	3197	1/1	0.92	0.09	48,48,48,48	0
54	MG	1a	3066	1/1	0.92	0.05	45,45,45,45	0
54	MG	1A	3037	1/1	0.92	0.09	39,39,39,39	0
54	MG	2A	3202	1/1	0.92	0.06	33,33,33,33	0
54	MG	2A	3204	1/1	0.92	0.09	50,50,50,50	0
54	MG	1Y	201	1/1	0.92	0.17	76,76,76,76	0
54	MG	1A	3376	1/1	0.92	0.12	36,36,36,36	0
54	MG	2A	3463	1/1	0.92	0.12	56,56,56,56	0
54	MG	2A	3213	1/1	0.92	0.06	44,44,44,44	0
54	MG	2A	3471	1/1	0.92	0.10	37,37,37,37	0
54	MG	1a	3178	1/1	0.92	0.12	84,84,84,84	0
54	MG	2A	3005	1/1	0.92	0.17	50,50,50,50	0
54	MG	1a	3071	1/1	0.92	0.15	52,52,52,52	0
54	MG	2A	3483	1/1	0.92	0.14	58,58,58,58	0
54	MG	1a	3181	1/1	0.92	0.11	70,70,70,70	0
54	MG	2P	201	1/1	0.92	0.28	57,57,57,57	0
54	MG	2A	3014	1/1	0.92	0.09	42,42,42,42	0
54	MG	1A	3172	1/1	0.92	0.07	30,30,30,30	0
54	MG	1A	4002	1/1	0.92	0.07	57,57,57,57	0
54	MG	2A	3231	1/1	0.92	0.17	59,59,59,59	0
54	MG	1a	3185	1/1	0.92	0.17	64,64,64,64	0
54	MG	2W	202	1/1	0.92	0.26	53,53,53,53	0
54	MG	2A	3234	1/1	0.92	0.17	58,58,58,58	0
54	MG	21	101	1/1	0.92	0.15	46,46,46,46	0
54	MG	1A	3210	1/1	0.92	0.08	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	4004	1/1	0.92	0.15	43,43,43,43	0
54	MG	27	101	1/1	0.92	0.11	42,42,42,42	0
54	MG	2A	3240	1/1	0.92	0.13	47,47,47,47	0
54	MG	1A	3585	1/1	0.92	0.11	54,54,54,54	0
54	MG	2A	3243	1/1	0.92	0.23	44,44,44,44	0
54	MG	2A	3244	1/1	0.92	0.11	45,45,45,45	0
54	MG	1A	4006	1/1	0.92	0.17	54,54,54,54	0
54	MG	1A	4007	1/1	0.92	0.11	41,41,41,41	0
54	MG	2a	3008	1/1	0.92	0.09	73,73,73,73	0
54	MG	1a	3083	1/1	0.92	0.18	47,47,47,47	0
54	MG	1A	3884	1/1	0.92	0.10	26,26,26,26	0
54	MG	1a	3087	1/1	0.92	0.12	54,54,54,54	0
54	MG	2A	3048	1/1	0.92	0.12	50,50,50,50	0
54	MG	2A	3255	1/1	0.92	0.20	52,52,52,52	0
54	MG	1a	3204	1/1	0.92	0.13	72,72,72,72	0
54	MG	2A	3517	1/1	0.92	0.10	50,50,50,50	0
54	MG	1A	3682	1/1	0.92	0.10	48,48,48,48	0
54	MG	2A	3521	1/1	0.92	0.09	57,57,57,57	0
54	MG	2A	3522	1/1	0.92	0.09	53,53,53,53	0
54	MG	2a	3023	1/1	0.92	0.23	67,67,67,67	0
54	MG	1a	3210	1/1	0.92	0.09	93,93,93,93	0
54	MG	2a	3026	1/1	0.92	0.12	52,52,52,52	0
54	MG	1A	3775	1/1	0.92	0.14	58,58,58,58	0
54	MG	1A	3892	1/1	0.92	0.08	15,15,15,15	0
54	MG	2a	3032	1/1	0.92	0.08	42,42,42,42	0
54	MG	2A	3271	1/1	0.92	0.12	22,22,22,22	0
54	MG	2A	3273	1/1	0.92	0.22	44,44,44,44	0
54	MG	2A	3536	1/1	0.92	0.14	63,63,63,63	0
54	MG	1a	3214	1/1	0.92	0.26	63,63,63,63	0
54	MG	1A	3893	1/1	0.92	0.09	35,35,35,35	0
54	MG	2A	3061	1/1	0.92	0.31	53,53,53,53	0
54	MG	2A	3063	1/1	0.92	0.09	56,56,56,56	0
54	MG	1A	3898	1/1	0.92	0.63	34,34,34,34	0
54	MG	2A	3070	1/1	0.92	0.27	53,53,53,53	0
54	MG	2a	3048	1/1	0.92	0.09	50,50,50,50	0
54	MG	2a	3049	1/1	0.92	0.10	47,47,47,47	0
54	MG	2A	3554	1/1	0.92	0.11	35,35,35,35	0
54	MG	1A	3173	1/1	0.92	0.14	45,45,45,45	0
54	MG	2A	3561	1/1	0.92	0.10	51,51,51,51	0
54	MG	1A	3901	1/1	0.92	0.20	42,42,42,42	0
54	MG	2A	3564	1/1	0.92	0.14	70,70,70,70	0
54	MG	1A	3440	1/1	0.92	0.10	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3567	1/1	0.92	0.09	53,53,53,53	0
54	MG	1A	3693	1/1	0.92	0.16	35,35,35,35	0
54	MG	1A	3521	1/1	0.92	0.10	48,48,48,48	0
54	MG	1A	3790	1/1	0.92	0.12	67,67,67,67	0
54	MG	2A	3299	1/1	0.92	0.12	46,46,46,46	0
54	MG	2A	3093	1/1	0.92	0.16	54,54,54,54	0
54	MG	2A	3579	1/1	0.92	0.09	40,40,40,40	0
54	MG	2A	3582	1/1	0.92	0.09	50,50,50,50	0
54	MG	2a	3072	1/1	0.92	0.09	58,58,58,58	0
54	MG	2a	3073	1/1	0.92	0.10	63,63,63,63	0
54	MG	2A	3095	1/1	0.92	0.07	35,35,35,35	0
54	MG	2A	3595	1/1	0.92	0.10	49,49,49,49	0
54	MG	1a	3225	1/1	0.92	0.10	39,39,39,39	0
54	MG	1A	3522	1/1	0.92	0.21	30,30,30,30	0
54	MG	2A	3603	1/1	0.92	0.08	27,27,27,27	0
54	MG	2a	3084	1/1	0.92	0.24	61,61,61,61	0
54	MG	2A	3318	1/1	0.92	0.09	38,38,38,38	0
54	MG	1A	3447	1/1	0.92	0.13	46,46,46,46	0
54	MG	2A	3323	1/1	0.92	0.08	47,47,47,47	0
54	MG	1D	309	1/1	0.92	0.13	42,42,42,42	0
54	MG	1A	3056	1/1	0.92	0.21	39,39,39,39	0
54	MG	2A	3329	1/1	0.92	0.14	25,25,25,25	0
54	MG	2a	3102	1/1	0.92	0.12	61,61,61,61	0
54	MG	1A	3315	1/1	0.92	0.09	32,32,32,32	0
54	MG	1A	3455	1/1	0.92	0.08	41,41,41,41	0
54	MG	1A	3702	1/1	0.92	0.08	22,22,22,22	0
54	MG	1A	3535	1/1	0.92	0.16	38,38,38,38	0
54	MG	1E	304	1/1	0.92	0.10	17,17,17,17	0
54	MG	2A	3352	1/1	0.92	0.15	52,52,52,52	0
54	MG	2A	3120	1/1	0.92	0.24	45,45,45,45	0
54	MG	1A	3625	1/1	0.92	0.12	47,47,47,47	0
54	MG	2A	3629	1/1	0.92	0.09	52,52,52,52	0
54	MG	1a	3130	1/1	0.92	0.11	52,52,52,52	0
54	MG	2a	3123	1/1	0.92	0.09	54,54,54,54	0
54	MG	2A	3359	1/1	0.92	0.14	44,44,44,44	0
54	MG	1a	3131	1/1	0.92	0.07	63,63,63,63	0
54	MG	1A	3004	1/1	0.92	0.08	48,48,48,48	0
54	MG	2a	3128	1/1	0.92	0.08	56,56,56,56	0
54	MG	1A	3349	1/1	0.92	0.11	27,27,27,27	0
54	MG	1A	3815	1/1	0.92	0.13	43,43,43,43	0
54	MG	2a	3147	1/1	0.92	0.09	73,73,73,73	0
54	MG	2A	3646	1/1	0.92	0.09	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3647	1/1	0.92	0.20	76,76,76,76	0
54	MG	2A	3372	1/1	0.92	0.11	30,30,30,30	0
54	MG	2A	3650	1/1	0.92	0.14	63,63,63,63	0
54	MG	1a	3136	1/1	0.92	0.17	63,63,63,63	0
54	MG	1F	309	1/1	0.92	0.08	30,30,30,30	0
54	MG	2a	3157	1/1	0.92	0.10	86,86,86,86	0
54	MG	1A	3405	1/1	0.92	0.15	49,49,49,49	0
54	MG	2A	3659	1/1	0.92	0.11	32,32,32,32	0
54	MG	1F	314	1/1	0.92	0.31	53,53,53,53	0
54	MG	2a	3165	1/1	0.92	0.09	74,74,74,74	0
54	MG	2A	3386	1/1	0.92	0.09	49,49,49,49	0
54	MG	2A	3675	1/1	0.92	0.08	46,46,46,46	0
54	MG	2A	3143	1/1	0.92	0.13	39,39,39,39	0
54	MG	1A	3470	1/1	0.92	0.08	17,17,17,17	0
54	MG	1A	3185	1/1	0.92	0.35	32,32,32,32	0
54	MG	2a	3179	1/1	0.92	0.09	61,61,61,61	0
54	MG	2A	3683	1/1	0.92	0.11	36,36,36,36	0
54	MG	1A	3478	1/1	0.92	0.10	18,18,18,18	0
54	MG	1G	204	1/1	0.92	0.10	46,46,46,46	0
54	MG	2A	3690	1/1	0.92	0.12	59,59,59,59	0
54	MG	2A	3695	1/1	0.92	0.10	48,48,48,48	0
54	MG	2A	3153	1/1	0.92	0.15	33,33,33,33	0
54	MG	2A	3408	1/1	0.92	0.14	51,51,51,51	0
54	MG	2a	3192	1/1	0.92	0.09	62,62,62,62	0
54	MG	1a	3270	1/1	0.92	0.09	53,53,53,53	0
54	MG	1A	3964	1/1	0.92	0.09	46,46,46,46	0
54	MG	2A	3705	1/1	0.92	0.15	42,42,42,42	0
54	MG	1H	4103	1/1	0.92	0.11	61,61,61,61	0
54	MG	1a	3047	1/1	0.92	0.16	44,44,44,44	0
54	MG	2A	3168	1/1	0.92	0.13	43,43,43,43	0
54	MG	1A	3187	1/1	0.92	0.18	31,31,31,31	0
54	MG	1A	3486	1/1	0.92	0.14	47,47,47,47	0
54	MG	2A	3723	1/1	0.92	0.06	43,43,43,43	0
54	MG	1A	3741	1/1	0.92	0.06	35,35,35,35	0
54	MG	1A	3563	1/1	0.92	0.08	55,55,55,55	0
54	MG	1A	3975	1/1	0.92	0.22	43,43,43,43	0
54	MG	1A	3116	1/1	0.92	0.13	31,31,31,31	0
54	MG	1a	3082	1/1	0.93	0.11	50,50,50,50	0
54	MG	2A	3725	1/1	0.93	0.10	52,52,52,52	0
54	MG	1A	3477	1/1	0.93	0.08	57,57,57,57	0
54	MG	1A	3594	1/1	0.93	0.40	31,31,31,31	0
54	MG	1a	3086	1/1	0.93	0.16	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3421	1/1	0.93	0.41	36,36,36,36	0
54	MG	2A	3424	1/1	0.93	0.15	63,63,63,63	0
54	MG	1A	3059	1/1	0.93	0.11	47,47,47,47	0
54	MG	1A	3369	1/1	0.93	0.14	57,57,57,57	0
54	MG	1A	3483	1/1	0.93	0.08	17,17,17,17	0
54	MG	2A	3167	1/1	0.93	0.16	40,40,40,40	0
54	MG	1A	3484	1/1	0.93	0.13	35,35,35,35	0
54	MG	2A	3169	1/1	0.93	0.18	48,48,48,48	0
54	MG	2A	3438	1/1	0.93	0.14	59,59,59,59	0
54	MG	1A	3752	1/1	0.93	0.14	40,40,40,40	0
54	MG	1A	3923	1/1	0.93	0.07	27,27,27,27	0
54	MG	2A	3441	1/1	0.93	0.21	41,41,41,41	0
54	MG	1A	3605	1/1	0.93	0.23	35,35,35,35	0
54	MG	1a	3095	1/1	0.93	0.15	58,58,58,58	0
54	MG	1A	3135	1/1	0.93	0.44	42,42,42,42	0
54	MG	2B	215	1/1	0.93	0.10	60,60,60,60	0
54	MG	1a	3255	1/1	0.93	0.17	55,55,55,55	0
54	MG	1Q	201	1/1	0.93	0.37	28,28,28,28	0
54	MG	2D	303	1/1	0.93	0.40	40,40,40,40	0
54	MG	2A	3186	1/1	0.93	0.13	47,47,47,47	0
54	MG	1a	3260	1/1	0.93	0.13	54,54,54,54	0
54	MG	1a	3099	1/1	0.93	0.10	43,43,43,43	0
54	MG	2A	3189	1/1	0.93	0.09	45,45,45,45	0
54	MG	2E	308	1/1	0.93	0.16	41,41,41,41	0
54	MG	2A	3454	1/1	0.93	0.09	54,54,54,54	0
54	MG	1A	3612	1/1	0.93	0.10	20,20,20,20	0
54	MG	1a	3102	1/1	0.93	0.11	63,63,63,63	0
54	MG	2A	3192	1/1	0.93	0.18	53,53,53,53	0
54	MG	1A	3375	1/1	0.93	0.09	37,37,37,37	0
54	MG	2O	201	1/1	0.93	0.07	40,40,40,40	0
54	MG	1A	3060	1/1	0.93	0.12	46,46,46,46	0
54	MG	2P	202	1/1	0.93	0.11	51,51,51,51	0
54	MG	1A	3502	1/1	0.93	0.10	19,19,19,19	0
54	MG	1A	3622	1/1	0.93	0.17	53,53,53,53	0
54	MG	2A	3466	1/1	0.93	0.17	50,50,50,50	0
54	MG	2T	202	1/1	0.93	0.09	50,50,50,50	0
54	MG	1A	3771	1/1	0.93	0.14	28,28,28,28	0
54	MG	1U	202	1/1	0.93	0.11	35,35,35,35	0
54	MG	1a	3116	1/1	0.93	0.09	53,53,53,53	0
54	MG	1A	3503	1/1	0.93	0.13	17,17,17,17	0
54	MG	1V	206	1/1	0.93	0.05	52,52,52,52	0
54	MG	1A	3953	1/1	0.93	0.12	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3209	1/1	0.93	0.10	45,45,45,45	0
54	MG	25	103	1/1	0.93	0.12	64,64,64,64	0
54	MG	1A	3029	1/1	0.93	0.12	33,33,33,33	0
54	MG	1A	3776	1/1	0.93	0.08	88,88,88,88	0
54	MG	1A	3103	1/1	0.93	0.48	32,32,32,32	0
54	MG	2A	3493	1/1	0.93	0.08	34,34,34,34	0
54	MG	2A	3218	1/1	0.93	0.19	55,55,55,55	0
54	MG	1a	3128	1/1	0.93	0.10	39,39,39,39	0
54	MG	1A	3195	1/1	0.93	0.06	29,29,29,29	0
54	MG	1A	3105	1/1	0.93	0.08	54,54,54,54	0
54	MG	1A	3967	1/1	0.93	0.11	52,52,52,52	0
54	MG	2a	3010	1/1	0.93	0.13	75,75,75,75	0
54	MG	2A	3226	1/1	0.93	0.16	41,41,41,41	0
54	MG	2A	3228	1/1	0.93	0.27	59,59,59,59	0
54	MG	1A	3783	1/1	0.93	0.09	48,48,48,48	0
54	MG	1A	3785	1/1	0.93	0.36	46,46,46,46	0
54	MG	1A	3281	1/1	0.93	0.23	44,44,44,44	0
54	MG	2A	3232	1/1	0.93	0.28	41,41,41,41	0
54	MG	1A	3642	1/1	0.93	0.18	48,48,48,48	0
54	MG	1A	3977	1/1	0.93	0.28	52,52,52,52	0
54	MG	1A	3107	1/1	0.93	0.48	25,25,25,25	0
54	MG	2A	3236	1/1	0.93	0.16	48,48,48,48	0
54	MG	1A	3153	1/1	0.93	0.07	26,26,26,26	0
54	MG	1A	3034	1/1	0.93	0.08	42,42,42,42	0
54	MG	2a	3028	1/1	0.93	0.15	74,74,74,74	0
54	MG	1A	3211	1/1	0.93	0.41	36,36,36,36	0
54	MG	1A	3286	1/1	0.93	0.12	53,53,53,53	0
54	MG	2a	3031	1/1	0.93	0.13	56,56,56,56	0
54	MG	2A	3007	1/1	0.93	0.08	41,41,41,41	0
54	MG	1A	3523	1/1	0.93	0.05	37,37,37,37	0
54	MG	2A	3525	1/1	0.93	0.09	53,53,53,53	0
54	MG	2A	3246	1/1	0.93	0.08	47,47,47,47	0
54	MG	2A	3012	1/1	0.93	0.18	52,52,52,52	0
54	MG	1A	3112	1/1	0.93	0.15	50,50,50,50	0
54	MG	1A	3067	1/1	0.93	0.06	14,14,14,14	0
54	MG	2a	3041	1/1	0.93	0.12	72,72,72,72	0
54	MG	2a	3042	1/1	0.93	0.16	64,64,64,64	0
54	MG	2A	3021	1/1	0.93	0.16	39,39,39,39	0
54	MG	1a	3153	1/1	0.93	0.09	54,54,54,54	0
54	MG	2A	3254	1/1	0.93	0.39	45,45,45,45	0
54	MG	1A	3810	1/1	0.93	0.18	51,51,51,51	0
54	MG	1A	3663	1/1	0.93	0.08	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3070	1/1	0.93	0.51	28,28,28,28	0
54	MG	1A	3424	1/1	0.93	0.13	17,17,17,17	0
54	MG	1a	3160	1/1	0.93	0.09	36,36,36,36	0
54	MG	2a	3055	1/1	0.93	0.09	51,51,51,51	0
54	MG	2a	3056	1/1	0.93	0.07	65,65,65,65	0
54	MG	2A	3265	1/1	0.93	0.10	49,49,49,49	0
54	MG	2A	3037	1/1	0.93	0.20	54,54,54,54	0
54	MG	2A	3268	1/1	0.93	0.10	54,54,54,54	0
54	MG	2A	3040	1/1	0.93	0.11	41,41,41,41	0
54	MG	2A	3041	1/1	0.93	0.07	23,23,23,23	0
54	MG	1A	3241	1/1	0.93	0.25	34,34,34,34	0
54	MG	1A	3304	1/1	0.93	0.16	33,33,33,33	0
54	MG	1A	3242	1/1	0.93	0.06	51,51,51,51	0
54	MG	1A	4008	1/1	0.93	0.11	46,46,46,46	0
54	MG	1A	4010	1/1	0.93	0.20	42,42,42,42	0
54	MG	1A	4011	1/1	0.93	0.11	53,53,53,53	0
54	MG	2A	3286	1/1	0.93	0.08	30,30,30,30	0
54	MG	1B	201	1/1	0.93	0.17	50,50,50,50	0
54	MG	2A	3583	1/1	0.93	0.10	73,73,73,73	0
54	MG	2A	3589	1/1	0.93	0.10	70,70,70,70	0
54	MG	2A	3591	1/1	0.93	0.09	35,35,35,35	0
54	MG	1A	3243	1/1	0.93	0.13	64,64,64,64	0
54	MG	1B	203	1/1	0.93	0.17	43,43,43,43	0
54	MG	2A	3597	1/1	0.93	0.10	36,36,36,36	0
54	MG	1A	3832	1/1	0.93	0.15	34,34,34,34	0
54	MG	1A	3837	1/1	0.93	0.11	17,17,17,17	0
54	MG	2a	3088	1/1	0.93	0.09	61,61,61,61	0
54	MG	1A	3545	1/1	0.93	0.07	39,39,39,39	0
54	MG	2A	3298	1/1	0.93	0.12	56,56,56,56	0
54	MG	1A	3075	1/1	0.93	0.08	37,37,37,37	0
54	MG	1B	215	1/1	0.93	0.09	52,52,52,52	0
54	MG	1A	3688	1/1	0.93	0.11	49,49,49,49	0
54	MG	1A	3318	1/1	0.93	0.12	30,30,30,30	0
54	MG	1A	3553	1/1	0.93	0.08	37,37,37,37	0
54	MG	1A	3246	1/1	0.93	0.33	40,40,40,40	0
54	MG	1a	3044	1/1	0.93	0.12	45,45,45,45	0
54	MG	1A	3445	1/1	0.93	0.07	30,30,30,30	0
54	MG	1B	226	1/1	0.93	0.17	65,65,65,65	0
54	MG	2A	3091	1/1	0.93	0.09	64,64,64,64	0
54	MG	1A	3446	1/1	0.93	0.08	40,40,40,40	0
54	MG	2a	3119	1/1	0.93	0.20	52,52,52,52	0
54	MG	1A	3854	1/1	0.93	0.07	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3333	1/1	0.93	0.14	58,58,58,58	0
54	MG	1B	229	1/1	0.93	0.17	49,49,49,49	0
54	MG	2A	3338	1/1	0.93	0.07	30,30,30,30	0
54	MG	2A	3340	1/1	0.93	0.15	38,38,38,38	0
54	MG	2A	3634	1/1	0.93	0.08	66,66,66,66	0
54	MG	1A	3320	1/1	0.93	0.09	19,19,19,19	0
54	MG	2A	3342	1/1	0.93	0.22	38,38,38,38	0
54	MG	2a	3132	1/1	0.93	0.09	73,73,73,73	0
54	MG	2A	3343	1/1	0.93	0.14	52,52,52,52	0
54	MG	2a	3146	1/1	0.93	0.17	64,64,64,64	0
54	MG	1D	302	1/1	0.93	0.78	23,23,23,23	0
54	MG	2A	3103	1/1	0.93	0.19	35,35,35,35	0
54	MG	1a	3203	1/1	0.93	0.12	70,70,70,70	0
54	MG	1A	3326	1/1	0.93	0.13	11,11,11,11	0
54	MG	1A	3329	1/1	0.93	0.12	44,44,44,44	0
54	MG	1a	3209	1/1	0.93	0.10	61,61,61,61	0
54	MG	2A	3652	1/1	0.93	0.07	48,48,48,48	0
54	MG	1D	311	1/1	0.93	0.16	33,33,33,33	0
54	MG	2A	3361	1/1	0.93	0.09	59,59,59,59	0
54	MG	2A	3656	1/1	0.93	0.10	35,35,35,35	0
54	MG	2a	3160	1/1	0.93	0.09	62,62,62,62	0
54	MG	1A	3126	1/1	0.93	0.16	41,41,41,41	0
54	MG	1A	3870	1/1	0.93	0.14	37,37,37,37	0
54	MG	2A	3669	1/1	0.93	0.09	52,52,52,52	0
54	MG	2A	3116	1/1	0.93	0.08	43,43,43,43	0
54	MG	2A	3370	1/1	0.93	0.12	58,58,58,58	0
54	MG	1A	3043	1/1	0.93	0.16	8,8,8,8	0
54	MG	1D	317	1/1	0.93	0.12	44,44,44,44	0
54	MG	2A	3679	1/1	0.93	0.12	51,51,51,51	0
54	MG	2A	3373	1/1	0.93	0.07	40,40,40,40	0
54	MG	2a	3182	1/1	0.93	0.25	70,70,70,70	0
54	MG	2A	3682	1/1	0.93	0.19	82,82,82,82	0
54	MG	2A	3375	1/1	0.93	0.13	38,38,38,38	0
54	MG	1A	3174	1/1	0.93	0.11	31,31,31,31	0
54	MG	1A	3460	1/1	0.93	0.09	29,29,29,29	0
54	MG	1A	3261	1/1	0.93	0.10	32,32,32,32	0
54	MG	2A	3693	1/1	0.93	0.22	47,47,47,47	0
54	MG	2A	3127	1/1	0.93	0.26	53,53,53,53	0
54	MG	2e	201	1/1	0.93	0.28	51,51,51,51	0
54	MG	1A	3886	1/1	0.93	0.13	22,22,22,22	0
54	MG	1A	3128	1/1	0.93	0.17	46,46,46,46	0
54	MG	1a	3221	1/1	0.93	0.12	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2r	101	1/1	0.93	0.11	67,67,67,67	0
54	MG	1A	3473	1/1	0.93	0.09	36,36,36,36	0
54	MG	1A	3088	1/1	0.93	0.47	41,41,41,41	0
54	MG	1A	3588	1/1	0.93	0.07	27,27,27,27	0
54	MG	1A	3591	1/1	0.93	0.11	50,50,50,50	0
54	MG	2A	3142	1/1	0.93	0.11	38,38,38,38	0
54	MG	2A	3712	1/1	0.93	0.18	78,78,78,78	0
54	MG	1F	313	1/1	0.93	0.09	39,39,39,39	0
54	MG	1A	3730	1/1	0.93	0.10	41,41,41,41	0
54	MG	2A	3721	1/1	0.93	0.10	43,43,43,43	0
54	MG	1A	3737	1/1	0.93	0.08	18,18,18,18	0
54	MG	1A	3386	1/1	0.94	0.08	19,19,19,19	0
54	MG	1A	3552	1/1	0.94	0.09	43,43,43,43	0
54	MG	2A	3717	1/1	0.94	0.10	48,48,48,48	0
54	MG	2A	3718	1/1	0.94	0.17	52,52,52,52	0
54	MG	1a	3232	1/1	0.94	0.11	54,54,54,54	0
54	MG	2A	3151	1/1	0.94	0.10	57,57,57,57	0
54	MG	1A	3042	1/1	0.94	0.08	25,25,25,25	0
54	MG	1A	3309	1/1	0.94	0.18	32,32,32,32	0
54	MG	2A	3154	1/1	0.94	0.12	34,34,34,34	0
54	MG	1A	3170	1/1	0.94	0.11	40,40,40,40	0
54	MG	1A	3200	1/1	0.94	0.10	33,33,33,33	0
54	MG	2A	3415	1/1	0.94	0.07	35,35,35,35	0
54	MG	2A	3416	1/1	0.94	0.18	60,60,60,60	0
54	MG	1a	3237	1/1	0.94	0.13	57,57,57,57	0
54	MG	2A	3420	1/1	0.94	0.08	46,46,46,46	0
54	MG	1A	3312	1/1	0.94	0.14	47,47,47,47	0
54	MG	2A	3166	1/1	0.94	0.14	46,46,46,46	0
54	MG	1N	202	1/1	0.94	0.15	61,61,61,61	0
54	MG	1A	3944	1/1	0.94	0.09	35,35,35,35	0
54	MG	2A	3430	1/1	0.94	0.12	54,54,54,54	0
54	MG	1a	3244	1/1	0.94	0.07	66,66,66,66	0
54	MG	2A	3171	1/1	0.94	0.11	40,40,40,40	0
54	MG	1A	3667	1/1	0.94	0.08	26,26,26,26	0
54	MG	1A	3947	1/1	0.94	0.09	31,31,31,31	0
54	MG	2A	3437	1/1	0.94	0.15	48,48,48,48	0
54	MG	1P	205	1/1	0.94	0.15	43,43,43,43	0
54	MG	2A	3180	1/1	0.94	0.07	72,72,72,72	0
54	MG	1A	3201	1/1	0.94	0.08	28,28,28,28	0
54	MG	1a	3096	1/1	0.94	0.11	59,59,59,59	0
54	MG	2A	3442	1/1	0.94	0.08	65,65,65,65	0
54	MG	1a	3253	1/1	0.94	0.08	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3952	1/1	0.94	0.13	34,34,34,34	0
54	MG	1Q	204	1/1	0.94	0.07	25,25,25,25	0
54	MG	1R	205	1/1	0.94	0.08	48,48,48,48	0
54	MG	1a	3262	1/1	0.94	0.08	86,86,86,86	0
54	MG	1a	3100	1/1	0.94	0.07	47,47,47,47	0
54	MG	1A	3793	1/1	0.94	0.15	23,23,23,23	0
54	MG	2A	3451	1/1	0.94	0.10	64,64,64,64	0
54	MG	1S	201	1/1	0.94	0.12	61,61,61,61	0
54	MG	1A	3795	1/1	0.94	0.08	31,31,31,31	0
54	MG	1A	3961	1/1	0.94	0.14	61,61,61,61	0
54	MG	2N	201	1/1	0.94	0.07	48,48,48,48	0
54	MG	1A	3407	1/1	0.94	0.08	30,30,30,30	0
54	MG	1A	3568	1/1	0.94	0.10	45,45,45,45	0
54	MG	1A	3317	1/1	0.94	0.15	56,56,56,56	0
54	MG	1A	3571	1/1	0.94	0.12	39,39,39,39	0
54	MG	1a	3115	1/1	0.94	0.07	35,35,35,35	0
54	MG	1U	205	1/1	0.94	0.37	63,63,63,63	0
54	MG	2R	202	1/1	0.94	0.07	34,34,34,34	0
54	MG	2A	3464	1/1	0.94	0.08	45,45,45,45	0
54	MG	1V	203	1/1	0.94	0.22	44,44,44,44	0
54	MG	1a	3118	1/1	0.94	0.09	43,43,43,43	0
54	MG	1A	3204	1/1	0.94	0.14	55,55,55,55	0
54	MG	1A	3968	1/1	0.94	0.10	35,35,35,35	0
54	MG	2Y	201	1/1	0.94	0.16	48,48,48,48	0
54	MG	1W	201	1/1	0.94	0.16	33,33,33,33	0
54	MG	2A	3478	1/1	0.94	0.11	49,49,49,49	0
54	MG	2A	3212	1/1	0.94	0.10	53,53,53,53	0
54	MG	1W	203	1/1	0.94	0.16	28,28,28,28	0
54	MG	1A	3143	1/1	0.94	0.09	37,37,37,37	0
54	MG	2A	3487	1/1	0.94	0.09	51,51,51,51	0
54	MG	2A	3217	1/1	0.94	0.06	42,42,42,42	0
54	MG	1A	3495	1/1	0.94	0.10	41,41,41,41	0
54	MG	1a	3129	1/1	0.94	0.09	43,43,43,43	0
54	MG	1l	202	1/1	0.94	0.09	61,61,61,61	0
54	MG	2A	3222	1/1	0.94	0.15	53,53,53,53	0
54	MG	1A	3578	1/1	0.94	0.10	51,51,51,51	0
54	MG	1A	3690	1/1	0.94	0.08	33,33,33,33	0
54	MG	1A	3415	1/1	0.94	0.09	20,20,20,20	0
54	MG	1l	101	1/1	0.94	0.26	46,46,46,46	0
54	MG	1a	3134	1/1	0.94	0.10	47,47,47,47	0
54	MG	1A	3978	1/1	0.94	0.18	42,42,42,42	0
54	MG	1A	3416	1/1	0.94	0.10	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3001	1/1	0.94	0.18	50,50,50,50	0
54	MG	1a	3137	1/1	0.94	0.17	52,52,52,52	0
54	MG	2A	3507	1/1	0.94	0.31	48,48,48,48	0
54	MG	1A	3133	1/1	0.94	0.07	47,47,47,47	0
54	MG	1A	3818	1/1	0.94	0.11	41,41,41,41	0
54	MG	1A	3983	1/1	0.94	0.08	37,37,37,37	0
54	MG	2A	3238	1/1	0.94	0.26	46,46,46,46	0
54	MG	2a	3025	1/1	0.94	0.15	49,49,49,49	0
54	MG	1A	3321	1/1	0.94	0.08	22,22,22,22	0
54	MG	2A	3011	1/1	0.94	0.16	38,38,38,38	0
54	MG	1A	3826	1/1	0.94	0.16	43,43,43,43	0
54	MG	1A	3420	1/1	0.94	0.06	17,17,17,17	0
54	MG	1A	3152	1/1	0.94	0.09	51,51,51,51	0
54	MG	1A	3831	1/1	0.94	0.17	26,26,26,26	0
54	MG	1a	3002	1/1	0.94	0.14	69,69,69,69	0
54	MG	1a	3151	1/1	0.94	0.16	46,46,46,46	0
54	MG	1A	3999	1/1	0.94	0.10	68,68,68,68	0
54	MG	2A	3526	1/1	0.94	0.08	26,26,26,26	0
54	MG	1A	3041	1/1	0.94	0.08	45,45,45,45	0
54	MG	2a	3038	1/1	0.94	0.13	56,56,56,56	0
54	MG	2A	3530	1/1	0.94	0.07	42,42,42,42	0
54	MG	1A	3833	1/1	0.94	0.20	59,59,59,59	0
54	MG	2A	3032	1/1	0.94	0.16	48,48,48,48	0
54	MG	2a	3044	1/1	0.94	0.12	65,65,65,65	0
54	MG	2A	3034	1/1	0.94	0.16	53,53,53,53	0
54	MG	2A	3534	1/1	0.94	0.19	88,88,88,88	0
54	MG	1A	3834	1/1	0.94	0.10	53,53,53,53	0
54	MG	1A	3593	1/1	0.94	0.10	23,23,23,23	0
54	MG	2A	3038	1/1	0.94	0.11	45,45,45,45	0
54	MG	2a	3050	1/1	0.94	0.18	46,46,46,46	0
54	MG	1A	3508	1/1	0.94	0.09	37,37,37,37	0
54	MG	1A	3839	1/1	0.94	0.24	33,33,33,33	0
54	MG	1A	3595	1/1	0.94	0.07	70,70,70,70	0
54	MG	2A	3551	1/1	0.94	0.09	62,62,62,62	0
54	MG	1A	3343	1/1	0.94	0.09	66,66,66,66	0
54	MG	1A	4009	1/1	0.94	0.11	33,33,33,33	0
54	MG	2A	3270	1/1	0.94	0.10	44,44,44,44	0
54	MG	1A	3428	1/1	0.94	0.11	34,34,34,34	0
54	MG	1A	3846	1/1	0.94	0.06	58,58,58,58	0
54	MG	2A	3050	1/1	0.94	0.19	43,43,43,43	0
54	MG	1A	3136	1/1	0.94	0.23	31,31,31,31	0
54	MG	1A	3713	1/1	0.94	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3171	1/1	0.94	0.06	70,70,70,70	0
54	MG	2a	3067	1/1	0.94	0.06	55,55,55,55	0
54	MG	1A	3715	1/1	0.94	0.36	43,43,43,43	0
54	MG	1B	205	1/1	0.94	0.09	46,46,46,46	0
54	MG	2a	3070	1/1	0.94	0.11	28,28,28,28	0
54	MG	1A	3852	1/1	0.94	0.07	33,33,33,33	0
54	MG	2A	3574	1/1	0.94	0.17	82,82,82,82	0
54	MG	1A	3717	1/1	0.94	0.19	38,38,38,38	0
54	MG	2A	3578	1/1	0.94	0.08	38,38,38,38	0
54	MG	2A	3060	1/1	0.94	0.11	40,40,40,40	0
54	MG	1A	3223	1/1	0.94	0.13	34,34,34,34	0
54	MG	2A	3062	1/1	0.94	0.14	48,48,48,48	0
54	MG	2A	3586	1/1	0.94	0.07	76,76,76,76	0
54	MG	2a	3080	1/1	0.94	0.21	42,42,42,42	0
54	MG	2A	3292	1/1	0.94	0.09	42,42,42,42	0
54	MG	1A	3235	1/1	0.94	0.23	26,26,26,26	0
54	MG	2A	3064	1/1	0.94	0.42	44,44,44,44	0
54	MG	1A	3356	1/1	0.94	0.09	25,25,25,25	0
54	MG	2a	3091	1/1	0.94	0.14	60,60,60,60	0
54	MG	1A	3155	1/1	0.94	0.27	38,38,38,38	0
54	MG	2A	3303	1/1	0.94	0.12	35,35,35,35	0
54	MG	1A	3186	1/1	0.94	0.15	54,54,54,54	0
54	MG	2a	3096	1/1	0.94	0.11	59,59,59,59	0
54	MG	1B	219	1/1	0.94	0.10	41,41,41,41	0
54	MG	2a	3100	1/1	0.94	0.16	33,33,33,33	0
54	MG	1A	3867	1/1	0.94	0.10	34,34,34,34	0
54	MG	2A	3312	1/1	0.94	0.08	36,36,36,36	0
54	MG	2A	3314	1/1	0.94	0.07	27,27,27,27	0
54	MG	2A	3079	1/1	0.94	0.14	48,48,48,48	0
54	MG	2a	3106	1/1	0.94	0.26	56,56,56,56	0
54	MG	2A	3082	1/1	0.94	0.39	46,46,46,46	0
54	MG	2A	3611	1/1	0.94	0.14	36,36,36,36	0
54	MG	2A	3319	1/1	0.94	0.08	38,38,38,38	0
54	MG	2A	3321	1/1	0.94	0.07	41,41,41,41	0
54	MG	1A	3731	1/1	0.94	0.17	30,30,30,30	0
54	MG	1B	224	1/1	0.94	0.14	44,44,44,44	0
54	MG	2A	3087	1/1	0.94	0.23	60,60,60,60	0
54	MG	1A	3733	1/1	0.94	0.08	25,25,25,25	0
54	MG	2A	3328	1/1	0.94	0.09	34,34,34,34	0
54	MG	1A	3616	1/1	0.94	0.13	52,52,52,52	0
54	MG	1A	3046	1/1	0.94	0.10	32,32,32,32	0
54	MG	2A	3094	1/1	0.94	0.19	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3530	1/1	0.94	0.05	32,32,32,32	0
54	MG	2A	3096	1/1	0.94	0.31	52,52,52,52	0
54	MG	1A	3158	1/1	0.94	0.21	47,47,47,47	0
54	MG	2A	3635	1/1	0.94	0.10	79,79,79,79	0
54	MG	2a	3139	1/1	0.94	0.18	74,74,74,74	0
54	MG	1A	3623	1/1	0.94	0.07	46,46,46,46	0
54	MG	2A	3639	1/1	0.94	0.08	65,65,65,65	0
54	MG	1a	3202	1/1	0.94	0.10	49,49,49,49	0
54	MG	2A	3105	1/1	0.94	0.16	60,60,60,60	0
54	MG	2A	3644	1/1	0.94	0.08	88,88,88,88	0
54	MG	1A	3087	1/1	0.94	0.46	40,40,40,40	0
54	MG	1A	3627	1/1	0.94	0.13	31,31,31,31	0
54	MG	2a	3155	1/1	0.94	0.08	41,41,41,41	0
54	MG	1A	3245	1/1	0.94	0.40	40,40,40,40	0
54	MG	1a	3208	1/1	0.94	0.13	52,52,52,52	0
54	MG	1A	3895	1/1	0.94	0.11	47,47,47,47	0
54	MG	1A	3454	1/1	0.94	0.08	45,45,45,45	0
54	MG	1a	3211	1/1	0.94	0.11	73,73,73,73	0
54	MG	1A	3537	1/1	0.94	0.20	43,43,43,43	0
54	MG	2A	3654	1/1	0.94	0.10	49,49,49,49	0
54	MG	2a	3166	1/1	0.94	0.08	59,59,59,59	0
54	MG	2A	3362	1/1	0.94	0.07	51,51,51,51	0
54	MG	2A	3366	1/1	0.94	0.09	24,24,24,24	0
54	MG	2A	3657	1/1	0.94	0.08	36,36,36,36	0
54	MG	1A	3190	1/1	0.94	0.09	55,55,55,55	0
54	MG	1A	3635	1/1	0.94	0.10	46,46,46,46	0
54	MG	2A	3663	1/1	0.94	0.09	52,52,52,52	0
54	MG	2a	3180	1/1	0.94	0.07	70,70,70,70	0
54	MG	1A	3766	1/1	0.94	0.10	33,33,33,33	0
54	MG	1A	3907	1/1	0.94	0.07	47,47,47,47	0
54	MG	2A	3124	1/1	0.94	0.62	43,43,43,43	0
54	MG	2a	3184	1/1	0.94	0.13	65,65,65,65	0
54	MG	1A	3299	1/1	0.94	0.06	25,25,25,25	0
54	MG	1A	3640	1/1	0.94	0.15	49,49,49,49	0
54	MG	2a	3188	1/1	0.94	0.17	57,57,57,57	0
54	MG	1A	3544	1/1	0.94	0.10	47,47,47,47	0
54	MG	1a	3070	1/1	0.94	0.10	55,55,55,55	0
54	MG	2A	3681	1/1	0.94	0.10	67,67,67,67	0
54	MG	1F	303	1/1	0.94	0.10	28,28,28,28	0
54	MG	2A	3379	1/1	0.94	0.12	53,53,53,53	0
54	MG	2A	3380	1/1	0.94	0.07	28,28,28,28	0
54	MG	1A	3918	1/1	0.94	0.06	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3164	1/1	0.94	0.33	26,26,26,26	0
54	MG	1A	3547	1/1	0.94	0.08	40,40,40,40	0
54	MG	2A	3390	1/1	0.94	0.08	56,56,56,56	0
54	MG	2A	3393	1/1	0.94	0.15	44,44,44,44	0
55	A1CRE	1A	4012	41/41	0.94	0.12	23,29,52,60	0
55	A1CRE	2A	3733	41/41	0.94	0.14	35,45,60,67	0
54	MG	2A	3394	1/1	0.94	0.08	32,32,32,32	0
56	MPD	18	105	8/8	0.94	0.14	24,26,28,33	0
54	MG	1A	3049	1/1	0.94	0.44	38,38,38,38	0
54	MG	1A	3924	1/1	0.94	0.09	35,35,35,35	0
54	MG	1A	3926	1/1	0.94	0.12	52,52,52,52	0
54	MG	2A	3399	1/1	0.94	0.10	33,33,33,33	0
54	MG	2A	3402	1/1	0.94	0.09	48,48,48,48	0
57	ARG	1B	231	12/12	0.94	0.14	29,40,45,46	0
54	MG	2A	3709	1/1	0.94	0.09	45,45,45,45	0
54	MG	2A	3145	1/1	0.94	0.09	51,51,51,51	0
54	MG	1A	3461	1/1	0.95	0.08	34,34,34,34	0
54	MG	1A	3368	1/1	0.95	0.07	56,56,56,56	0
54	MG	2A	3210	1/1	0.95	0.13	58,58,58,58	0
54	MG	1A	3219	1/1	0.95	0.08	27,27,27,27	0
54	MG	1y	202	1/1	0.95	0.07	67,67,67,67	0
54	MG	1A	3687	1/1	0.95	0.28	47,47,47,47	0
54	MG	2A	3455	1/1	0.95	0.09	43,43,43,43	0
54	MG	2A	3214	1/1	0.95	0.19	49,49,49,49	0
54	MG	11	104	1/1	0.95	0.12	33,33,33,33	0
54	MG	1A	3819	1/1	0.95	0.10	39,39,39,39	0
54	MG	1A	3984	1/1	0.95	0.07	80,80,80,80	0
54	MG	2A	3461	1/1	0.95	0.06	54,54,54,54	0
54	MG	15	101	1/1	0.95	0.22	32,32,32,32	0
54	MG	2B	219	1/1	0.95	0.12	76,76,76,76	0
54	MG	2D	301	1/1	0.95	0.20	47,47,47,47	0
54	MG	1A	3821	1/1	0.95	0.06	31,31,31,31	0
54	MG	2A	3008	1/1	0.95	0.09	32,32,32,32	0
54	MG	2D	305	1/1	0.95	0.15	40,40,40,40	0
54	MG	1A	3822	1/1	0.95	0.07	35,35,35,35	0
54	MG	17	103	1/1	0.95	0.11	52,52,52,52	0
54	MG	2E	302	1/1	0.95	0.15	33,33,33,33	0
54	MG	2E	303	1/1	0.95	0.07	39,39,39,39	0
54	MG	17	104	1/1	0.95	0.10	32,32,32,32	0
54	MG	2E	305	1/1	0.95	0.07	28,28,28,28	0
54	MG	1A	3472	1/1	0.95	0.08	28,28,28,28	0
54	MG	1A	3570	1/1	0.95	0.18	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3476	1/1	0.95	0.06	51,51,51,51	0
54	MG	2A	3020	1/1	0.95	0.06	29,29,29,29	0
54	MG	1A	3992	1/1	0.95	0.15	33,33,33,33	0
54	MG	1A	3371	1/1	0.95	0.12	40,40,40,40	0
54	MG	1A	3998	1/1	0.95	0.18	44,44,44,44	0
54	MG	1A	3177	1/1	0.95	0.45	25,25,25,25	0
54	MG	1a	3004	1/1	0.95	0.08	55,55,55,55	0
54	MG	2A	3028	1/1	0.95	0.07	38,38,38,38	0
54	MG	1A	3178	1/1	0.95	0.56	29,29,29,29	0
54	MG	2A	3491	1/1	0.95	0.11	54,54,54,54	0
54	MG	1A	3179	1/1	0.95	0.09	40,40,40,40	0
54	MG	1A	3377	1/1	0.95	0.06	19,19,19,19	0
54	MG	2T	201	1/1	0.95	0.08	51,51,51,51	0
54	MG	1A	3378	1/1	0.95	0.08	18,18,18,18	0
54	MG	1A	3380	1/1	0.95	0.07	23,23,23,23	0
54	MG	1A	3581	1/1	0.95	0.07	31,31,31,31	0
54	MG	2A	3039	1/1	0.95	0.18	40,40,40,40	0
54	MG	1A	3232	1/1	0.95	0.36	29,29,29,29	0
54	MG	2A	3247	1/1	0.95	0.12	39,39,39,39	0
54	MG	1A	3287	1/1	0.95	0.12	14,14,14,14	0
54	MG	1a	3015	1/1	0.95	0.10	68,68,68,68	0
54	MG	25	101	1/1	0.95	0.15	44,44,44,44	0
54	MG	2A	3505	1/1	0.95	0.10	27,27,27,27	0
54	MG	1A	3707	1/1	0.95	0.06	83,83,83,83	0
54	MG	1a	3165	1/1	0.95	0.11	51,51,51,51	0
54	MG	28	101	1/1	0.95	0.16	48,48,48,48	0
54	MG	1A	3586	1/1	0.95	0.11	40,40,40,40	0
54	MG	2A	3047	1/1	0.95	0.09	47,47,47,47	0
54	MG	1A	3490	1/1	0.95	0.06	34,34,34,34	0
54	MG	1A	3182	1/1	0.95	0.15	33,33,33,33	0
54	MG	1A	3150	1/1	0.95	0.09	30,30,30,30	0
54	MG	1A	3849	1/1	0.95	0.23	43,43,43,43	0
54	MG	2a	3007	1/1	0.95	0.12	41,41,41,41	0
54	MG	1A	3130	1/1	0.95	0.06	43,43,43,43	0
54	MG	1a	3025	1/1	0.95	0.06	54,54,54,54	0
54	MG	1a	3026	1/1	0.95	0.17	43,43,43,43	0
54	MG	1A	3012	1/1	0.95	0.17	23,23,23,23	0
54	MG	1A	3301	1/1	0.95	0.12	46,46,46,46	0
54	MG	1a	3029	1/1	0.95	0.14	49,49,49,49	0
54	MG	1A	3718	1/1	0.95	0.10	37,37,37,37	0
54	MG	1A	3596	1/1	0.95	0.13	44,44,44,44	0
54	MG	1B	210	1/1	0.95	0.17	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	3184	1/1	0.95	0.08	65,65,65,65	0
54	MG	2A	3279	1/1	0.95	0.21	44,44,44,44	0
54	MG	2A	3065	1/1	0.95	0.17	31,31,31,31	0
54	MG	1B	211	1/1	0.95	0.14	59,59,59,59	0
54	MG	2A	3282	1/1	0.95	0.16	54,54,54,54	0
54	MG	2A	3069	1/1	0.95	0.16	30,30,30,30	0
54	MG	1A	3721	1/1	0.95	0.20	42,42,42,42	0
54	MG	2A	3538	1/1	0.95	0.07	65,65,65,65	0
54	MG	1a	3187	1/1	0.95	0.07	69,69,69,69	0
54	MG	2A	3540	1/1	0.95	0.10	86,86,86,86	0
54	MG	1B	216	1/1	0.95	0.07	38,38,38,38	0
54	MG	1A	3724	1/1	0.95	0.10	38,38,38,38	0
54	MG	1a	3191	1/1	0.95	0.15	47,47,47,47	0
54	MG	1A	3020	1/1	0.95	0.28	32,32,32,32	0
54	MG	2A	3552	1/1	0.95	0.10	76,76,76,76	0
54	MG	1a	3041	1/1	0.95	0.16	55,55,55,55	0
54	MG	2A	3294	1/1	0.95	0.10	50,50,50,50	0
54	MG	2A	3555	1/1	0.95	0.09	26,26,26,26	0
54	MG	2A	3556	1/1	0.95	0.08	70,70,70,70	0
54	MG	2A	3557	1/1	0.95	0.12	28,28,28,28	0
54	MG	1A	3726	1/1	0.95	0.08	41,41,41,41	0
54	MG	2a	3043	1/1	0.95	0.14	45,45,45,45	0
54	MG	2A	3297	1/1	0.95	0.15	33,33,33,33	0
54	MG	1A	3072	1/1	0.95	0.07	34,34,34,34	0
54	MG	2A	3088	1/1	0.95	0.06	44,44,44,44	0
54	MG	2A	3300	1/1	0.95	0.07	51,51,51,51	0
54	MG	2A	3089	1/1	0.95	0.21	49,49,49,49	0
54	MG	2A	3304	1/1	0.95	0.07	34,34,34,34	0
54	MG	2A	3090	1/1	0.95	0.05	59,59,59,59	0
54	MG	2A	3307	1/1	0.95	0.07	44,44,44,44	0
54	MG	2A	3572	1/1	0.95	0.08	55,55,55,55	0
54	MG	1A	3134	1/1	0.95	0.07	24,24,24,24	0
54	MG	1a	3201	1/1	0.95	0.10	58,58,58,58	0
54	MG	1A	3044	1/1	0.95	0.32	26,26,26,26	0
54	MG	1a	3046	1/1	0.95	0.23	56,56,56,56	0
54	MG	1A	3247	1/1	0.95	0.21	63,63,63,63	0
54	MG	2A	3580	1/1	0.95	0.07	50,50,50,50	0
54	MG	2A	3581	1/1	0.95	0.09	32,32,32,32	0
54	MG	1A	3606	1/1	0.95	0.14	31,31,31,31	0
54	MG	2A	3097	1/1	0.95	0.21	39,39,39,39	0
54	MG	2a	3064	1/1	0.95	0.05	51,51,51,51	0
54	MG	1A	3734	1/1	0.95	0.31	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3100	1/1	0.95	0.31	61,61,61,61	0
54	MG	1a	3050	1/1	0.95	0.15	55,55,55,55	0
54	MG	1a	3052	1/1	0.95	0.13	39,39,39,39	0
54	MG	2A	3104	1/1	0.95	0.12	26,26,26,26	0
54	MG	1A	3735	1/1	0.95	0.07	39,39,39,39	0
54	MG	1A	3512	1/1	0.95	0.13	20,20,20,20	0
54	MG	1A	3891	1/1	0.95	0.07	27,27,27,27	0
54	MG	1A	3739	1/1	0.95	0.07	36,36,36,36	0
54	MG	1A	3191	1/1	0.95	0.22	50,50,50,50	0
54	MG	2A	3336	1/1	0.95	0.09	38,38,38,38	0
54	MG	1a	3060	1/1	0.95	0.24	62,62,62,62	0
54	MG	1A	3414	1/1	0.95	0.09	20,20,20,20	0
54	MG	2A	3608	1/1	0.95	0.09	77,77,77,77	0
54	MG	2A	3609	1/1	0.95	0.09	55,55,55,55	0
54	MG	1A	3253	1/1	0.95	0.14	38,38,38,38	0
54	MG	1A	3743	1/1	0.95	0.14	45,45,45,45	0
54	MG	1A	3617	1/1	0.95	0.09	38,38,38,38	0
54	MG	2A	3613	1/1	0.95	0.07	50,50,50,50	0
54	MG	2A	3119	1/1	0.95	0.11	49,49,49,49	0
54	MG	1A	3746	1/1	0.95	0.10	31,31,31,31	0
54	MG	1A	3519	1/1	0.95	0.06	29,29,29,29	0
54	MG	1A	3011	1/1	0.95	0.08	40,40,40,40	0
54	MG	2a	3095	1/1	0.95	0.08	46,46,46,46	0
54	MG	1A	3162	1/1	0.95	0.33	30,30,30,30	0
54	MG	2A	3125	1/1	0.95	0.29	52,52,52,52	0
54	MG	2A	3357	1/1	0.95	0.06	28,28,28,28	0
54	MG	2A	3621	1/1	0.95	0.05	32,32,32,32	0
54	MG	1A	3118	1/1	0.95	0.23	30,30,30,30	0
54	MG	2A	3623	1/1	0.95	0.07	76,76,76,76	0
54	MG	1A	3758	1/1	0.95	0.12	18,18,18,18	0
54	MG	2A	3128	1/1	0.95	0.14	52,52,52,52	0
54	MG	1A	3915	1/1	0.95	0.09	45,45,45,45	0
54	MG	2A	3130	1/1	0.95	0.17	51,51,51,51	0
54	MG	2a	3109	1/1	0.95	0.11	55,55,55,55	0
54	MG	2a	3111	1/1	0.95	0.08	39,39,39,39	0
54	MG	1A	3917	1/1	0.95	0.25	43,43,43,43	0
54	MG	2a	3114	1/1	0.95	0.19	71,71,71,71	0
54	MG	2A	3133	1/1	0.95	0.09	35,35,35,35	0
54	MG	1A	3526	1/1	0.95	0.11	42,42,42,42	0
54	MG	1A	3919	1/1	0.95	0.14	55,55,55,55	0
54	MG	1a	3075	1/1	0.95	0.21	50,50,50,50	0
54	MG	1A	3263	1/1	0.95	0.17	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3138	1/1	0.95	0.12	48,48,48,48	0
54	MG	1A	3423	1/1	0.95	0.09	54,54,54,54	0
54	MG	2A	3141	1/1	0.95	0.07	43,43,43,43	0
54	MG	1A	3529	1/1	0.95	0.10	17,17,17,17	0
54	MG	1A	3630	1/1	0.95	0.12	43,43,43,43	0
54	MG	2A	3381	1/1	0.95	0.07	31,31,31,31	0
54	MG	1A	3101	1/1	0.95	0.14	23,23,23,23	0
54	MG	2a	3135	1/1	0.95	0.07	48,48,48,48	0
54	MG	1F	316	1/1	0.95	0.04	51,51,51,51	0
54	MG	1A	3325	1/1	0.95	0.07	22,22,22,22	0
54	MG	2a	3143	1/1	0.95	0.09	48,48,48,48	0
54	MG	2A	3389	1/1	0.95	0.07	41,41,41,41	0
54	MG	2A	3148	1/1	0.95	0.09	49,49,49,49	0
54	MG	1A	3930	1/1	0.95	0.16	27,27,27,27	0
54	MG	2A	3150	1/1	0.95	0.14	47,47,47,47	0
54	MG	1A	3931	1/1	0.95	0.09	26,26,26,26	0
54	MG	1A	3932	1/1	0.95	0.25	24,24,24,24	0
54	MG	2A	3666	1/1	0.95	0.09	62,62,62,62	0
54	MG	1a	3249	1/1	0.95	0.10	48,48,48,48	0
54	MG	1A	3077	1/1	0.95	0.36	28,28,28,28	0
54	MG	2A	3674	1/1	0.95	0.10	50,50,50,50	0
54	MG	2A	3401	1/1	0.95	0.16	51,51,51,51	0
54	MG	2A	3155	1/1	0.95	0.06	51,51,51,51	0
54	MG	1A	3534	1/1	0.95	0.09	31,31,31,31	0
54	MG	1A	3637	1/1	0.95	0.06	34,34,34,34	0
54	MG	1A	3938	1/1	0.95	0.10	55,55,55,55	0
54	MG	1A	3269	1/1	0.95	0.16	30,30,30,30	0
54	MG	1A	3330	1/1	0.95	0.12	25,25,25,25	0
54	MG	1a	3259	1/1	0.95	0.18	87,87,87,87	0
54	MG	2A	3686	1/1	0.95	0.15	63,63,63,63	0
54	MG	1A	3645	1/1	0.95	0.21	43,43,43,43	0
54	MG	2a	3176	1/1	0.95	0.07	81,81,81,81	0
54	MG	2A	3688	1/1	0.95	0.09	48,48,48,48	0
54	MG	1A	3646	1/1	0.95	0.07	20,20,20,20	0
54	MG	1A	3945	1/1	0.95	0.12	52,52,52,52	0
54	MG	1A	3331	1/1	0.95	0.08	36,36,36,36	0
54	MG	2A	3694	1/1	0.95	0.20	66,66,66,66	0
54	MG	1A	3339	1/1	0.95	0.07	33,33,33,33	0
54	MG	1A	3080	1/1	0.95	0.28	29,29,29,29	0
54	MG	2A	3178	1/1	0.95	0.07	44,44,44,44	0
54	MG	2a	3186	1/1	0.95	0.06	67,67,67,67	0
54	MG	2A	3419	1/1	0.95	0.10	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3348	1/1	0.95	0.07	35,35,35,35	0
54	MG	1A	3106	1/1	0.95	0.30	20,20,20,20	0
54	MG	1A	3144	1/1	0.95	0.23	40,40,40,40	0
54	MG	1a	3105	1/1	0.95	0.07	53,53,53,53	0
54	MG	1A	3957	1/1	0.95	0.16	48,48,48,48	0
54	MG	2A	3427	1/1	0.95	0.06	51,51,51,51	0
54	MG	2e	202	1/1	0.95	0.06	73,73,73,73	0
54	MG	1A	3794	1/1	0.95	0.30	56,56,56,56	0
54	MG	1A	3273	1/1	0.95	0.14	30,30,30,30	0
54	MG	2l	201	1/1	0.95	0.25	48,48,48,48	0
54	MG	2o	101	1/1	0.95	0.06	48,48,48,48	0
54	MG	1U	201	1/1	0.95	0.10	20,20,20,20	0
54	MG	1e	202	1/1	0.95	0.21	59,59,59,59	0
54	MG	2A	3434	1/1	0.95	0.07	38,38,38,38	0
54	MG	1A	3148	1/1	0.95	0.14	30,30,30,30	0
54	MG	2A	3722	1/1	0.95	0.13	42,42,42,42	0
54	MG	1A	3129	1/1	0.95	0.10	35,35,35,35	0
54	MG	1A	3361	1/1	0.95	0.12	38,38,38,38	0
54	MG	1A	3554	1/1	0.95	0.16	63,63,63,63	0
54	MG	1A	3363	1/1	0.95	0.06	32,32,32,32	0
54	MG	1A	3214	1/1	0.95	0.35	34,34,34,34	0
54	MG	1W	202	1/1	0.95	0.08	34,34,34,34	0
54	MG	1a	3122	1/1	0.95	0.09	35,35,35,35	0
54	MG	1A	3674	1/1	0.95	0.08	52,52,52,52	0
54	MG	1A	3215	1/1	0.95	0.26	26,26,26,26	0
54	MG	1A	3216	1/1	0.95	0.15	47,47,47,47	0
58	ZN	14	501	1/1	0.95	0.12	126,126,126,126	0
54	MG	1A	3812	1/1	0.95	0.09	31,31,31,31	0
54	MG	1A	3540	1/1	0.96	0.05	26,26,26,26	0
54	MG	1A	3934	1/1	0.96	0.07	52,52,52,52	0
54	MG	1Q	206	1/1	0.96	0.24	39,39,39,39	0
54	MG	1R	201	1/1	0.96	0.28	31,31,31,31	0
54	MG	1R	202	1/1	0.96	0.11	47,47,47,47	0
54	MG	2B	204	1/1	0.96	0.07	56,56,56,56	0
54	MG	1A	3542	1/1	0.96	0.08	32,32,32,32	0
54	MG	2A	3198	1/1	0.96	0.08	45,45,45,45	0
54	MG	1o	101	1/1	0.96	0.08	61,61,61,61	0
54	MG	1o	102	1/1	0.96	0.06	29,29,29,29	0
54	MG	1A	3099	1/1	0.96	0.08	38,38,38,38	0
54	MG	1A	3207	1/1	0.96	0.10	30,30,30,30	0
54	MG	1A	3449	1/1	0.96	0.10	65,65,65,65	0
54	MG	2A	3206	1/1	0.96	0.15	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3208	1/1	0.96	0.14	51,51,51,51	0
54	MG	1A	3546	1/1	0.96	0.07	46,46,46,46	0
54	MG	1A	3787	1/1	0.96	0.12	55,55,55,55	0
54	MG	1A	3653	1/1	0.96	0.08	50,50,50,50	0
54	MG	1A	3452	1/1	0.96	0.07	40,40,40,40	0
54	MG	1A	3030	1/1	0.96	0.07	26,26,26,26	0
54	MG	1A	3657	1/1	0.96	0.10	49,49,49,49	0
54	MG	2A	3215	1/1	0.96	0.06	45,45,45,45	0
54	MG	1U	204	1/1	0.96	0.15	30,30,30,30	0
54	MG	1a	3127	1/1	0.96	0.10	65,65,65,65	0
54	MG	2A	3469	1/1	0.96	0.09	49,49,49,49	0
54	MG	2A	3470	1/1	0.96	0.11	31,31,31,31	0
54	MG	1A	3658	1/1	0.96	0.21	27,27,27,27	0
54	MG	2A	3009	1/1	0.96	0.12	39,39,39,39	0
54	MG	1A	3951	1/1	0.96	0.07	28,28,28,28	0
54	MG	2A	3221	1/1	0.96	0.13	56,56,56,56	0
54	MG	1A	3251	1/1	0.96	0.44	33,33,33,33	0
54	MG	2F	304	1/1	0.96	0.18	45,45,45,45	0
54	MG	1A	3374	1/1	0.96	0.11	37,37,37,37	0
54	MG	2A	3482	1/1	0.96	0.09	32,32,32,32	0
54	MG	1A	3798	1/1	0.96	0.07	36,36,36,36	0
54	MG	2A	3485	1/1	0.96	0.09	46,46,46,46	0
54	MG	2A	3015	1/1	0.96	0.18	43,43,43,43	0
54	MG	2A	3227	1/1	0.96	0.31	50,50,50,50	0
54	MG	1A	3799	1/1	0.96	0.08	50,50,50,50	0
54	MG	2A	3019	1/1	0.96	0.12	40,40,40,40	0
54	MG	1A	3015	1/1	0.96	0.26	37,37,37,37	0
54	MG	1A	3801	1/1	0.96	0.07	20,20,20,20	0
54	MG	2Q	203	1/1	0.96	0.10	47,47,47,47	0
54	MG	1A	3665	1/1	0.96	0.07	20,20,20,20	0
54	MG	10	101	1/1	0.96	0.09	34,34,34,34	0
54	MG	1A	3255	1/1	0.96	0.10	33,33,33,33	0
54	MG	1a	3139	1/1	0.96	0.07	43,43,43,43	0
54	MG	2A	3026	1/1	0.96	0.08	51,51,51,51	0
54	MG	2A	3237	1/1	0.96	0.22	44,44,44,44	0
54	MG	1A	3459	1/1	0.96	0.08	50,50,50,50	0
54	MG	2A	3029	1/1	0.96	0.11	43,43,43,43	0
54	MG	2A	3030	1/1	0.96	0.06	25,25,25,25	0
54	MG	2A	3503	1/1	0.96	0.09	50,50,50,50	0
54	MG	1A	3966	1/1	0.96	0.09	43,43,43,43	0
54	MG	2A	3242	1/1	0.96	0.09	47,47,47,47	0
54	MG	1A	3305	1/1	0.96	0.18	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3033	1/1	0.96	0.06	43,43,43,43	0
54	MG	2A	3508	1/1	0.96	0.15	48,48,48,48	0
54	MG	1A	3183	1/1	0.96	0.22	29,29,29,29	0
54	MG	1a	3145	1/1	0.96	0.09	56,56,56,56	0
54	MG	1A	3463	1/1	0.96	0.08	39,39,39,39	0
54	MG	13	101	1/1	0.96	0.25	23,23,23,23	0
54	MG	1A	3970	1/1	0.96	0.06	38,38,38,38	0
54	MG	1A	3379	1/1	0.96	0.07	11,11,11,11	0
54	MG	1A	3679	1/1	0.96	0.22	25,25,25,25	0
54	MG	1A	3680	1/1	0.96	0.10	44,44,44,44	0
54	MG	1A	3814	1/1	0.96	0.07	42,42,42,42	0
54	MG	2A	3520	1/1	0.96	0.15	44,44,44,44	0
54	MG	1a	3155	1/1	0.96	0.09	61,61,61,61	0
54	MG	2A	3258	1/1	0.96	0.23	44,44,44,44	0
54	MG	17	101	1/1	0.96	0.27	26,26,26,26	0
54	MG	2A	3524	1/1	0.96	0.06	52,52,52,52	0
54	MG	2A	3046	1/1	0.96	0.12	47,47,47,47	0
54	MG	2a	3015	1/1	0.96	0.08	50,50,50,50	0
54	MG	1A	3565	1/1	0.96	0.08	39,39,39,39	0
54	MG	2A	3528	1/1	0.96	0.05	24,24,24,24	0
54	MG	2a	3018	1/1	0.96	0.09	45,45,45,45	0
54	MG	1A	3123	1/1	0.96	0.04	21,21,21,21	0
54	MG	1A	3471	1/1	0.96	0.10	24,24,24,24	0
54	MG	1A	3685	1/1	0.96	0.17	27,27,27,27	0
54	MG	18	103	1/1	0.96	0.10	45,45,45,45	0
54	MG	1A	3982	1/1	0.96	0.14	52,52,52,52	0
54	MG	1A	3260	1/1	0.96	0.05	67,67,67,67	0
54	MG	1A	3125	1/1	0.96	0.07	26,26,26,26	0
54	MG	1A	3384	1/1	0.96	0.06	17,17,17,17	0
54	MG	1a	3003	1/1	0.96	0.09	55,55,55,55	0
54	MG	1A	3314	1/1	0.96	0.08	25,25,25,25	0
54	MG	1A	3691	1/1	0.96	0.22	53,53,53,53	0
54	MG	1A	3829	1/1	0.96	0.18	42,42,42,42	0
54	MG	2A	3542	1/1	0.96	0.09	62,62,62,62	0
54	MG	2A	3543	1/1	0.96	0.08	58,58,58,58	0
54	MG	1A	3140	1/1	0.96	0.28	30,30,30,30	0
54	MG	2A	3548	1/1	0.96	0.10	54,54,54,54	0
54	MG	1A	3694	1/1	0.96	0.06	24,24,24,24	0
54	MG	1a	3009	1/1	0.96	0.08	52,52,52,52	0
54	MG	2a	3039	1/1	0.96	0.18	55,55,55,55	0
54	MG	2A	3066	1/1	0.96	0.16	47,47,47,47	0
54	MG	2A	3067	1/1	0.96	0.18	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3576	1/1	0.96	0.21	51,51,51,51	0
54	MG	1A	3316	1/1	0.96	0.06	35,35,35,35	0
54	MG	1A	3398	1/1	0.96	0.09	30,30,30,30	0
54	MG	1A	4001	1/1	0.96	0.13	45,45,45,45	0
54	MG	2A	3072	1/1	0.96	0.16	52,52,52,52	0
54	MG	1A	3836	1/1	0.96	0.20	38,38,38,38	0
54	MG	2A	3295	1/1	0.96	0.10	58,58,58,58	0
54	MG	1A	3102	1/1	0.96	0.13	28,28,28,28	0
54	MG	1A	3485	1/1	0.96	0.17	40,40,40,40	0
54	MG	2A	3080	1/1	0.96	0.18	49,49,49,49	0
54	MG	1A	3084	1/1	0.96	0.10	34,34,34,34	0
54	MG	1a	3020	1/1	0.96	0.06	48,48,48,48	0
54	MG	2A	3302	1/1	0.96	0.17	50,50,50,50	0
54	MG	1A	3583	1/1	0.96	0.10	30,30,30,30	0
54	MG	2A	3085	1/1	0.96	0.09	32,32,32,32	0
54	MG	2A	3305	1/1	0.96	0.08	28,28,28,28	0
54	MG	2A	3576	1/1	0.96	0.08	57,57,57,57	0
54	MG	2a	3060	1/1	0.96	0.15	45,45,45,45	0
54	MG	1A	3704	1/1	0.96	0.08	43,43,43,43	0
54	MG	1A	3843	1/1	0.96	0.11	55,55,55,55	0
54	MG	1a	3189	1/1	0.96	0.10	55,55,55,55	0
54	MG	1A	3086	1/1	0.96	0.17	28,28,28,28	0
54	MG	2A	3311	1/1	0.96	0.07	32,32,32,32	0
54	MG	1A	3026	1/1	0.96	0.47	28,28,28,28	0
54	MG	1A	3225	1/1	0.96	0.19	28,28,28,28	0
54	MG	1A	3587	1/1	0.96	0.24	33,33,33,33	0
54	MG	2A	3588	1/1	0.96	0.07	39,39,39,39	0
54	MG	1A	3496	1/1	0.96	0.07	17,17,17,17	0
54	MG	1A	3850	1/1	0.96	0.08	56,56,56,56	0
54	MG	1a	3030	1/1	0.96	0.12	50,50,50,50	0
54	MG	1A	3589	1/1	0.96	0.05	23,23,23,23	0
54	MG	1a	3033	1/1	0.96	0.12	53,53,53,53	0
54	MG	1A	3497	1/1	0.96	0.07	56,56,56,56	0
54	MG	2A	3599	1/1	0.96	0.11	68,68,68,68	0
54	MG	1A	3498	1/1	0.96	0.07	34,34,34,34	0
54	MG	1a	3205	1/1	0.96	0.05	40,40,40,40	0
54	MG	1A	3716	1/1	0.96	0.08	36,36,36,36	0
54	MG	2a	3081	1/1	0.96	0.08	48,48,48,48	0
54	MG	2a	3082	1/1	0.96	0.09	61,61,61,61	0
54	MG	2a	3083	1/1	0.96	0.17	56,56,56,56	0
54	MG	1A	3322	1/1	0.96	0.11	31,31,31,31	0
54	MG	2a	3085	1/1	0.96	0.07	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3331	1/1	0.96	0.06	43,43,43,43	0
54	MG	2A	3332	1/1	0.96	0.06	22,22,22,22	0
54	MG	2A	3106	1/1	0.96	0.09	45,45,45,45	0
54	MG	2A	3107	1/1	0.96	0.07	42,42,42,42	0
54	MG	1A	3858	1/1	0.96	0.17	56,56,56,56	0
54	MG	1A	3410	1/1	0.96	0.07	11,11,11,11	0
54	MG	1B	212	1/1	0.96	0.06	47,47,47,47	0
54	MG	1A	3226	1/1	0.96	0.06	33,33,33,33	0
54	MG	1A	3412	1/1	0.96	0.06	23,23,23,23	0
54	MG	2a	3097	1/1	0.96	0.06	48,48,48,48	0
54	MG	1A	3227	1/1	0.96	0.24	43,43,43,43	0
54	MG	2A	3114	1/1	0.96	0.12	36,36,36,36	0
54	MG	2a	3101	1/1	0.96	0.06	31,31,31,31	0
54	MG	1A	3868	1/1	0.96	0.07	47,47,47,47	0
54	MG	2A	3351	1/1	0.96	0.10	33,33,33,33	0
54	MG	1A	3869	1/1	0.96	0.17	41,41,41,41	0
54	MG	2A	3353	1/1	0.96	0.07	47,47,47,47	0
54	MG	2A	3117	1/1	0.96	0.13	38,38,38,38	0
54	MG	1A	3598	1/1	0.96	0.30	34,34,34,34	0
54	MG	1A	3599	1/1	0.96	0.31	28,28,28,28	0
54	MG	2A	3624	1/1	0.96	0.15	79,79,79,79	0
54	MG	2A	3625	1/1	0.96	0.06	53,53,53,53	0
54	MG	2a	3112	1/1	0.96	0.07	57,57,57,57	0
54	MG	2A	3628	1/1	0.96	0.09	67,67,67,67	0
54	MG	1B	222	1/1	0.96	0.12	57,57,57,57	0
54	MG	2A	3358	1/1	0.96	0.06	62,62,62,62	0
54	MG	1A	3231	1/1	0.96	0.24	34,34,34,34	0
54	MG	2a	3118	1/1	0.96	0.09	53,53,53,53	0
54	MG	2A	3122	1/1	0.96	0.12	42,42,42,42	0
54	MG	1A	3874	1/1	0.96	0.07	20,20,20,20	0
54	MG	1A	3145	1/1	0.96	0.07	39,39,39,39	0
54	MG	1a	3223	1/1	0.96	0.05	56,56,56,56	0
54	MG	1A	3878	1/1	0.96	0.08	40,40,40,40	0
54	MG	1A	3881	1/1	0.96	0.11	58,58,58,58	0
54	MG	1a	3056	1/1	0.96	0.10	77,77,77,77	0
54	MG	2a	3127	1/1	0.96	0.17	59,59,59,59	0
54	MG	1A	3882	1/1	0.96	0.18	47,47,47,47	0
54	MG	1A	3276	1/1	0.96	0.08	44,44,44,44	0
54	MG	1D	301	1/1	0.96	0.28	34,34,34,34	0
54	MG	2A	3374	1/1	0.96	0.07	39,39,39,39	0
54	MG	2A	3132	1/1	0.96	0.15	35,35,35,35	0
54	MG	1A	3885	1/1	0.96	0.21	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3142	1/1	0.96	0.07	59,59,59,59	0
54	MG	1D	303	1/1	0.96	0.13	33,33,33,33	0
54	MG	1D	304	1/1	0.96	0.15	44,44,44,44	0
54	MG	1A	3277	1/1	0.96	0.33	37,37,37,37	0
54	MG	1A	3233	1/1	0.96	0.33	28,28,28,28	0
54	MG	1A	3419	1/1	0.96	0.10	19,19,19,19	0
54	MG	2a	3150	1/1	0.96	0.08	63,63,63,63	0
54	MG	1A	3610	1/1	0.96	0.06	23,23,23,23	0
54	MG	1a	3238	1/1	0.96	0.06	40,40,40,40	0
54	MG	2A	3661	1/1	0.96	0.11	51,51,51,51	0
54	MG	2a	3154	1/1	0.96	0.07	62,62,62,62	0
54	MG	2A	3388	1/1	0.96	0.07	52,52,52,52	0
54	MG	1A	3234	1/1	0.96	0.11	49,49,49,49	0
54	MG	1A	3421	1/1	0.96	0.07	13,13,13,13	0
54	MG	2A	3667	1/1	0.96	0.07	35,35,35,35	0
54	MG	1A	3894	1/1	0.96	0.06	18,18,18,18	0
54	MG	1A	3614	1/1	0.96	0.10	30,30,30,30	0
54	MG	1A	3280	1/1	0.96	0.06	54,54,54,54	0
54	MG	1a	3247	1/1	0.96	0.08	64,64,64,64	0
54	MG	1A	3520	1/1	0.96	0.07	46,46,46,46	0
54	MG	2A	3677	1/1	0.96	0.07	51,51,51,51	0
54	MG	2a	3168	1/1	0.96	0.08	83,83,83,83	0
54	MG	2a	3169	1/1	0.96	0.10	55,55,55,55	0
54	MG	1A	3171	1/1	0.96	0.21	35,35,35,35	0
54	MG	2A	3400	1/1	0.96	0.06	39,39,39,39	0
54	MG	1A	3073	1/1	0.96	0.14	20,20,20,20	0
54	MG	1A	3745	1/1	0.96	0.06	36,36,36,36	0
54	MG	1A	3906	1/1	0.96	0.15	55,55,55,55	0
54	MG	2a	3178	1/1	0.96	0.08	56,56,56,56	0
54	MG	1F	305	1/1	0.96	0.18	34,34,34,34	0
54	MG	2A	3685	1/1	0.96	0.08	45,45,45,45	0
54	MG	1A	3239	1/1	0.96	0.18	28,28,28,28	0
54	MG	2A	3156	1/1	0.96	0.08	47,47,47,47	0
54	MG	1a	3256	1/1	0.96	0.07	31,31,31,31	0
54	MG	2A	3158	1/1	0.96	0.08	40,40,40,40	0
54	MG	2A	3162	1/1	0.96	0.15	44,44,44,44	0
54	MG	1A	3358	1/1	0.96	0.08	57,57,57,57	0
54	MG	1F	310	1/1	0.96	0.06	31,31,31,31	0
54	MG	1F	311	1/1	0.96	0.21	37,37,37,37	0
54	MG	1a	3084	1/1	0.96	0.12	57,57,57,57	0
54	MG	1A	3909	1/1	0.96	0.06	44,44,44,44	0
54	MG	2A	3700	1/1	0.96	0.07	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3701	1/1	0.96	0.11	47,47,47,47	0
54	MG	1A	3014	1/1	0.96	0.06	32,32,32,32	0
54	MG	1A	3626	1/1	0.96	0.20	21,21,21,21	0
54	MG	2f	201	1/1	0.96	0.12	42,42,42,42	0
54	MG	2A	3170	1/1	0.96	0.12	48,48,48,48	0
54	MG	1A	3430	1/1	0.96	0.05	20,20,20,20	0
54	MG	1A	3433	1/1	0.96	0.16	40,40,40,40	0
54	MG	1A	3436	1/1	0.96	0.12	41,41,41,41	0
54	MG	1A	3091	1/1	0.96	0.11	37,37,37,37	0
54	MG	1A	3763	1/1	0.96	0.07	19,19,19,19	0
54	MG	2A	3715	1/1	0.96	0.14	42,42,42,42	0
54	MG	2A	3428	1/1	0.96	0.07	53,53,53,53	0
54	MG	1A	3362	1/1	0.96	0.06	26,26,26,26	0
54	MG	1A	3533	1/1	0.96	0.05	22,22,22,22	0
54	MG	2A	3719	1/1	0.96	0.06	30,30,30,30	0
54	MG	1A	3151	1/1	0.96	0.29	31,31,31,31	0
54	MG	1A	3925	1/1	0.96	0.14	41,41,41,41	0
54	MG	1A	3022	1/1	0.96	0.21	33,33,33,33	0
54	MG	1e	203	1/1	0.96	0.14	43,43,43,43	0
54	MG	2A	3436	1/1	0.96	0.10	46,46,46,46	0
54	MG	1A	3444	1/1	0.96	0.07	37,37,37,37	0
54	MG	1P	202	1/1	0.96	0.52	22,22,22,22	0
54	MG	1A	3290	1/1	0.96	0.27	39,39,39,39	0
54	MG	1A	3203	1/1	0.96	0.04	33,33,33,33	0
54	MG	1A	3539	1/1	0.96	0.11	34,34,34,34	0
58	ZN	2n	501	1/1	0.96	0.07	105,105,105,105	0
54	MG	1A	3861	1/1	0.97	0.06	18,18,18,18	0
54	MG	1A	3450	1/1	0.97	0.07	31,31,31,31	0
54	MG	2D	306	1/1	0.97	0.12	46,46,46,46	0
54	MG	1A	3003	1/1	0.97	0.06	22,22,22,22	0
54	MG	2A	3257	1/1	0.97	0.09	48,48,48,48	0
54	MG	1A	3262	1/1	0.97	0.05	29,29,29,29	0
54	MG	2A	3259	1/1	0.97	0.08	48,48,48,48	0
54	MG	1a	3011	1/1	0.97	0.07	53,53,53,53	0
54	MG	1A	3866	1/1	0.97	0.07	27,27,27,27	0
54	MG	2A	3500	1/1	0.97	0.07	45,45,45,45	0
54	MG	1A	3085	1/1	0.97	0.40	28,28,28,28	0
54	MG	2F	303	1/1	0.97	0.06	44,44,44,44	0
54	MG	1A	3264	1/1	0.97	0.06	34,34,34,34	0
54	MG	2A	3264	1/1	0.97	0.06	33,33,33,33	0
54	MG	1B	204	1/1	0.97	0.07	39,39,39,39	0
54	MG	1A	3736	1/1	0.97	0.08	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3267	1/1	0.97	0.08	29,29,29,29	0
54	MG	1A	3313	1/1	0.97	0.06	20,20,20,20	0
54	MG	2A	3269	1/1	0.97	0.05	24,24,24,24	0
54	MG	1A	3265	1/1	0.97	0.30	22,22,22,22	0
54	MG	2A	3073	1/1	0.97	0.08	46,46,46,46	0
54	MG	2A	3074	1/1	0.97	0.11	40,40,40,40	0
54	MG	2Q	201	1/1	0.97	0.09	45,45,45,45	0
54	MG	2A	3513	1/1	0.97	0.05	45,45,45,45	0
54	MG	2A	3075	1/1	0.97	0.06	42,42,42,42	0
54	MG	2A	3076	1/1	0.97	0.10	50,50,50,50	0
54	MG	1A	3050	1/1	0.97	0.24	26,26,26,26	0
54	MG	2A	3278	1/1	0.97	0.09	29,29,29,29	0
54	MG	1A	3157	1/1	0.97	0.19	39,39,39,39	0
54	MG	2A	3519	1/1	0.97	0.06	53,53,53,53	0
54	MG	1A	3224	1/1	0.97	0.08	32,32,32,32	0
54	MG	2V	201	1/1	0.97	0.16	48,48,48,48	0
54	MG	2W	201	1/1	0.97	0.24	35,35,35,35	0
54	MG	1A	3462	1/1	0.97	0.05	45,45,45,45	0
54	MG	2A	3081	1/1	0.97	0.33	39,39,39,39	0
54	MG	1A	3392	1/1	0.97	0.05	15,15,15,15	0
54	MG	20	101	1/1	0.97	0.12	40,40,40,40	0
54	MG	20	102	1/1	0.97	0.09	59,59,59,59	0
54	MG	1a	3193	1/1	0.97	0.09	56,56,56,56	0
54	MG	2A	3287	1/1	0.97	0.07	31,31,31,31	0
54	MG	1B	213	1/1	0.97	0.08	44,44,44,44	0
54	MG	1A	3633	1/1	0.97	0.06	30,30,30,30	0
54	MG	2A	3086	1/1	0.97	0.07	49,49,49,49	0
54	MG	1A	3465	1/1	0.97	0.09	9,9,9,9	0
54	MG	1A	3747	1/1	0.97	0.07	43,43,43,43	0
54	MG	1a	3199	1/1	0.97	0.09	44,44,44,44	0
54	MG	1A	3467	1/1	0.97	0.06	20,20,20,20	0
54	MG	1A	3111	1/1	0.97	0.27	32,32,32,32	0
54	MG	2A	3535	1/1	0.97	0.07	57,57,57,57	0
54	MG	1A	3888	1/1	0.97	0.05	25,25,25,25	0
54	MG	1a	3032	1/1	0.97	0.10	29,29,29,29	0
54	MG	1A	3751	1/1	0.97	0.06	60,60,60,60	0
54	MG	1A	3638	1/1	0.97	0.10	37,37,37,37	0
54	MG	1A	3396	1/1	0.97	0.07	21,21,21,21	0
54	MG	2A	3301	1/1	0.97	0.13	44,44,44,44	0
54	MG	1A	3641	1/1	0.97	0.16	37,37,37,37	0
54	MG	1A	3550	1/1	0.97	0.05	46,46,46,46	0
54	MG	1A	3643	1/1	0.97	0.06	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3545	1/1	0.97	0.06	60,60,60,60	0
54	MG	1A	3762	1/1	0.97	0.26	38,38,38,38	0
54	MG	2A	3102	1/1	0.97	0.06	40,40,40,40	0
54	MG	1A	3551	1/1	0.97	0.13	44,44,44,44	0
54	MG	1A	3159	1/1	0.97	0.14	38,38,38,38	0
54	MG	1A	3051	1/1	0.97	0.20	34,34,34,34	0
54	MG	2A	3310	1/1	0.97	0.09	52,52,52,52	0
54	MG	1A	3114	1/1	0.97	0.21	34,34,34,34	0
54	MG	1A	3904	1/1	0.97	0.06	50,50,50,50	0
54	MG	1A	3905	1/1	0.97	0.07	52,52,52,52	0
54	MG	1D	305	1/1	0.97	0.09	21,21,21,21	0
54	MG	1D	306	1/1	0.97	0.23	26,26,26,26	0
54	MG	2a	3027	1/1	0.97	0.07	60,60,60,60	0
54	MG	1A	3768	1/1	0.97	0.10	35,35,35,35	0
54	MG	2A	3320	1/1	0.97	0.08	22,22,22,22	0
54	MG	2A	3565	1/1	0.97	0.06	57,57,57,57	0
54	MG	1A	3474	1/1	0.97	0.08	23,23,23,23	0
54	MG	1D	310	1/1	0.97	0.07	39,39,39,39	0
54	MG	1a	3051	1/1	0.97	0.29	53,53,53,53	0
54	MG	2A	3324	1/1	0.97	0.06	26,26,26,26	0
54	MG	1A	3475	1/1	0.97	0.07	25,25,25,25	0
54	MG	1a	3053	1/1	0.97	0.11	50,50,50,50	0
54	MG	1D	313	1/1	0.97	0.13	40,40,40,40	0
54	MG	1A	3561	1/1	0.97	0.07	33,33,33,33	0
54	MG	2A	3575	1/1	0.97	0.10	64,64,64,64	0
54	MG	1A	3052	1/1	0.97	0.14	32,32,32,32	0
54	MG	1A	3911	1/1	0.97	0.09	43,43,43,43	0
54	MG	1a	3231	1/1	0.97	0.12	66,66,66,66	0
54	MG	1A	3773	1/1	0.97	0.07	33,33,33,33	0
54	MG	1A	3913	1/1	0.97	0.07	37,37,37,37	0
54	MG	2A	3335	1/1	0.97	0.04	50,50,50,50	0
54	MG	1A	3053	1/1	0.97	0.29	26,26,26,26	0
54	MG	2A	3337	1/1	0.97	0.07	59,59,59,59	0
54	MG	2A	3585	1/1	0.97	0.10	63,63,63,63	0
54	MG	1A	3036	1/1	0.97	0.07	22,22,22,22	0
54	MG	1A	3481	1/1	0.97	0.05	53,53,53,53	0
54	MG	1A	3092	1/1	0.97	0.19	33,33,33,33	0
54	MG	2A	3590	1/1	0.97	0.05	33,33,33,33	0
54	MG	1E	309	1/1	0.97	0.08	52,52,52,52	0
54	MG	2a	3054	1/1	0.97	0.05	42,42,42,42	0
54	MG	1F	301	1/1	0.97	0.13	28,28,28,28	0
54	MG	1A	3660	1/1	0.97	0.06	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3347	1/1	0.97	0.09	64,64,64,64	0
54	MG	1A	3921	1/1	0.97	0.12	61,61,61,61	0
54	MG	1a	3242	1/1	0.97	0.10	76,76,76,76	0
54	MG	1A	3093	1/1	0.97	0.06	34,34,34,34	0
54	MG	2A	3602	1/1	0.97	0.06	43,43,43,43	0
54	MG	1F	306	1/1	0.97	0.13	28,28,28,28	0
54	MG	1A	3124	1/1	0.97	0.04	21,21,21,21	0
54	MG	1A	3333	1/1	0.97	0.05	17,17,17,17	0
54	MG	1A	3335	1/1	0.97	0.12	34,34,34,34	0
54	MG	1A	3789	1/1	0.97	0.05	43,43,43,43	0
54	MG	2A	3139	1/1	0.97	0.21	45,45,45,45	0
54	MG	1A	3666	1/1	0.97	0.07	42,42,42,42	0
54	MG	1A	3929	1/1	0.97	0.07	55,55,55,55	0
54	MG	1A	3338	1/1	0.97	0.06	21,21,21,21	0
54	MG	2A	3364	1/1	0.97	0.08	62,62,62,62	0
54	MG	1a	3254	1/1	0.97	0.06	59,59,59,59	0
54	MG	2A	3144	1/1	0.97	0.12	46,46,46,46	0
54	MG	1a	3077	1/1	0.97	0.08	44,44,44,44	0
54	MG	1a	3078	1/1	0.97	0.07	42,42,42,42	0
54	MG	1A	3792	1/1	0.97	0.07	29,29,29,29	0
54	MG	1A	3573	1/1	0.97	0.07	30,30,30,30	0
54	MG	2a	3078	1/1	0.97	0.25	46,46,46,46	0
54	MG	1A	3489	1/1	0.97	0.08	26,26,26,26	0
54	MG	1A	3575	1/1	0.97	0.05	38,38,38,38	0
54	MG	1G	203	1/1	0.97	0.18	66,66,66,66	0
54	MG	1A	3675	1/1	0.97	0.08	36,36,36,36	0
54	MG	1H	4101	1/1	0.97	0.06	50,50,50,50	0
54	MG	1A	3074	1/1	0.97	0.10	28,28,28,28	0
54	MG	1A	3937	1/1	0.97	0.08	40,40,40,40	0
54	MG	2A	3627	1/1	0.97	0.19	64,64,64,64	0
54	MG	1A	3492	1/1	0.97	0.04	41,41,41,41	0
54	MG	1A	3146	1/1	0.97	0.16	18,18,18,18	0
54	MG	2a	3089	1/1	0.97	0.13	61,61,61,61	0
54	MG	1a	3090	1/1	0.97	0.15	39,39,39,39	0
54	MG	2A	3159	1/1	0.97	0.18	71,71,71,71	0
54	MG	2A	3633	1/1	0.97	0.06	41,41,41,41	0
54	MG	2A	3160	1/1	0.97	0.18	50,50,50,50	0
54	MG	1O	201	1/1	0.97	0.06	36,36,36,36	0
54	MG	1A	3940	1/1	0.97	0.05	36,36,36,36	0
54	MG	1A	3345	1/1	0.97	0.05	20,20,20,20	0
54	MG	2A	3392	1/1	0.97	0.06	51,51,51,51	0
54	MG	1A	3346	1/1	0.97	0.05	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1P	203	1/1	0.97	0.30	26,26,26,26	0
54	MG	1A	3943	1/1	0.97	0.05	35,35,35,35	0
54	MG	1A	3804	1/1	0.97	0.23	22,22,22,22	0
54	MG	1A	3347	1/1	0.97	0.07	11,11,11,11	0
54	MG	1A	3206	1/1	0.97	0.09	45,45,45,45	0
54	MG	1A	3684	1/1	0.97	0.08	38,38,38,38	0
54	MG	1A	3500	1/1	0.97	0.06	18,18,18,18	0
54	MG	1A	3686	1/1	0.97	0.05	34,34,34,34	0
54	MG	2A	3403	1/1	0.97	0.10	29,29,29,29	0
54	MG	1A	3032	1/1	0.97	0.11	42,42,42,42	0
54	MG	2A	3176	1/1	0.97	0.07	44,44,44,44	0
54	MG	1R	203	1/1	0.97	0.10	28,28,28,28	0
54	MG	1l	201	1/1	0.97	0.12	48,48,48,48	0
54	MG	2A	3658	1/1	0.97	0.06	30,30,30,30	0
54	MG	1R	204	1/1	0.97	0.19	43,43,43,43	0
54	MG	1A	3008	1/1	0.97	0.08	32,32,32,32	0
54	MG	1A	3209	1/1	0.97	0.23	36,36,36,36	0
54	MG	1R	207	1/1	0.97	0.05	20,20,20,20	0
54	MG	2a	3121	1/1	0.97	0.15	71,71,71,71	0
54	MG	2A	3664	1/1	0.97	0.06	57,57,57,57	0
54	MG	1a	3113	1/1	0.97	0.08	38,38,38,38	0
54	MG	1R	208	1/1	0.97	0.07	39,39,39,39	0
54	MG	2A	3668	1/1	0.97	0.05	61,61,61,61	0
54	MG	1A	3354	1/1	0.97	0.08	18,18,18,18	0
54	MG	2A	3672	1/1	0.97	0.08	32,32,32,32	0
54	MG	1A	3958	1/1	0.97	0.11	44,44,44,44	0
54	MG	2a	3129	1/1	0.97	0.09	65,65,65,65	0
54	MG	2a	3130	1/1	0.97	0.05	48,48,48,48	0
54	MG	1A	3959	1/1	0.97	0.10	41,41,41,41	0
54	MG	1A	3001	1/1	0.97	0.05	28,28,28,28	0
54	MG	2a	3133	1/1	0.97	0.07	65,65,65,65	0
54	MG	2a	3134	1/1	0.97	0.10	51,51,51,51	0
54	MG	1A	3590	1/1	0.97	0.14	48,48,48,48	0
54	MG	1A	3248	1/1	0.97	0.46	30,30,30,30	0
54	MG	2a	3138	1/1	0.97	0.07	53,53,53,53	0
54	MG	2A	3422	1/1	0.97	0.05	56,56,56,56	0
54	MG	2a	3140	1/1	0.97	0.06	73,73,73,73	0
54	MG	1A	3695	1/1	0.97	0.18	26,26,26,26	0
54	MG	2A	3003	1/1	0.97	0.08	32,32,32,32	0
54	MG	1A	3427	1/1	0.97	0.13	51,51,51,51	0
54	MG	1U	203	1/1	0.97	0.45	35,35,35,35	0
54	MG	1A	3509	1/1	0.97	0.07	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3429	1/1	0.97	0.11	48,48,48,48	0
54	MG	1A	3359	1/1	0.97	0.05	34,34,34,34	0
54	MG	1V	201	1/1	0.97	0.26	23,23,23,23	0
54	MG	1A	3288	1/1	0.97	0.09	15,15,15,15	0
54	MG	2A	3203	1/1	0.97	0.09	25,25,25,25	0
54	MG	1A	3048	1/1	0.97	0.18	35,35,35,35	0
54	MG	1A	3828	1/1	0.97	0.09	43,43,43,43	0
54	MG	1A	3514	1/1	0.97	0.06	38,38,38,38	0
54	MG	2A	3207	1/1	0.97	0.07	46,46,46,46	0
54	MG	1A	3432	1/1	0.97	0.08	38,38,38,38	0
54	MG	2A	3016	1/1	0.97	0.12	41,41,41,41	0
54	MG	1A	3292	1/1	0.97	0.45	28,28,28,28	0
54	MG	2A	3018	1/1	0.97	0.21	31,31,31,31	0
54	MG	1A	3976	1/1	0.97	0.07	46,46,46,46	0
54	MG	2A	3703	1/1	0.97	0.07	39,39,39,39	0
54	MG	1A	3600	1/1	0.97	0.32	22,22,22,22	0
54	MG	2A	3444	1/1	0.97	0.07	22,22,22,22	0
54	MG	1A	3212	1/1	0.97	0.48	35,35,35,35	0
54	MG	2A	3707	1/1	0.97	0.09	63,63,63,63	0
54	MG	1A	3602	1/1	0.97	0.26	27,27,27,27	0
54	MG	10	104	1/1	0.97	0.07	34,34,34,34	0
54	MG	2A	3710	1/1	0.97	0.10	56,56,56,56	0
54	MG	1A	3835	1/1	0.97	0.13	42,42,42,42	0
54	MG	10	106	1/1	0.97	0.08	56,56,56,56	0
54	MG	1A	3294	1/1	0.97	0.05	26,26,26,26	0
54	MG	1A	3710	1/1	0.97	0.09	33,33,33,33	0
54	MG	1A	3252	1/1	0.97	0.30	40,40,40,40	0
54	MG	1A	3366	1/1	0.97	0.11	24,24,24,24	0
54	MG	1A	3213	1/1	0.97	0.19	33,33,33,33	0
54	MG	2A	3224	1/1	0.97	0.15	41,41,41,41	0
54	MG	1A	3607	1/1	0.97	0.10	48,48,48,48	0
54	MG	1A	3608	1/1	0.97	0.10	38,38,38,38	0
54	MG	1A	3990	1/1	0.97	0.12	38,38,38,38	0
54	MG	15	103	1/1	0.97	0.27	36,36,36,36	0
54	MG	1A	3844	1/1	0.97	0.05	33,33,33,33	0
54	MG	1A	3441	1/1	0.97	0.05	29,29,29,29	0
54	MG	1A	3993	1/1	0.97	0.07	26,26,26,26	0
54	MG	17	102	1/1	0.97	0.29	29,29,29,29	0
54	MG	2A	3729	1/1	0.97	0.07	37,37,37,37	0
54	MG	1A	3994	1/1	0.97	0.06	34,34,34,34	0
54	MG	1A	3180	1/1	0.97	0.19	30,30,30,30	0
54	MG	2A	3468	1/1	0.97	0.13	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3997	1/1	0.97	0.12	53,53,53,53	0
54	MG	1A	3256	1/1	0.97	0.13	60,60,60,60	0
54	MG	1A	3720	1/1	0.97	0.05	27,27,27,27	0
54	MG	2A	3472	1/1	0.97	0.16	56,56,56,56	0
54	MG	1A	3081	1/1	0.97	0.29	28,28,28,28	0
54	MG	19	101	1/1	0.97	0.04	45,45,45,45	0
54	MG	1A	3722	1/1	0.97	0.04	30,30,30,30	0
54	MG	2A	3477	1/1	0.97	0.09	32,32,32,32	0
54	MG	2B	209	1/1	0.97	0.09	62,62,62,62	0
54	MG	2A	3049	1/1	0.97	0.11	46,46,46,46	0
54	MG	1A	3082	1/1	0.97	0.10	34,34,34,34	0
54	MG	1a	3167	1/1	0.97	0.08	75,75,75,75	0
54	MG	1A	3615	1/1	0.97	0.09	16,16,16,16	0
54	MG	1A	3218	1/1	0.97	0.06	36,36,36,36	0
54	MG	1a	3170	1/1	0.97	0.08	55,55,55,55	0
54	MG	1A	3307	1/1	0.97	0.25	30,30,30,30	0
54	MG	1A	3728	1/1	0.97	0.07	40,40,40,40	0
54	MG	2A	3058	1/1	0.97	0.09	33,33,33,33	0
58	ZN	1Y	202	1/1	0.97	0.07	97,97,97,97	0
54	MG	2B	220	1/1	0.97	0.06	66,66,66,66	0
54	MG	1A	3619	1/1	0.97	0.06	24,24,24,24	0
54	MG	1a	3174	1/1	0.97	0.06	53,53,53,53	0
54	MG	1A	3196	1/1	0.98	0.04	34,34,34,34	0
54	MG	1A	3197	1/1	0.98	0.07	41,41,41,41	0
54	MG	2A	3563	1/1	0.98	0.06	55,55,55,55	0
54	MG	11	102	1/1	0.98	0.07	36,36,36,36	0
54	MG	1A	3024	1/1	0.98	0.13	20,20,20,20	0
54	MG	2X	101	1/1	0.98	0.09	45,45,45,45	0
54	MG	1A	3013	1/1	0.98	0.07	25,25,25,25	0
54	MG	2A	3360	1/1	0.98	0.08	41,41,41,41	0
54	MG	1y	203	1/1	0.98	0.14	44,44,44,44	0
54	MG	1y	204	1/1	0.98	0.06	68,68,68,68	0
54	MG	2A	3363	1/1	0.98	0.05	50,50,50,50	0
54	MG	2A	3571	1/1	0.98	0.09	28,28,28,28	0
54	MG	1A	3855	1/1	0.98	0.09	45,45,45,45	0
54	MG	2A	3365	1/1	0.98	0.08	50,50,50,50	0
54	MG	1A	3510	1/1	0.98	0.04	22,22,22,22	0
54	MG	1A	3323	1/1	0.98	0.04	13,13,13,13	0
54	MG	1A	3860	1/1	0.98	0.04	23,23,23,23	0
54	MG	2A	3177	1/1	0.98	0.12	39,39,39,39	0
54	MG	2A	3004	1/1	0.98	0.07	38,38,38,38	0
54	MG	2A	3179	1/1	0.98	0.06	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	15	102	1/1	0.98	0.20	24,24,24,24	0
54	MG	1A	3058	1/1	0.98	0.06	13,13,13,13	0
54	MG	1A	3117	1/1	0.98	0.17	27,27,27,27	0
54	MG	1A	3328	1/1	0.98	0.04	23,23,23,23	0
54	MG	2A	3584	1/1	0.98	0.08	57,57,57,57	0
54	MG	2A	3184	1/1	0.98	0.40	41,41,41,41	0
54	MG	2A	3377	1/1	0.98	0.05	32,32,32,32	0
54	MG	1a	3143	1/1	0.98	0.05	61,61,61,61	0
54	MG	1A	3202	1/1	0.98	0.15	38,38,38,38	0
54	MG	1A	3732	1/1	0.98	0.05	29,29,29,29	0
54	MG	1A	3009	1/1	0.98	0.14	23,23,23,23	0
54	MG	2A	3013	1/1	0.98	0.11	22,22,22,22	0
54	MG	2A	3594	1/1	0.98	0.05	54,54,54,54	0
54	MG	1a	3147	1/1	0.98	0.07	55,55,55,55	0
54	MG	2A	3384	1/1	0.98	0.05	31,31,31,31	0
54	MG	2A	3385	1/1	0.98	0.07	51,51,51,51	0
54	MG	1A	3518	1/1	0.98	0.10	38,38,38,38	0
54	MG	2a	3022	1/1	0.98	0.24	55,55,55,55	0
54	MG	1A	3119	1/1	0.98	0.10	33,33,33,33	0
54	MG	2A	3601	1/1	0.98	0.04	39,39,39,39	0
54	MG	1A	3332	1/1	0.98	0.06	22,22,22,22	0
54	MG	1A	3205	1/1	0.98	0.37	35,35,35,35	0
54	MG	2A	3391	1/1	0.98	0.07	28,28,28,28	0
54	MG	1A	3010	1/1	0.98	0.12	28,28,28,28	0
54	MG	1A	3336	1/1	0.98	0.11	42,42,42,42	0
54	MG	1a	3154	1/1	0.98	0.06	42,42,42,42	0
54	MG	2A	3395	1/1	0.98	0.08	25,25,25,25	0
54	MG	1A	3524	1/1	0.98	0.06	37,37,37,37	0
54	MG	1A	3337	1/1	0.98	0.14	37,37,37,37	0
54	MG	2A	3200	1/1	0.98	0.05	33,33,33,33	0
54	MG	1A	3880	1/1	0.98	0.07	29,29,29,29	0
54	MG	1A	3121	1/1	0.98	0.11	28,28,28,28	0
54	MG	1A	3122	1/1	0.98	0.11	39,39,39,39	0
54	MG	1A	3883	1/1	0.98	0.10	38,38,38,38	0
54	MG	1A	3341	1/1	0.98	0.05	18,18,18,18	0
54	MG	1A	3061	1/1	0.98	0.07	18,18,18,18	0
54	MG	1B	214	1/1	0.98	0.06	42,42,42,42	0
54	MG	1A	3344	1/1	0.98	0.04	20,20,20,20	0
54	MG	1A	3434	1/1	0.98	0.09	38,38,38,38	0
54	MG	1A	3161	1/1	0.98	0.08	20,20,20,20	0
54	MG	2A	3035	1/1	0.98	0.11	41,41,41,41	0
54	MG	1A	3028	1/1	0.98	0.21	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3163	1/1	0.98	0.14	28,28,28,28	0
54	MG	1A	3755	1/1	0.98	0.05	28,28,28,28	0
54	MG	2A	3626	1/1	0.98	0.04	57,57,57,57	0
54	MG	1A	3063	1/1	0.98	0.07	35,35,35,35	0
54	MG	1A	3639	1/1	0.98	0.15	46,46,46,46	0
54	MG	1A	3759	1/1	0.98	0.10	39,39,39,39	0
54	MG	2A	3417	1/1	0.98	0.09	37,37,37,37	0
54	MG	1A	3165	1/1	0.98	0.20	32,32,32,32	0
54	MG	1A	3350	1/1	0.98	0.07	45,45,45,45	0
54	MG	1A	3900	1/1	0.98	0.07	53,53,53,53	0
54	MG	1A	3090	1/1	0.98	0.13	31,31,31,31	0
54	MG	1A	3167	1/1	0.98	0.07	29,29,29,29	0
54	MG	1A	3541	1/1	0.98	0.05	39,39,39,39	0
54	MG	2A	3640	1/1	0.98	0.07	53,53,53,53	0
54	MG	1a	3179	1/1	0.98	0.06	65,65,65,65	0
54	MG	1A	3016	1/1	0.98	0.27	25,25,25,25	0
54	MG	1A	3169	1/1	0.98	0.05	22,22,22,22	0
54	MG	1A	3357	1/1	0.98	0.07	12,12,12,12	0
54	MG	1A	3649	1/1	0.98	0.05	45,45,45,45	0
54	MG	1A	3220	1/1	0.98	0.27	34,34,34,34	0
54	MG	1A	3066	1/1	0.98	0.06	30,30,30,30	0
54	MG	2A	3649	1/1	0.98	0.09	54,54,54,54	0
54	MG	1A	3451	1/1	0.98	0.08	13,13,13,13	0
54	MG	1A	3017	1/1	0.98	0.29	17,17,17,17	0
54	MG	1A	3094	1/1	0.98	0.16	30,30,30,30	0
54	MG	1A	3095	1/1	0.98	0.26	21,21,21,21	0
54	MG	1D	312	1/1	0.98	0.09	18,18,18,18	0
54	MG	1A	3914	1/1	0.98	0.13	30,30,30,30	0
54	MG	1A	3068	1/1	0.98	0.06	27,27,27,27	0
54	MG	1A	3916	1/1	0.98	0.10	51,51,51,51	0
54	MG	1a	3194	1/1	0.98	0.05	62,62,62,62	0
54	MG	1A	3175	1/1	0.98	0.07	32,32,32,32	0
54	MG	2A	3660	1/1	0.98	0.04	63,63,63,63	0
54	MG	1A	3780	1/1	0.98	0.04	28,28,28,28	0
54	MG	1A	3781	1/1	0.98	0.04	20,20,20,20	0
54	MG	1E	301	1/1	0.98	0.19	34,34,34,34	0
54	MG	1A	3659	1/1	0.98	0.05	51,51,51,51	0
54	MG	2A	3665	1/1	0.98	0.06	59,59,59,59	0
54	MG	1a	3200	1/1	0.98	0.13	71,71,71,71	0
54	MG	1E	303	1/1	0.98	0.28	25,25,25,25	0
54	MG	1A	3457	1/1	0.98	0.04	40,40,40,40	0
54	MG	1A	3784	1/1	0.98	0.04	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3670	1/1	0.98	0.05	62,62,62,62	0
54	MG	2a	3090	1/1	0.98	0.13	73,73,73,73	0
54	MG	2A	3671	1/1	0.98	0.05	35,35,35,35	0
54	MG	1A	3097	1/1	0.98	0.17	21,21,21,21	0
54	MG	1E	308	1/1	0.98	0.07	29,29,29,29	0
54	MG	1A	3662	1/1	0.98	0.14	57,57,57,57	0
54	MG	1A	3230	1/1	0.98	0.23	29,29,29,29	0
54	MG	1F	302	1/1	0.98	0.16	27,27,27,27	0
54	MG	1A	3289	1/1	0.98	0.17	33,33,33,33	0
54	MG	1A	3559	1/1	0.98	0.17	25,25,25,25	0
54	MG	2a	3099	1/1	0.98	0.06	44,44,44,44	0
54	MG	1A	3928	1/1	0.98	0.12	47,47,47,47	0
54	MG	2A	3458	1/1	0.98	0.11	46,46,46,46	0
54	MG	1A	3560	1/1	0.98	0.08	37,37,37,37	0
54	MG	1A	3098	1/1	0.98	0.08	13,13,13,13	0
54	MG	1A	3668	1/1	0.98	0.08	49,49,49,49	0
54	MG	2A	3684	1/1	0.98	0.05	41,41,41,41	0
54	MG	1A	3670	1/1	0.98	0.07	52,52,52,52	0
54	MG	1A	3291	1/1	0.98	0.37	30,30,30,30	0
54	MG	1A	3796	1/1	0.98	0.04	38,38,38,38	0
54	MG	1A	3370	1/1	0.98	0.04	22,22,22,22	0
54	MG	2a	3110	1/1	0.98	0.10	42,42,42,42	0
54	MG	1A	3673	1/1	0.98	0.06	26,26,26,26	0
54	MG	1A	3464	1/1	0.98	0.06	34,34,34,34	0
54	MG	2A	3691	1/1	0.98	0.05	43,43,43,43	0
54	MG	2A	3692	1/1	0.98	0.19	37,37,37,37	0
54	MG	1A	3069	1/1	0.98	0.34	43,43,43,43	0
54	MG	1A	3676	1/1	0.98	0.05	24,24,24,24	0
54	MG	1A	3566	1/1	0.98	0.09	23,23,23,23	0
54	MG	1A	3803	1/1	0.98	0.15	41,41,41,41	0
54	MG	2A	3272	1/1	0.98	0.04	45,45,45,45	0
54	MG	2A	3699	1/1	0.98	0.10	54,54,54,54	0
54	MG	1A	3047	1/1	0.98	0.07	26,26,26,26	0
54	MG	2A	3274	1/1	0.98	0.09	37,37,37,37	0
54	MG	1A	3137	1/1	0.98	0.38	28,28,28,28	0
54	MG	1A	3469	1/1	0.98	0.07	19,19,19,19	0
54	MG	2A	3480	1/1	0.98	0.05	68,68,68,68	0
54	MG	2A	3098	1/1	0.98	0.16	48,48,48,48	0
54	MG	1A	3181	1/1	0.98	0.07	40,40,40,40	0
54	MG	1A	3808	1/1	0.98	0.09	18,18,18,18	0
54	MG	1A	3297	1/1	0.98	0.05	51,51,51,51	0
54	MG	1A	3298	1/1	0.98	0.15	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3950	1/1	0.98	0.04	23,23,23,23	0
54	MG	1A	3236	1/1	0.98	0.53	24,24,24,24	0
54	MG	1A	3071	1/1	0.98	0.22	27,27,27,27	0
54	MG	2A	3714	1/1	0.98	0.07	30,30,30,30	0
54	MG	1A	3031	1/1	0.98	0.05	25,25,25,25	0
54	MG	1A	3240	1/1	0.98	0.35	25,25,25,25	0
54	MG	1A	3303	1/1	0.98	0.25	29,29,29,29	0
54	MG	1A	3018	1/1	0.98	0.16	26,26,26,26	0
54	MG	2a	3141	1/1	0.98	0.06	60,60,60,60	0
54	MG	1A	3479	1/1	0.98	0.04	14,14,14,14	0
54	MG	1Q	202	1/1	0.98	0.21	30,30,30,30	0
54	MG	1Q	203	1/1	0.98	0.07	43,43,43,43	0
54	MG	1a	3243	1/1	0.98	0.07	46,46,46,46	0
54	MG	1A	3960	1/1	0.98	0.08	38,38,38,38	0
54	MG	1Q	205	1/1	0.98	0.04	15,15,15,15	0
54	MG	1A	3480	1/1	0.98	0.06	27,27,27,27	0
54	MG	2A	3501	1/1	0.98	0.07	45,45,45,45	0
54	MG	1Q	207	1/1	0.98	0.09	33,33,33,33	0
54	MG	1A	3820	1/1	0.98	0.04	27,27,27,27	0
54	MG	1A	3692	1/1	0.98	0.11	39,39,39,39	0
54	MG	1A	3385	1/1	0.98	0.05	11,11,11,11	0
54	MG	1A	3823	1/1	0.98	0.33	36,36,36,36	0
54	MG	1A	3582	1/1	0.98	0.05	34,34,34,34	0
54	MG	1A	3104	1/1	0.98	0.12	23,23,23,23	0
54	MG	1A	3388	1/1	0.98	0.05	25,25,25,25	0
54	MG	1A	3391	1/1	0.98	0.14	15,15,15,15	0
54	MG	1A	3306	1/1	0.98	0.04	14,14,14,14	0
54	MG	2a	3162	1/1	0.98	0.07	59,59,59,59	0
54	MG	2a	3163	1/1	0.98	0.08	61,61,61,61	0
54	MG	2a	3164	1/1	0.98	0.04	68,68,68,68	0
54	MG	1a	3258	1/1	0.98	0.04	58,58,58,58	0
54	MG	1A	3971	1/1	0.98	0.06	20,20,20,20	0
54	MG	1A	3019	1/1	0.98	0.18	19,19,19,19	0
54	MG	1a	3261	1/1	0.98	0.06	46,46,46,46	0
54	MG	1A	3973	1/1	0.98	0.12	22,22,22,22	0
54	MG	2A	3313	1/1	0.98	0.06	21,21,21,21	0
54	MG	1A	3487	1/1	0.98	0.04	14,14,14,14	0
54	MG	2a	3174	1/1	0.98	0.07	62,62,62,62	0
54	MG	2A	3315	1/1	0.98	0.09	27,27,27,27	0
54	MG	1A	3394	1/1	0.98	0.04	15,15,15,15	0
54	MG	2A	3317	1/1	0.98	0.06	33,33,33,33	0
54	MG	1a	3265	1/1	0.98	0.06	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3395	1/1	0.98	0.06	13,13,13,13	0
54	MG	2B	217	1/1	0.98	0.07	61,61,61,61	0
54	MG	1A	3005	1/1	0.98	0.06	23,23,23,23	0
54	MG	1A	3491	1/1	0.98	0.08	44,44,44,44	0
54	MG	1a	3106	1/1	0.98	0.06	40,40,40,40	0
54	MG	2A	3527	1/1	0.98	0.07	31,31,31,31	0
54	MG	2D	302	1/1	0.98	0.06	43,43,43,43	0
54	MG	1A	3021	1/1	0.98	0.08	26,26,26,26	0
54	MG	1A	3493	1/1	0.98	0.10	36,36,36,36	0
54	MG	2A	3325	1/1	0.98	0.04	32,32,32,32	0
54	MG	1a	3109	1/1	0.98	0.04	31,31,31,31	0
54	MG	1d	303	1/1	0.98	0.06	73,73,73,73	0
54	MG	1a	3110	1/1	0.98	0.07	35,35,35,35	0
54	MG	1A	3494	1/1	0.98	0.07	36,36,36,36	0
54	MG	1a	3112	1/1	0.98	0.05	39,39,39,39	0
54	MG	1V	202	1/1	0.98	0.14	28,28,28,28	0
54	MG	1A	3108	1/1	0.98	0.29	36,36,36,36	0
54	MG	2E	306	1/1	0.98	0.12	59,59,59,59	0
54	MG	1e	204	1/1	0.98	0.04	43,43,43,43	0
54	MG	1A	3840	1/1	0.98	0.06	29,29,29,29	0
54	MG	1V	205	1/1	0.98	0.09	43,43,43,43	0
54	MG	1A	3109	1/1	0.98	0.05	28,28,28,28	0
54	MG	1A	3985	1/1	0.98	0.12	8,8,8,8	0
54	MG	1A	3006	1/1	0.98	0.06	19,19,19,19	0
54	MG	2A	3339	1/1	0.98	0.07	26,26,26,26	0
54	MG	1A	3079	1/1	0.98	0.07	45,45,45,45	0
54	MG	2A	3546	1/1	0.98	0.07	27,27,27,27	0
54	MG	2A	3547	1/1	0.98	0.05	54,54,54,54	0
54	MG	1A	3714	1/1	0.98	0.09	38,38,38,38	0
54	MG	1A	3193	1/1	0.98	0.06	33,33,33,33	0
54	MG	2A	3550	1/1	0.98	0.05	43,43,43,43	0
54	MG	1a	3123	1/1	0.98	0.06	61,61,61,61	0
54	MG	1A	3406	1/1	0.98	0.04	29,29,29,29	0
54	MG	1m	201	1/1	0.98	0.04	65,65,65,65	0
54	MG	1A	3194	1/1	0.98	0.12	29,29,29,29	0
54	MG	2R	201	1/1	0.98	0.07	37,37,37,37	0
54	MG	2A	3161	1/1	0.98	0.19	40,40,40,40	0
54	MG	1A	3408	1/1	0.98	0.04	17,17,17,17	0
58	ZN	15	107	1/1	0.98	0.04	64,64,64,64	0
58	ZN	1n	103	1/1	0.98	0.04	74,74,74,74	0
58	ZN	2Y	202	1/1	0.98	0.07	109,109,109,109	0
54	MG	1A	3023	1/1	0.98	0.21	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	ZN	25	104	1/1	0.98	0.06	87,87,87,87	0
58	ZN	29	501	1/1	0.98	0.04	67,67,67,67	0
54	MG	1A	3254	1/1	0.98	0.06	26,26,26,26	0
54	MG	1A	3324	1/1	0.99	0.04	17,17,17,17	0
54	MG	1A	3738	1/1	0.99	0.03	26,26,26,26	0
54	MG	2a	3115	1/1	0.99	0.05	65,65,65,65	0
54	MG	1A	3308	1/1	0.99	0.26	23,23,23,23	0
54	MG	1A	3045	1/1	0.99	0.06	11,11,11,11	0
54	MG	2A	3713	1/1	0.99	0.07	51,51,51,51	0
54	MG	2A	3423	1/1	0.99	0.03	39,39,39,39	0
54	MG	2A	3172	1/1	0.99	0.07	46,46,46,46	0
54	MG	1A	3431	1/1	0.99	0.07	33,33,33,33	0
54	MG	2A	3253	1/1	0.99	0.09	17,17,17,17	0
54	MG	1A	3501	1/1	0.99	0.03	13,13,13,13	0
54	MG	1a	3245	1/1	0.99	0.04	53,53,53,53	0
54	MG	2A	3256	1/1	0.99	0.04	24,24,24,24	0
54	MG	1D	308	1/1	0.99	0.05	28,28,28,28	0
54	MG	1A	3399	1/1	0.99	0.03	17,17,17,17	0
54	MG	1A	3327	1/1	0.99	0.03	18,18,18,18	0
54	MG	1A	3401	1/1	0.99	0.04	15,15,15,15	0
54	MG	1A	3372	1/1	0.99	0.04	21,21,21,21	0
54	MG	2A	3346	1/1	0.99	0.04	53,53,53,53	0
54	MG	1A	3249	1/1	0.99	0.08	37,37,37,37	0
54	MG	2A	3348	1/1	0.99	0.03	20,20,20,20	0
54	MG	2A	3349	1/1	0.99	0.04	34,34,34,34	0
54	MG	1A	3859	1/1	0.99	0.02	28,28,28,28	0
54	MG	2a	3136	1/1	0.99	0.05	56,56,56,56	0
54	MG	1A	3988	1/1	0.99	0.05	39,39,39,39	0
54	MG	2A	3630	1/1	0.99	0.03	43,43,43,43	0
54	MG	2A	3027	1/1	0.99	0.03	22,22,22,22	0
54	MG	1A	3618	1/1	0.99	0.06	18,18,18,18	0
54	MG	1A	3749	1/1	0.99	0.04	19,19,19,19	0
54	MG	1A	3703	1/1	0.99	0.03	13,13,13,13	0
54	MG	1A	3863	1/1	0.99	0.04	36,36,36,36	0
54	MG	2a	3144	1/1	0.99	0.08	40,40,40,40	0
54	MG	2a	3145	1/1	0.99	0.06	51,51,51,51	0
54	MG	1A	3404	1/1	0.99	0.04	19,19,19,19	0
54	MG	2A	3637	1/1	0.99	0.03	33,33,33,33	0
54	MG	2A	3638	1/1	0.99	0.05	40,40,40,40	0
54	MG	1A	3217	1/1	0.99	0.11	28,28,28,28	0
54	MG	1A	3995	1/1	0.99	0.10	21,21,21,21	0
54	MG	1A	3753	1/1	0.99	0.03	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1E	306	1/1	0.99	0.09	13,13,13,13	0
54	MG	2A	3643	1/1	0.99	0.03	38,38,38,38	0
54	MG	1A	3754	1/1	0.99	0.03	25,25,25,25	0
54	MG	1A	3706	1/1	0.99	0.07	29,29,29,29	0
54	MG	1A	3238	1/1	0.99	0.10	19,19,19,19	0
54	MG	1a	3266	1/1	0.99	0.04	53,53,53,53	0
54	MG	1A	3757	1/1	0.99	0.04	17,17,17,17	0
54	MG	10	102	1/1	0.99	0.09	33,33,33,33	0
54	MG	1A	3352	1/1	0.99	0.04	35,35,35,35	0
54	MG	1A	3443	1/1	0.99	0.04	15,15,15,15	0
54	MG	2A	3283	1/1	0.99	0.06	29,29,29,29	0
54	MG	1A	3873	1/1	0.99	0.07	28,28,28,28	0
54	MG	2A	3285	1/1	0.99	0.05	31,31,31,31	0
54	MG	1A	3624	1/1	0.99	0.10	22,22,22,22	0
54	MG	1A	3876	1/1	0.99	0.04	33,33,33,33	0
54	MG	1A	3054	1/1	0.99	0.27	29,29,29,29	0
54	MG	1F	308	1/1	0.99	0.12	29,29,29,29	0
54	MG	2A	3559	1/1	0.99	0.03	46,46,46,46	0
54	MG	2a	3170	1/1	0.99	0.09	47,47,47,47	0
54	MG	2A	3560	1/1	0.99	0.05	19,19,19,19	0
54	MG	1A	3228	1/1	0.99	0.05	25,25,25,25	0
54	MG	2a	3173	1/1	0.99	0.08	57,57,57,57	0
54	MG	1A	3879	1/1	0.99	0.04	21,21,21,21	0
54	MG	1A	3669	1/1	0.99	0.08	36,36,36,36	0
54	MG	2E	307	1/1	0.99	0.04	25,25,25,25	0
54	MG	1A	3355	1/1	0.99	0.03	30,30,30,30	0
54	MG	1A	3765	1/1	0.99	0.07	32,32,32,32	0
54	MG	2F	302	1/1	0.99	0.10	37,37,37,37	0
54	MG	1A	3268	1/1	0.99	0.28	25,25,25,25	0
54	MG	2A	3473	1/1	0.99	0.07	42,42,42,42	0
54	MG	1A	3334	1/1	0.99	0.04	27,27,27,27	0
54	MG	2A	3057	1/1	0.99	0.03	26,26,26,26	0
54	MG	1a	3207	1/1	0.99	0.05	53,53,53,53	0
54	MG	1A	3382	1/1	0.99	0.02	27,27,27,27	0
54	MG	2A	3387	1/1	0.99	0.05	20,20,20,20	0
54	MG	2A	3479	1/1	0.99	0.05	42,42,42,42	0
54	MG	1A	3948	1/1	0.99	0.08	51,51,51,51	0
54	MG	15	105	1/1	0.99	0.04	35,35,35,35	0
54	MG	1A	3229	1/1	0.99	0.32	25,25,25,25	0
54	MG	1A	3064	1/1	0.99	0.04	24,24,24,24	0
54	MG	1A	3556	1/1	0.99	0.08	10,10,10,10	0
54	MG	1A	3889	1/1	0.99	0.05	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3634	1/1	0.99	0.13	25,25,25,25	0
54	MG	1A	3557	1/1	0.99	0.07	35,35,35,35	0
54	MG	1A	3955	1/1	0.99	0.07	13,13,13,13	0
54	MG	1A	3774	1/1	0.99	0.07	44,44,44,44	0
54	MG	1A	3723	1/1	0.99	0.05	31,31,31,31	0
54	MG	1A	3147	1/1	0.99	0.09	29,29,29,29	0
54	MG	1A	3040	1/1	0.99	0.13	34,34,34,34	0
54	MG	2A	3587	1/1	0.99	0.04	38,38,38,38	0
54	MG	1A	3896	1/1	0.99	0.07	20,20,20,20	0
54	MG	1A	3897	1/1	0.99	0.08	46,46,46,46	0
54	MG	1A	3387	1/1	0.99	0.05	22,22,22,22	0
54	MG	1A	3779	1/1	0.99	0.04	78,78,78,78	0
54	MG	2A	3592	1/1	0.99	0.05	41,41,41,41	0
54	MG	2A	3405	1/1	0.99	0.08	33,33,33,33	0
54	MG	1A	3258	1/1	0.99	0.07	21,21,21,21	0
54	MG	1A	3525	1/1	0.99	0.09	44,44,44,44	0
54	MG	2A	3596	1/1	0.99	0.03	25,25,25,25	0
54	MG	2A	3697	1/1	0.99	0.07	61,61,61,61	0
54	MG	1A	3389	1/1	0.99	0.05	32,32,32,32	0
54	MG	1B	223	1/1	0.99	0.05	42,42,42,42	0
54	MG	1A	3390	1/1	0.99	0.10	12,12,12,12	0
54	MG	1A	3340	1/1	0.99	0.08	34,34,34,34	0
54	MG	1A	3644	1/1	0.99	0.04	22,22,22,22	0
54	MG	2a	3001	1/1	0.99	0.07	52,52,52,52	0
54	MG	1A	3786	1/1	0.99	0.10	45,45,45,45	0
54	MG	1A	3113	1/1	0.99	0.15	27,27,27,27	0
54	MG	1A	3342	1/1	0.99	0.06	23,23,23,23	0
54	MG	1A	3083	1/1	0.99	0.06	32,32,32,32	0
58	ZN	26	501	1/1	0.99	0.02	51,51,51,51	0
54	MG	1a	3016	1/1	0.99	0.03	76,76,76,76	0
54	MG	1A	3078	1/1	0.99	0.28	27,27,27,27	0
59	SF4	1d	306	8/8	0.99	0.04	57,64,71,75	0
59	SF4	2d	501	8/8	0.99	0.04	55,77,84,87	0
54	MG	1A	3816	1/1	1.00	0.03	27,27,27,27	0
54	MG	1A	3857	1/1	1.00	0.03	20,20,20,20	0
54	MG	1A	3435	1/1	1.00	0.02	19,19,19,19	0
54	MG	1a	3124	1/1	1.00	0.03	36,36,36,36	0
54	MG	1A	3466	1/1	1.00	0.03	34,34,34,34	0
54	MG	1A	3442	1/1	1.00	0.02	17,17,17,17	0
54	MG	1A	3956	1/1	1.00	0.04	20,20,20,20	0
54	MG	1A	3295	1/1	1.00	0.02	31,31,31,31	0
58	ZN	16	501	1/1	1.00	0.03	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	ZN	19	103	1/1	1.00	0.01	42,42,42,42	0
54	MG	2A	3344	1/1	1.00	0.03	18,18,18,18	0
54	MG	1A	3422	1/1	1.00	0.05	21,21,21,21	0
54	MG	1A	3611	1/1	1.00	0.03	22,22,22,22	0
54	MG	2A	3467	1/1	1.00	0.04	26,26,26,26	0
54	MG	2A	3484	1/1	1.00	0.02	25,25,25,25	0
54	MG	1A	3875	1/1	1.00	0.02	32,32,32,32	0
54	MG	1A	3654	1/1	1.00	0.07	34,34,34,34	0
54	MG	1A	3515	1/1	1.00	0.03	17,17,17,17	0
54	MG	1A	3825	1/1	1.00	0.02	13,13,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.