Full wwPDB X-ray Structure Validation Report ⓘ

Jul 29, 2024 – 11:34 PM EDT

PDB ID	:	8VTY
Title	:	Crystal structure of the wild-type Thermus thermophilus 70S ribosome in complex with ciprofloxacin and protein Y at 2.60A resolution
Authors	:	Aleksandrova, E.V.; Ma, C.-X.; Klepacki, D.; Alizadeh, F.; Vazquez-Laslop, N.; Liang, J.-H.; Polikanov, Y.S.; Mankin, A.S.
Deposited on	:	2024-01-27
Resolution	:	2.60 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 ⓘ) were used in the production of this report:

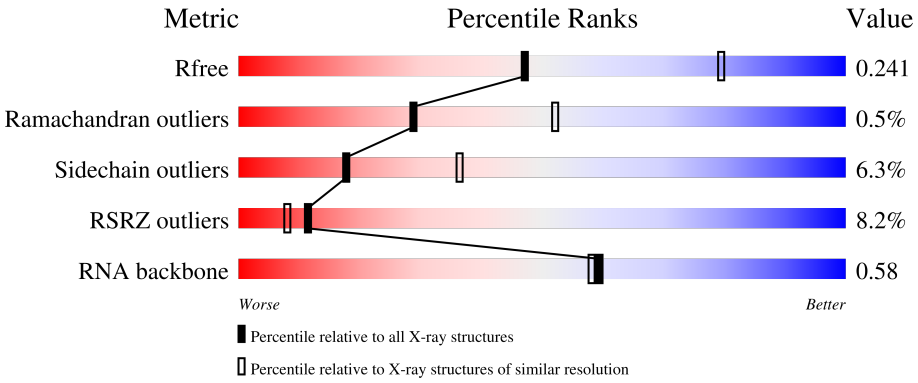
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.60 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}	130704	3163 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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	4% 84% 14% ·
1	2A	2915	5% 82% 17% ·
2	1B	121	92% 7% ·
2	2B	121	2% 87% 12% ·

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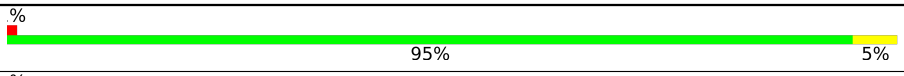
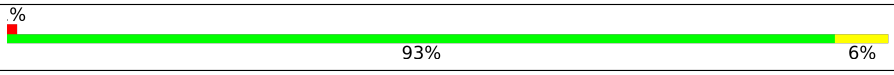
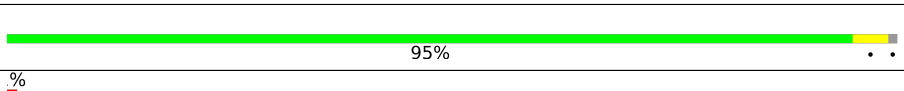
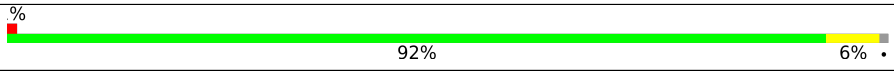
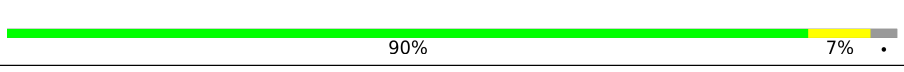
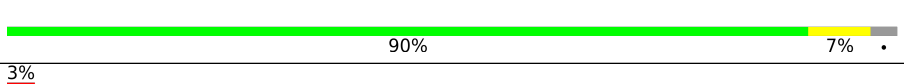
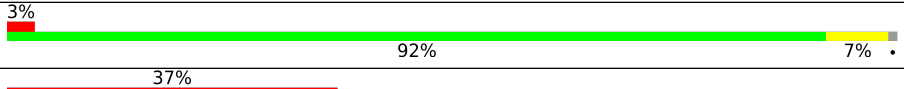
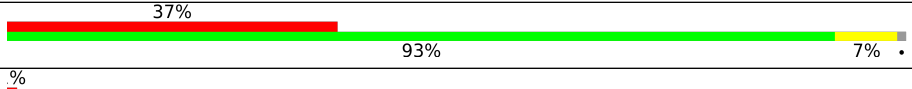
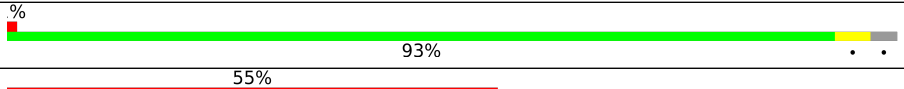
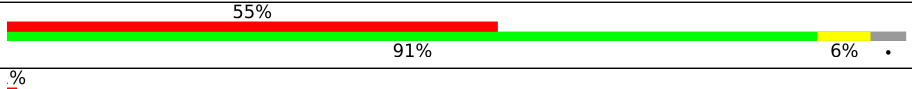
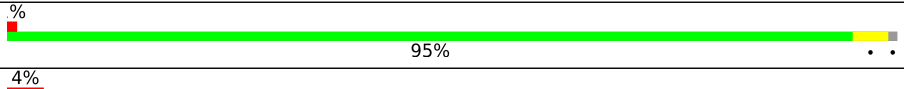
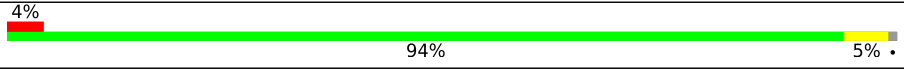
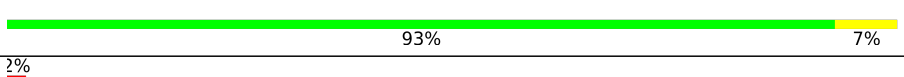
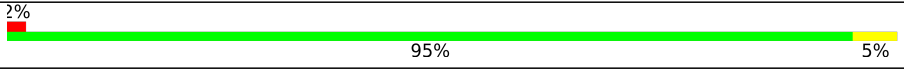
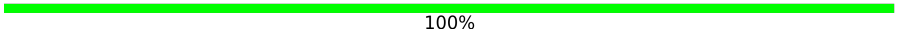
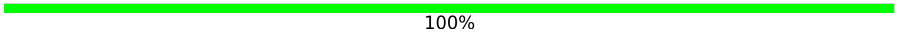
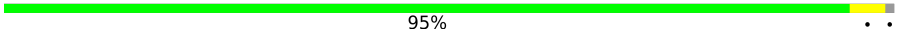
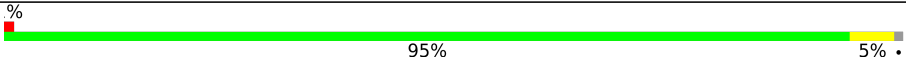
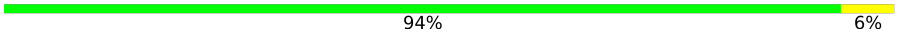
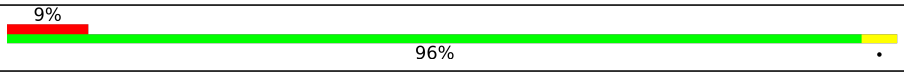
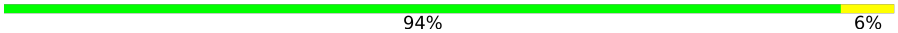
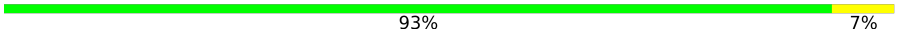
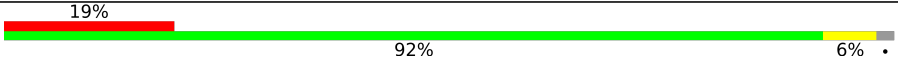
Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

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Mol	Chain	Length	Quality of chain
15	2T	146	88% 10%
16	1U	118	94%
16	2U	118	96%
17	1V	101	97%
17	2V	101	91% 8%
18	1W	113	96%
18	2W	113	96%
19	1X	96	94% 5%
19	2X	96	3% 96%
20	1Y	110	91% 6%
20	2Y	110	93% 5%
21	1Z	206	92% 7%
21	2Z	206	10% 92% 5%
22	10	85	89% 9%
22	20	85	14% 91% 9%
23	11	98	95%
23	21	98	95%
24	12	72	94%
24	22	72	89% 8%
25	13	60	93% 5%
25	23	60	3% 93% 5%
26	14	71	17% 89% 6%
26	24	71	49% 85% 13%
27	15	60	95%
27	25	60	97%

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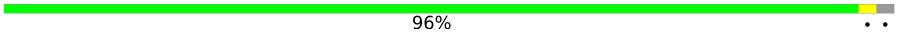
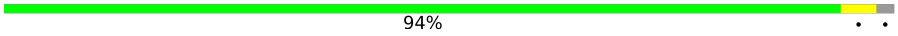
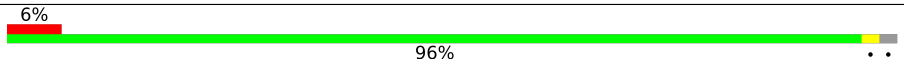
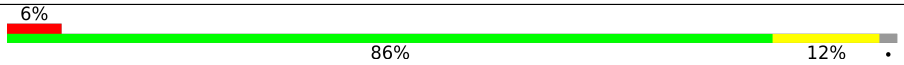
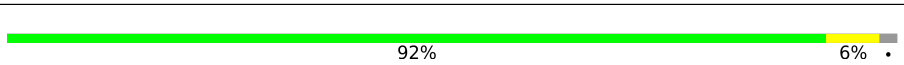
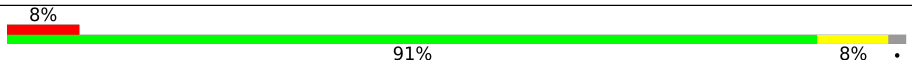
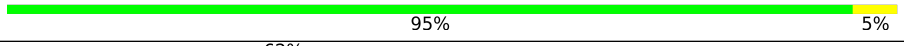
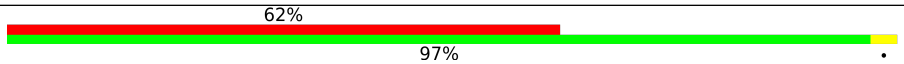
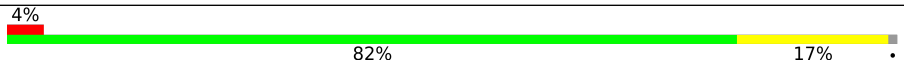
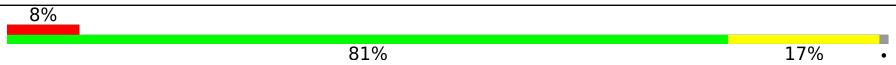
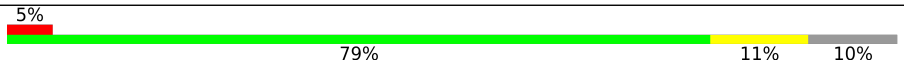
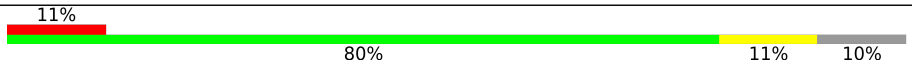
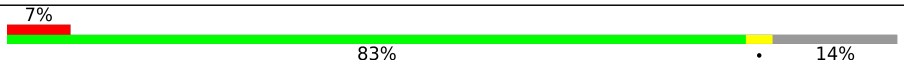
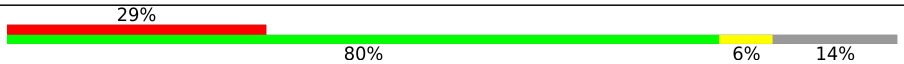
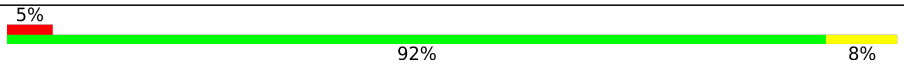
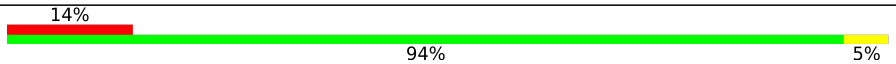
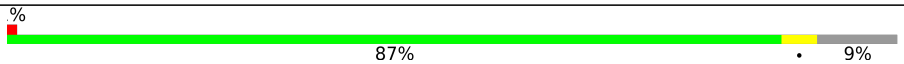
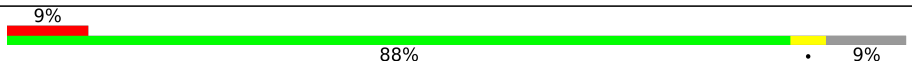
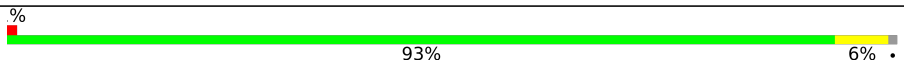
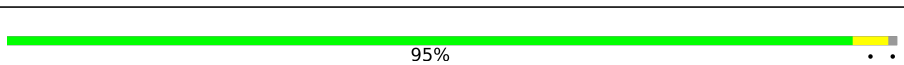
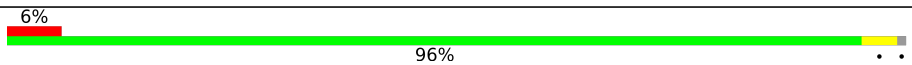
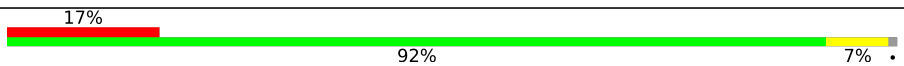
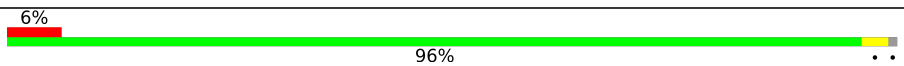
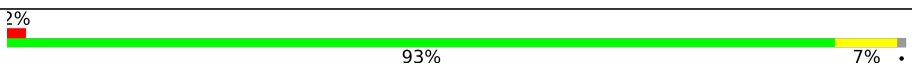
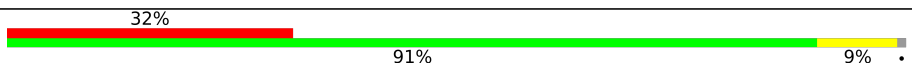
Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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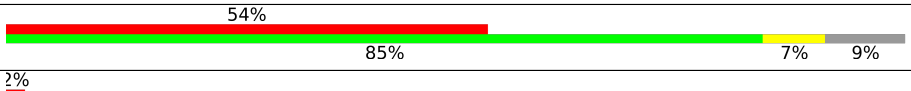
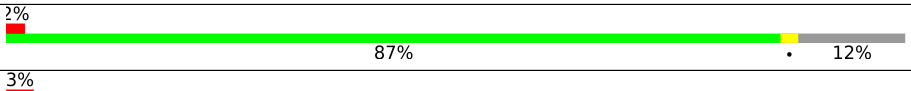
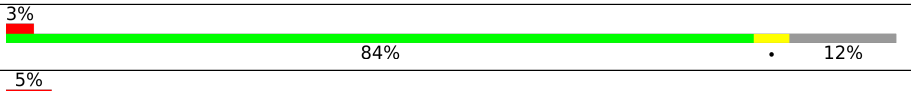
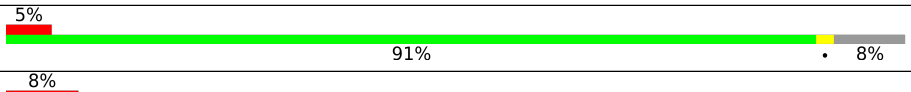
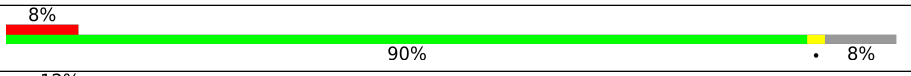
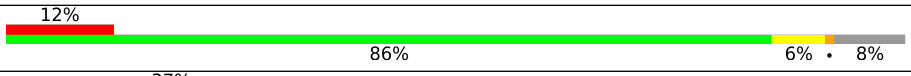
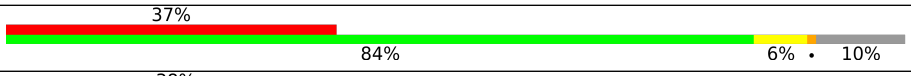
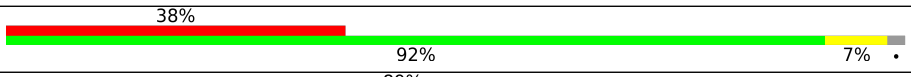
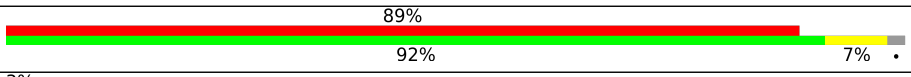
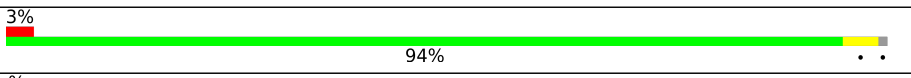
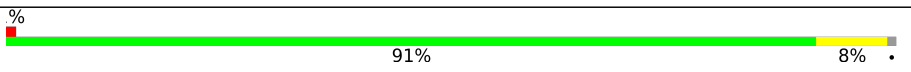
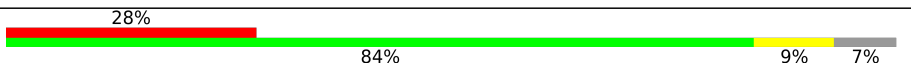
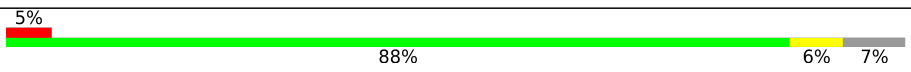
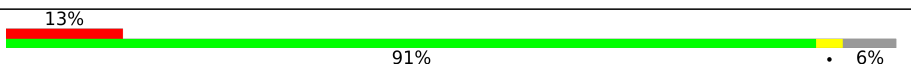
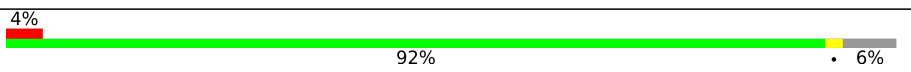
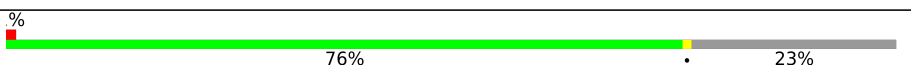
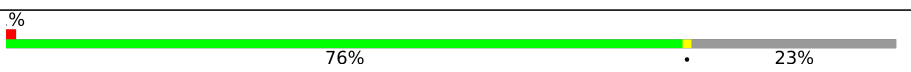
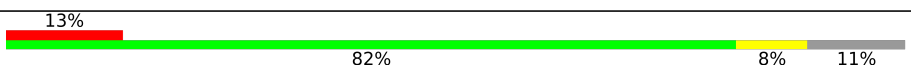
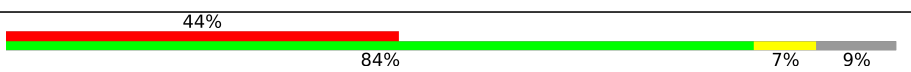
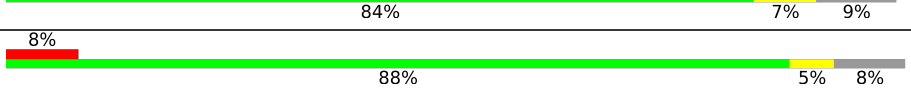
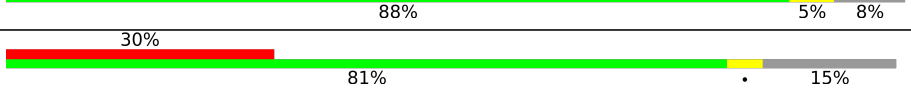
Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	

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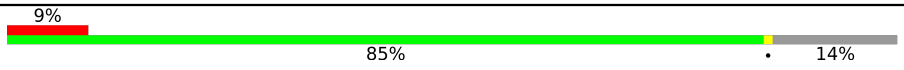
Mol	Chain	Length	Quality of chain
53	1y	113	
53	2y	113	

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	3270	-	-	-	X
54	MG	1A	3310	-	-	-	X
54	MG	1A	3641	-	-	-	X
54	MG	1A	3688	-	-	-	X
54	MG	1A	3703	-	-	-	X
54	MG	1A	3704	-	-	-	X
54	MG	1A	3996	-	-	-	X
54	MG	1A	4051	-	-	-	X
54	MG	1B	207	-	-	-	X
54	MG	1E	306	-	-	-	X
54	MG	1a	1795	-	-	-	X
54	MG	2A	3034	-	-	-	X
54	MG	2A	3042	-	-	-	X
54	MG	2A	3080	-	-	-	X
54	MG	2A	3162	-	-	-	X
54	MG	2A	3190	-	-	-	X
54	MG	2A	3202	-	-	-	X
54	MG	2A	3206	-	-	-	X
54	MG	2A	3524	-	-	-	X
54	MG	2A	3707	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 297563 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 933	C 588	N 171	O 170	S 4	0	0	0

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

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

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

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

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

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

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

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

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

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

- 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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1A	1056	Total 1056	Mg 1056	0	0
54	1B	29	Total 29	Mg 29	0	0
54	1D	18	Total 18	Mg 18	0	0
54	1E	9	Total 9	Mg 9	0	0
54	1F	19	Total 19	Mg 19	0	0
54	1G	4	Total 4	Mg 4	0	0
54	1H	3	Total 3	Mg 3	0	0
54	1N	5	Total 5	Mg 5	0	0
54	1O	1	Total 1	Mg 1	0	0
54	1P	6	Total 6	Mg 6	0	0
54	1Q	5	Total 5	Mg 5	0	0
54	1R	6	Total 6	Mg 6	0	0
54	1T	5	Total 5	Mg 5	0	0
54	1U	7	Total 7	Mg 7	0	0
54	1V	6	Total 6	Mg 6	0	0
54	1W	3	Total 3	Mg 3	0	0
54	1Z	1	Total 1	Mg 1	0	0
54	10	7	Total 7	Mg 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	11	5	Total Mg 5 5	0	0
54	13	4	Total Mg 4 4	0	0
54	14	1	Total Mg 1 1	0	0
54	15	8	Total Mg 8 8	0	0
54	17	7	Total Mg 7 7	0	0
54	18	3	Total Mg 3 3	0	0
54	19	2	Total Mg 2 2	0	0
54	1a	277	Total Mg 277 277	0	0
54	1b	1	Total Mg 1 1	0	0
54	1d	5	Total Mg 5 5	0	0
54	1e	2	Total Mg 2 2	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	1k	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	3	Total Mg 3 3	0	0
54	1o	1	Total Mg 1 1	0	0
54	1t	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	1y	4	Total Mg 4 4	0	0
54	2A	741	Total Mg 741 741	0	0
54	2B	18	Total Mg 18 18	0	0
54	2D	12	Total Mg 12 12	0	0
54	2E	7	Total Mg 7 7	0	0
54	2F	4	Total Mg 4 4	0	0
54	2G	3	Total Mg 3 3	0	0
54	2N	1	Total Mg 1 1	0	0
54	2O	2	Total Mg 2 2	0	0
54	2Q	3	Total Mg 3 3	0	0
54	2R	3	Total Mg 3 3	0	0
54	2T	3	Total Mg 3 3	0	0
54	2V	3	Total Mg 3 3	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	3	Total Mg 3 3	0	0
54	21	1	Total Mg 1 1	0	0
54	23	2	Total Mg 2 2	0	0
54	25	1	Total Mg 1 1	0	0
54	27	1	Total Mg 1 1	0	0

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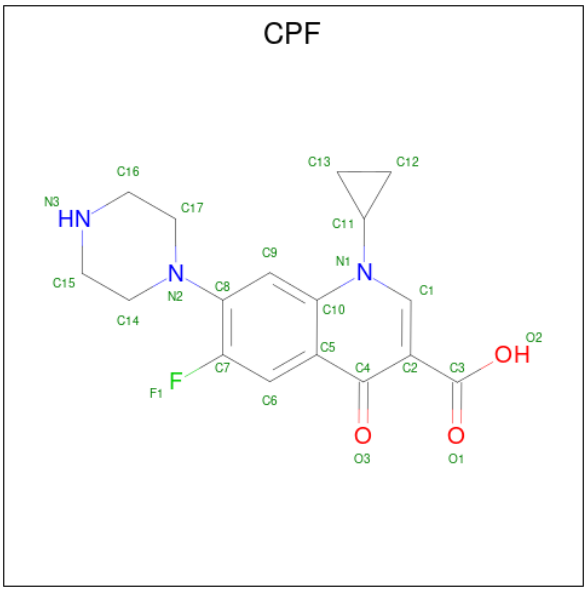
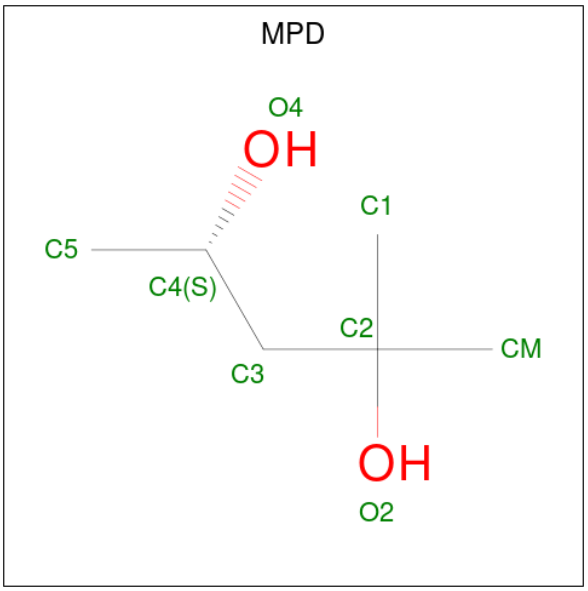
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	28	2	Total Mg 2 2	0	0
54	2a	195	Total Mg 195 195	0	0
54	2d	1	Total Mg 1 1	0	0
54	2e	1	Total Mg 1 1	0	0
54	2f	2	Total Mg 2 2	0	0
54	2j	1	Total Mg 1 1	0	0
54	2k	1	Total Mg 1 1	0	0
54	2n	1	Total Mg 1 1	0	0
54	2o	1	Total Mg 1 1	0	0
54	2p	1	Total Mg 1 1	0	0
54	2r	1	Total Mg 1 1	0	0
54	2t	1	Total Mg 1 1	0	0

- Molecule 55 is 1-CYCLOPROPYL-6-FLUORO-4-OXO-7-PIPERAZIN-1-YL-1,4-DIHYDR OQUINOLINE-3-CARBOXYLIC ACID (three-letter code: CPF) (formula: $C_{17}H_{18}FN_3O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
55	1A	1	Total	C	F	N	O	0	0
			24	17	1	3	3		
55	2A	1	Total	C	F	N	O	0	0
			24	17	1	3	3		

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



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

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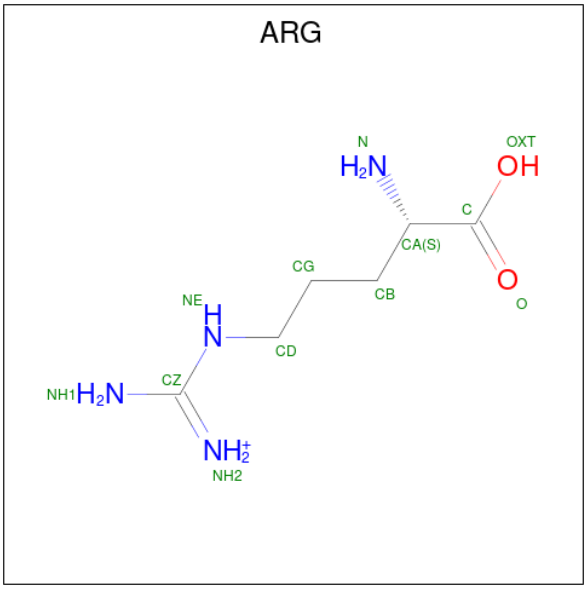
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1O	1	Total C O 8 6 2	0	0
56	18	1	Total C O 8 6 2	0	0
56	1a	1	Total C O 8 6 2	0	0
56	2A	1	Total C O 8 6 2	0	0
56	2A	1	Total C O 8 6 2	0	0
56	2B	1	Total C O 8 6 2	0	0

- Molecule 57 is ARGININE (three-letter code: 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 (three-letter code: ZN) (formula: Zn).

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

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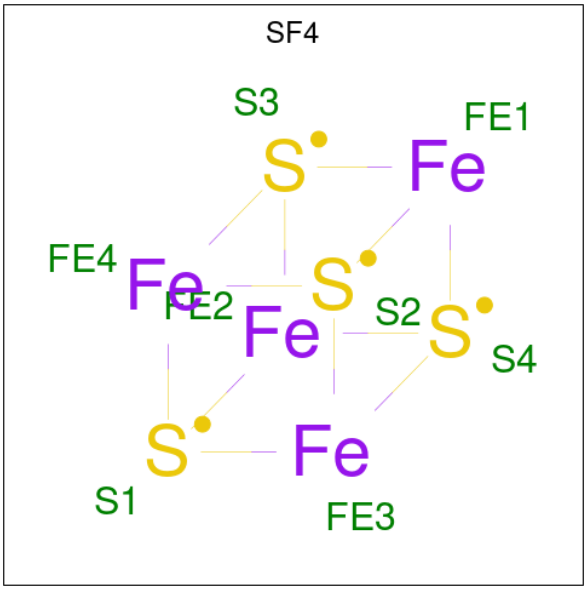
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	14	1	Total Zn 1 1	0	0
58	15	1	Total Zn 1 1	0	0
58	16	1	Total Zn 1 1	0	0
58	19	1	Total Zn 1 1	0	0
58	1n	1	Total Zn 1 1	0	0
58	2Y	1	Total Zn 1 1	0	0
58	24	1	Total Zn 1 1	0	0
58	25	1	Total Zn 1 1	0	0
58	26	1	Total Zn 1 1	0	0
58	29	1	Total Zn 1 1	0	0
58	2n	1	Total Zn 1 1	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1A	3927	Total O 3927 3927	0	0
60	1B	89	Total O 89 89	0	0
60	1D	110	Total O 110 110	0	0
60	1E	72	Total O 72 72	0	0
60	1F	67	Total O 67 67	0	0
60	1G	16	Total O 16 16	0	0
60	1H	14	Total O 14 14	0	0
60	1I	5	Total O 5 5	0	0
60	1N	52	Total O 52 52	0	0
60	1O	25	Total O 25 25	0	0
60	1P	65	Total O 65 65	0	0
60	1Q	41	Total O 41 41	0	0
60	1R	32	Total O 32 32	0	0
60	1S	8	Total O 8 8	0	0
60	1T	36	Total O 36 36	0	0
60	1U	43	Total O 43 43	0	0
60	1V	36	Total O 36 36	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	17	Total O 17 17	0	0
60	1Z	11	Total O 11 11	0	0
60	10	25	Total O 25 25	0	0
60	11	28	Total O 28 28	0	0
60	12	13	Total O 13 13	0	0
60	13	25	Total O 25 25	0	0
60	14	3	Total O 3 3	0	0
60	15	28	Total O 28 28	0	0
60	16	20	Total O 20 20	0	0
60	17	13	Total O 13 13	0	0
60	18	28	Total O 28 28	0	0
60	19	8	Total O 8 8	0	0
60	1a	496	Total O 496 496	0	0
60	1b	1	Total O 1 1	0	0
60	1c	1	Total O 1 1	0	0
60	1d	9	Total O 9 9	0	0
60	1e	10	Total O 10 10	0	0
60	1f	1	Total O 1 1	0	0
60	1h	1	Total O 1 1	0	0
60	1j	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1k	1	Total O 1 1	0	0
60	1l	4	Total O 4 4	0	0
60	1o	4	Total O 4 4	0	0
60	1p	1	Total O 1 1	0	0
60	1y	5	Total O 5 5	0	0
60	2A	2249	Total O 2249 2249	0	0
60	2B	42	Total O 42 42	0	0
60	2D	47	Total O 47 47	0	0
60	2E	28	Total O 28 28	0	0
60	2F	23	Total O 23 23	0	0
60	2G	4	Total O 4 4	0	0
60	2H	1	Total O 1 1	0	0
60	2N	6	Total O 6 6	0	0
60	2O	15	Total O 15 15	0	0
60	2P	21	Total O 21 21	0	0
60	2Q	18	Total O 18 18	0	0
60	2R	22	Total O 22 22	0	0
60	2S	2	Total O 2 2	0	0
60	2T	12	Total O 12 12	0	0
60	2U	16	Total O 16 16	0	0
60	2V	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	2W	19	Total O 19 19	0	0
60	2X	8	Total O 8 8	0	0
60	2Y	4	Total O 4 4	0	0
60	2Z	8	Total O 8 8	0	0
60	20	10	Total O 10 10	0	0
60	21	17	Total O 17 17	0	0
60	22	2	Total O 2 2	0	0
60	23	2	Total O 2 2	0	0
60	25	7	Total O 7 7	0	0
60	26	6	Total O 6 6	0	0
60	27	9	Total O 9 9	0	0
60	28	15	Total O 15 15	0	0
60	2a	404	Total O 404 404	0	0
60	2d	3	Total O 3 3	0	0
60	2e	3	Total O 3 3	0	0
60	2f	3	Total O 3 3	0	0
60	2j	2	Total O 2 2	0	0
60	2l	5	Total O 5 5	0	0
60	2o	2	Total O 2 2	0	0
60	2p	1	Total O 1 1	0	0
60	2q	1	Total O 1 1	0	0

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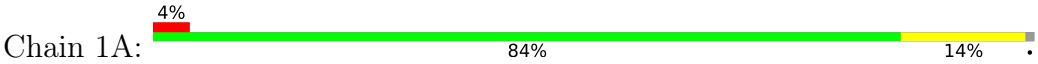
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	2r	3	Total O 3 3	0	0
60	2t	3	Total O 3 3	0	0
60	2u	1	Total O 1 1	0	0
60	2y	1	Total O 1 1	0	0

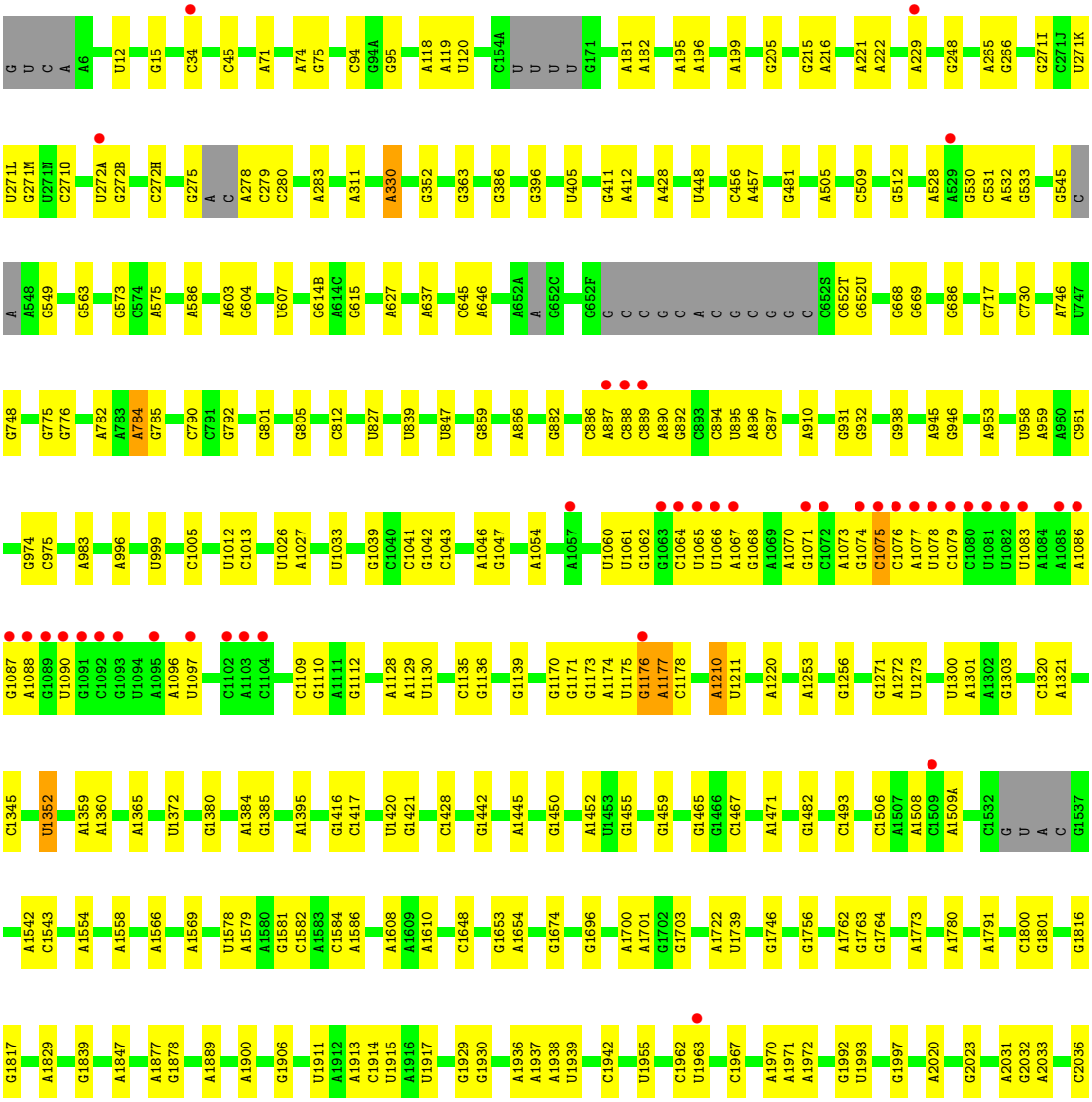
3 Residue-property plots (i)

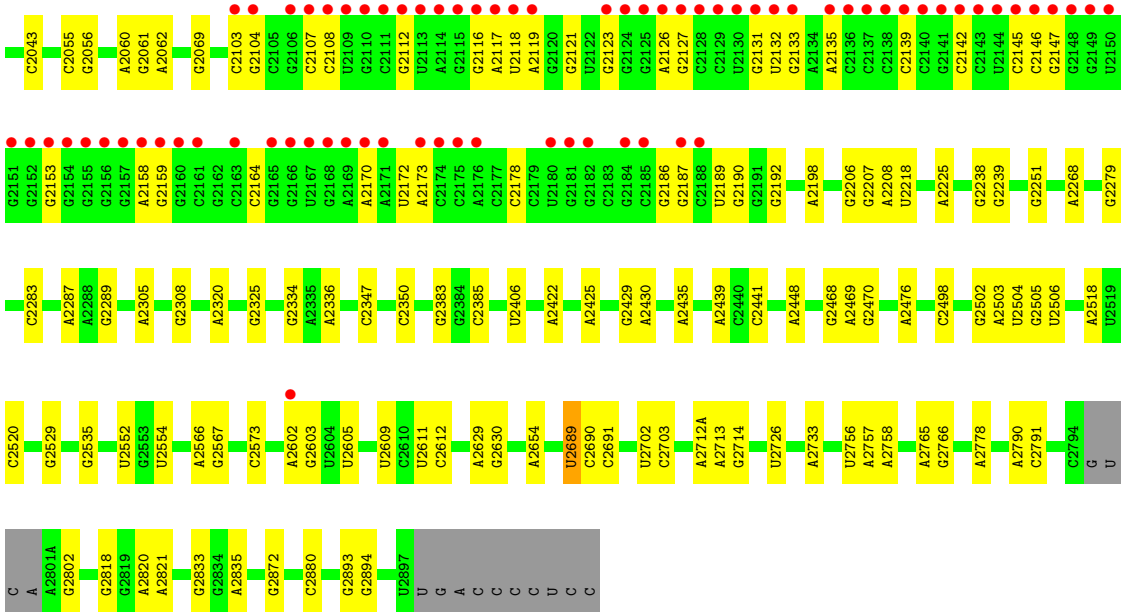
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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:

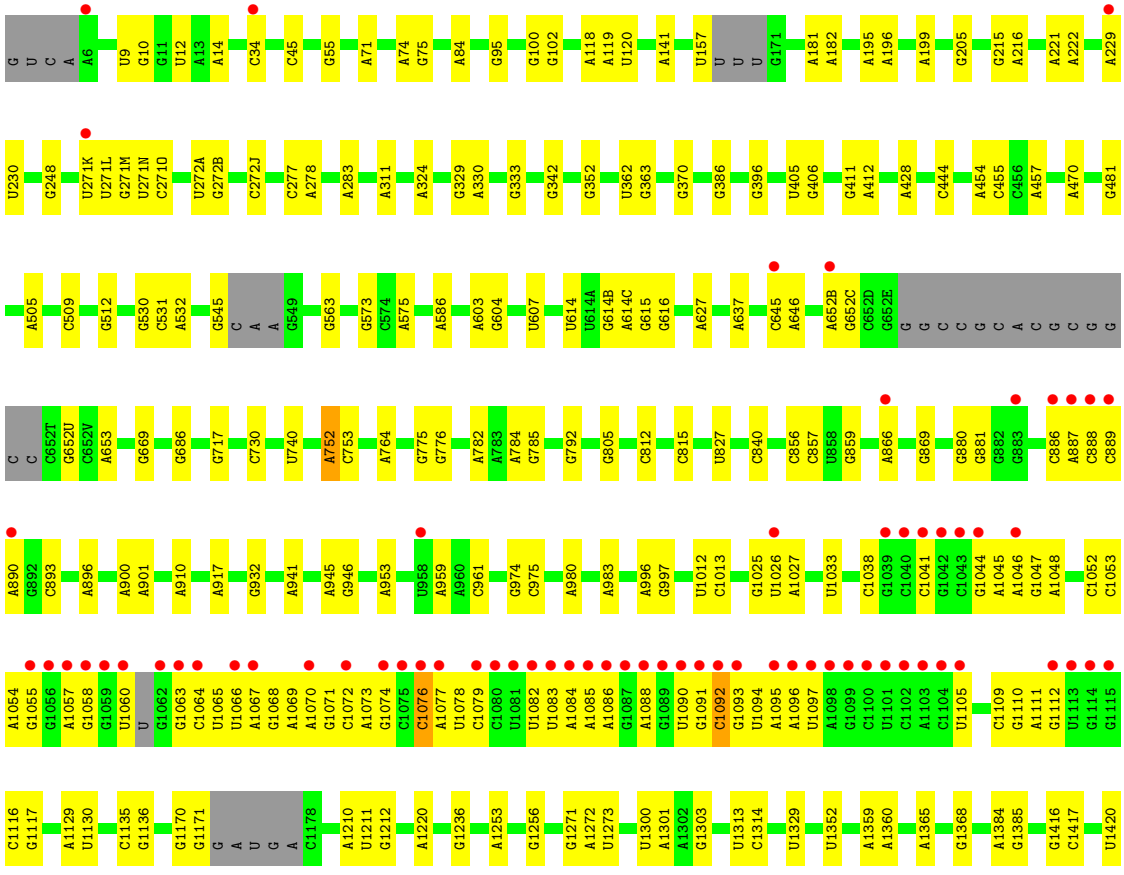


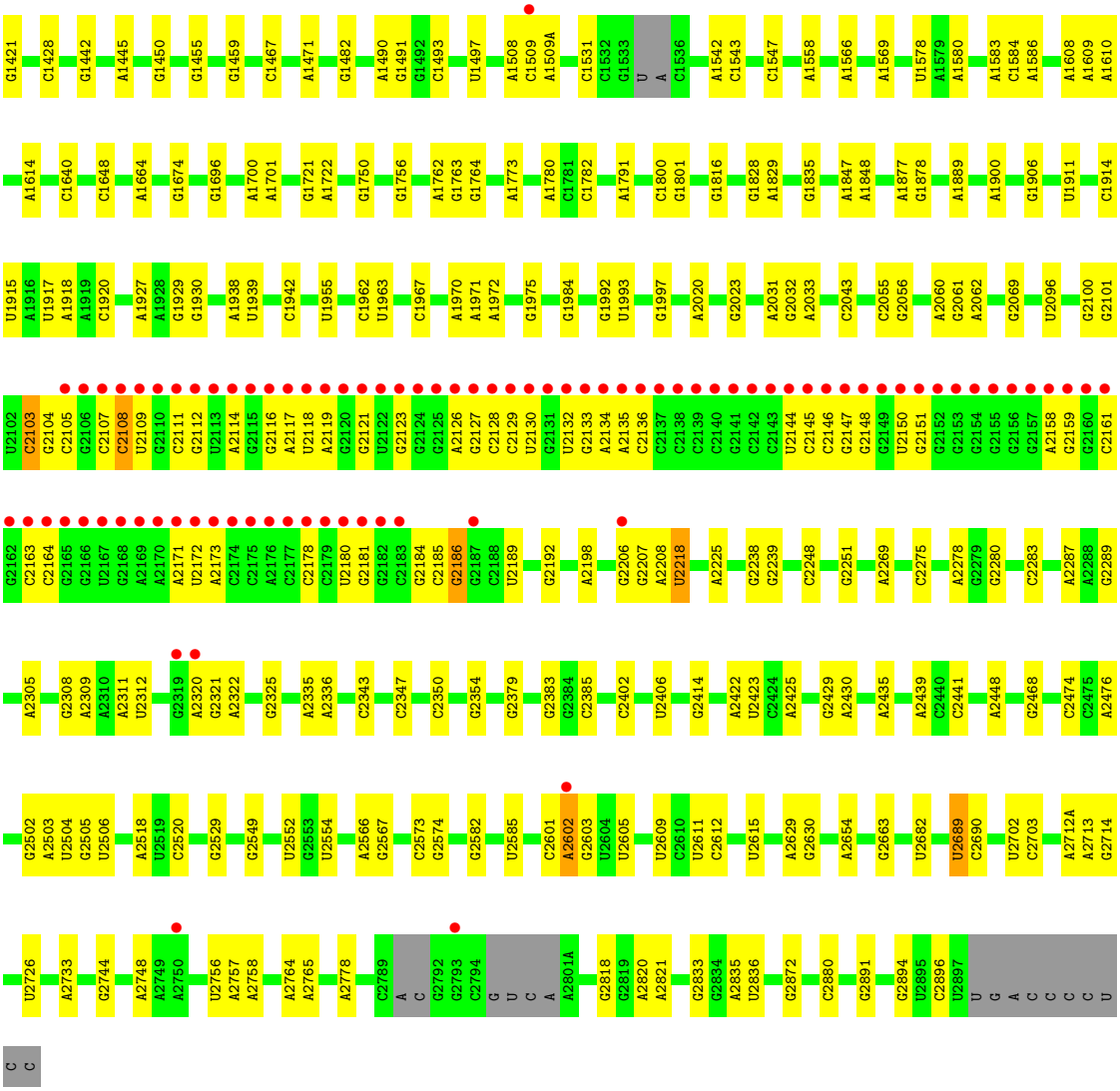




• Molecule 1: 23S Ribosomal RNA

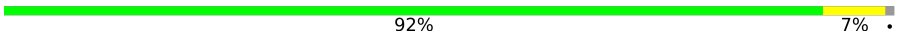
Chain 2A:





• Molecule 2: 5S Ribosomal RNA

Chain 1B:

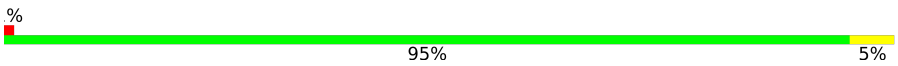


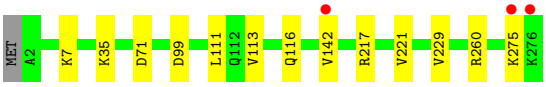
• Molecule 2: 5S Ribosomal RNA

Chain 2B:

• Molecule 3: 50S ribosomal protein L2

Chain 1D:

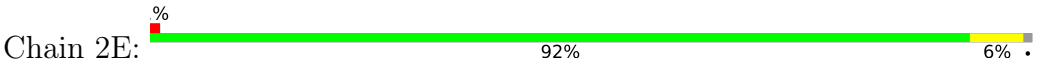


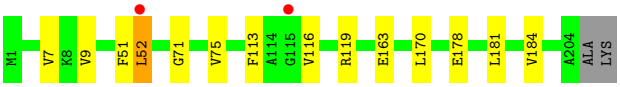


• Molecule 3: 50S ribosomal protein L2

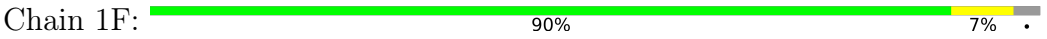
• Molecule 4: 50S ribosomal protein L3

• Molecule 4: 50S ribosomal protein L3

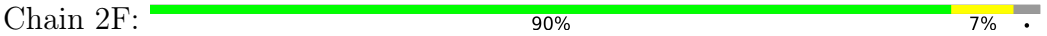




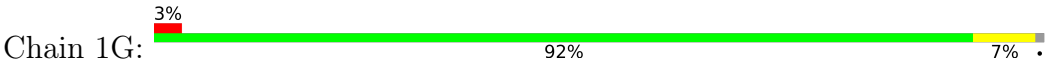
• Molecule 5: 50S ribosomal protein L4

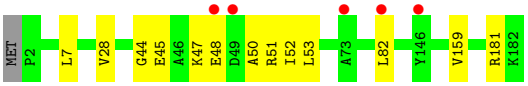


• Molecule 5: 50S ribosomal protein L4

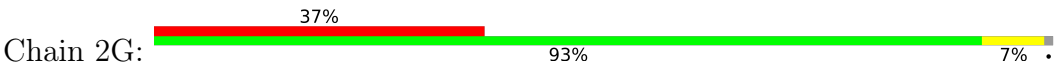


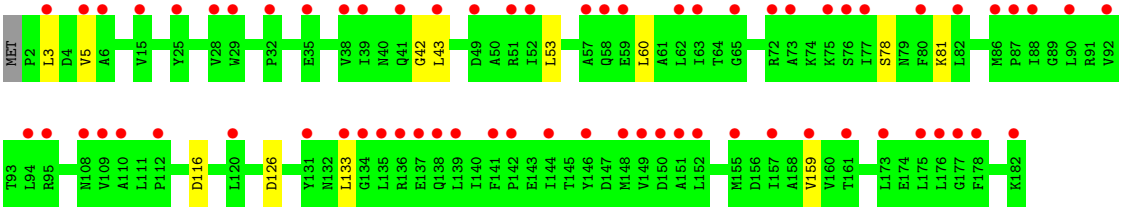
• Molecule 6: 50S ribosomal protein L5





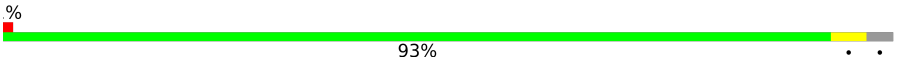
• Molecule 6: 50S ribosomal protein L5

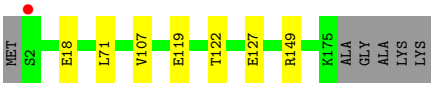




• Molecule 7: 50S ribosomal protein L6

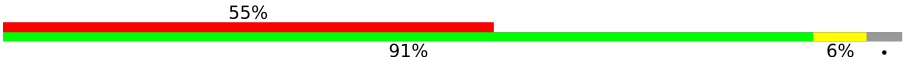
Chain 1H:

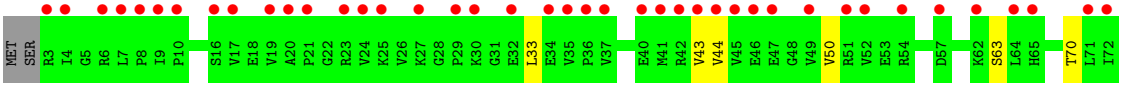


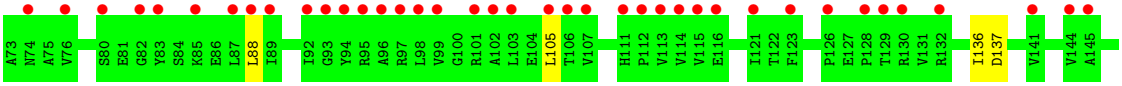


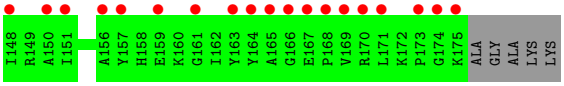
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



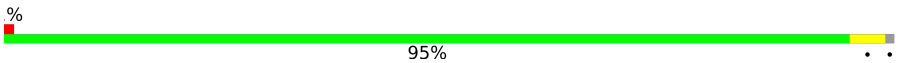


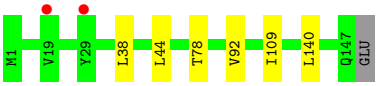




• Molecule 8: 50S ribosomal protein L9

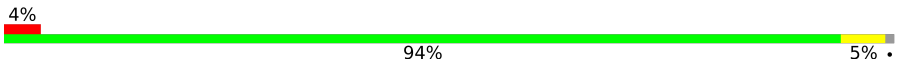
Chain 1I:

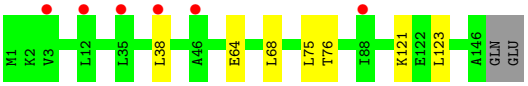




• Molecule 8: 50S ribosomal protein L9

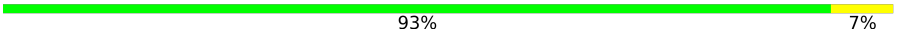
Chain 2I:





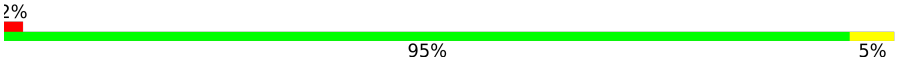
• Molecule 9: 50S ribosomal protein L13

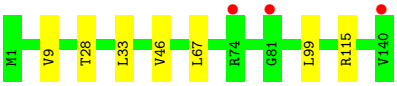
Chain 1N:



• Molecule 9: 50S ribosomal protein L13

Chain 2N:





• Molecule 10: 50S ribosomal protein L14

Chain 1O:

There are no outlier residues recorded for this chain.

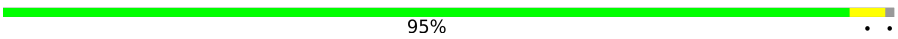
• Molecule 10: 50S ribosomal protein L14

Chain 2O:

There are no outlier residues recorded for this chain.

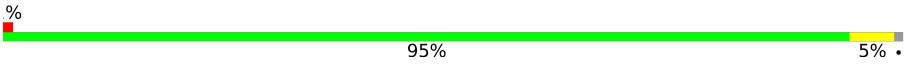
• Molecule 11: 50S ribosomal protein L15

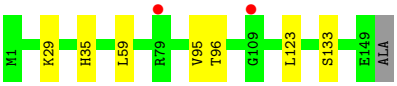
Chain 1P:



• Molecule 11: 50S ribosomal protein L15

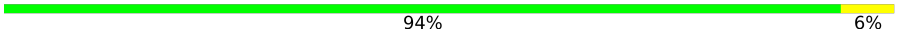
Chain 2P:





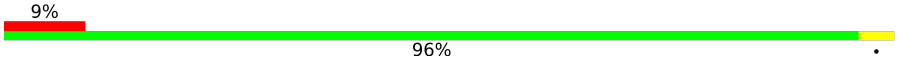
• Molecule 12: 50S ribosomal protein L16

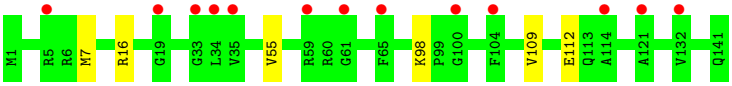
Chain 1Q:



• Molecule 12: 50S ribosomal protein L16

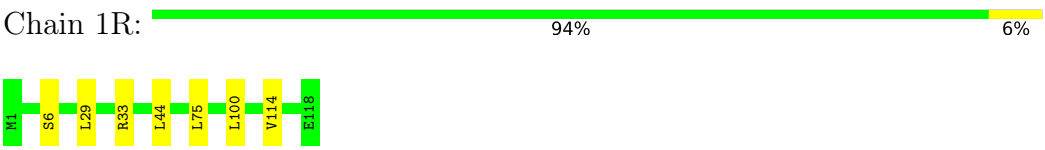
Chain 2Q:





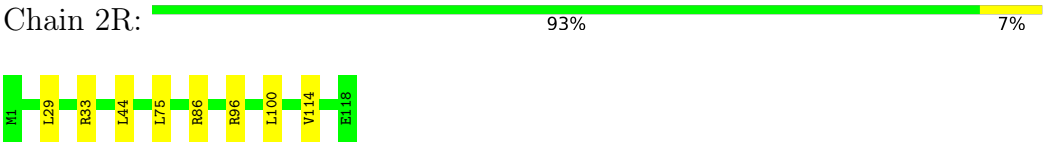
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



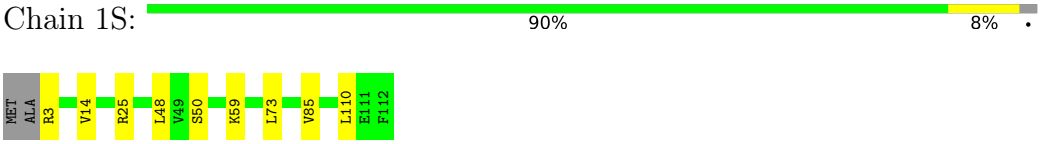
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



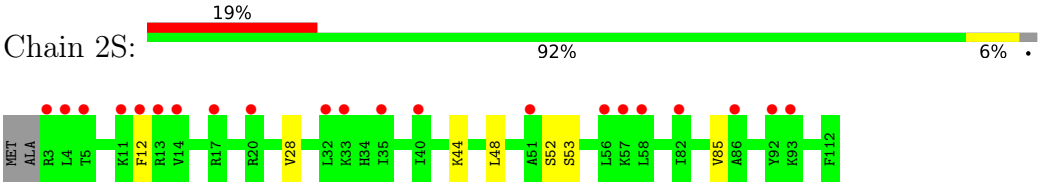
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



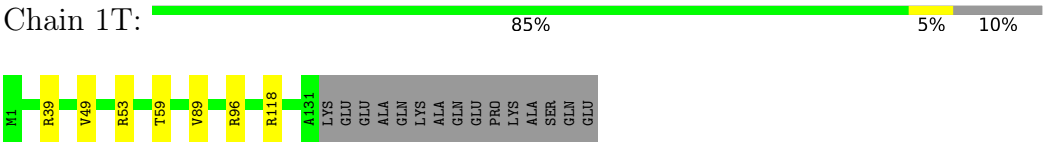
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



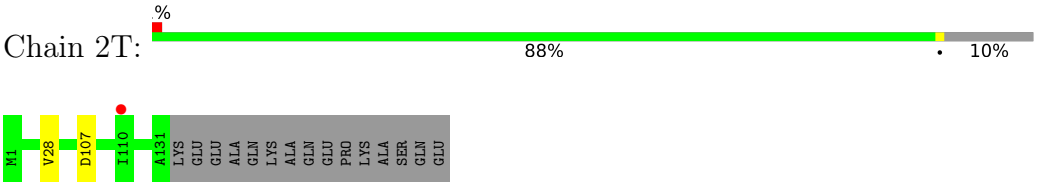
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



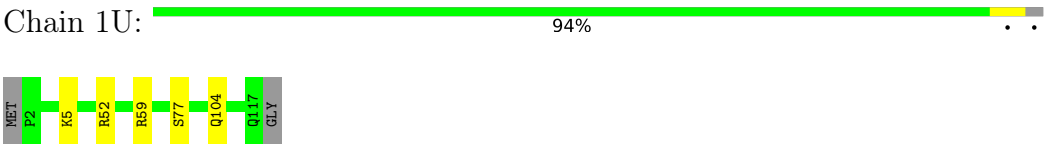
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



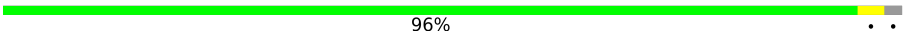
• Molecule 16: 50S ribosomal protein L20

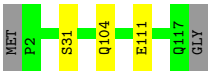
Chain 1U:



• Molecule 16: 50S ribosomal protein L20

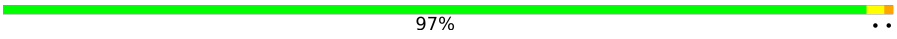
Chain 2U:





• Molecule 17: 50S ribosomal protein L21

Chain 1V:

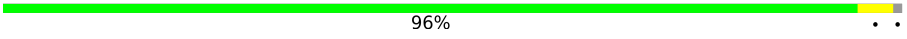


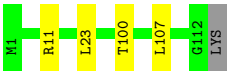
• Molecule 17: 50S ribosomal protein L21

Chain 2V:

• Molecule 18: 50S ribosomal protein L22

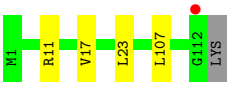
Chain 1W:





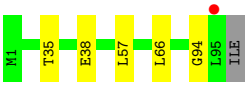
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



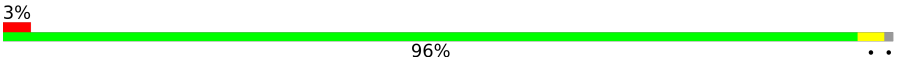
• Molecule 19: 50S ribosomal protein L23

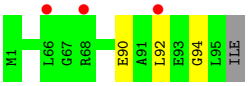
Chain 1X:



• Molecule 19: 50S ribosomal protein L23

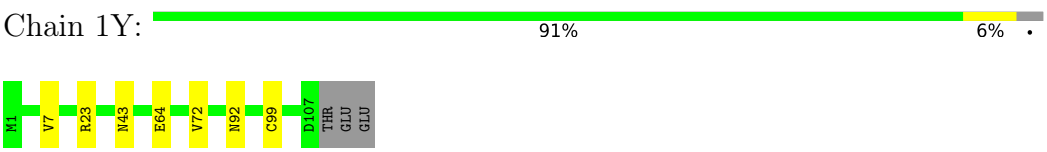
Chain 2X:





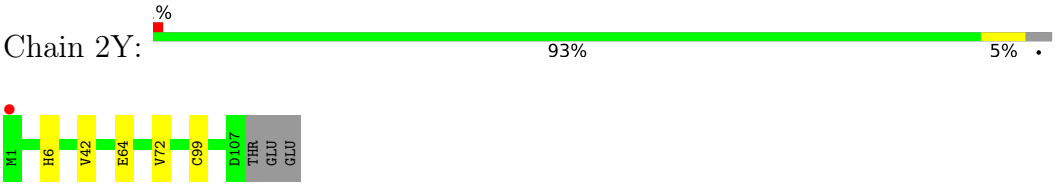
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



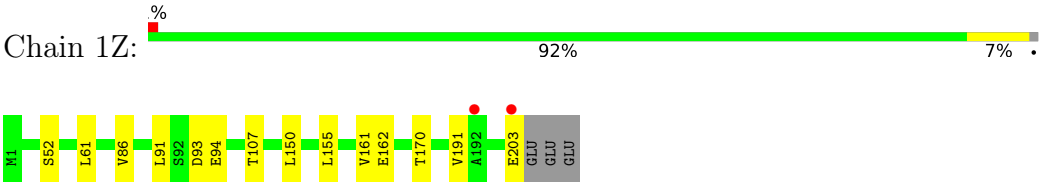
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



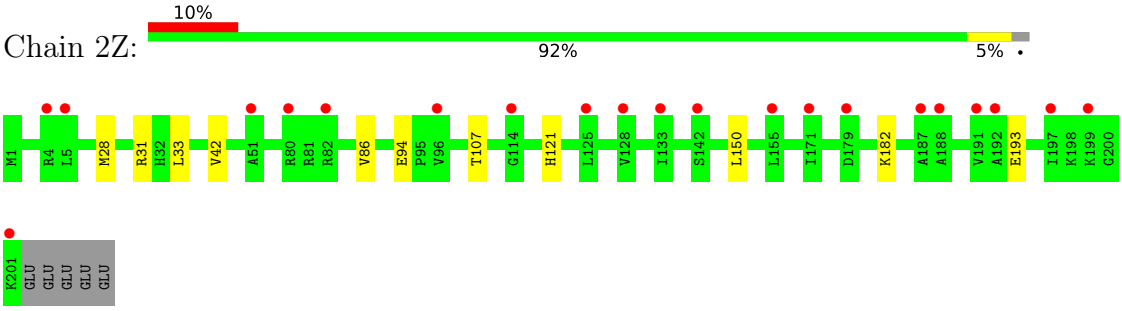
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



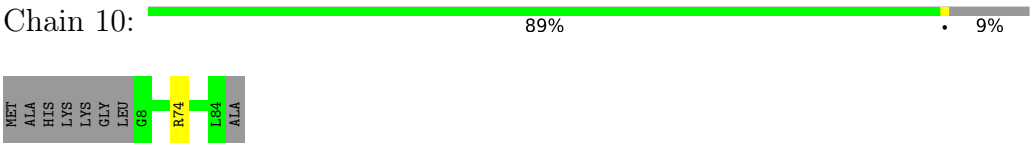
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:



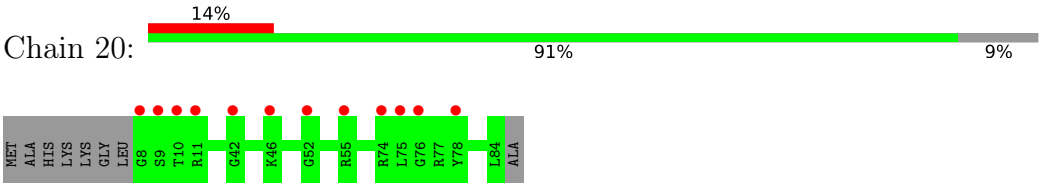
• Molecule 22: 50S ribosomal protein L27

Chain 10:



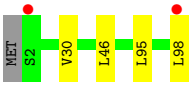
• Molecule 22: 50S ribosomal protein L27

Chain 20:



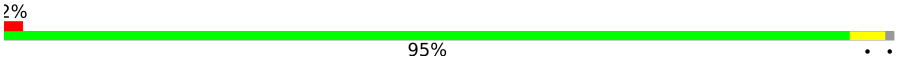
• Molecule 23: 50S ribosomal protein L28

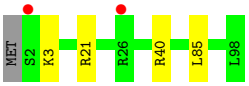
Chain 11:



• Molecule 23: 50S ribosomal protein L28

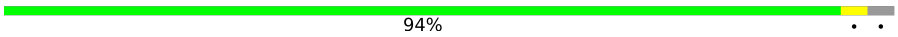
Chain 21:

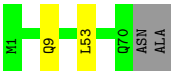




• Molecule 24: 50S ribosomal protein L29

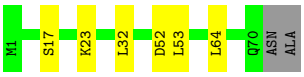
Chain 12:





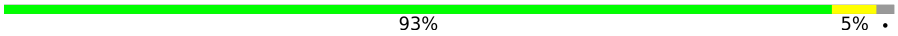
• Molecule 24: 50S ribosomal protein L29

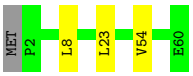
Chain 22:



• Molecule 25: 50S ribosomal protein L30

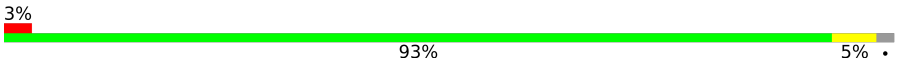
Chain 13:

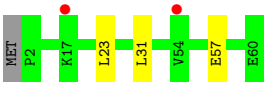




• Molecule 25: 50S ribosomal protein L30

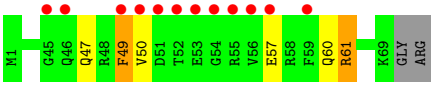
Chain 23:





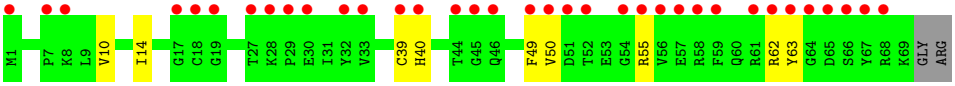
• Molecule 26: 50S ribosomal protein L31

Chain 14:



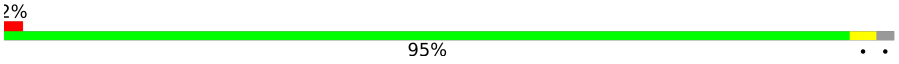
• Molecule 26: 50S ribosomal protein L31

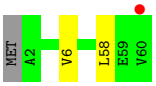
Chain 24:



• Molecule 27: 50S ribosomal protein L32

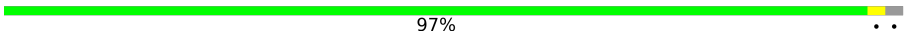
Chain 15:

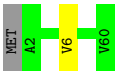




• Molecule 27: 50S ribosomal protein L32

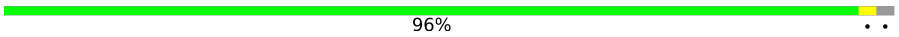
Chain 25:





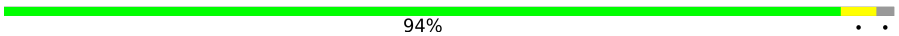
• Molecule 28: 50S ribosomal protein L33

Chain 16:



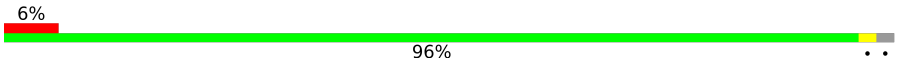
• Molecule 28: 50S ribosomal protein L33

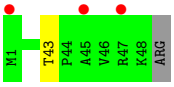
Chain 26:



• Molecule 29: 50S ribosomal protein L34

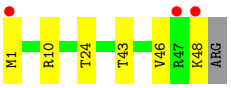
Chain 17:





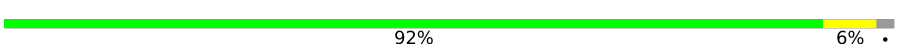
• Molecule 29: 50S ribosomal protein L34

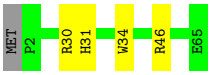
Chain 27:



• Molecule 30: 50S ribosomal protein L35

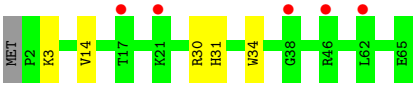
Chain 18:





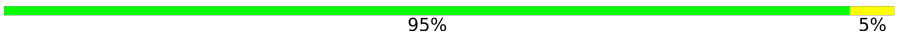
• Molecule 30: 50S ribosomal protein L35

Chain 28:



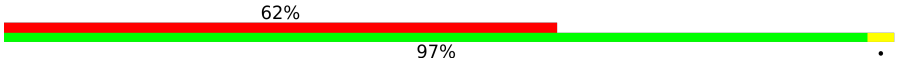
• Molecule 31: 50S ribosomal protein L36

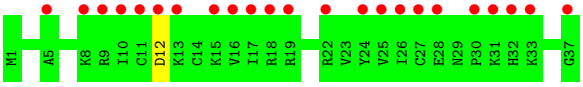
Chain 19:



• Molecule 31: 50S ribosomal protein L36

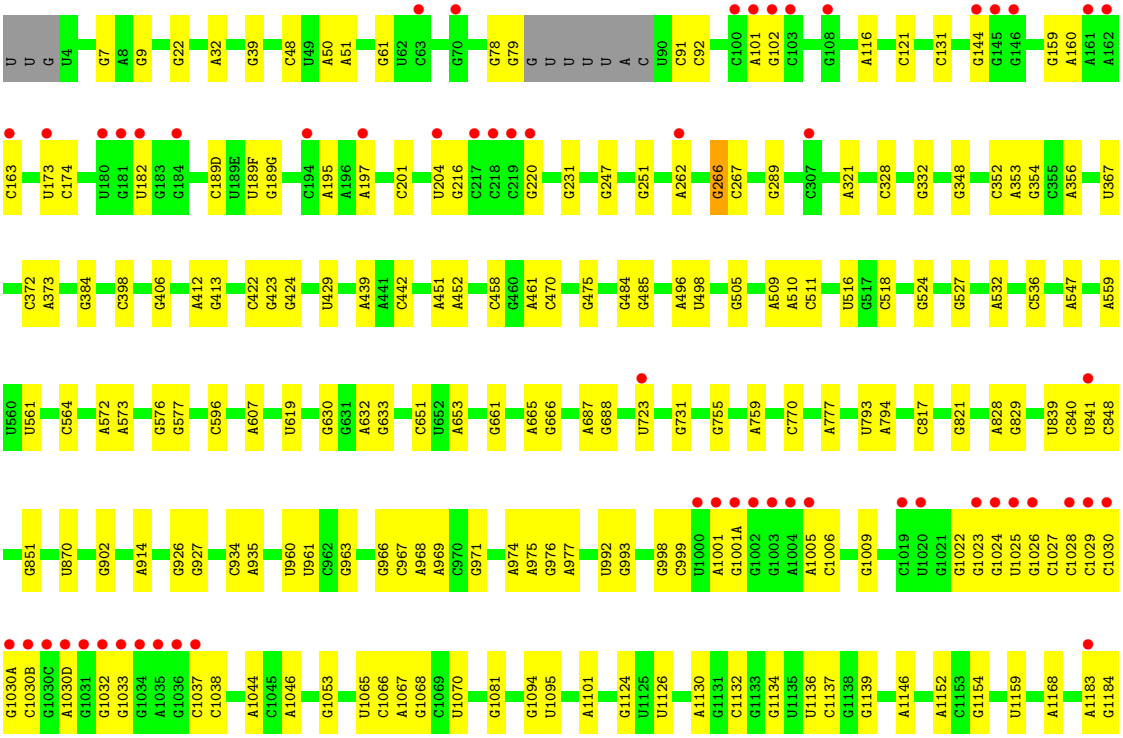
Chain 29:

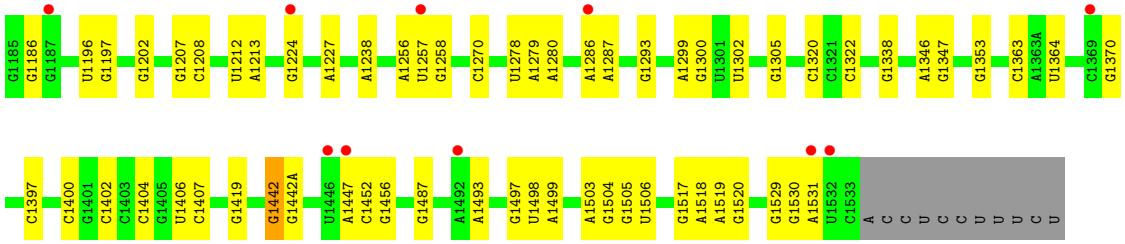




• Molecule 32: 16S Ribosomal RNA

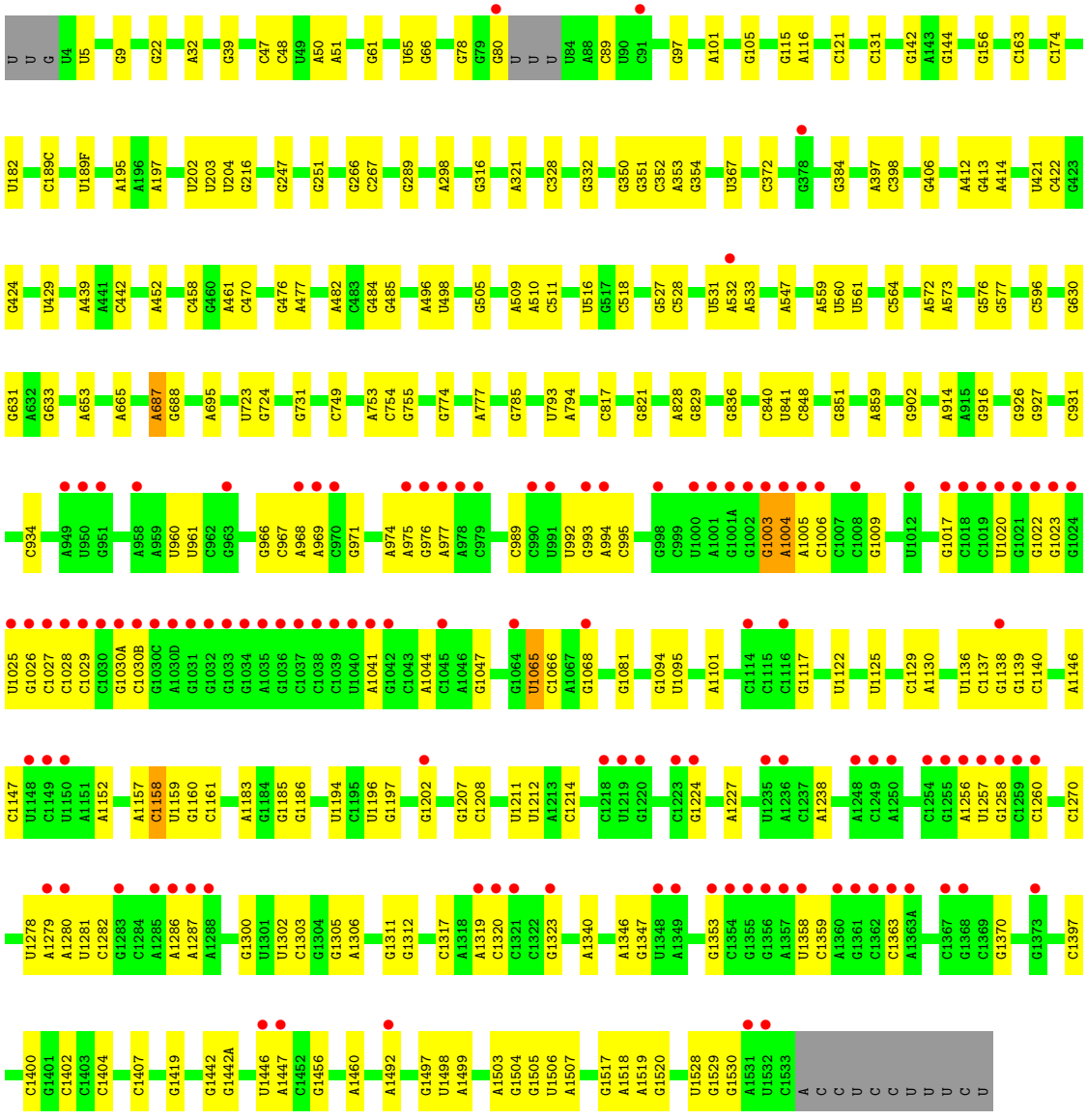
Chain 1a:





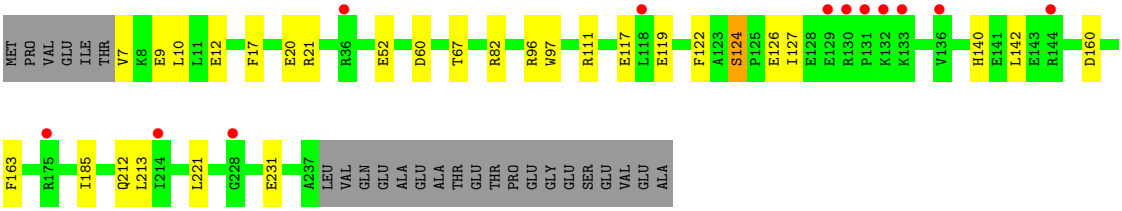
• Molecule 32: 16S Ribosomal RNA

Chain 2a:



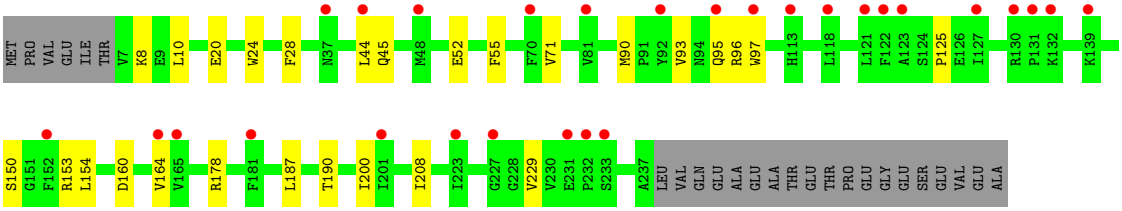
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



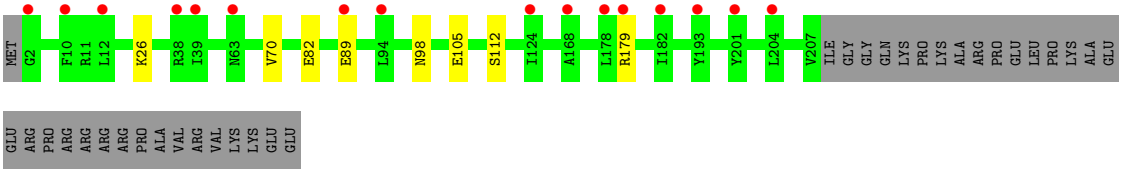
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



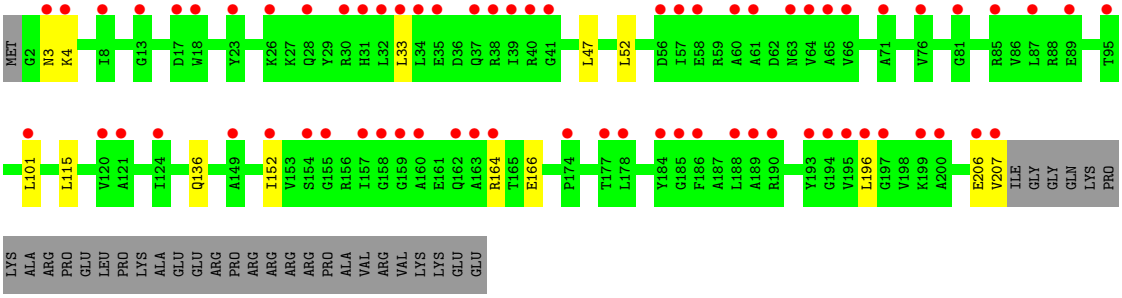
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



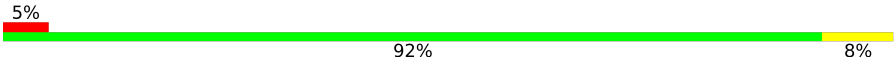
• Molecule 34: 30S ribosomal protein S3

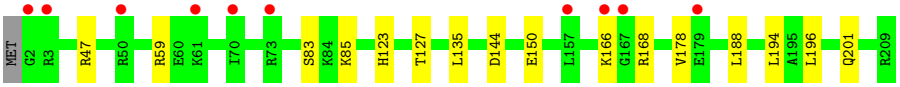
Chain 2c:



• Molecule 35: 30S ribosomal protein S4

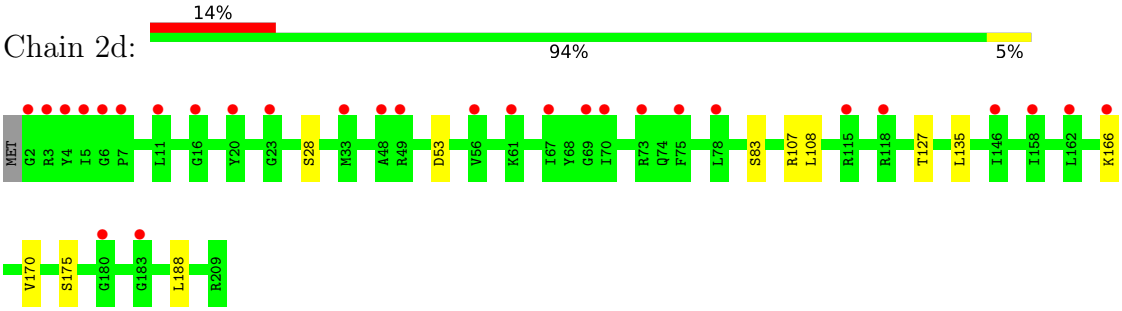
Chain 1d:





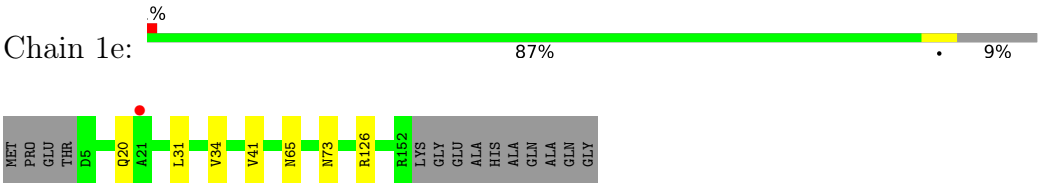
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



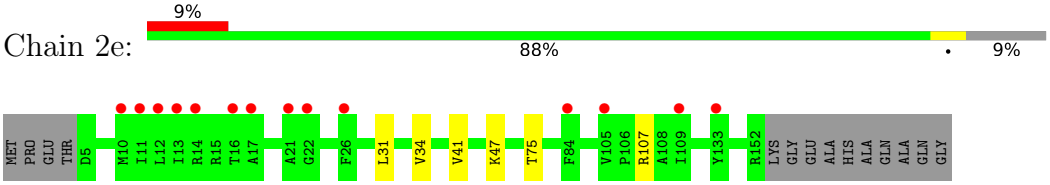
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



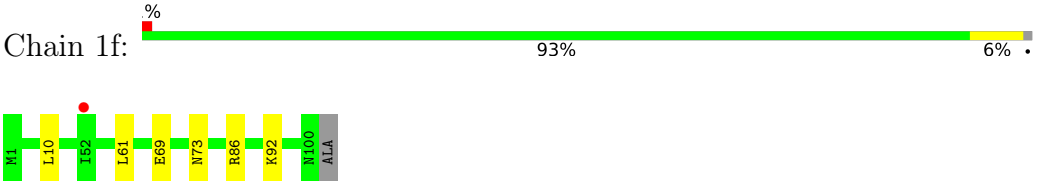
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



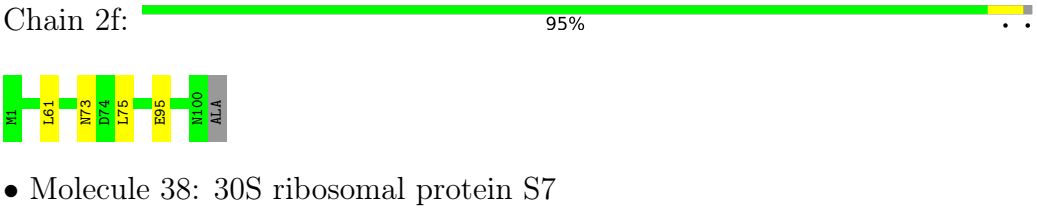
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



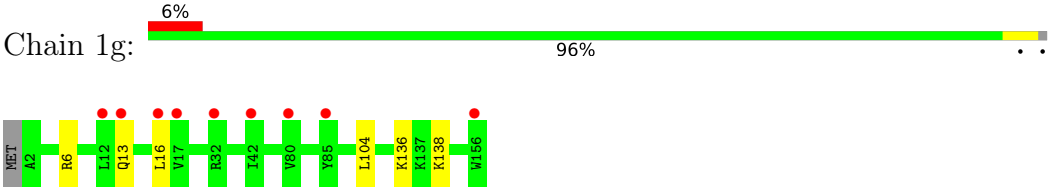
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



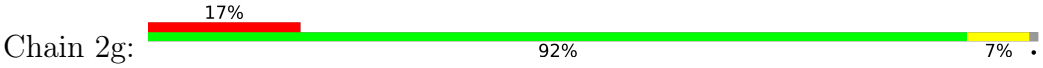
• Molecule 38: 30S ribosomal protein S7

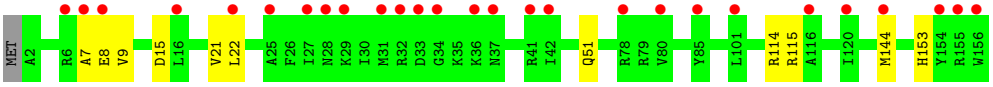
Chain 1g:



• Molecule 38: 30S ribosomal protein S7

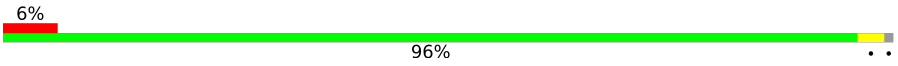
Chain 2g:

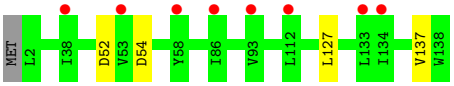




• Molecule 39: 30S ribosomal protein S8

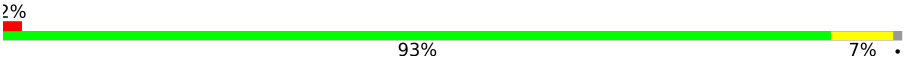
Chain 1h:

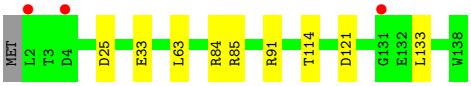




• Molecule 39: 30S ribosomal protein S8

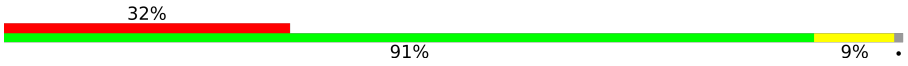
Chain 2h:

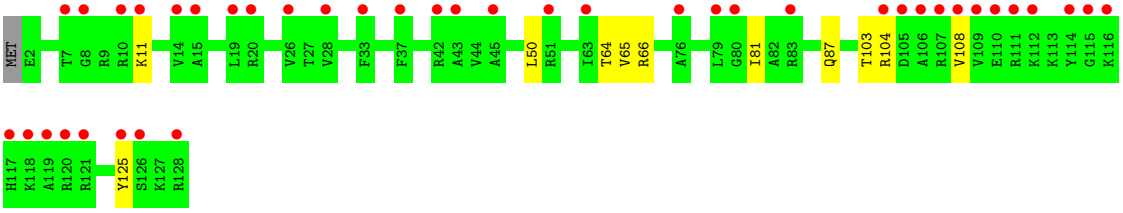




• Molecule 40: 30S ribosomal protein S9

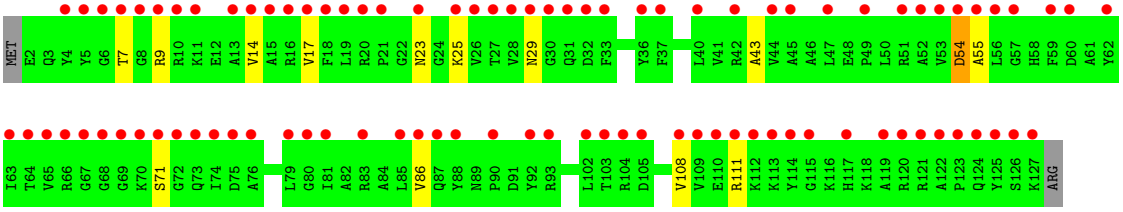
Chain 1i:





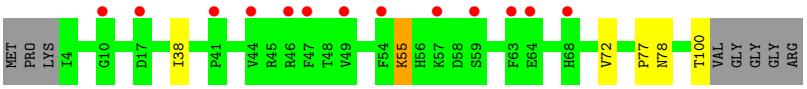
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



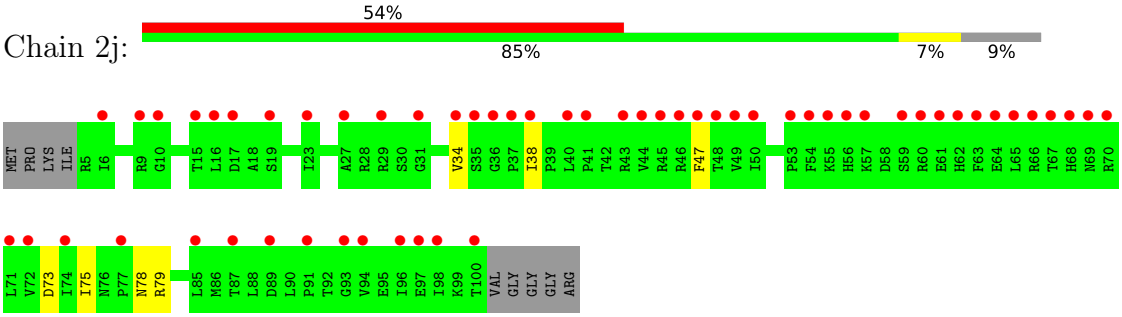
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



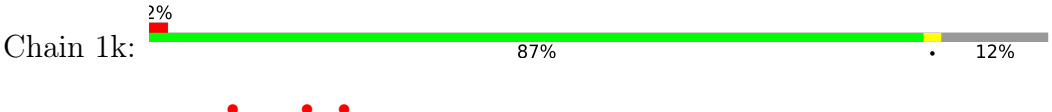
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



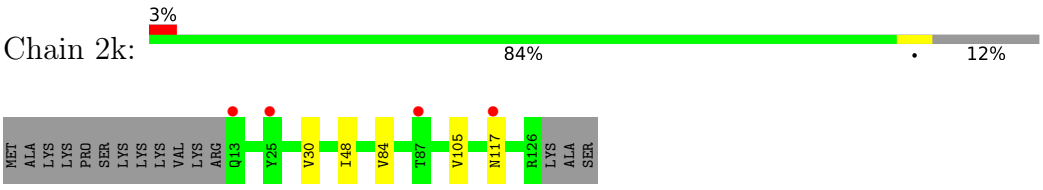
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



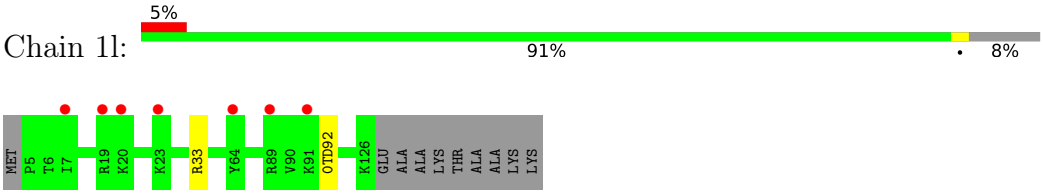
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



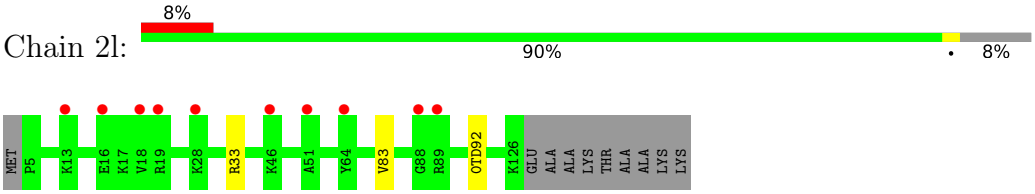
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



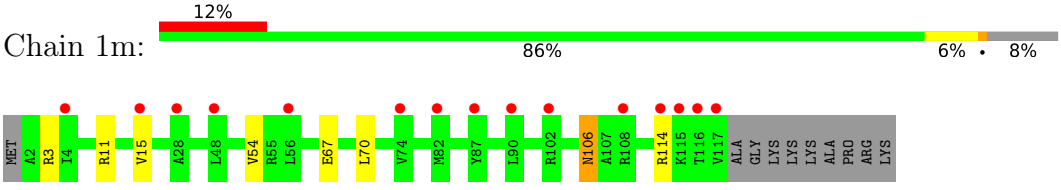
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



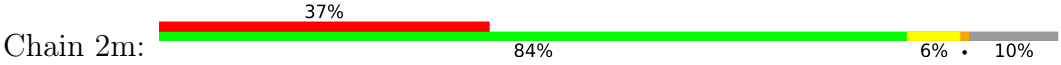
• Molecule 44: 30S ribosomal protein S13

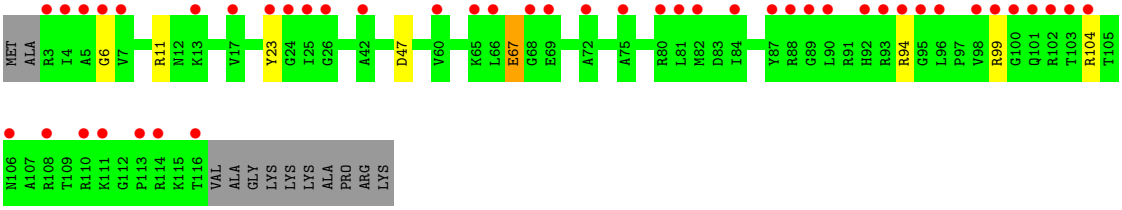
Chain 1m:



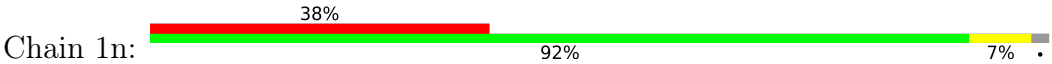
• Molecule 44: 30S ribosomal protein S13

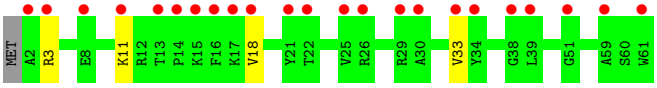
Chain 2m:



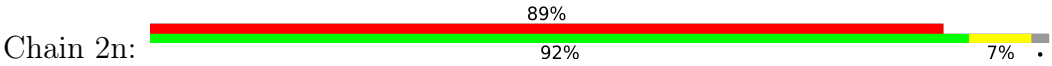


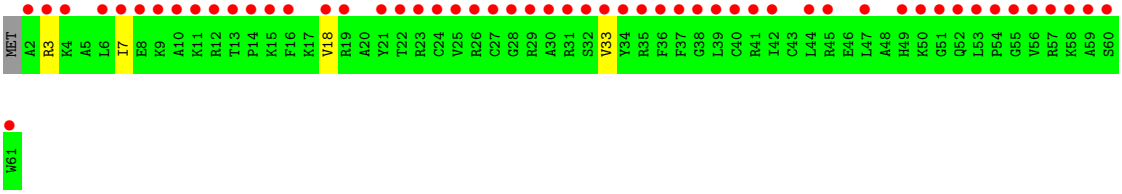
• Molecule 45: 30S ribosomal protein S14 type Z



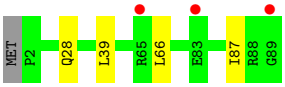


• Molecule 45: 30S ribosomal protein S14 type Z

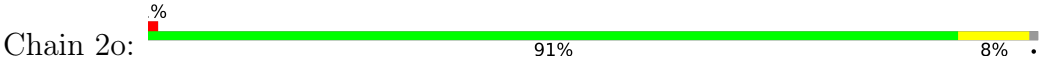




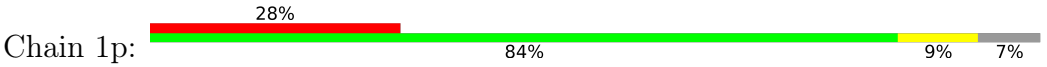
• Molecule 46: 30S ribosomal protein S15

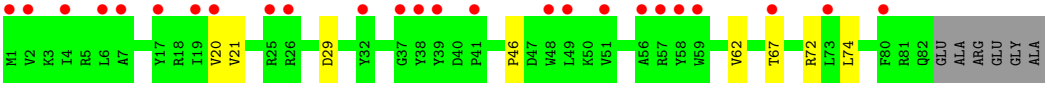


• Molecule 46: 30S ribosomal protein S15



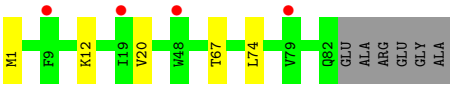
• Molecule 47: 30S ribosomal protein S16





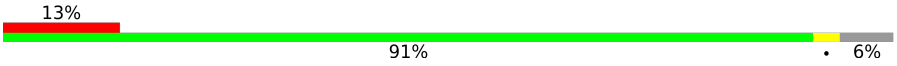
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



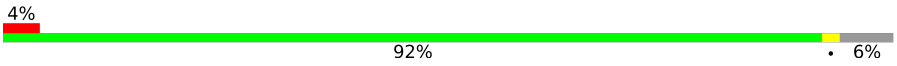
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



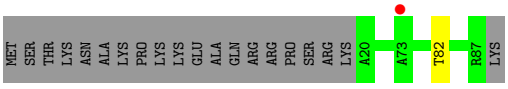
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



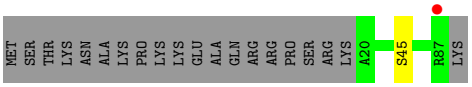
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



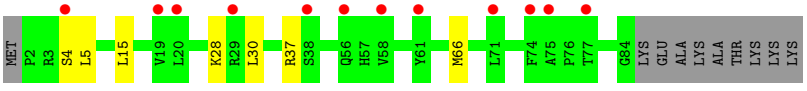
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



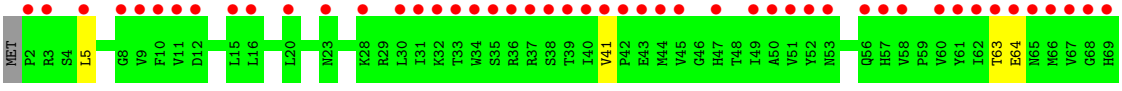
• Molecule 50: 30S ribosomal protein S19

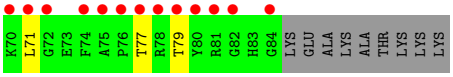
Chain 1s:



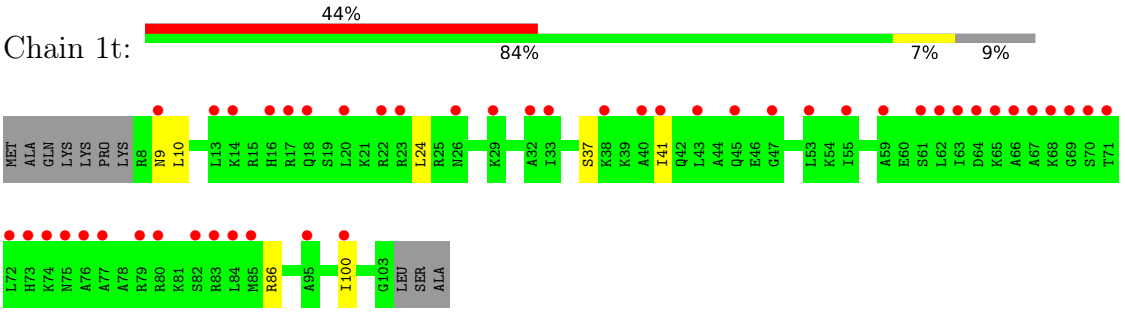
• Molecule 50: 30S ribosomal protein S19

Chain 2s:

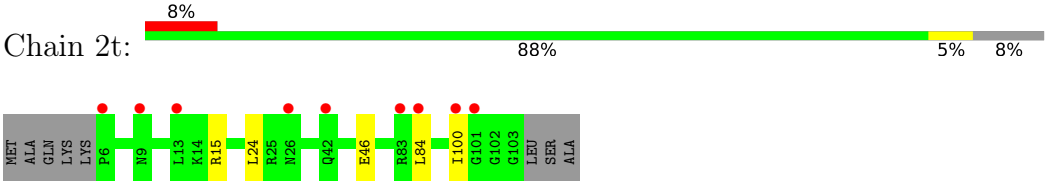




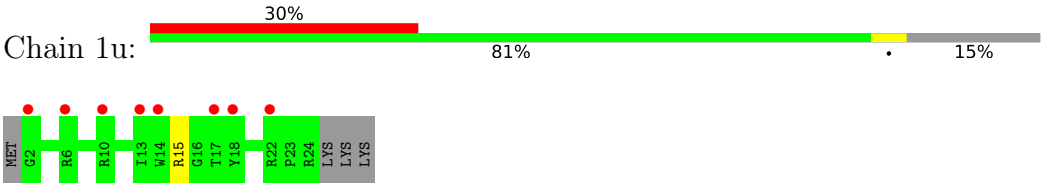
• Molecule 51: 30S ribosomal protein S20



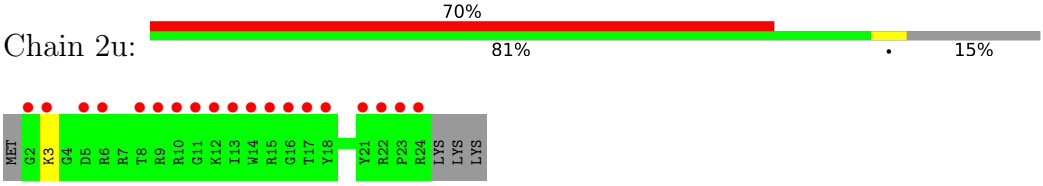
• Molecule 51: 30S ribosomal protein S20



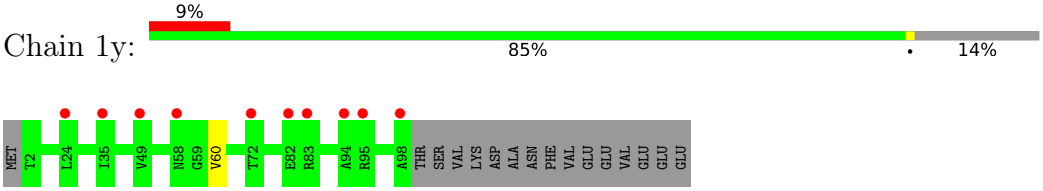
• Molecule 52: 30S ribosomal protein Thx



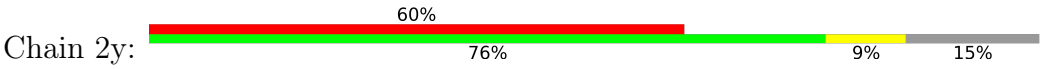
• Molecule 52: 30S ribosomal protein Thx

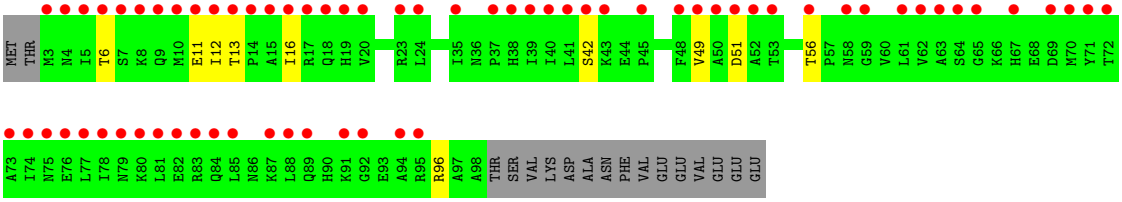


• Molecule 53: Ribosome-associated inhibitor A



• Molecule 53: Ribosome-associated inhibitor A




MET
THR
M3
N4
I5
T6
S7
K8
Q9
M10
E11
I12
T13
P14
A15
I16
R17
Q18
H19
V20
R23
L24
T35
N36
P37
H38
I39
I40
L41
S42
K43
E44
P45
F48
V49
A50
D51
A52
T53
T56
P57
N58
G59
V60
L61
V62
A63
S64
G65
K66
H67
E68
D69
M70
Y71
T72
A73
I74
N75
E76
L77
I78
N79
K80
L81
E82
R83
Q84
L85
N86
K87
L88
Q89
H90
K91
G92
E93
A94
R95
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	209.90Å 449.76Å 620.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.00 – 2.60 190.21 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (122.00-2.60) 99.8 (190.21-2.60)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.203 , 0.241 0.204 , 0.241	Depositor DCC
R_{free} test set	88927 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	53.0	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	297563	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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: M2G, SF4, 2MA, MPD, ZN, CPF, 5MC, 4OC, PSU, UR3, MA6, 2MG, OMU, G7M, 5MU, MG, OMC, 0TD, OMG

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	0.32	0/69031	0.80	20/107754 (0.0%)
1	2A	0.27	2/68903 (0.0%)	0.78	33/107552 (0.0%)
2	1B	0.26	0/2876	0.74	0/4486
2	2B	0.23	0/2878	0.72	0/4490
3	1D	0.28	0/2181	0.51	0/2940
3	2D	0.27	0/2186	0.48	0/2944
4	1E	0.28	0/1592	0.49	0/2149
4	2E	0.27	0/1592	0.48	0/2149
5	1F	0.27	0/1619	0.46	0/2193
5	2F	0.26	0/1615	0.47	0/2188
6	1G	0.26	0/1451	0.44	0/1961
6	2G	0.25	0/1449	0.43	0/1957
7	1H	0.27	0/1356	0.45	0/1834
7	2H	0.25	0/1350	0.45	0/1826
8	1I	0.25	0/1109	0.46	0/1512
8	2I	0.25	0/1091	0.45	0/1490
9	1N	0.27	0/1148	0.46	0/1547
9	2N	0.25	0/1144	0.43	0/1543
10	1O	0.29	0/943	0.52	0/1269
10	2O	0.28	0/943	0.50	0/1269
11	1P	0.28	0/1152	0.49	0/1533
11	2P	0.27	0/1152	0.48	0/1533
12	1Q	0.28	0/1143	0.46	0/1527
12	2Q	0.26	0/1143	0.43	0/1527
13	1R	0.25	0/982	0.46	0/1312
13	2R	0.24	0/982	0.45	0/1312
14	1S	0.26	0/887	0.45	0/1180
14	2S	0.26	0/880	0.46	0/1172
15	1T	0.27	0/1105	0.48	0/1477
15	2T	0.25	0/1097	0.46	0/1468
16	1U	0.27	0/977	0.43	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.25	0/977	0.39	0/1301
17	1V	0.29	0/786	0.49	0/1053
17	2V	0.27	0/782	0.49	0/1049
18	1W	0.29	0/897	0.46	0/1205
18	2W	0.26	0/897	0.44	0/1205
19	1X	0.29	0/764	0.49	0/1025
19	2X	0.26	0/764	0.47	0/1025
20	1Y	0.29	0/823	0.48	0/1099
20	2Y	0.26	0/823	0.47	0/1100
21	1Z	0.26	0/1620	0.44	0/2200
21	2Z	0.25	0/1590	0.45	0/2162
22	10	0.28	0/616	0.47	0/821
22	20	0.27	0/616	0.48	0/821
23	11	0.26	0/761	0.47	0/1013
23	21	0.27	0/766	0.47	0/1018
24	12	0.24	0/590	0.41	0/781
24	22	0.24	0/594	0.38	0/785
25	13	0.27	0/474	0.47	0/635
25	23	0.25	0/469	0.43	0/630
26	14	0.26	0/559	0.49	0/754
26	24	0.29	0/549	0.51	0/741
27	15	0.27	0/473	0.52	0/639
27	25	0.26	0/469	0.46	0/635
28	16	0.26	0/460	0.48	0/613
28	26	0.24	0/456	0.44	0/608
29	17	0.27	0/426	0.46	0/561
29	27	0.26	0/426	0.46	0/561
30	18	0.26	0/525	0.48	0/691
30	28	0.26	0/525	0.45	0/691
31	19	0.27	0/310	0.47	0/407
31	29	0.26	0/310	0.46	0/407
32	1a	0.24	0/35795	0.77	3/55864 (0.0%)
32	2a	0.24	0/35890	0.77	16/56012 (0.0%)
33	1b	0.25	0/1876	0.44	0/2533
33	2b	0.26	0/1860	0.45	0/2518
34	1c	0.25	0/1582	0.43	0/2137
34	2c	0.25	0/1566	0.44	0/2119
35	1d	0.25	0/1695	0.44	0/2274
35	2d	0.25	0/1698	0.42	0/2277
36	1e	0.26	0/1149	0.48	0/1548
36	2e	0.26	0/1149	0.47	0/1548
37	1f	0.26	0/827	0.45	0/1120
37	2f	0.25	0/829	0.46	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.24	0/1254	0.38	0/1683
38	2g	0.25	0/1248	0.39	0/1676
39	1h	0.25	0/1118	0.45	0/1506
39	2h	0.25	0/1108	0.45	0/1494
40	1i	0.26	0/1005	0.44	0/1351
40	2i	0.25	0/985	0.43	0/1329
41	1j	0.24	0/732	0.44	0/993
41	2j	0.25	0/723	0.46	0/984
42	1k	0.26	0/849	0.46	0/1150
42	2k	0.25	0/848	0.46	0/1149
43	1l	0.25	0/937	0.47	0/1260
43	2l	0.25	0/937	0.49	0/1260
44	1m	0.24	0/924	0.44	0/1242
44	2m	0.25	0/905	0.45	0/1217
45	1n	0.26	0/501	0.43	0/664
45	2n	0.25	0/501	0.43	0/664
46	1o	0.24	0/739	0.38	0/985
46	2o	0.24	0/739	0.41	0/985
47	1p	0.25	0/697	0.48	0/939
47	2p	0.23	0/693	0.45	0/935
48	1q	0.25	0/836	0.47	0/1117
48	2q	0.25	0/836	0.45	0/1117
49	1r	0.24	0/560	0.44	0/746
49	2r	0.26	0/560	0.44	0/746
50	1s	0.24	0/663	0.47	0/895
50	2s	0.26	0/660	0.46	0/893
51	1t	0.25	0/734	0.39	0/969
51	2t	0.25	0/736	0.37	0/976
52	1u	0.23	0/203	0.44	0/266
52	2u	0.26	0/203	0.51	0/266
53	1y	0.24	0/776	0.42	0/1048
53	2y	0.24	0/761	0.41	0/1030
All	All	0.27	2/309941 (0.0%)	0.71	72/463239 (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
11	1P	0	1
11	2P	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	1b	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2104	G	N1-C2	-6.63	1.32	1.37
1	2A	2104	G	C6-N1	-5.58	1.35	1.39

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2185	C	N1-C2-O2	15.57	128.25	118.90
1	2A	2104	G	C5-C6-O6	15.02	137.61	128.60
1	2A	2104	G	N3-C2-N2	14.90	130.33	119.90
1	2A	2104	G	N1-C2-N2	-12.83	104.66	116.20
1	2A	2185	C	C2-N3-C4	10.85	125.33	119.90
1	2A	2104	G	C6-N1-C2	9.45	130.77	125.10
32	2a	1158	C	C2-N1-C1'	8.67	128.33	118.80
32	2a	1158	C	N1-C2-O2	8.48	123.99	118.90
1	2A	2104	G	N1-C6-O6	-8.26	114.94	119.90
1	2A	2104	G	C5-C6-N1	-8.12	107.44	111.50
1	1A	512	G	O4'-C1'-N9	8.03	114.62	108.20
1	1A	999	U	O5'-P-OP2	-7.94	98.55	105.70
1	2A	2185	C	N3-C4-N4	-7.42	112.81	118.00
1	2A	2185	C	N3-C2-O2	-7.33	116.77	121.90
1	1A	1086	A	N1-C6-N6	-7.22	114.27	118.60
1	1A	2036	C	O5'-P-OP1	-7.20	99.22	105.70
1	2A	2185	C	C5-C4-N4	7.17	125.22	120.20
32	2a	1158	C	N3-C2-O2	-7.10	116.93	121.90
32	2a	1003	G	N3-C4-C5	-7.05	125.07	128.60
1	1A	801	G	O5'-P-OP2	-7.01	99.39	105.70
1	2A	2185	C	C5-C6-N1	6.93	124.47	121.00
32	2a	1158	C	C6-N1-C2	-6.72	117.61	120.30
1	2A	1092	C	N1-C2-O2	6.52	122.81	118.90
1	2A	2104	G	C2-N3-C4	-6.30	108.75	111.90
1	1A	1074	G	N3-C2-N2	6.27	124.29	119.90
1	2A	2185	C	C4-C5-C6	-6.27	114.27	117.40
32	2a	1004	A	O4'-C1'-N9	6.18	113.15	108.20
1	2A	1614	A	O5'-P-OP1	-6.16	100.15	105.70
1	1A	1352	U	O5'-P-OP1	-6.11	100.20	105.70
1	2A	1092	C	C2-N1-C1'	6.06	125.47	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2185	C	N1-C2-N3	-6.03	114.98	119.20
1	2A	512	G	O4'-C1'-N9	5.97	112.98	108.20
1	2A	2689	U	N3-C2-O2	-5.91	118.06	122.20
32	2a	754	C	C2-N1-C1'	5.84	125.22	118.80
1	1A	1064	C	N1-C2-O2	5.72	122.33	118.90
1	1A	1176	G	OP1-P-O3'	5.68	117.70	105.20
1	1A	330	A	N1-C2-N3	5.66	132.13	129.30
32	2a	1158	C	C6-N1-C1'	-5.65	114.02	120.80
1	2A	1076	C	OP1-P-O3'	5.64	117.61	105.20
32	2a	1003	G	N3-C4-N9	5.62	129.37	126.00
1	2A	2108	C	N1-C2-O2	5.61	122.27	118.90
1	1A	1064	C	C2-N3-C4	5.60	122.70	119.90
1	1A	330	A	C2-N3-C4	-5.52	107.84	110.60
1	1A	1075	C	N1-C2-O2	5.51	122.21	118.90
32	2a	1065	U	P-O3'-C3'	5.51	126.31	119.70
1	1A	1372	U	C5-C4-O4	-5.50	122.60	125.90
1	1A	1177	A	O5'-P-OP1	-5.50	100.75	105.70
1	2A	1092	C	C6-N1-C2	-5.49	118.11	120.30
1	2A	1092	C	C5-C6-N1	5.47	123.73	121.00
1	2A	2186	G	C5-C6-O6	5.43	131.86	128.60
1	1A	847	U	C2-N1-C1'	5.35	124.12	117.70
1	2A	1313	U	C2-N1-C1'	5.32	124.08	117.70
1	1A	2689	U	N3-C2-O2	-5.32	118.48	122.20
32	2a	1003	G	C4-N9-C1'	5.24	133.31	126.50
32	1a	1067	A	P-O3'-C3'	5.23	125.97	119.70
1	1A	1372	U	N3-C4-O4	5.22	123.06	119.40
32	2a	560	U	C2-N1-C1'	5.19	123.92	117.70
1	2A	1076	C	P-O3'-C3'	5.16	125.89	119.70
32	1a	266	G	P-O3'-C3'	5.15	125.88	119.70
1	2A	2103	C	C2-N3-C4	5.13	122.47	119.90
32	2a	687	A	P-O3'-C3'	5.13	125.86	119.70
1	1A	1210	A	P-O3'-C3'	5.13	125.86	119.70
32	2a	65	U	P-O3'-C3'	5.12	125.85	119.70
32	1a	1442	G	N3-C4-C5	-5.12	126.04	128.60
1	2A	2218	U	N1-C2-O2	5.12	126.38	122.80
1	2A	614	U	C2-N1-C1'	5.11	123.83	117.70
32	2a	1158	C	C5-C6-N1	5.10	123.55	121.00
1	2A	752	A	P-O3'-C3'	5.10	125.82	119.70
1	2A	2602	A	OP1-P-O3'	5.09	116.41	105.20
1	1A	784	A	O4'-C1'-N9	5.09	112.27	108.20
32	2a	115	G	P-O3'-C3'	5.07	125.78	119.70
1	2A	2248	C	O5'-P-OP2	-5.02	101.18	105.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
33	1b	231	GLU	Peptide
11	2P	35	HIS	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	261 (96%)	12 (4%)	0	100 100
3	2D	273/276 (99%)	262 (96%)	10 (4%)	1 (0%)	34 57
4	1E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29 52
4	2E	202/206 (98%)	193 (96%)	7 (4%)	2 (1%)	15 32
5	1F	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	29 52
5	2F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	29 52
6	1G	179/182 (98%)	171 (96%)	4 (2%)	4 (2%)	6 12
6	2G	179/182 (98%)	164 (92%)	12 (7%)	3 (2%)	9 18
7	1H	172/180 (96%)	161 (94%)	11 (6%)	0	100 100
7	2H	171/180 (95%)	155 (91%)	16 (9%)	0	100 100
8	1I	145/148 (98%)	132 (91%)	13 (9%)	0	100 100
8	2I	144/148 (97%)	134 (93%)	10 (7%)	0	100 100
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100 100
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	22	43
11	2P	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
12	1Q	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22	43
12	2Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
14	1S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
14	2S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
15	1T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
15	2T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	32
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	15	32
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	14	30
19	2X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	14	30
20	1Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
20	2Y	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
21	1Z	201/206 (98%)	191 (95%)	9 (4%)	1 (0%)	29	52
21	2Z	199/206 (97%)	186 (94%)	13 (6%)	0	100	100
22	10	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
22	20	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
23	11	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	30
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
26	14	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1 1
26	24	67/71 (94%)	51 (76%)	13 (19%)	3 (4%)	2 3
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
29	17	46/49 (94%)	46 (100%)	0	0	100 100
29	27	46/49 (94%)	46 (100%)	0	0	100 100
30	18	62/65 (95%)	62 (100%)	0	0	100 100
30	28	62/65 (95%)	62 (100%)	0	0	100 100
31	19	35/37 (95%)	35 (100%)	0	0	100 100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
33	1b	229/256 (90%)	198 (86%)	26 (11%)	5 (2%)	6 12
33	2b	229/256 (90%)	201 (88%)	22 (10%)	6 (3%)	5 9
34	1c	204/239 (85%)	190 (93%)	14 (7%)	0	100 100
34	2c	204/239 (85%)	175 (86%)	28 (14%)	1 (0%)	29 52
35	1d	206/209 (99%)	198 (96%)	8 (4%)	0	100 100
35	2d	206/209 (99%)	198 (96%)	8 (4%)	0	100 100
36	1e	146/162 (90%)	139 (95%)	7 (5%)	0	100 100
36	2e	146/162 (90%)	142 (97%)	4 (3%)	0	100 100
37	1f	98/101 (97%)	96 (98%)	2 (2%)	0	100 100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100 100
38	1g	153/156 (98%)	148 (97%)	5 (3%)	0	100 100
38	2g	153/156 (98%)	146 (95%)	6 (4%)	1 (1%)	22 43
39	1h	135/138 (98%)	129 (96%)	6 (4%)	0	100 100
39	2h	135/138 (98%)	127 (94%)	8 (6%)	0	100 100
40	1i	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	19 39
40	2i	124/128 (97%)	109 (88%)	12 (10%)	3 (2%)	6 10
41	1j	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	4 6
41	2j	94/105 (90%)	82 (87%)	9 (10%)	3 (3%)	4 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
42	1k	112/129 (87%)	105 (94%)	7 (6%)	0	100 100
42	2k	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	17 35
43	1l	119/132 (90%)	117 (98%)	2 (2%)	0	100 100
43	2l	119/132 (90%)	113 (95%)	6 (5%)	0	100 100
44	1m	114/126 (90%)	104 (91%)	8 (7%)	2 (2%)	8 16
44	2m	112/126 (89%)	97 (87%)	12 (11%)	3 (3%)	5 8
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%)	79 (92%)	6 (7%)	1 (1%)	13 27
46	2o	86/89 (97%)	79 (92%)	5 (6%)	2 (2%)	6 11
47	1p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	12 24
47	2p	80/88 (91%)	74 (92%)	6 (8%)	0	100 100
48	1q	97/105 (92%)	91 (94%)	5 (5%)	1 (1%)	15 32
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100 100
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100 100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100 100
50	1s	81/93 (87%)	74 (91%)	7 (9%)	0	100 100
50	2s	81/93 (87%)	69 (85%)	12 (15%)	0	100 100
51	1t	94/106 (89%)	88 (94%)	6 (6%)	0	100 100
51	2t	96/106 (91%)	91 (95%)	5 (5%)	0	100 100
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
52	2u	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2 2
53	1y	95/113 (84%)	95 (100%)	0	0	100 100
53	2y	94/113 (83%)	92 (98%)	2 (2%)	0	100 100
All	All	11629/12354 (94%)	10978 (94%)	588 (5%)	63 (0%)	29 52

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	1b	21	ARG
33	1b	124	SER
44	1m	67	GLU
44	1m	106	ASN
5	2F	130	ALA

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Mol	Chain	Res	Type
26	24	62	ARG
5	1F	130	ALA
6	1G	50	ALA
19	1X	94	GLY
21	1Z	52	SER
26	14	57	GLU
33	1b	17	PHE
41	1j	55	LYS
4	2E	71	GLY
6	2G	78	SER
17	2V	79	VAL
19	2X	94	GLY
26	24	63	TYR
40	2i	43	ALA
40	2i	54	ASP
41	2j	79	ARG
46	2o	88	ARG
40	1i	11	LYS
41	1j	77	PRO
41	1j	78	ASN
6	2G	81	LYS
23	21	3	LYS
33	2b	95	GLN
34	2c	4	LYS
38	2g	7	ALA
40	2i	55	ALA
44	2m	23	TYR
4	1E	52	LEU
11	1P	29	LYS
26	14	61	ARG
33	1b	20	GLU
48	1q	68	ARG
33	2b	10	LEU
33	2b	20	GLU
33	2b	125	PRO
41	2j	78	ASN
6	1G	51	ARG
12	1Q	59	ARG
26	14	47	GLN
26	14	49	PHE
46	1o	87	ILE
47	1p	46	PRO

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Mol	Chain	Res	Type
6	2G	42	GLY
26	24	55	ARG
33	2b	190	THR
41	2j	75	ILE
46	2o	87	ILE
6	1G	48	GLU
33	1b	127	ILE
4	2E	52	LEU
33	2b	150	SER
44	2m	67	GLU
52	2u	3	LYS
44	2m	6	GLY
6	1G	44	GLY
42	2k	105	VAL
17	1V	79	VAL
3	2D	125	ILE

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%)	201 (94%)	13 (6%)	18	38
3	2D	215/218 (99%)	199 (93%)	16 (7%)	13	28
4	1E	164/166 (99%)	155 (94%)	9 (6%)	21	43
4	2E	164/166 (99%)	151 (92%)	13 (8%)	12	24
5	1F	160/166 (96%)	147 (92%)	13 (8%)	11	23
5	2F	159/166 (96%)	145 (91%)	14 (9%)	10	19
6	1G	144/156 (92%)	135 (94%)	9 (6%)	18	36
6	2G	142/156 (91%)	133 (94%)	9 (6%)	18	36
7	1H	144/148 (97%)	137 (95%)	7 (5%)	25	48
7	2H	143/148 (97%)	133 (93%)	10 (7%)	15	30
8	1I	111/124 (90%)	105 (95%)	6 (5%)	22	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	2I	108/124 (87%)	101 (94%)	7 (6%)	17 34
9	1N	119/119 (100%)	109 (92%)	10 (8%)	11 21
9	2N	118/119 (99%)	111 (94%)	7 (6%)	19 39
10	1O	100/100 (100%)	100 (100%)	0	100 100
10	2O	100/100 (100%)	100 (100%)	0	100 100
11	1P	115/116 (99%)	111 (96%)	4 (4%)	36 62
11	2P	115/116 (99%)	109 (95%)	6 (5%)	23 46
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	18 36
12	2Q	111/111 (100%)	105 (95%)	6 (5%)	22 44
13	1R	101/101 (100%)	94 (93%)	7 (7%)	15 31
13	2R	101/101 (100%)	93 (92%)	8 (8%)	12 24
14	1S	87/88 (99%)	78 (90%)	9 (10%)	7 13
14	2S	85/88 (97%)	78 (92%)	7 (8%)	11 22
15	1T	115/127 (91%)	108 (94%)	7 (6%)	18 38
15	2T	113/127 (89%)	111 (98%)	2 (2%)	59 80
16	1U	93/94 (99%)	88 (95%)	5 (5%)	22 44
16	2U	93/94 (99%)	90 (97%)	3 (3%)	39 65
17	1V	81/82 (99%)	78 (96%)	3 (4%)	34 60
17	2V	80/82 (98%)	71 (89%)	9 (11%)	6 10
18	1W	90/92 (98%)	86 (96%)	4 (4%)	28 53
18	2W	90/92 (98%)	86 (96%)	4 (4%)	28 53
19	1X	77/78 (99%)	73 (95%)	4 (5%)	23 46
19	2X	77/78 (99%)	75 (97%)	2 (3%)	46 72
20	1Y	86/91 (94%)	79 (92%)	7 (8%)	11 23
20	2Y	86/91 (94%)	81 (94%)	5 (6%)	20 40
21	1Z	169/179 (94%)	156 (92%)	13 (8%)	13 25
21	2Z	165/179 (92%)	154 (93%)	11 (7%)	16 33
22	10	61/67 (91%)	60 (98%)	1 (2%)	62 82
22	20	61/67 (91%)	61 (100%)	0	100 100
23	11	79/83 (95%)	75 (95%)	4 (5%)	24 46
23	21	81/83 (98%)	78 (96%)	3 (4%)	34 60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	12	65/67 (97%)	63 (97%)	2 (3%)	40 66
24	22	66/67 (98%)	60 (91%)	6 (9%)	9 18
25	13	51/52 (98%)	48 (94%)	3 (6%)	19 39
25	23	50/52 (96%)	47 (94%)	3 (6%)	19 39
26	14	58/63 (92%)	54 (93%)	4 (7%)	15 31
26	24	54/63 (86%)	48 (89%)	6 (11%)	6 11
27	15	51/52 (98%)	49 (96%)	2 (4%)	32 58
27	25	50/52 (96%)	49 (98%)	1 (2%)	55 78
28	16	51/52 (98%)	50 (98%)	1 (2%)	55 78
28	26	50/52 (96%)	48 (96%)	2 (4%)	31 57
29	17	41/42 (98%)	40 (98%)	1 (2%)	49 74
29	27	41/42 (98%)	35 (85%)	6 (15%)	3 5
30	18	54/55 (98%)	50 (93%)	4 (7%)	13 28
30	28	54/55 (98%)	49 (91%)	5 (9%)	9 17
31	19	34/34 (100%)	32 (94%)	2 (6%)	19 39
31	29	34/34 (100%)	33 (97%)	1 (3%)	42 68
33	1b	191/220 (87%)	167 (87%)	24 (13%)	4 8
33	2b	187/220 (85%)	166 (89%)	21 (11%)	6 10
34	1c	144/188 (77%)	136 (94%)	8 (6%)	21 42
34	2c	140/188 (74%)	127 (91%)	13 (9%)	9 17
35	1d	171/181 (94%)	155 (91%)	16 (9%)	8 17
35	2d	172/181 (95%)	161 (94%)	11 (6%)	17 35
36	1e	114/123 (93%)	107 (94%)	7 (6%)	18 38
36	2e	114/123 (93%)	108 (95%)	6 (5%)	22 45
37	1f	85/90 (94%)	79 (93%)	6 (7%)	14 29
37	2f	85/90 (94%)	81 (95%)	4 (5%)	26 50
38	1g	120/127 (94%)	114 (95%)	6 (5%)	24 47
38	2g	119/127 (94%)	109 (92%)	10 (8%)	11 21
39	1h	116/119 (98%)	112 (97%)	4 (3%)	37 63
39	2h	114/119 (96%)	105 (92%)	9 (8%)	12 24
40	1i	91/99 (92%)	81 (89%)	10 (11%)	6 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	2i	88/99 (89%)	76 (86%)	12 (14%)	3 6
41	1j	68/92 (74%)	64 (94%)	4 (6%)	19 39
41	2j	68/92 (74%)	64 (94%)	4 (6%)	19 39
42	1k	83/99 (84%)	81 (98%)	2 (2%)	49 74
42	2k	83/99 (84%)	79 (95%)	4 (5%)	25 49
43	1l	96/108 (89%)	95 (99%)	1 (1%)	76 90
43	2l	96/108 (89%)	94 (98%)	2 (2%)	53 77
44	1m	90/101 (89%)	83 (92%)	7 (8%)	12 25
44	2m	87/101 (86%)	81 (93%)	6 (7%)	15 31
45	1n	49/50 (98%)	45 (92%)	4 (8%)	11 22
45	2n	49/50 (98%)	45 (92%)	4 (8%)	11 22
46	1o	78/80 (98%)	75 (96%)	3 (4%)	33 59
46	2o	78/80 (98%)	73 (94%)	5 (6%)	17 35
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7 14
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13 28
48	1q	94/97 (97%)	92 (98%)	2 (2%)	53 77
48	2q	94/97 (97%)	92 (98%)	2 (2%)	53 77
49	1r	59/77 (77%)	58 (98%)	1 (2%)	60 81
49	2r	59/77 (77%)	58 (98%)	1 (2%)	60 81
50	1s	68/80 (85%)	61 (90%)	7 (10%)	7 13
50	2s	67/80 (84%)	60 (90%)	7 (10%)	7 13
51	1t	71/82 (87%)	64 (90%)	7 (10%)	8 15
51	2t	70/82 (85%)	65 (93%)	5 (7%)	14 29
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21 42
52	2u	18/22 (82%)	18 (100%)	0	100 100
53	1y	82/98 (84%)	81 (99%)	1 (1%)	71 87
53	2y	79/98 (81%)	69 (87%)	10 (13%)	4 8
All	All	9524/10260 (93%)	8922 (94%)	602 (6%)	18 36

All (602) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	7	LYS

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Mol	Chain	Res	Type
3	1D	35	LYS
3	1D	71	ASP
3	1D	99	ASP
3	1D	111	LEU
3	1D	113	VAL
3	1D	116	GLN
3	1D	142	VAL
3	1D	217	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	260	ARG
3	1D	275	LYS
4	1E	9	VAL
4	1E	52	LEU
4	1E	75	VAL
4	1E	93	VAL
4	1E	116	VAL
4	1E	119	ARG
4	1E	163	GLU
4	1E	181	LEU
4	1E	184	VAL
5	1F	12	LEU
5	1F	18	ARG
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	110	LEU
5	1F	125	LEU
5	1F	132	VAL
5	1F	140	LEU
5	1F	158	THR
5	1F	162	LEU
5	1F	192	LEU
5	1F	197	ASP
6	1G	7	LEU
6	1G	28	VAL
6	1G	45	GLU
6	1G	47	LYS
6	1G	52	ILE
6	1G	53	LEU
6	1G	82	LEU
6	1G	159	VAL

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Mol	Chain	Res	Type
6	1G	181	ARG
7	1H	18	GLU
7	1H	71	LEU
7	1H	107	VAL
7	1H	119	GLU
7	1H	122	THR
7	1H	127	GLU
7	1H	149	ARG
8	1I	38	LEU
8	1I	44	LEU
8	1I	78	THR
8	1I	92	VAL
8	1I	109	ILE
8	1I	140	LEU
9	1N	5	VAL
9	1N	12	ARG
9	1N	14	VAL
9	1N	33	LEU
9	1N	48	MET
9	1N	61	ARG
9	1N	62	VAL
9	1N	67	LEU
9	1N	121	LYS
9	1N	133	GLN
11	1P	59	LEU
11	1P	95	VAL
11	1P	99	LEU
11	1P	119	GLU
12	1Q	7	MET
12	1Q	16	ARG
12	1Q	21	THR
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	112	GLU
12	1Q	133	ARG
13	1R	6	SER
13	1R	29	LEU
13	1R	33	ARG
13	1R	44	LEU
13	1R	75	LEU
13	1R	100	LEU
13	1R	114	VAL

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Mol	Chain	Res	Type
14	1S	3	ARG
14	1S	14	VAL
14	1S	25	ARG
14	1S	48	LEU
14	1S	50	SER
14	1S	59	LYS
14	1S	73	LEU
14	1S	85	VAL
14	1S	110	LEU
15	1T	39	ARG
15	1T	49	VAL
15	1T	53	ARG
15	1T	59	THR
15	1T	89	VAL
15	1T	96	ARG
15	1T	118	ARG
16	1U	5	LYS
16	1U	52	ARG
16	1U	59	ARG
16	1U	77	SER
16	1U	104	GLN
17	1V	44	LYS
17	1V	51	VAL
17	1V	79	VAL
18	1W	11	ARG
18	1W	23	LEU
18	1W	100	THR
18	1W	107	LEU
19	1X	35	THR
19	1X	38	GLU
19	1X	57	LEU
19	1X	66	LEU
20	1Y	7	VAL
20	1Y	23	ARG
20	1Y	43	ASN
20	1Y	64	GLU
20	1Y	72	VAL
20	1Y	92	ASN
20	1Y	99	CYS
21	1Z	61	LEU
21	1Z	86	VAL
21	1Z	91	LEU

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Mol	Chain	Res	Type
21	1Z	93	ASP
21	1Z	94	GLU
21	1Z	107	THR
21	1Z	150	LEU
21	1Z	155	LEU
21	1Z	161	VAL
21	1Z	162	GLU
21	1Z	170	THR
21	1Z	191	VAL
21	1Z	203	GLU
22	10	74	ARG
23	11	30	VAL
23	11	46	LEU
23	11	95	LEU
23	11	98	LEU
24	12	9	GLN
24	12	53	LEU
25	13	8	LEU
25	13	23	LEU
25	13	54	VAL
26	14	49	PHE
26	14	50	VAL
26	14	60	GLN
26	14	61	ARG
27	15	6	VAL
27	15	58	LEU
28	16	52	VAL
29	17	43	THR
30	18	30	ARG
30	18	31	HIS
30	18	34	TRP
30	18	46	ARG
31	19	17	ILE
31	19	33	LYS
33	1b	7	VAL
33	1b	9	GLU
33	1b	10	LEU
33	1b	12	GLU
33	1b	52	GLU
33	1b	60	ASP
33	1b	67	THR
33	1b	82	ARG

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Mol	Chain	Res	Type
33	1b	96	ARG
33	1b	97	TRP
33	1b	111	ARG
33	1b	117	GLU
33	1b	119	GLU
33	1b	122	PHE
33	1b	124	SER
33	1b	126	GLU
33	1b	140	HIS
33	1b	142	LEU
33	1b	160	ASP
33	1b	163	PHE
33	1b	185	ILE
33	1b	212	GLN
33	1b	213	LEU
33	1b	221	LEU
34	1c	26	LYS
34	1c	70	VAL
34	1c	82	GLU
34	1c	89	GLU
34	1c	98	ASN
34	1c	105	GLU
34	1c	112	SER
34	1c	179	ARG
35	1d	47	ARG
35	1d	59	ARG
35	1d	83	SER
35	1d	85	LYS
35	1d	123	HIS
35	1d	127	THR
35	1d	135	LEU
35	1d	144	ASP
35	1d	150	GLU
35	1d	166	LYS
35	1d	168	ARG
35	1d	178	VAL
35	1d	188	LEU
35	1d	194	LEU
35	1d	196	LEU
35	1d	201	GLN
36	1e	20	GLN
36	1e	31	LEU

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Mol	Chain	Res	Type
36	1e	34	VAL
36	1e	41	VAL
36	1e	65	ASN
36	1e	73	ASN
36	1e	126	ARG
37	1f	10	LEU
37	1f	61	LEU
37	1f	69	GLU
37	1f	73	ASN
37	1f	86	ARG
37	1f	92	LYS
38	1g	6	ARG
38	1g	13	GLN
38	1g	16	LEU
38	1g	104	LEU
38	1g	136	LYS
38	1g	138	LYS
39	1h	52	ASP
39	1h	54	ASP
39	1h	127	LEU
39	1h	137	VAL
40	1i	50	LEU
40	1i	64	THR
40	1i	65	VAL
40	1i	66	ARG
40	1i	81	ILE
40	1i	87	GLN
40	1i	103	THR
40	1i	104	ARG
40	1i	108	VAL
40	1i	125	TYR
41	1j	38	ILE
41	1j	55	LYS
41	1j	72	VAL
41	1j	100	THR
42	1k	16	SER
42	1k	96	ARG
43	1l	33	ARG
44	1m	3	ARG
44	1m	11	ARG
44	1m	15	VAL
44	1m	54	VAL

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Mol	Chain	Res	Type
44	1m	70	LEU
44	1m	106	ASN
44	1m	114	ARG
45	1n	3	ARG
45	1n	11	LYS
45	1n	18	VAL
45	1n	33	VAL
46	1o	28	GLN
46	1o	39	LEU
46	1o	66	LEU
47	1p	20	VAL
47	1p	21	VAL
47	1p	29	ASP
47	1p	62	VAL
47	1p	67	THR
47	1p	72	ARG
47	1p	74	LEU
48	1q	45	HIS
48	1q	86	GLU
49	1r	82	THR
50	1s	4	SER
50	1s	5	LEU
50	1s	15	LEU
50	1s	28	LYS
50	1s	30	LEU
50	1s	37	ARG
50	1s	66	MET
51	1t	9	ASN
51	1t	10	LEU
51	1t	24	LEU
51	1t	37	SER
51	1t	41	ILE
51	1t	86	ARG
51	1t	100	ILE
52	1u	15	ARG
53	1y	60	VAL
3	2D	3	VAL
3	2D	61	LEU
3	2D	99	ASP
3	2D	103	ARG
3	2D	113	VAL
3	2D	116	GLN

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Mol	Chain	Res	Type
3	2D	138	VAL
3	2D	155	LEU
3	2D	173	VAL
3	2D	193	VAL
3	2D	211	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	274	ARG
4	2E	7	VAL
4	2E	9	VAL
4	2E	51	PHE
4	2E	52	LEU
4	2E	75	VAL
4	2E	113	PHE
4	2E	116	VAL
4	2E	119	ARG
4	2E	163	GLU
4	2E	170	LEU
4	2E	178	GLU
4	2E	181	LEU
4	2E	184	VAL
5	2F	20	LEU
5	2F	23	ASP
5	2F	27	GLU
5	2F	33	LEU
5	2F	57	VAL
5	2F	74	ARG
5	2F	107	LYS
5	2F	140	LEU
5	2F	168	ARG
5	2F	170	LEU
5	2F	183	VAL
5	2F	197	ASP
5	2F	201	VAL
5	2F	203	GLN
6	2G	3	LEU
6	2G	5	VAL
6	2G	43	LEU
6	2G	53	LEU
6	2G	60	LEU

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Mol	Chain	Res	Type
6	2G	116	ASP
6	2G	126	ASP
6	2G	133	LEU
6	2G	159	VAL
7	2H	33	LEU
7	2H	43	VAL
7	2H	44	VAL
7	2H	50	VAL
7	2H	63	SER
7	2H	70	THR
7	2H	88	LEU
7	2H	105	LEU
7	2H	136	ILE
7	2H	137	ASP
8	2I	38	LEU
8	2I	64	GLU
8	2I	68	LEU
8	2I	75	LEU
8	2I	76	THR
8	2I	121	LYS
8	2I	123	LEU
9	2N	9	VAL
9	2N	28	THR
9	2N	33	LEU
9	2N	46	VAL
9	2N	67	LEU
9	2N	99	LEU
9	2N	115	ARG
11	2P	29	LYS
11	2P	59	LEU
11	2P	95	VAL
11	2P	96	THR
11	2P	123	LEU
11	2P	133	SER
12	2Q	7	MET
12	2Q	16	ARG
12	2Q	55	VAL
12	2Q	98	LYS
12	2Q	109	VAL
12	2Q	112	GLU
13	2R	29	LEU
13	2R	33	ARG

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Mol	Chain	Res	Type
13	2R	44	LEU
13	2R	75	LEU
13	2R	86	ARG
13	2R	96	ARG
13	2R	100	LEU
13	2R	114	VAL
14	2S	12	PHE
14	2S	28	VAL
14	2S	44	LYS
14	2S	48	LEU
14	2S	52	SER
14	2S	53	SER
14	2S	85	VAL
15	2T	28	VAL
15	2T	107	ASP
16	2U	31	SER
16	2U	104	GLN
16	2U	111	GLU
17	2V	13	ARG
17	2V	32	THR
17	2V	35	LEU
17	2V	46	VAL
17	2V	51	VAL
17	2V	62	LEU
17	2V	71	LEU
17	2V	72	VAL
17	2V	79	VAL
18	2W	11	ARG
18	2W	17	VAL
18	2W	23	LEU
18	2W	107	LEU
19	2X	90	GLU
19	2X	92	LEU
20	2Y	6	HIS
20	2Y	42	VAL
20	2Y	64	GLU
20	2Y	72	VAL
20	2Y	99	CYS
21	2Z	28	MET
21	2Z	31	ARG
21	2Z	33	LEU
21	2Z	42	VAL

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Mol	Chain	Res	Type
21	2Z	86	VAL
21	2Z	94	GLU
21	2Z	107	THR
21	2Z	121	HIS
21	2Z	150	LEU
21	2Z	182	LYS
21	2Z	193	GLU
23	21	21	ARG
23	21	40	ARG
23	21	85	LEU
24	22	17	SER
24	22	23	LYS
24	22	32	LEU
24	22	52	ASP
24	22	53	LEU
24	22	64	LEU
25	23	23	LEU
25	23	31	LEU
25	23	57	GLU
26	24	10	VAL
26	24	14	ILE
26	24	39	CYS
26	24	40	HIS
26	24	49	PHE
26	24	50	VAL
27	25	6	VAL
28	26	14	THR
28	26	48	VAL
29	27	1	MET
29	27	10	ARG
29	27	24	THR
29	27	43	THR
29	27	46	VAL
29	27	48	LYS
30	28	3	LYS
30	28	14	VAL
30	28	30	ARG
30	28	31	HIS
30	28	34	TRP
31	29	12	ASP
33	2b	8	LYS
33	2b	24	TRP

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Mol	Chain	Res	Type
33	2b	28	PHE
33	2b	44	LEU
33	2b	45	GLN
33	2b	52	GLU
33	2b	55	PHE
33	2b	71	VAL
33	2b	90	MET
33	2b	93	VAL
33	2b	96	ARG
33	2b	97	TRP
33	2b	153	ARG
33	2b	154	LEU
33	2b	160	ASP
33	2b	164	VAL
33	2b	178	ARG
33	2b	187	LEU
33	2b	200	ILE
33	2b	208	ILE
33	2b	229	VAL
34	2c	3	ASN
34	2c	33	LEU
34	2c	47	LEU
34	2c	52	LEU
34	2c	101	LEU
34	2c	115	LEU
34	2c	136	GLN
34	2c	152	ILE
34	2c	164	ARG
34	2c	166	GLU
34	2c	196	LEU
34	2c	206	GLU
34	2c	207	VAL
35	2d	28	SER
35	2d	53	ASP
35	2d	83	SER
35	2d	107	ARG
35	2d	108	LEU
35	2d	127	THR
35	2d	135	LEU
35	2d	166	LYS
35	2d	170	VAL
35	2d	175	SER

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Mol	Chain	Res	Type
35	2d	188	LEU
36	2e	31	LEU
36	2e	34	VAL
36	2e	41	VAL
36	2e	47	LYS
36	2e	75	THR
36	2e	107	ARG
37	2f	61	LEU
37	2f	73	ASN
37	2f	75	LEU
37	2f	95	GLU
38	2g	8	GLU
38	2g	9	VAL
38	2g	15	ASP
38	2g	21	VAL
38	2g	22	LEU
38	2g	51	GLN
38	2g	114	ARG
38	2g	115	ARG
38	2g	144	MET
38	2g	153	HIS
39	2h	25	ASP
39	2h	33	GLU
39	2h	63	LEU
39	2h	84	ARG
39	2h	85	ARG
39	2h	91	ARG
39	2h	114	THR
39	2h	121	ASP
39	2h	133	LEU
40	2i	7	THR
40	2i	9	ARG
40	2i	14	VAL
40	2i	17	VAL
40	2i	23	ASN
40	2i	25	LYS
40	2i	29	ASN
40	2i	54	ASP
40	2i	71	SER
40	2i	86	VAL
40	2i	108	VAL
40	2i	111	ARG

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Mol	Chain	Res	Type
41	2j	34	VAL
41	2j	38	ILE
41	2j	47	PHE
41	2j	73	ASP
42	2k	30	VAL
42	2k	48	ILE
42	2k	84	VAL
42	2k	117	ASN
43	2l	33	ARG
43	2l	83	VAL
44	2m	11	ARG
44	2m	47	ASP
44	2m	67	GLU
44	2m	94	ARG
44	2m	99	ARG
44	2m	104	ARG
45	2n	3	ARG
45	2n	7	ILE
45	2n	18	VAL
45	2n	33	VAL
46	2o	3	ILE
46	2o	5	LYS
46	2o	39	LEU
46	2o	64	ARG
46	2o	84	LYS
47	2p	1	MET
47	2p	12	LYS
47	2p	20	VAL
47	2p	67	THR
47	2p	74	LEU
48	2q	53	LEU
48	2q	86	GLU
49	2r	45	SER
50	2s	5	LEU
50	2s	41	VAL
50	2s	63	THR
50	2s	64	GLU
50	2s	71	LEU
50	2s	77	THR
50	2s	79	THR
51	2t	15	ARG
51	2t	24	LEU

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Mol	Chain	Res	Type
51	2t	46	GLU
51	2t	84	LEU
51	2t	100	ILE
53	2y	6	THR
53	2y	11	GLU
53	2y	12	ILE
53	2y	13	THR
53	2y	16	ILE
53	2y	42	SER
53	2y	49	VAL
53	2y	51	ASP
53	2y	56	THR
53	2y	96	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	253	GLN
4	1E	48	GLN
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
8	1I	104	GLN
9	1N	133	GLN
10	1O	3	GLN
12	1Q	89	ASN
13	1R	24	GLN
14	1S	68	GLN
15	1T	58	ASN
15	1T	123	GLN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
20	1Y	43	ASN
20	1Y	92	ASN
21	1Z	73	GLN
21	1Z	151	HIS
23	11	56	GLN
25	13	32	GLN
34	1c	6	HIS

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Mol	Chain	Res	Type
34	1c	37	GLN
34	1c	102	ASN
34	1c	104	GLN
34	1c	162	GLN
35	1d	123	HIS
35	1d	129	ASN
36	1e	20	GLN
36	1e	73	ASN
37	1f	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	86	GLN
38	1g	110	GLN
38	1g	148	ASN
38	1g	153	HIS
40	1i	3	GLN
40	1i	34	ASN
40	1i	73	GLN
40	1i	87	GLN
41	1j	56	HIS
41	1j	84	GLN
42	1k	93	GLN
43	1l	99	HIS
46	1o	13	GLN
46	1o	28	GLN
47	1p	16	HIS
48	1q	45	HIS
50	1s	83	HIS
51	1t	18	GLN
53	1y	38	HIS
3	2D	126	GLN
3	2D	253	GLN
4	2E	48	GLN
5	2F	69	HIS
6	2G	41	GLN
6	2G	132	ASN
8	2I	43	ASN
9	2N	133	GLN
12	2Q	13	GLN
13	2R	24	GLN
15	2T	58	ASN

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Mol	Chain	Res	Type
17	2V	64	HIS
18	2W	60	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	65	GLN
21	2Z	151	HIS
25	23	32	GLN
26	24	20	ASN
26	24	40	HIS
26	24	46	GLN
30	28	35	GLN
33	2b	19	HIS
33	2b	146	GLN
33	2b	224	GLN
34	2c	6	HIS
34	2c	136	GLN
34	2c	139	GLN
34	2c	176	HIS
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	201	GLN
36	2e	38	GLN
36	2e	73	ASN
37	2f	73	ASN
38	2g	13	GLN
38	2g	28	ASN
38	2g	51	GLN
38	2g	86	GLN
38	2g	97	GLN
39	2h	15	ASN
40	2i	29	ASN
41	2j	69	ASN
43	2l	8	ASN
43	2l	99	HIS
46	2o	28	GLN
47	2p	16	HIS
48	2q	16	GLN
48	2q	93	GLN
50	2s	14	HIS

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Mol	Chain	Res	Type
50	2s	83	HIS
53	2y	9	GLN
53	2y	46	GLN
53	2y	58	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	395 (13%)	27 (0%)
1	2A	2857/2915 (98%)	460 (16%)	32 (1%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	119/121 (98%)	15 (12%)	0
32	1a	1494/1521 (98%)	241 (16%)	0
32	2a	1498/1521 (98%)	253 (16%)	0
All	All	8951/9114 (98%)	1373 (15%)	59 (0%)

All (1373) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	94	C
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	181	A
1	1A	182	A
1	1A	196	A
1	1A	199	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

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Mol	Chain	Res	Type
1	1A	248	G
1	1A	265	A
1	1A	271(I)	G
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(O)	C
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(H)	C
1	1A	275	G
1	1A	279	C
1	1A	280	C
1	1A	283	A
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	456	C
1	1A	457	A
1	1A	481	G
1	1A	505	A
1	1A	509	C
1	1A	528	A
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	575	A
1	1A	586	A
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	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	668	G
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	748	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	827	U
1	1A	859	G
1	1A	866	A
1	1A	882	G
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	892	G
1	1A	894	C
1	1A	896	A
1	1A	897	C
1	1A	910	A
1	1A	931	G
1	1A	932	G
1	1A	938	G

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Mol	Chain	Res	Type
1	1A	945	A
1	1A	946	G
1	1A	953	A
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	996	A
1	1A	1005	C
1	1A	1012	U
1	1A	1013	C
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1039	G
1	1A	1041	C
1	1A	1042	G
1	1A	1043	C
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1060	U
1	1A	1061	U
1	1A	1062	G
1	1A	1065	U
1	1A	1066	U
1	1A	1068	G
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	1087	G
1	1A	1088	A
1	1A	1090	U
1	1A	1096	A

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Mol	Chain	Res	Type
1	1A	1097	U
1	1A	1109	C
1	1A	1110	G
1	1A	1112	G
1	1A	1128	A
1	1A	1129	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1139	G
1	1A	1170	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	1220	A
1	1A	1253	A
1	1A	1256	G
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	1320	C
1	1A	1321	A
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1395	A
1	1A	1416	G
1	1A	1417	C

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Mol	Chain	Res	Type
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	1459	G
1	1A	1465	G
1	1A	1467	C
1	1A	1471	A
1	1A	1482	G
1	1A	1493	C
1	1A	1506	C
1	1A	1508	A
1	1A	1509(A)	A
1	1A	1542	A
1	1A	1543	C
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1579	A
1	1A	1581	G
1	1A	1582	C
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1610	A
1	1A	1648	C
1	1A	1654	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1746	G
1	1A	1756	G
1	1A	1762	A

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Mol	Chain	Res	Type
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1817	G
1	1A	1829	A
1	1A	1839	G
1	1A	1847	A
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
1	1A	1914	C
1	1A	1929	G
1	1A	1930	G
1	1A	1936	A
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
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	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A

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Mol	Chain	Res	Type
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	2112	G
1	1A	2116	G
1	1A	2117	A
1	1A	2118	U
1	1A	2119	A
1	1A	2121	G
1	1A	2123	G
1	1A	2126	A
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2135	A
1	1A	2139	C
1	1A	2142	C
1	1A	2145	C
1	1A	2146	C
1	1A	2147	G
1	1A	2153	G
1	1A	2158	A
1	1A	2159	G
1	1A	2164	C
1	1A	2170	A
1	1A	2173	A
1	1A	2178	C
1	1A	2186	G
1	1A	2187	G
1	1A	2189	U
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	2218	U

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Mol	Chain	Res	Type
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2279	G
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
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2422	A
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2469	A
1	1A	2470	G
1	1A	2476	A
1	1A	2498	C
1	1A	2502	G
1	1A	2504	U
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2520	C
1	1A	2529	G
1	1A	2535	G
1	1A	2554	U
1	1A	2566	A

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Mol	Chain	Res	Type
1	1A	2567	G
1	1A	2573	C
1	1A	2602	A
1	1A	2603	G
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2757	A
1	1A	2758	A
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
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	2872	G
1	1A	2880	C
1	1A	2893	G
1	1A	2894	G
2	1B	2	C
2	1B	13	A
2	1B	45	A
2	1B	53	A
2	1B	56	G

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Mol	Chain	Res	Type
2	1B	73	A
2	1B	85	G
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	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	61	G
32	1a	78	G
32	1a	79	G
32	1a	91	C
32	1a	92	C
32	1a	101	A
32	1a	102	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	159	G
32	1a	160	A
32	1a	163	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	189(D)	C
32	1a	189(F)	U
32	1a	189(G)	G
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	204	U
32	1a	216	G
32	1a	220	G
32	1a	231	G
32	1a	247	G
32	1a	251	G
32	1a	262	A

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Mol	Chain	Res	Type
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	356	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	398	C
32	1a	406	G
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	442	C
32	1a	451	A
32	1a	452	A
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	475	G
32	1a	484	G
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	524	G
32	1a	532	A

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Mol	Chain	Res	Type
32	1a	536	C
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	564	C
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	619	U
32	1a	630	G
32	1a	632	A
32	1a	633	G
32	1a	651	C
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	666	G
32	1a	687	A
32	1a	688	G
32	1a	723	U
32	1a	731	G
32	1a	755	G
32	1a	759	A
32	1a	770	C
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	829	G
32	1a	839	U
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	851	G
32	1a	870	U
32	1a	902	G
32	1a	914	A

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Mol	Chain	Res	Type
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	963	G
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	998	G
32	1a	999	C
32	1a	1001	A
32	1a	1001(A)	G
32	1a	1005	A
32	1a	1006	C
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
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(B)	C
32	1a	1030(D)	A
32	1a	1032	G
32	1a	1033	G
32	1a	1037	C
32	1a	1038	C
32	1a	1044	A
32	1a	1046	A
32	1a	1053	G

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Mol	Chain	Res	Type
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1070	U
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1124	G
32	1a	1126	U
32	1a	1130	A
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G
32	1a	1159	U
32	1a	1168	A
32	1a	1183	A
32	1a	1184	G
32	1a	1186	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1208	C
32	1a	1212	U
32	1a	1213	A
32	1a	1224	G
32	1a	1227	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A

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Mol	Chain	Res	Type
32	1a	1293	G
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1397	C
32	1a	1406	U
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1487	G
32	1a	1493	A
32	1a	1497	G
32	1a	1499	A
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
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	14	A
1	2A	34	C
1	2A	45	C
1	2A	55	G
1	2A	71	A

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Mol	Chain	Res	Type
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	141	A
1	2A	157	U
1	2A	181	A
1	2A	182	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	229	A
1	2A	230	U
1	2A	248	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	272(J)	C
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	311	A
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	342	G
1	2A	352	G
1	2A	362	U

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Mol	Chain	Res	Type
1	2A	363	G
1	2A	370	G
1	2A	386	G
1	2A	396	G
1	2A	405	U
1	2A	406	G
1	2A	411	G
1	2A	412	A
1	2A	428	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	470	A
1	2A	481	G
1	2A	505	A
1	2A	509	C
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	545	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	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	627	A
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	669	G
1	2A	686	G

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Mol	Chain	Res	Type
1	2A	717	G
1	2A	730	C
1	2A	740	U
1	2A	752	A
1	2A	753	C
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	805	G
1	2A	812	C
1	2A	815	C
1	2A	827	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	880	G
1	2A	881	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	900	A
1	2A	901	A
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	980	A

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Mol	Chain	Res	Type
1	2A	983	A
1	2A	996	A
1	2A	997	G
1	2A	1012	U
1	2A	1013	C
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
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	1048	A
1	2A	1052	C
1	2A	1053	C
1	2A	1054	A
1	2A	1055	G
1	2A	1058	G
1	2A	1060	U
1	2A	1063	G
1	2A	1064	C
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	1072	C
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

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Mol	Chain	Res	Type
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	1095	A
1	2A	1096	A
1	2A	1097	U
1	2A	1105	U
1	2A	1109	C
1	2A	1110	G
1	2A	1111	A
1	2A	1112	G
1	2A	1116	C
1	2A	1117	G
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1170	G
1	2A	1171	G
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1236	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1329	U
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G

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Mol	Chain	Res	Type
1	2A	1384	A
1	2A	1385	G
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C
1	2A	1648	C
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A

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Mol	Chain	Res	Type
1	2A	1721	G
1	2A	1722	A
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	1816	G
1	2A	1828	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1918	A
1	2A	1927	A
1	2A	1929	G
1	2A	1930	G
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1975	G
1	2A	1984	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G

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Mol	Chain	Res	Type
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	2069	G
1	2A	2096	U
1	2A	2100	G
1	2A	2101	G
1	2A	2103	C
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2109	U
1	2A	2111	C
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
1	2A	2123	G
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	2130	U
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2144	U
1	2A	2145	C
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G

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Mol	Chain	Res	Type
1	2A	2150	U
1	2A	2151	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2163	C
1	2A	2164	C
1	2A	2172	U
1	2A	2173	A
1	2A	2178	C
1	2A	2180	U
1	2A	2181	G
1	2A	2184	G
1	2A	2186	G
1	2A	2189	U
1	2A	2192	G
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	2238	G
1	2A	2239	G
1	2A	2269	A
1	2A	2275	C
1	2A	2278	A
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A
1	2A	2311	A
1	2A	2312	U
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2335	A
1	2A	2336	A

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Mol	Chain	Res	Type
1	2A	2343	C
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2402	C
1	2A	2406	U
1	2A	2414	G
1	2A	2422	A
1	2A	2423	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2468	G
1	2A	2474	C
1	2A	2476	A
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2549	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2574	G
1	2A	2582	G
1	2A	2585	U
1	2A	2602	A
1	2A	2603	G
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C

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Mol	Chain	Res	Type
1	2A	2615	U
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2663	G
1	2A	2682	U
1	2A	2689	U
1	2A	2690	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	2744	G
1	2A	2748	A
1	2A	2757	A
1	2A	2758	A
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2836	U
1	2A	2872	G
1	2A	2880	C
1	2A	2891	G
1	2A	2894	G
1	2A	2896	C
2	2B	2	C
2	2B	7	G
2	2B	9	G
2	2B	13	A
2	2B	30	C
2	2B	33	G
2	2B	35	U
2	2B	45	A
2	2B	51	G

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Mol	Chain	Res	Type
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	106	G
2	2B	109	C
2	2B	110	G
32	2a	5	U
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	61	G
32	2a	66	G
32	2a	78	G
32	2a	80	G
32	2a	89	C
32	2a	97	G
32	2a	101	A
32	2a	105	G
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	142	G
32	2a	144	G
32	2a	156	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(C)	C
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G

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Mol	Chain	Res	Type
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	298	A
32	2a	316	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	414	A
32	2a	421	U
32	2a	422	C
32	2a	424	G
32	2a	429	U
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	458	C
32	2a	461	A
32	2a	470	C
32	2a	476	G
32	2a	477	A
32	2a	482	A
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A

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Mol	Chain	Res	Type
32	2a	511	C
32	2a	518	C
32	2a	528	C
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	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	630	G
32	2a	631	G
32	2a	633	G
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	774	G
32	2a	777	A
32	2a	785	G
32	2a	793	U
32	2a	794	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	829	G
32	2a	836	G
32	2a	840	C
32	2a	841	U
32	2a	848	C

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Mol	Chain	Res	Type
32	2a	851	G
32	2a	859	A
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	995	C
32	2a	1003	G
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	1029	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1041	A
32	2a	1044	A
32	2a	1047	G

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Mol	Chain	Res	Type
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1117	G
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1160	G
32	2a	1161	C
32	2a	1183	A
32	2a	1185	G
32	2a	1186	G
32	2a	1194	U
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1208	C
32	2a	1211	U
32	2a	1212	U
32	2a	1214	C
32	2a	1224	G
32	2a	1227	A
32	2a	1238	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G

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Mol	Chain	Res	Type
32	2a	1260	C
32	2a	1270	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1281	U
32	2a	1282	C
32	2a	1286	A
32	2a	1287	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1311	G
32	2a	1312	G
32	2a	1317	C
32	2a	1319	A
32	2a	1320	C
32	2a	1323	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1358	U
32	2a	1359	C
32	2a	1363	C
32	2a	1370	G
32	2a	1397	C
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1456	G
32	2a	1460	A
32	2a	1492	A
32	2a	1497	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1505	G

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Mol	Chain	Res	Type
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1520	G
32	2a	1528	U
32	2a	1529	G
32	2a	1530	G

All (59) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	195	A
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	746	A
1	1A	827	U
1	1A	839	U
1	1A	895	U
1	1A	974	G
1	1A	1065	U
1	1A	1067	A
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1442	G
1	1A	1608	A
1	1A	1653	G
1	1A	2126	A
1	1A	2172	U
1	1A	2406	U
1	1A	2430	A
1	1A	2602	A
1	1A	2689	U
1	1A	2756	U
1	1A	2893	G
1	2A	9	U
1	2A	195	A
1	2A	196	A
1	2A	271(M)	G

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Mol	Chain	Res	Type
1	2A	277	C
1	2A	645	C
1	2A	752	A
1	2A	764	A
1	2A	827	U
1	2A	840	C
1	2A	856	C
1	2A	900	A
1	2A	1053	C
1	2A	1057	A
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A
1	2A	1076	C
1	2A	1210	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	2406	U
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	UR3	1a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.45	1 (3%)
43	0TD	2l	92	43	7,9,10	4.60	1 (14%)	6,11,13	1.28	1 (16%)
1	PSU	2A	1917	1	18,21,22	1.34	2 (11%)	22,30,33	1.83	3 (13%)
32	5MC	2a	1400	32	18,22,23	0.96	2 (11%)	26,32,35	1.19	2 (7%)
1	OMC	2A	1920	1	19,22,23	0.82	0	26,31,34	0.95	1 (3%)
1	PSU	1A	1911	1	18,21,22	1.32	2 (11%)	22,30,33	1.89	4 (18%)
32	PSU	2a	516	32,54	18,21,22	1.34	2 (11%)	22,30,33	1.93	5 (22%)
1	5MU	1A	1915	1,54	19,22,23	1.46	5 (26%)	28,32,35	2.15	8 (28%)
32	MA6	1a	1518	32	18,26,27	0.78	0	19,38,41	1.34	2 (10%)
32	4OC	1a	1402	32	20,23,24	0.75	0	26,32,35	0.97	1 (3%)
32	PSU	1a	516	32,54	18,21,22	1.35	2 (11%)	22,30,33	1.83	3 (13%)
1	PSU	2A	1911	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)
1	5MU	2A	1915	1	19,22,23	1.45	4 (21%)	28,32,35	2.17	8 (28%)
1	2MA	2A	2503	1,54	17,25,26	1.04	1 (5%)	17,37,40	0.94	2 (11%)
43	0TD	1l	92	43	7,9,10	4.76	1 (14%)	6,11,13	6.93	2 (33%)
32	2MG	2a	1207	32	18,26,27	0.90	1 (5%)	16,38,41	1.08	1 (6%)
32	5MC	1a	1400	32	18,22,23	0.98	2 (11%)	26,32,35	1.14	2 (7%)
32	G7M	2a	527	32,54	20,26,27	1.27	2 (10%)	17,39,42	0.57	0
32	5MC	2a	1404	32	18,22,23	0.97	2 (11%)	26,32,35	1.11	3 (11%)
32	5MC	2a	1407	32	18,22,23	0.99	2 (11%)	26,32,35	1.15	3 (11%)
32	MA6	2a	1519	32	18,26,27	0.79	0	19,38,41	1.47	2 (10%)
1	OMU	1A	2552	1,54	19,22,23	1.22	2 (10%)	26,31,34	1.67	5 (19%)
32	MA6	2a	1518	32	18,26,27	0.78	0	19,38,41	1.37	2 (10%)
32	MA6	1a	1519	32	18,26,27	0.78	0	19,38,41	1.41	2 (10%)
32	5MC	1a	1404	32	18,22,23	0.96	2 (11%)	26,32,35	1.10	2 (7%)
32	G7M	1a	527	32,54	20,26,27	1.20	2 (10%)	17,39,42	0.56	0
32	5MC	2a	967	32	18,22,23	0.98	2 (11%)	26,32,35	1.10	2 (7%)
1	OMG	1A	2251	1,54	18,26,27	0.96	1 (5%)	19,38,41	1.06	2 (10%)
1	2MA	1A	2503	1,54	17,25,26	1.01	1 (5%)	17,37,40	0.97	2 (11%)
1	PSU	1A	2605	1	18,21,22	1.35	2 (11%)	22,30,33	1.87	4 (18%)
32	2MG	1a	1207	32,54	18,26,27	0.96	1 (5%)	16,38,41	1.38	3 (18%)
1	5MU	1A	1939	1,54	19,22,23	1.43	5 (26%)	28,32,35	2.09	6 (21%)
1	5MU	2A	1939	1	19,22,23	1.41	5 (26%)	28,32,35	2.15	6 (21%)
1	OMG	2A	2251	1,54	18,26,27	0.93	1 (5%)	19,38,41	1.13	2 (10%)
1	OMU	2A	2552	1,54	19,22,23	1.16	2 (10%)	26,31,34	1.76	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	2A	2605	1	18,21,22	1.30	2 (11%)	22,30,33	1.94	3 (13%)
32	M2G	1a	966	32	20,27,28	1.40	3 (15%)	22,40,43	0.94	2 (9%)
1	5MC	2A	1942	1	18,22,23	0.96	2 (11%)	26,32,35	1.15	2 (7%)
32	M2G	2a	966	32	20,27,28	1.42	3 (15%)	22,40,43	1.00	2 (9%)
1	5MC	1A	1962	1	18,22,23	0.96	2 (11%)	26,32,35	1.20	3 (11%)
32	5MC	1a	1407	32	18,22,23	0.97	2 (11%)	26,32,35	1.14	3 (11%)
32	5MC	1a	967	32	18,22,23	0.98	2 (11%)	26,32,35	1.12	2 (7%)
1	OMC	1A	1920	1	19,22,23	0.81	0	26,31,34	0.83	0
32	4OC	2a	1402	32	20,23,24	0.77	0	26,32,35	1.01	1 (3%)
1	5MC	2A	1962	1,54	18,22,23	0.96	2 (11%)	26,32,35	1.15	2 (7%)
32	UR3	2a	1498	32	19,22,23	1.00	1 (5%)	26,32,35	1.43	2 (7%)
1	PSU	1A	1917	1,54	18,21,22	1.33	2 (11%)	22,30,33	1.83	3 (13%)
1	5MC	1A	1942	1,54	18,22,23	0.99	2 (11%)	26,32,35	1.11	2 (7%)

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	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	1/9/27/28	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1,54	-	2/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
32	4OC	1a	1402	32	-	4/9/29/30	0/2/2/2
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2
1	2MA	2A	2503	1,54	-	2/3/25/26	0/3/3/3
43	0TD	1l	92	43	-	3/7/12/14	-
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	G7M	2a	527	32,54	-	3/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1404	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	-	2/7/29/30	0/3/3/3
1	OMU	1A	2552	1,54	-	0/9/27/28	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	MA6	1a	1519	32	-	2/7/29/30	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,54	-	1/3/25/26	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,54	-	0/5/27/28	0/3/3/3
1	2MA	1A	2503	1,54	-	2/3/25/26	0/3/3/3
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32,54	-	0/5/27/28	0/3/3/3
1	5MU	1A	1939	1,54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,54	-	0/5/27/28	0/3/3/3
1	OMU	2A	2552	1,54	-	0/9/27/28	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
1	5MC	2A	1962	1,54	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1,54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1,54	-	0/7/25/26	0/2/2/2

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.25	1.69	1.82
43	2l	92	0TD	CB-SB	-11.85	1.70	1.82
32	2a	966	M2G	C2-N3	4.50	1.36	1.30
32	1a	966	M2G	C2-N3	4.35	1.36	1.30
32	2a	527	G7M	C5-C4	3.68	1.46	1.39
32	1a	527	G7M	C5-C4	3.60	1.46	1.39
32	1a	516	PSU	C6-C5	3.33	1.39	1.35
1	1A	1917	PSU	C6-C5	3.32	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1911	PSU	C6-C5	3.29	1.39	1.35
1	2A	1917	PSU	C6-C5	3.23	1.39	1.35
32	2a	516	PSU	C6-C5	3.17	1.39	1.35
1	1A	1911	PSU	C6-C5	3.13	1.39	1.35
32	2a	1407	5MC	C6-C5	3.01	1.39	1.34
1	2A	2605	PSU	C6-C5	3.00	1.38	1.35
1	1A	1939	5MU	C6-C5	2.95	1.39	1.34
32	1a	1400	5MC	C6-C5	2.90	1.39	1.34
1	1A	1915	5MU	C2-N1	2.86	1.43	1.38
32	2a	1404	5MC	C6-C5	2.85	1.39	1.34
32	1a	1407	5MC	C6-C5	2.84	1.39	1.34
1	1A	1939	5MU	C4-N3	-2.84	1.33	1.38
32	2a	966	M2G	C2-N2	2.84	1.40	1.35
32	2a	967	5MC	C6-C5	2.83	1.39	1.34
1	2A	1939	5MU	C6-C5	2.83	1.39	1.34
1	2A	1915	5MU	C6-C5	2.82	1.39	1.34
1	1A	2605	PSU	C6-C5	2.82	1.38	1.35
1	1A	2605	PSU	C4-N3	-2.82	1.33	1.38
1	2A	1915	5MU	C2-N1	2.81	1.43	1.38
32	1a	1404	5MC	C6-C5	2.81	1.39	1.34
32	1a	967	5MC	C6-C5	2.78	1.39	1.34
1	2A	1962	5MC	C6-C5	2.78	1.39	1.34
1	1A	1942	5MC	C6-C5	2.77	1.39	1.34
1	1A	1915	5MU	C4-N3	-2.75	1.33	1.38
1	1A	1915	5MU	C6-C5	2.75	1.39	1.34
1	2A	1942	5MC	C6-C5	2.70	1.39	1.34
32	2a	1400	5MC	C6-C5	2.69	1.39	1.34
1	2A	1911	PSU	C4-N3	-2.66	1.33	1.38
32	1a	966	M2G	C2-N2	2.66	1.40	1.35
1	2A	1915	5MU	C4-N3	-2.65	1.33	1.38
1	2A	1939	5MU	C4-N3	-2.63	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.61	1.33	1.38
32	2a	516	PSU	C4-N3	-2.60	1.34	1.38
1	1A	2251	OMG	C6-N1	-2.59	1.34	1.37
1	2A	1917	PSU	C4-N3	-2.57	1.34	1.38
1	2A	2605	PSU	C4-N3	-2.56	1.34	1.38
1	1A	1917	PSU	C4-N3	-2.55	1.34	1.38
32	1a	516	PSU	C4-N3	-2.54	1.34	1.38
1	2A	1939	5MU	C4-C5	2.54	1.49	1.44
1	1A	1911	PSU	C4-N3	-2.53	1.34	1.38
1	1A	2552	OMU	C4-N3	-2.52	1.34	1.38
32	1a	966	M2G	C6-N1	-2.50	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1962	5MC	C6-C5	2.48	1.38	1.34
1	2A	2552	OMU	C4-N3	-2.45	1.34	1.38
32	2a	527	G7M	C6-N1	-2.44	1.34	1.37
1	1A	1942	5MC	C6-N1	-2.43	1.33	1.38
1	2A	2503	2MA	C2-N3	2.42	1.36	1.31
1	2A	1915	5MU	C4-C5	2.33	1.48	1.44
1	2A	2251	OMG	C6-N1	-2.33	1.34	1.37
32	1a	527	G7M	C6-N1	-2.33	1.34	1.37
32	1a	1207	2MG	C6-N1	-2.32	1.34	1.37
32	1a	1400	5MC	C6-N1	-2.29	1.34	1.38
1	1A	1915	5MU	C4-C5	2.29	1.48	1.44
1	1A	1939	5MU	C6-N1	-2.29	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.26	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.26	1.33	1.38
1	2A	1942	5MC	C6-N1	-2.25	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.25	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.22	1.34	1.38
32	2a	966	M2G	C6-N1	-2.20	1.34	1.37
32	1a	967	5MC	C6-N1	-2.20	1.34	1.38
1	1A	2503	2MA	C2-N3	2.20	1.35	1.31
32	2a	1404	5MC	C6-N1	-2.16	1.34	1.38
1	1A	1939	5MU	C4-C5	2.16	1.48	1.44
32	2a	1207	2MG	C6-N1	-2.16	1.34	1.37
1	1A	2552	OMU	C2-N3	-2.16	1.34	1.38
32	2a	967	5MC	C6-N1	-2.15	1.34	1.38
32	1a	1498	UR3	C6-C5	2.13	1.40	1.35
32	1a	1404	5MC	C6-N1	-2.13	1.34	1.38
32	2a	1498	UR3	C6-C5	2.10	1.39	1.35
1	2A	2552	OMU	C2-N3	-2.08	1.34	1.38
1	1A	1915	5MU	C6-N1	-2.05	1.34	1.38
32	1a	1407	5MC	C6-N1	-2.04	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.01	1.34	1.38
1	2A	1939	5MU	C2-N1	2.01	1.41	1.38

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	-16.69	72.24	102.44
32	2a	516	PSU	N1-C2-N3	6.00	121.93	115.13
32	1a	1498	UR3	C4-N3-C2	-5.99	118.92	124.56
1	2A	1911	PSU	N1-C2-N3	5.96	121.89	115.13
32	2a	1498	UR3	C4-N3-C2	-5.95	118.96	124.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2605	PSU	N1-C2-N3	5.92	121.84	115.13
1	1A	2605	PSU	N1-C2-N3	5.87	121.78	115.13
1	1A	1911	PSU	N1-C2-N3	5.85	121.76	115.13
1	2A	1917	PSU	N1-C2-N3	5.77	121.67	115.13
32	1a	516	PSU	N1-C2-N3	5.76	121.66	115.13
1	1A	1917	PSU	N1-C2-N3	5.75	121.65	115.13
1	2A	1939	5MU	C4-N3-C2	-5.43	120.32	127.35
1	1A	1939	5MU	C4-N3-C2	-5.23	120.58	127.35
1	2A	1939	5MU	N3-C2-N1	5.10	121.67	114.89
1	1A	1939	5MU	N3-C2-N1	5.07	121.61	114.89
1	1A	1915	5MU	N3-C2-N1	5.03	121.57	114.89
1	2A	1915	5MU	N3-C2-N1	5.02	121.56	114.89
1	2A	1915	5MU	C4-N3-C2	-4.79	121.15	127.35
32	2a	1519	MA6	N3-C2-N1	-4.79	121.20	128.68
32	2a	1518	MA6	N3-C2-N1	-4.76	121.24	128.68
1	1A	1915	5MU	C4-N3-C2	-4.75	121.21	127.35
1	2A	2552	OMU	C4-N3-C2	-4.73	120.34	126.58
32	1a	1519	MA6	N3-C2-N1	-4.60	121.49	128.68
32	1a	1518	MA6	N3-C2-N1	-4.60	121.50	128.68
1	1A	1939	5MU	C5-C4-N3	4.58	119.22	115.31
1	2A	1939	5MU	C5-C4-N3	4.48	119.14	115.31
1	1A	2552	OMU	C4-N3-C2	-4.40	120.78	126.58
1	2A	1939	5MU	C5-C6-N1	-4.18	119.03	123.34
1	2A	1915	5MU	C5-C4-N3	4.18	118.88	115.31
1	1A	2552	OMU	N3-C2-N1	4.17	120.43	114.89
1	2A	2605	PSU	C4-N3-C2	-4.15	120.36	126.34
1	1A	1939	5MU	C5-C6-N1	-4.12	119.10	123.34
1	1A	1915	5MU	C5-C4-N3	4.11	118.82	115.31
32	2a	516	PSU	C4-N3-C2	-4.08	120.47	126.34
1	2A	2552	OMU	N3-C2-N1	4.07	120.30	114.89
1	1A	2605	PSU	C4-N3-C2	-4.04	120.52	126.34
1	1A	1911	PSU	C4-N3-C2	-4.02	120.55	126.34
1	2A	1911	PSU	C4-N3-C2	-3.86	120.77	126.34
1	1A	1915	5MU	C1'-N1-C2	3.86	124.55	117.57
1	2A	1915	5MU	C1'-N1-C2	3.82	124.49	117.57
1	1A	1917	PSU	C4-N3-C2	-3.82	120.84	126.34
1	2A	1939	5MU	O4-C4-C5	-3.79	120.51	124.90
1	1A	1939	5MU	O4-C4-C5	-3.78	120.52	124.90
32	1a	516	PSU	C4-N3-C2	-3.77	120.91	126.34
1	2A	2552	OMU	C5-C4-N3	3.76	120.46	114.84
32	2a	1400	5MC	C5-C6-N1	-3.76	119.47	123.34
32	1a	1400	5MC	C5-C6-N1	-3.73	119.50	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1942	5MC	C5-C6-N1	-3.71	119.52	123.34
1	2A	1917	PSU	C4-N3-C2	-3.66	121.06	126.34
1	2A	1915	5MU	O4-C4-C5	-3.65	120.67	124.90
1	1A	1962	5MC	C5-C6-N1	-3.62	119.61	123.34
1	1A	1942	5MC	C5-C6-N1	-3.61	119.63	123.34
1	1A	1915	5MU	O4-C4-C5	-3.53	120.81	124.90
1	2A	1962	5MC	C5-C6-N1	-3.45	119.79	123.34
32	2a	967	5MC	C5-C6-N1	-3.44	119.80	123.34
1	1A	1911	PSU	O2-C2-N1	-3.42	119.02	122.79
1	2A	2605	PSU	O2-C2-N1	-3.42	119.03	122.79
1	1A	2552	OMU	C5-C4-N3	3.41	119.95	114.84
32	1a	1407	5MC	C5-C6-N1	-3.41	119.83	123.34
32	1a	967	5MC	C5-C6-N1	-3.37	119.87	123.34
32	1a	1404	5MC	C5-C6-N1	-3.37	119.87	123.34
32	2a	516	PSU	O2-C2-N1	-3.36	119.09	122.79
1	2A	1917	PSU	O2-C2-N1	-3.34	119.11	122.79
32	2a	1404	5MC	C5-C6-N1	-3.32	119.93	123.34
32	2a	1407	5MC	C5-C6-N1	-3.27	119.97	123.34
32	2a	1519	MA6	C4-C5-N7	-3.25	106.01	109.40
1	1A	1917	PSU	O2-C2-N1	-3.24	119.23	122.79
1	2A	2552	OMU	O4-C4-C5	-3.17	119.58	125.16
32	1a	1519	MA6	C4-C5-N7	-3.16	106.10	109.40
1	1A	2605	PSU	O2-C2-N1	-3.16	119.32	122.79
1	2A	1939	5MU	O2-C2-N1	-3.11	118.65	122.79
32	1a	516	PSU	O2-C2-N1	-3.09	119.39	122.79
1	1A	1915	5MU	C1'-N1-C6	-3.07	116.02	121.12
1	2A	1911	PSU	O2-C2-N1	-3.06	119.42	122.79
1	2A	1915	5MU	C1'-N1-C6	-3.05	116.05	121.12
32	2a	1518	MA6	C4-C5-N7	-2.86	106.42	109.40
1	1A	2552	OMU	O4-C4-C5	-2.84	120.17	125.16
32	1a	1518	MA6	C4-C5-N7	-2.79	106.49	109.40
1	2A	2552	OMU	O2-C2-N1	-2.79	119.08	122.79
1	1A	1915	5MU	C5-C6-N1	-2.78	120.48	123.34
1	1A	1915	5MU	O2-C2-N3	-2.74	116.40	121.50
1	2A	1915	5MU	C5-C6-N1	-2.72	120.54	123.34
32	1a	1402	4OC	C6-C5-C4	2.71	120.28	116.96
32	2a	1407	5MC	C5-C4-N3	-2.71	118.75	121.67
1	1A	1939	5MU	O2-C2-N1	-2.60	119.33	122.79
32	1a	1207	2MG	C8-N7-C5	2.58	107.91	102.99
32	2a	1404	5MC	C5-C4-N3	-2.58	118.89	121.67
32	1a	1400	5MC	C5-C4-N3	-2.57	118.90	121.67
32	1a	1404	5MC	C5-C4-N3	-2.52	118.95	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	967	5MC	C5-C4-N3	-2.51	118.97	121.67
1	2A	1942	5MC	C5-C4-N3	-2.49	118.99	121.67
1	1A	2251	OMG	C8-N7-C5	2.48	107.71	102.99
1	2A	1920	OMC	O2-C2-N3	-2.48	118.30	122.33
32	1a	967	5MC	C5-C4-N3	-2.47	119.01	121.67
32	2a	1207	2MG	C8-N7-C5	2.46	107.68	102.99
1	2A	1915	5MU	O2-C2-N3	-2.45	116.94	121.50
32	2a	1400	5MC	C5-C4-N3	-2.41	119.08	121.67
1	2A	2503	2MA	C8-N7-C5	2.40	107.55	102.99
1	2A	2503	2MA	C5-C6-N1	2.38	118.13	114.02
32	1a	1407	5MC	C5-C4-N3	-2.34	119.15	121.67
1	1A	1962	5MC	CM5-C5-C6	-2.34	119.73	122.85
32	2a	1407	5MC	O2-C2-N3	-2.33	118.55	122.33
1	2A	1962	5MC	C5-C4-N3	-2.32	119.17	121.67
1	2A	2251	OMG	C5-C6-N1	2.31	118.03	113.95
43	1l	92	0TD	OD2-CG-CB	2.28	118.08	113.15
1	1A	1942	5MC	C5-C4-N3	-2.28	119.21	121.67
32	1a	966	M2G	C5-C6-N1	2.28	117.98	113.95
32	1a	1207	2MG	C5-C6-N1	2.28	117.97	113.95
1	2A	2251	OMG	C8-N7-C5	2.27	107.32	102.99
32	2a	1402	4OC	C6-C5-C4	2.27	119.74	116.96
32	1a	1407	5MC	O2-C2-N3	-2.27	118.64	122.33
1	1A	2552	OMU	O2-C2-N1	-2.27	119.77	122.79
1	1A	2503	2MA	C8-N7-C5	2.25	107.27	102.99
32	2a	516	PSU	O4'-C1'-C2'	2.25	108.31	105.14
32	2a	966	M2G	C5-C6-N1	2.24	117.92	113.95
32	1a	966	M2G	C8-N7-C5	2.24	107.25	102.99
32	2a	966	M2G	C8-N7-C5	2.23	107.24	102.99
1	1A	1962	5MC	C5-C4-N3	-2.22	119.28	121.67
43	2l	92	0TD	OD2-CG-CB	2.21	117.93	113.15
1	1A	2605	PSU	C5-C6-N1	-2.21	118.79	122.11
1	1A	2503	2MA	C5-C6-N1	2.20	117.82	114.02
1	1A	2251	OMG	C5-C6-N1	2.19	117.81	113.95
32	2a	1498	UR3	C3U-N3-C4	2.19	121.01	117.89
32	2a	516	PSU	C5-C6-N1	-2.08	118.98	122.11
32	1a	1207	2MG	O3'-C3'-C2'	2.08	118.54	111.82
1	1A	1911	PSU	C5-C6-N1	-2.06	119.02	122.11
32	2a	1404	5MC	O2-C2-N3	-2.00	119.07	122.33

There are no chirality outliers.

All (32) 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
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
43	2l	92	0TD	O-C-CA-CB
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
32	1a	1402	4OC	O4'-C4'-C5'-O5'
43	2l	92	0TD	SB-CB-CG-OD1
1	1A	2503	2MA	C4'-C5'-O5'-P
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C2'-O2'-CM2
32	2a	1400	5MC	O4'-C4'-C5'-O5'
43	1l	92	0TD	SB-CB-CG-OD2
1	2A	1917	PSU	O4'-C4'-C5'-O5'
1	2A	2503	2MA	C3'-C4'-C5'-O5'
32	1a	1402	4OC	C1'-C2'-O2'-CM2
43	1l	92	0TD	CG-CB-SB-CSB
43	1l	92	0TD	SB-CB-CG-OD1
1	2A	1920	OMC	C2'-C1'-N1-C2
1	1A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1400	5MC	C3'-C4'-C5'-O5'
32	2a	527	G7M	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2572 ligands modelled in this entry, 2559 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	1O	202	-	7,7,7	0.28	0	9,10,10	0.19	0
56	MPD	2B	219	-	7,7,7	0.29	0	9,10,10	0.22	0
56	MPD	18	104	-	7,7,7	0.27	0	9,10,10	0.24	0
56	MPD	1A	4058	-	7,7,7	0.31	0	9,10,10	0.36	0
55	CPF	2A	3741	54	27,27,27	2.10	5 (18%)	40,40,40	2.27	14 (35%)
56	MPD	2A	3744	-	7,7,7	0.27	0	9,10,10	0.20	0
55	CPF	1A	4056	54	27,27,27	2.13	5 (18%)	40,40,40	1.85	11 (27%)
56	MPD	2A	3743	-	7,7,7	0.30	0	9,10,10	0.29	0
56	MPD	1a	1878	-	7,7,7	0.36	0	9,10,10	0.38	0
57	ARG	1F	320	-	10,11,11	0.73	1 (10%)	11,13,13	1.05	2 (18%)
59	SF4	1d	306	35	0,12,12	-	-	-		
57	ARG	1B	230	54	10,11,11	0.74	1 (10%)	11,13,13	1.10	2 (18%)
59	SF4	2d	302	35	0,12,12	-	-	-		

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	1O	202	-	-	1/5/5/5	-
56	MPD	2B	219	-	-	3/5/5/5	-
56	MPD	18	104	-	-	3/5/5/5	-
56	MPD	1A	4058	-	-	2/5/5/5	-
55	CPF	2A	3741	54	-	6/12/22/22	0/4/4/4
56	MPD	2A	3744	-	-	3/5/5/5	-
55	CPF	1A	4056	54	-	9/12/22/22	0/4/4/4
56	MPD	2A	3743	-	-	0/5/5/5	-
56	MPD	1a	1878	-	-	4/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	ARG	1F	320	-	-	2/11/11/11	-
59	SF4	1d	306	35	-	-	0/6/5/5
57	ARG	1B	230	54	-	2/11/11/11	-
59	SF4	2d	302	35	-	-	0/6/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1A	4056	CPF	C2-C3	-5.21	1.39	1.48
55	2A	3741	CPF	C2-C3	-5.18	1.40	1.48
55	1A	4056	CPF	C10-N1	-5.03	1.34	1.40
55	2A	3741	CPF	C5-C4	-4.99	1.38	1.48
55	2A	3741	CPF	C10-N1	-4.82	1.34	1.40
55	1A	4056	CPF	C5-C4	-4.74	1.39	1.48
55	1A	4056	CPF	C1-N1	3.89	1.40	1.34
55	2A	3741	CPF	C1-N1	3.69	1.40	1.34
55	1A	4056	CPF	C8-N2	-3.13	1.34	1.41
55	2A	3741	CPF	C8-N2	-2.71	1.35	1.41
57	1B	230	ARG	OXT-C	-2.15	1.23	1.30
57	1F	320	ARG	OXT-C	-2.08	1.23	1.30

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2A	3741	CPF	F1-C7-C8	6.29	124.15	118.42
55	2A	3741	CPF	C6-C7-C8	-4.74	119.43	123.34
55	1A	4056	CPF	C2-C1-N1	-4.42	119.54	124.49
55	2A	3741	CPF	C9-C8-N2	-4.33	116.11	122.52
55	2A	3741	CPF	C7-C8-N2	4.05	125.28	120.47
55	1A	4056	CPF	C6-C7-C8	-3.97	120.06	123.34
55	2A	3741	CPF	C14-N2-C17	3.87	120.07	111.52
55	1A	4056	CPF	C14-N2-C17	3.85	120.03	111.52
55	2A	3741	CPF	C2-C1-N1	-3.75	120.28	124.49
55	1A	4056	CPF	C9-C8-C7	3.36	119.75	116.48
55	2A	3741	CPF	C5-C4-C2	3.34	119.83	115.59
55	2A	3741	CPF	C13-C11-N1	-3.26	113.95	118.84
55	1A	4056	CPF	C5-C4-C2	3.26	119.73	115.59
55	2A	3741	CPF	C17-N2-C8	2.97	123.31	116.27
55	1A	4056	CPF	C5-C10-N1	2.90	120.94	118.81
57	1B	230	ARG	OXT-C-O	-2.85	117.63	124.09
55	1A	4056	CPF	C13-C11-N1	-2.76	114.70	118.84
55	2A	3741	CPF	C12-C11-N1	-2.60	114.94	118.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	1F	320	ARG	OXT-C-O	-2.53	118.35	124.09
55	1A	4056	CPF	C9-C8-N2	-2.46	118.88	122.52
55	1A	4056	CPF	C12-C11-N1	-2.32	115.35	118.84
57	1F	320	ARG	OXT-C-CA	2.26	121.08	113.38
55	2A	3741	CPF	O2-C3-C2	2.23	121.38	115.83
55	1A	4056	CPF	O2-C3-C2	2.21	121.33	115.83
55	2A	3741	CPF	O3-C4-C5	-2.17	118.04	121.56
55	2A	3741	CPF	C9-C8-C7	2.17	118.59	116.48
57	1B	230	ARG	OXT-C-CA	2.15	120.72	113.38
55	2A	3741	CPF	O2-C3-O1	-2.07	118.87	123.61
55	1A	4056	CPF	O2-C3-O1	-2.02	118.98	123.61

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	1A	4056	CPF	C1-C2-C3-O2
55	1A	4056	CPF	C4-C2-C3-O2
55	1A	4056	CPF	C1-C2-C3-O1
55	1A	4056	CPF	C4-C2-C3-O1
55	1A	4056	CPF	C7-C8-N2-C17
55	2A	3741	CPF	C12-C11-N1-C1
56	1O	202	MPD	C2-C3-C4-C5
56	18	104	MPD	C2-C3-C4-O4
56	1a	1878	MPD	C2-C3-C4-O4
56	2A	3744	MPD	C2-C3-C4-C5
56	2B	219	MPD	C2-C3-C4-C5
55	2A	3741	CPF	C13-C11-N1-C1
55	2A	3741	CPF	C12-C11-N1-C10
55	2A	3741	CPF	C9-C8-N2-C17
57	1B	230	ARG	CA-CB-CG-CD
55	1A	4056	CPF	C13-C11-N1-C1
55	2A	3741	CPF	C7-C8-N2-C17
55	2A	3741	CPF	C13-C11-N1-C10
57	1B	230	ARG	NE-CD-CG-CB
55	1A	4056	CPF	C13-C11-N1-C10
55	1A	4056	CPF	C9-C8-N2-C17
57	1F	320	ARG	CA-CB-CG-CD
56	18	104	MPD	C2-C3-C4-C5
56	18	104	MPD	CM-C2-C3-C4
56	1a	1878	MPD	CM-C2-C3-C4
56	2A	3744	MPD	C1-C2-C3-C4

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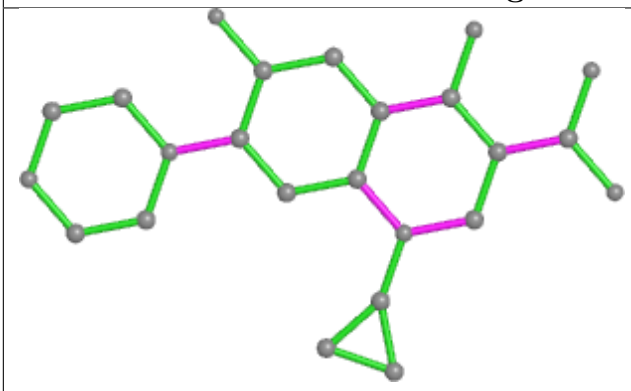
Mol	Chain	Res	Type	Atoms
55	1A	4056	CPF	C7-C8-N2-C14
57	1F	320	ARG	NE-CD-CG-CB
56	1a	1878	MPD	O2-C2-C3-C4
56	2B	219	MPD	O2-C2-C3-C4
56	1A	4058	MPD	C2-C3-C4-C5
56	1a	1878	MPD	C2-C3-C4-C5
56	1A	4058	MPD	C2-C3-C4-O4
56	2A	3744	MPD	C2-C3-C4-O4
56	2B	219	MPD	C2-C3-C4-O4

There are no ring outliers.

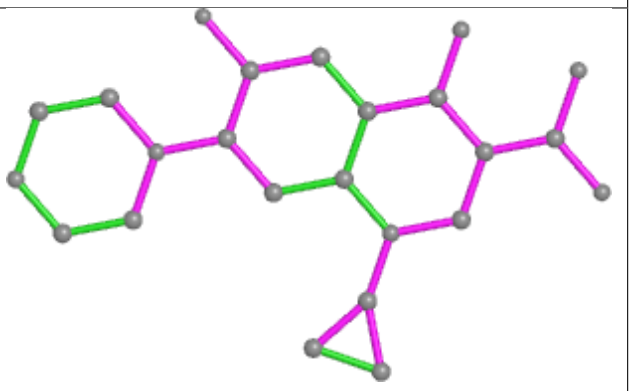
No monomer is involved in short contacts.

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.

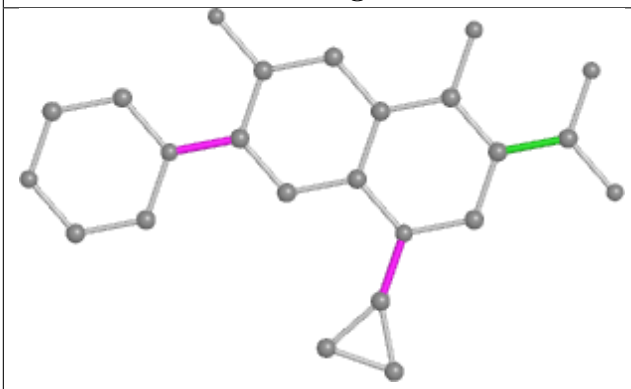
Ligand CPF 2A 3741



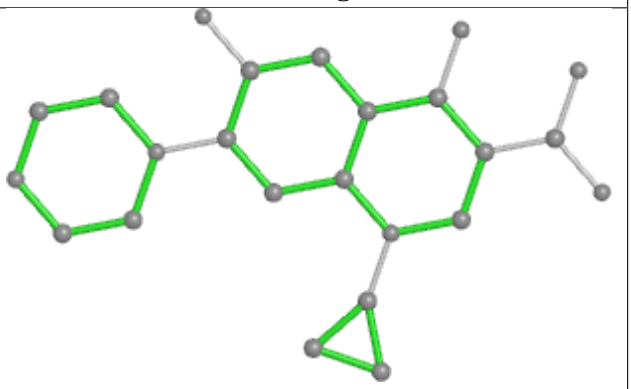
Bond lengths



Bond angles

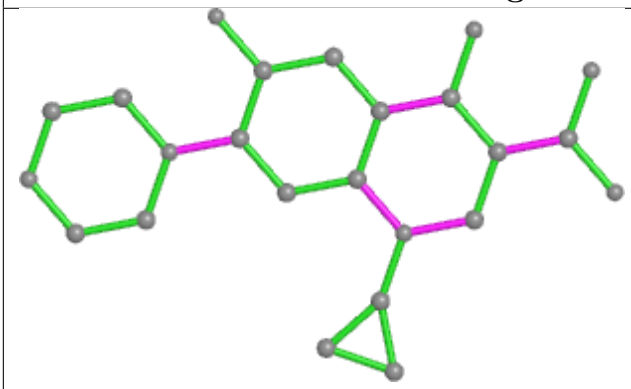


Torsions

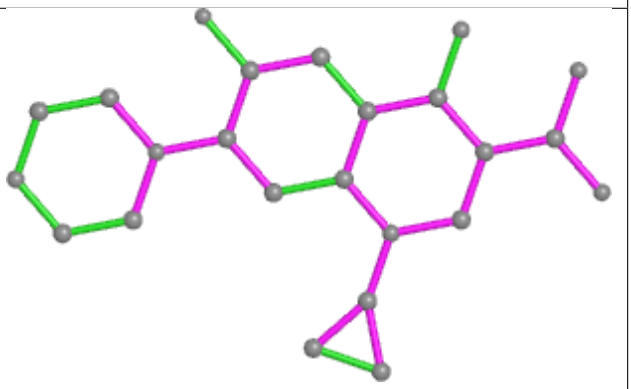


Rings

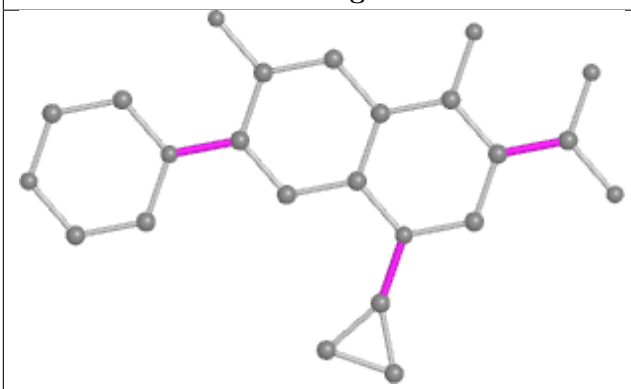
Ligand CPF 1A 4056



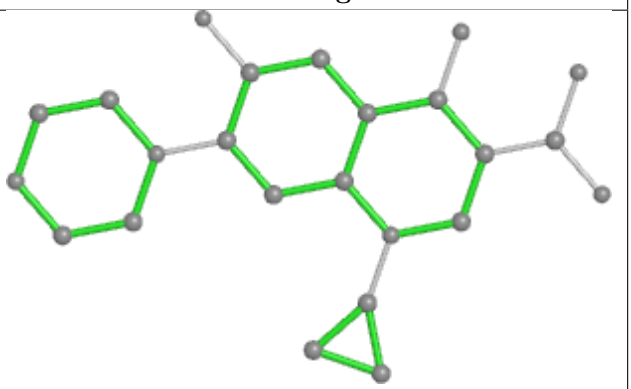
Bond lengths



Bond angles



Torsions



Rings

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%)	0.56	116 (4%) 37 30	24, 40, 97, 109	0
1	2A	2856/2915 (97%)	0.51	156 (5%) 25 19	31, 57, 100, 110	0
2	1B	120/121 (99%)	0.25	0 100 100	38, 56, 70, 88	0
2	2B	120/121 (99%)	0.17	2 (1%) 70 66	62, 82, 89, 98	0
3	1D	275/276 (99%)	0.47	3 (1%) 80 78	25, 39, 55, 76	0
3	2D	275/276 (99%)	0.56	2 (0%) 87 86	32, 50, 63, 78	0
4	1E	204/206 (99%)	0.47	0 100 100	23, 42, 64, 78	0
4	2E	204/206 (99%)	0.35	2 (0%) 82 80	36, 57, 73, 81	0
5	1F	203/210 (96%)	0.30	0 100 100	22, 45, 71, 89	0
5	2F	203/210 (96%)	0.32	0 100 100	35, 64, 79, 89	0
6	1G	181/182 (99%)	0.17	5 (2%) 53 46	53, 70, 82, 91	0
6	2G	181/182 (99%)	1.66	68 (37%) 0 0	77, 87, 94, 98	0
7	1H	174/180 (96%)	0.32	1 (0%) 89 88	41, 56, 69, 74	0
7	2H	173/180 (96%)	2.26	99 (57%) 0 0	72, 84, 90, 95	0
8	1I	147/148 (99%)	0.25	2 (1%) 75 71	45, 71, 83, 86	0
8	2I	146/148 (98%)	0.19	6 (4%) 37 30	53, 75, 86, 91	0
9	1N	140/140 (100%)	0.59	0 100 100	30, 43, 64, 79	0
9	2N	140/140 (100%)	0.33	3 (2%) 63 58	48, 64, 78, 86	0
10	1O	122/122 (100%)	0.30	0 100 100	31, 43, 62, 68	0
10	2O	122/122 (100%)	0.29	0 100 100	46, 55, 68, 75	0
11	1P	149/150 (99%)	0.28	0 100 100	24, 48, 68, 81	0
11	2P	149/150 (99%)	0.53	2 (1%) 77 73	39, 66, 83, 88	0
12	1Q	141/141 (100%)	0.40	0 100 100	31, 43, 57, 71	0
12	2Q	141/141 (100%)	0.86	13 (9%) 9 6	47, 65, 76, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	0.41	0 100 100	29, 41, 55, 63	0
13	2R	118/118 (100%)	0.40	0 100 100	40, 54, 64, 70	0
14	1S	110/112 (98%)	0.33	0 100 100	43, 55, 67, 72	0
14	2S	110/112 (98%)	0.88	21 (19%) 1 0	67, 76, 82, 89	0
15	1T	131/146 (89%)	0.23	0 100 100	38, 47, 70, 81	0
15	2T	131/146 (89%)	0.30	1 (0%) 86 84	47, 59, 76, 86	0
16	1U	116/118 (98%)	0.56	0 100 100	28, 35, 49, 65	0
16	2U	116/118 (98%)	0.40	0 100 100	42, 59, 72, 80	0
17	1V	101/101 (100%)	0.39	0 100 100	27, 46, 63, 71	0
17	2V	101/101 (100%)	0.31	0 100 100	41, 69, 77, 84	0
18	1W	112/113 (99%)	0.54	0 100 100	28, 36, 54, 84	0
18	2W	112/113 (99%)	0.58	1 (0%) 84 82	41, 50, 66, 91	0
19	1X	95/96 (98%)	0.64	1 (1%) 80 78	31, 42, 66, 77	0
19	2X	95/96 (98%)	0.48	3 (3%) 47 40	45, 60, 77, 86	0
20	1Y	107/110 (97%)	0.47	0 100 100	37, 51, 68, 78	0
20	2Y	107/110 (97%)	0.42	1 (0%) 84 82	59, 70, 79, 90	0
21	1Z	203/206 (98%)	0.15	2 (0%) 82 80	44, 62, 75, 86	0
21	2Z	201/206 (97%)	0.89	21 (10%) 6 4	68, 79, 85, 92	0
22	10	77/85 (90%)	0.47	0 100 100	32, 41, 60, 65	0
22	20	77/85 (90%)	0.84	12 (15%) 2 1	50, 65, 74, 77	0
23	11	97/98 (98%)	0.55	2 (2%) 63 58	32, 45, 69, 75	0
23	21	97/98 (98%)	0.48	2 (2%) 63 58	41, 55, 76, 80	0
24	12	70/72 (97%)	0.55	0 100 100	40, 51, 62, 83	0
24	22	70/72 (97%)	0.20	0 100 100	61, 70, 77, 79	0
25	13	59/60 (98%)	0.43	0 100 100	31, 42, 66, 72	0
25	23	59/60 (98%)	0.70	2 (3%) 45 38	51, 62, 80, 84	0
26	14	69/71 (97%)	0.57	12 (17%) 1 0	64, 83, 95, 98	0
26	24	69/71 (97%)	2.16	35 (50%) 0 0	85, 92, 99, 103	0
27	15	59/60 (98%)	0.52	1 (1%) 70 66	26, 40, 63, 74	0
27	25	59/60 (98%)	0.27	0 100 100	35, 52, 69, 79	0
28	16	53/54 (98%)	0.13	0 100 100	38, 46, 60, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.42	0 100 100	53, 62, 71, 74	0
29	17	48/49 (97%)	0.75	3 (6%) 20 15	25, 32, 61, 66	0
29	27	48/49 (97%)	0.76	3 (6%) 20 15	34, 41, 69, 77	0
30	18	64/65 (98%)	0.52	0 100 100	29, 37, 46, 54	0
30	28	64/65 (98%)	0.88	5 (7%) 13 9	48, 56, 63, 72	0
31	19	37/37 (100%)	0.54	0 100 100	35, 45, 60, 63	0
31	29	37/37 (100%)	2.38	23 (62%) 0 0	61, 70, 79, 81	0
32	1a	1488/1521 (97%)	0.41	67 (4%) 33 26	39, 73, 96, 110	0
32	2a	1492/1521 (98%)	0.52	121 (8%) 12 8	47, 77, 98, 109	0
33	1b	231/256 (90%)	0.29	12 (5%) 27 21	69, 81, 90, 96	0
33	2b	231/256 (90%)	0.59	28 (12%) 4 2	74, 85, 93, 98	0
34	1c	206/239 (86%)	0.60	16 (7%) 13 9	65, 76, 87, 89	0
34	2c	206/239 (86%)	1.60	69 (33%) 0 0	78, 86, 91, 96	0
35	1d	208/209 (99%)	0.45	10 (4%) 30 24	59, 74, 82, 89	0
35	2d	208/209 (99%)	0.99	29 (13%) 2 1	62, 72, 81, 84	0
36	1e	148/162 (91%)	0.36	1 (0%) 87 86	49, 68, 77, 90	0
36	2e	148/162 (91%)	0.52	14 (9%) 8 5	57, 73, 82, 93	0
37	1f	100/101 (99%)	0.06	1 (1%) 82 80	51, 68, 78, 82	0
37	2f	100/101 (99%)	0.03	0 100 100	56, 69, 78, 84	0
38	1g	155/156 (99%)	0.46	9 (5%) 23 17	68, 75, 83, 90	0
38	2g	155/156 (99%)	0.97	27 (17%) 1 0	76, 84, 89, 92	0
39	1h	137/138 (99%)	0.64	8 (5%) 23 17	58, 70, 78, 80	0
39	2h	137/138 (99%)	0.44	3 (2%) 62 56	62, 74, 81, 83	0
40	1i	127/128 (99%)	1.35	41 (32%) 0 0	66, 81, 87, 89	0
40	2i	126/128 (98%)	3.05	92 (73%) 0 0	77, 88, 93, 94	0
41	1j	97/105 (92%)	0.70	13 (13%) 3 2	65, 81, 90, 94	0
41	2j	96/105 (91%)	2.55	57 (59%) 0 0	79, 89, 93, 97	0
42	1k	114/129 (88%)	0.32	3 (2%) 56 50	46, 66, 76, 81	0
42	2k	114/129 (88%)	0.36	4 (3%) 44 36	60, 73, 82, 86	0
43	1l	121/132 (91%)	0.54	7 (5%) 23 17	51, 62, 73, 79	0
43	2l	121/132 (91%)	0.57	10 (8%) 11 8	56, 67, 76, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	116/126 (92%)	0.88	15 (12%) 3 2	68, 79, 84, 90	0
44	2m	114/126 (90%)	1.79	46 (40%) 0 0	80, 88, 93, 95	0
45	1n	60/61 (98%)	1.96	23 (38%) 0 0	67, 76, 83, 86	0
45	2n	60/61 (98%)	4.14	54 (90%) 0 0	80, 87, 93, 97	0
46	1o	88/89 (98%)	0.52	3 (3%) 45 38	47, 69, 80, 82	0
46	2o	88/89 (98%)	0.22	1 (1%) 80 78	58, 73, 81, 86	0
47	1p	82/88 (93%)	1.66	25 (30%) 0 0	62, 74, 83, 88	0
47	2p	82/88 (93%)	0.66	4 (4%) 29 23	62, 70, 80, 83	0
48	1q	99/105 (94%)	1.09	14 (14%) 2 1	57, 71, 80, 84	0
48	2q	99/105 (94%)	0.57	4 (4%) 38 31	55, 72, 79, 82	0
49	1r	68/88 (77%)	0.20	1 (1%) 73 70	58, 67, 80, 86	0
49	2r	68/88 (77%)	0.19	1 (1%) 73 70	62, 71, 82, 84	0
50	1s	83/93 (89%)	0.86	12 (14%) 2 1	71, 81, 87, 90	0
50	2s	83/93 (89%)	3.12	61 (73%) 0 0	79, 91, 95, 96	0
51	1t	96/106 (90%)	2.07	47 (48%) 0 0	64, 75, 86, 90	0
51	2t	98/106 (92%)	0.95	9 (9%) 9 6	60, 73, 84, 87	0
52	1u	23/27 (85%)	1.77	8 (34%) 0 0	72, 77, 81, 81	0
52	2u	23/27 (85%)	3.51	19 (82%) 0 0	80, 86, 89, 90	0
53	1y	97/113 (85%)	0.76	10 (10%) 6 4	59, 69, 78, 84	0
53	2y	96/113 (84%)	3.21	68 (70%) 0 0	73, 83, 88, 91	0
All	All	20766/21468 (96%)	0.63	1698 (8%) 11 8	22, 65, 92, 110	0

All (1698) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1076	C	11.4
1	1A	2602	A	9.1
1	2A	2153	G	9.0
45	2n	13	THR	8.8
1	2A	2139	C	8.5
1	2A	2147	G	8.4
40	2i	63	ILE	8.1
40	2i	109	VAL	8.1
32	2a	1030(A)	G	7.9
1	1A	1087	G	7.8

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Mol	Chain	Res	Type	RSRZ
52	2u	16	GLY	7.7
44	2m	102	ARG	7.5
1	2A	2140	C	7.5
1	2A	1076	C	7.4
1	2A	2174	C	7.4
41	2j	67	THR	7.4
45	2n	38	GLY	7.3
1	2A	2142	C	7.3
1	2A	1046	A	7.3
45	2n	55	GLY	7.3
45	2n	29	ARG	7.3
40	2i	66	ARG	7.3
32	2a	1030(B)	C	7.2
1	1A	1090	U	7.1
1	1A	1064	C	7.1
32	1a	1030(B)	C	7.1
1	1A	2147	G	7.1
1	1A	2141	G	7.0
32	2a	1001(A)	G	7.0
45	2n	35	ARG	6.9
26	24	49	PHE	6.9
41	2j	45	ARG	6.9
45	2n	2	ALA	6.8
40	2i	67	GLY	6.8
7	2H	165	ALA	6.8
32	2a	1257	U	6.8
1	2A	2106	G	6.8
23	11	2	SER	6.7
53	2y	73	ALA	6.7
1	2A	2152	G	6.7
1	2A	2146	C	6.5
20	2Y	1	MET	6.5
45	2n	34	TYR	6.5
1	2A	2154	G	6.5
32	2a	1036	G	6.5
41	2j	47	PHE	6.4
1	2A	1509	C	6.4
1	1A	1089	G	6.4
32	2a	1286	A	6.4
45	2n	25	VAL	6.4
1	2A	2148	G	6.4
40	2i	36	TYR	6.3

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Mol	Chain	Res	Type	RSRZ
53	2y	9	GLN	6.3
1	2A	2126	A	6.3
53	2y	38	HIS	6.3
53	2y	41	LEU	6.2
7	2H	115	VAL	6.2
53	2y	40	ILE	6.2
1	2A	2125	G	6.2
53	2y	71	TYR	6.2
40	2i	69	GLY	6.2
1	2A	2107	C	6.2
40	2i	76	ALA	6.2
6	2G	62	LEU	6.2
1	2A	2118	U	6.2
40	2i	7	THR	6.1
51	1t	66	ALA	6.1
41	2j	6	ILE	6.1
1	1A	1075	C	6.1
7	2H	82	GLY	6.1
1	2A	2162	G	6.1
7	2H	128	PRO	6.1
50	2s	40	ILE	6.1
1	2A	2116	G	6.1
32	1a	1031	G	6.0
53	2y	63	ALA	6.0
7	2H	103	LEU	6.0
53	2y	58	ASN	6.0
6	2G	152	LEU	6.0
45	2n	39	LEU	6.0
1	1A	1091	G	6.0
1	2A	2124	G	6.0
53	2y	77	LEU	6.0
1	2A	2138	C	5.9
41	2j	44	VAL	5.9
41	2j	65	LEU	5.9
52	2u	14	TRP	5.9
45	2n	10	ALA	5.9
1	2A	2132	U	5.9
40	2i	18	PHE	5.9
1	1A	2144	U	5.9
32	2a	1001	A	5.9
40	2i	75	ASP	5.9
1	1A	2145	C	5.8

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Mol	Chain	Res	Type	RSRZ
1	2A	2141	G	5.8
50	2s	11	VAL	5.8
1	1A	1067	A	5.8
40	2i	127	LYS	5.8
6	2G	39	ILE	5.8
41	2j	72	VAL	5.8
6	2G	146	TYR	5.7
1	1A	2142	C	5.7
32	2a	1030(C)	G	5.7
1	2A	2145	C	5.7
41	2j	62	HIS	5.7
1	1A	2132	U	5.7
1	2A	2179	C	5.7
53	2y	88	LEU	5.7
32	1a	162	A	5.7
40	2i	65	VAL	5.7
1	1A	1080	C	5.7
26	24	63	TYR	5.7
1	1A	888	C	5.6
50	2s	15	LEU	5.6
40	2i	126	SER	5.6
32	2a	1532	U	5.6
45	2n	59	ALA	5.6
1	2A	2169	A	5.6
50	2s	69	HIS	5.6
40	2i	102	LEU	5.6
32	1a	1001(A)	G	5.6
34	2c	155	GLY	5.6
45	2n	37	PHE	5.5
50	2s	30	LEU	5.5
26	24	45	GLY	5.5
53	2y	8	LYS	5.5
53	2y	5	ILE	5.5
41	2j	48	THR	5.5
45	2n	6	LEU	5.5
45	2n	11	LYS	5.5
40	2i	17	VAL	5.5
1	2A	2173	A	5.5
41	2j	46	ARG	5.5
1	2A	2111	C	5.5
32	1a	1030(D)	A	5.5
1	2A	2155	G	5.4

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Mol	Chain	Res	Type	RSRZ
1	2A	2168	G	5.4
1	2A	1085	A	5.4
50	2s	45	VAL	5.4
1	2A	2151	G	5.4
50	2s	49	ILE	5.4
44	2m	116	THR	5.4
41	2j	34	VAL	5.4
53	2y	10	MET	5.4
45	2n	14	PRO	5.4
1	1A	1066	U	5.4
50	2s	16	LEU	5.4
32	1a	1030(C)	G	5.4
1	2A	1075	C	5.4
52	2u	13	ILE	5.3
50	2s	9	VAL	5.3
41	2j	10	GLY	5.3
41	2j	40	LEU	5.3
32	2a	1531	A	5.3
45	2n	12	ARG	5.3
44	2m	17	VAL	5.3
1	1A	1509	C	5.2
41	2j	68	HIS	5.3
45	2n	54	PRO	5.2
47	1p	17	TYR	5.2
45	2n	30	ALA	5.2
38	2g	41	ARG	5.2
1	1A	2140	C	5.2
1	1A	1074	G	5.2
32	2a	1031	G	5.2
40	2i	14	VAL	5.2
50	2s	71	LEU	5.2
53	2y	67	HIS	5.2
53	2y	51	ASP	5.2
1	1A	1065	U	5.2
35	1d	2	GLY	5.2
1	2A	1064	C	5.2
1	2A	2110	G	5.1
32	2a	1354	C	5.1
50	2s	10	PHE	5.1
53	2y	52	ALA	5.1
1	1A	1078	U	5.1
41	2j	66	ARG	5.1

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Mol	Chain	Res	Type	RSRZ
1	2A	2165	G	5.1
34	2c	23	TYR	5.1
50	2s	42	PRO	5.1
1	2A	2134	A	5.0
32	1a	1447	A	5.0
40	1i	126	SER	5.0
34	2c	157	ILE	5.0
50	2s	62	ILE	5.0
53	2y	48	PHE	5.0
32	1a	1532	U	5.0
1	2A	2137	C	5.0
7	2H	166	GLY	5.0
40	2i	72	GLY	5.0
38	2g	32	ARG	5.0
40	2i	42	ARG	5.0
1	1A	1088	A	4.9
1	1A	2115	G	5.0
1	1A	2143	C	4.9
32	1a	1030	C	4.9
41	1j	10	GLY	4.9
44	1m	115	LYS	4.9
51	1t	72	LEU	4.9
40	2i	88	TYR	4.9
1	2A	2143	C	4.9
51	1t	76	ALA	4.9
53	2y	20	VAL	4.9
1	2A	2159	G	4.9
32	2a	1033	G	4.9
40	1i	79	LEU	4.9
53	1y	95	ARG	4.9
1	2A	2170	A	4.9
41	2j	63	PHE	4.9
6	2G	87	PRO	4.9
34	2c	196	LEU	4.9
42	2k	13	GLN	4.9
45	1n	2	ALA	4.9
32	1a	1001	A	4.9
50	2s	39	THR	4.9
50	2s	53	ASN	4.8
21	2Z	125	LEU	4.8
32	2a	1030	C	4.8
32	2a	1034	G	4.8

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Mol	Chain	Res	Type	RSRZ
1	2A	2150	U	4.8
45	2n	33	VAL	4.8
6	2G	157	ILE	4.8
1	2A	2135	A	4.8
26	24	27	THR	4.8
1	2A	2144	U	4.8
48	1q	98	LEU	4.8
53	2y	15	ALA	4.7
1	2A	888	C	4.7
51	1t	67	ALA	4.7
1	1A	2117	A	4.7
38	2g	42	ILE	4.7
40	2i	6	GLY	4.7
53	2y	80	LYS	4.7
1	2A	2176	A	4.7
44	2m	5	ALA	4.7
1	2A	1104	C	4.7
32	1a	1257	U	4.7
7	2H	102	ALA	4.7
32	2a	1021	G	4.7
32	2a	1035	A	4.7
45	2n	44	LEU	4.7
1	2A	2160	G	4.7
26	24	57	GLU	4.7
6	2G	136	ARG	4.7
1	1A	2113	U	4.7
45	2n	56	VAL	4.7
52	2u	22	ARG	4.6
1	1A	2116	G	4.6
44	2m	84	ILE	4.6
53	2y	39	ILE	4.6
32	2a	1030(D)	A	4.6
52	2u	15	ARG	4.6
7	2H	25	LYS	4.6
52	2u	12	LYS	4.6
52	2u	9	ARG	4.6
53	2y	78	ILE	4.6
1	2A	1067	A	4.6
41	2j	64	GLU	4.6
40	2i	125	TYR	4.6
44	2m	87	TYR	4.6
45	2n	21	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
45	2n	15	LYS	4.6
1	2A	2108	C	4.6
1	2A	2136	C	4.6
53	2y	64	SER	4.6
7	2H	49	VAL	4.6
1	2A	1079	C	4.6
35	2d	70	ILE	4.6
50	2s	34	TRP	4.6
50	2s	82	GLY	4.6
12	2Q	65	PHE	4.6
40	2i	5	TYR	4.6
32	2a	1002	G	4.5
44	2m	42	ALA	4.5
1	1A	2146	C	4.5
1	1A	2167	U	4.5
32	1a	1492	A	4.5
32	2a	1357	A	4.5
7	2H	105	LEU	4.5
1	2A	1083	U	4.5
1	1A	2108	C	4.5
32	1a	1286	A	4.5
53	2y	49	VAL	4.5
40	2i	79	LEU	4.5
50	2s	74	PHE	4.5
53	2y	4	ASN	4.5
26	24	19	GLY	4.5
38	2g	34	GLY	4.5
45	1n	18	VAL	4.5
47	1p	19	ILE	4.5
53	2y	65	GLY	4.5
26	24	44	THR	4.5
1	2A	2133	G	4.5
32	1a	1036	G	4.5
50	2s	79	THR	4.4
40	1i	14	VAL	4.4
36	2e	12	LEU	4.4
40	1i	106	ALA	4.4
7	2H	35	VAL	4.4
53	2y	45	PRO	4.4
6	2G	133	LEU	4.4
32	2a	1026	G	4.4
26	24	51	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	1A	1081	U	4.4
1	2A	2130	U	4.4
1	2A	2167	U	4.4
50	2s	60	VAL	4.4
51	1t	9	ASN	4.4
34	2c	152	ILE	4.4
50	2s	63	THR	4.4
31	29	13	LYS	4.4
32	2a	1040	U	4.4
34	2c	87	LEU	4.4
38	1g	16	LEU	4.4
1	1A	2107	C	4.4
1	2A	2161	C	4.4
1	1A	2159	G	4.4
1	2A	2149	G	4.4
23	21	2	SER	4.4
41	2j	19	SER	4.4
53	2y	7	SER	4.4
40	2i	29	ASN	4.4
1	1A	1093	G	4.4
1	2A	1099	G	4.4
40	2i	62	TYR	4.4
1	1A	2114	A	4.4
34	2c	124	ILE	4.4
50	2s	35	SER	4.3
35	2d	2	GLY	4.3
1	1A	2161	C	4.3
40	1i	128	ARG	4.3
40	2i	92	TYR	4.3
40	2i	114	TYR	4.3
1	2A	2109	U	4.3
1	2A	2172	U	4.3
1	2A	229	A	4.3
45	2n	61	TRP	4.3
52	2u	6	ARG	4.3
40	1i	109	VAL	4.3
50	2s	80	TYR	4.3
44	1m	4	ILE	4.3
53	2y	42	SER	4.3
1	1A	2155	G	4.3
1	2A	1091	G	4.3
1	2A	2131	G	4.3

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Mol	Chain	Res	Type	RSRZ
32	1a	204	U	4.3
44	2m	89	GLY	4.3
7	2H	171	LEU	4.3
1	1A	1092	C	4.3
50	2s	50	ALA	4.3
26	24	40	HIS	4.3
1	2A	2175	C	4.3
47	1p	6	LEU	4.3
53	2y	62	VAL	4.3
14	2S	35	ILE	4.3
1	2A	2157	G	4.3
33	1b	131	PRO	4.3
51	1t	70	SER	4.3
34	2c	190	ARG	4.2
40	2i	73	GLN	4.2
45	2n	8	GLU	4.2
45	2n	49	HIS	4.2
50	2s	41	VAL	4.2
26	14	52	THR	4.2
40	2i	33	PHE	4.2
35	2d	5	ILE	4.2
45	2n	7	ILE	4.2
38	2g	156	TRP	4.2
40	2i	108	VAL	4.2
47	1p	1	MET	4.2
50	2s	51	VAL	4.2
50	2s	67	VAL	4.2
53	2y	50	ALA	4.2
1	1A	1102	C	4.2
50	2s	47	HIS	4.2
1	1A	2153	G	4.2
52	2u	2	GLY	4.2
6	2G	3	LEU	4.2
1	2A	2119	A	4.2
1	1A	2150	U	4.1
53	2y	70	MET	4.1
52	2u	11	GLY	4.1
1	2A	1103	A	4.1
32	1a	1531	A	4.1
32	2a	1358	U	4.1
34	2c	65	ALA	4.1
52	2u	17	THR	4.1

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Mol	Chain	Res	Type	RSRZ
38	1g	12	LEU	4.1
40	2i	85	LEU	4.1
32	2a	994	A	4.1
33	2b	227	GLY	4.1
45	2n	36	PHE	4.1
6	2G	120	LEU	4.1
7	2H	6	ARG	4.1
51	1t	18	GLN	4.1
52	2u	10	ARG	4.1
48	1q	99	SER	4.1
34	2c	33	LEU	4.1
1	1A	1077	A	4.1
1	1A	1086	A	4.1
45	2n	18	VAL	4.1
26	24	39	CYS	4.0
41	2j	96	ILE	4.0
53	2y	12	ILE	4.0
34	1c	193	TYR	4.0
50	2s	12	ASP	4.0
1	1A	1103	A	4.0
1	2A	1043	C	4.0
1	2A	2156	G	4.0
41	2j	41	PRO	4.0
41	2j	23	ILE	4.0
32	2a	1029	C	4.0
21	2Z	51	ALA	4.0
51	1t	95	ALA	4.0
31	29	37	GLY	4.0
32	2a	1287	A	4.0
41	2j	98	ILE	4.0
45	2n	41	ARG	4.0
1	2A	2121	G	4.0
45	1n	61	TRP	4.0
40	2i	113	LYS	4.0
45	2n	3	ARG	4.0
6	2G	135	LEU	4.0
40	2i	20	ARG	4.0
1	1A	2129	C	4.0
1	2A	1056	G	3.9
26	14	49	PHE	3.9
52	1u	14	TRP	3.9
26	24	50	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
40	2i	115	GLY	3.9
1	1A	1063	G	3.9
50	2s	77	THR	3.9
26	24	68	ARG	3.9
45	2n	42	ILE	3.9
32	2a	1249	C	3.9
32	2a	1202	G	3.9
7	2H	101	ARG	3.9
44	2m	6	GLY	3.9
50	2s	66	MET	3.9
36	2e	22	GLY	3.9
33	2b	122	PHE	3.9
31	29	16	VAL	3.9
51	1t	71	THR	3.9
1	2A	652(B)	A	3.9
7	2H	164	TYR	3.9
50	2s	61	TYR	3.9
34	1c	2	GLY	3.9
45	2n	16	PHE	3.9
51	1t	55	ILE	3.9
45	1n	59	ALA	3.9
38	2g	155	ARG	3.9
44	1m	56	LEU	3.9
53	2y	3	MET	3.9
38	2g	154	TYR	3.9
1	2A	1095	A	3.9
1	1A	1072	C	3.9
50	2s	20	LEU	3.8
32	1a	1033	G	3.8
32	2a	1032	G	3.8
50	2s	76	PRO	3.8
12	2Q	59	ARG	3.8
32	1a	1037	C	3.8
53	2y	24	LEU	3.8
40	2i	110	GLU	3.8
1	1A	2149	G	3.8
8	2I	35	LEU	3.8
26	14	50	VAL	3.8
39	2h	2	LEU	3.8
1	2A	1088	A	3.8
32	2a	1028	C	3.8
7	2H	41	MET	3.8

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Mol	Chain	Res	Type	RSRZ
45	2n	40	CYS	3.8
53	2y	14	PRO	3.8
1	2A	2120	G	3.8
32	1a	1032	G	3.8
7	2H	95	ARG	3.8
6	2G	76	SER	3.8
1	1A	2106	G	3.8
40	1i	112	LYS	3.8
50	2s	31	ILE	3.8
40	2i	53	VAL	3.8
43	2l	18	VAL	3.8
14	2S	5	THR	3.8
51	1t	20	LEU	3.8
40	2i	9	ARG	3.8
1	2A	2602	A	3.8
32	2a	1041	A	3.8
51	1t	74	LYS	3.8
52	2u	23	PRO	3.8
34	2c	81	GLY	3.8
34	2c	159	GLY	3.8
41	1j	46	ARG	3.7
1	2A	2127	G	3.7
45	2n	53	LEU	3.7
45	2n	24	CYS	3.7
31	29	25	VAL	3.7
32	2a	1349	A	3.7
40	2i	90	PRO	3.7
53	2y	84	GLN	3.7
40	2i	81	ILE	3.7
34	2c	207	VAL	3.7
32	1a	220	G	3.7
31	29	9	ARG	3.7
45	2n	45	ARG	3.7
26	14	59	PHE	3.7
33	1b	130	ARG	3.7
44	2m	110	ARG	3.7
53	2y	61	LEU	3.7
34	2c	37	GLN	3.7
53	2y	72	THR	3.7
51	1t	14	LYS	3.7
34	2c	189	ALA	3.7
51	1t	59	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
51	1t	73	HIS	3.7
32	2a	1037	C	3.7
7	2H	8	PRO	3.7
7	2H	97	ARG	3.7
32	2a	1027	C	3.7
51	1t	69	GLY	3.7
26	24	30	GLU	3.7
26	24	65	ASP	3.7
32	2a	1023	G	3.7
32	2a	1283	G	3.7
44	2m	114	ARG	3.6
50	2s	81	ARG	3.6
36	2e	21	ALA	3.6
31	29	31	LYS	3.6
34	2c	162	GLN	3.6
43	2l	19	ARG	3.6
35	2d	11	LEU	3.6
41	1j	54	PHE	3.6
26	24	64	GLY	3.6
45	1n	25	VAL	3.6
52	1u	18	TYR	3.6
1	2A	1090	U	3.6
45	1n	17	LYS	3.6
32	2a	1149	C	3.6
32	2a	1321	C	3.6
19	2X	68	ARG	3.6
7	2H	157	TYR	3.6
7	2H	106	THR	3.6
50	2s	52	TYR	3.6
34	2c	32	LEU	3.6
1	2A	2123	G	3.6
26	24	56	VAL	3.6
40	2i	71	SER	3.6
1	2A	2128	C	3.6
7	2H	71	LEU	3.6
29	27	47	ARG	3.6
45	2n	57	ARG	3.6
7	2H	4	ILE	3.6
40	1i	28	VAL	3.6
45	1n	8	GLU	3.6
53	2y	87	LYS	3.6
7	2H	27	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
31	29	30	PRO	3.5
1	2A	1058	G	3.5
34	1c	10	PHE	3.5
32	1a	1446	U	3.5
35	1d	166	LYS	3.5
38	2g	120	ILE	3.5
51	1t	83	ARG	3.5
53	1y	35	ILE	3.5
32	2a	1373	G	3.5
41	2j	27	ALA	3.5
50	2s	84	GLY	3.5
7	2H	159	GLU	3.5
53	2y	11	GLU	3.5
21	2Z	187	ALA	3.5
34	2c	200	ALA	3.5
1	1A	2119	A	3.5
1	1A	2133	G	3.5
32	2a	1003	G	3.5
32	1a	1029	C	3.5
31	29	10	ILE	3.5
53	2y	16	ILE	3.5
1	2A	1081	U	3.5
53	2y	17	ARG	3.5
35	2d	69	GLY	3.5
7	2H	129	THR	3.5
32	2a	1356	G	3.5
53	2y	6	THR	3.5
32	2a	1006	C	3.5
40	2i	8	GLY	3.5
53	2y	74	ILE	3.5
1	1A	2173	A	3.5
40	2i	122	ALA	3.5
40	2i	19	LEU	3.5
40	2i	64	THR	3.5
45	2n	47	LEU	3.5
29	27	48	LYS	3.4
44	2m	95	GLY	3.4
1	1A	2154	G	3.4
53	2y	75	ASN	3.4
40	2i	44	VAL	3.4
50	2s	8	GLY	3.4
1	1A	2169	A	3.4

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Mol	Chain	Res	Type	RSRZ
1	1A	2174	C	3.4
1	2A	889	C	3.4
1	2A	1086	A	3.4
33	1b	133	LYS	3.4
33	2b	139	LYS	3.4
7	2H	132	ARG	3.4
40	2i	21	PRO	3.4
50	2s	3	ARG	3.4
32	1a	1030(A)	G	3.4
41	2j	71	LEU	3.4
38	1g	156	TRP	3.4
26	24	67	TYR	3.4
35	1d	3	ARG	3.4
40	2i	121	ARG	3.4
34	2c	66	VAL	3.4
45	1n	51	GLY	3.4
45	2n	60	SER	3.4
50	2s	75	ALA	3.4
31	29	12	ASP	3.4
6	2G	142	PRO	3.4
32	1a	182	U	3.4
47	1p	73	LEU	3.4
48	1q	37	LYS	3.4
1	1A	1079	C	3.4
7	2H	130	ARG	3.4
1	2A	1089	G	3.4
31	29	11	CYS	3.4
7	2H	45	VAL	3.4
12	2Q	100	GLY	3.4
32	2a	1219	U	3.4
35	2d	180	GLY	3.4
32	1a	63	C	3.4
32	1a	163	C	3.4
1	1A	229	A	3.4
1	2A	2117	A	3.4
1	1A	2168	G	3.4
40	2i	30	GLY	3.4
51	1t	47	GLY	3.4
45	2n	52	GLN	3.4
1	2A	1026	U	3.4
11	2P	79	ARG	3.4
44	2m	80	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
40	2i	83	ARG	3.4
7	2H	148	ILE	3.3
32	2a	1220	G	3.3
29	17	1	MET	3.3
1	2A	2105	C	3.3
50	2s	56	GLN	3.3
34	2c	188	LEU	3.3
7	2H	113	VAL	3.3
1	2A	1098	A	3.3
1	1A	2156	G	3.3
1	2A	1082	U	3.3
32	2a	1255	G	3.3
34	2c	26	LYS	3.3
40	1i	110	GLU	3.3
6	2G	155	MET	3.3
1	2A	1059	G	3.3
6	2G	131	TYR	3.3
34	2c	8	ILE	3.3
34	2c	35	GLU	3.3
35	2d	158	ILE	3.3
6	2G	58	GLN	3.3
50	1s	29	ARG	3.3
1	2A	2113	U	3.3
32	2a	1150	U	3.3
14	2S	92	TYR	3.3
40	2i	4	TYR	3.3
40	2i	26	VAL	3.3
41	1j	49	VAL	3.3
41	2j	89	ASP	3.3
52	2u	18	TYR	3.3
1	2A	1080	C	3.3
33	2b	97	TRP	3.3
34	2c	149	ALA	3.3
47	1p	7	ALA	3.3
7	2H	21	PRO	3.3
6	2G	139	LEU	3.3
40	2i	56	LEU	3.3
50	2s	44	MET	3.3
7	2H	169	VAL	3.3
34	2c	184	TYR	3.3
7	2H	123	PHE	3.3
33	2b	37	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
34	1c	38	ARG	3.3
53	2y	23	ARG	3.3
1	1A	2137	C	3.3
1	2A	2129	C	3.3
32	1a	1028	C	3.3
36	2e	13	ILE	3.3
40	2i	119	ALA	3.3
1	2A	1087	G	3.3
6	2G	141	PHE	3.2
7	2H	40	GLU	3.2
6	2G	29	TRP	3.2
7	2H	57	ASP	3.2
26	14	55	ARG	3.2
41	2j	43	ARG	3.2
50	2s	33	THR	3.2
7	2H	94	TYR	3.2
14	2S	3	ARG	3.2
53	2y	69	ASP	3.2
8	2I	38	LEU	3.2
26	14	56	VAL	3.2
40	2i	28	VAL	3.2
35	2d	146	ILE	3.2
30	28	46	ARG	3.2
34	2c	28	GLN	3.2
51	1t	80	ARG	3.2
7	2H	98	LEU	3.2
12	2Q	19	GLY	3.2
27	15	60	VAL	3.2
32	2a	1005	A	3.2
32	2a	1248	A	3.2
31	29	24	TYR	3.2
36	2e	109	ILE	3.2
40	2i	124	GLN	3.2
42	1k	25	TYR	3.2
48	1q	38	ARG	3.2
45	1n	15	LYS	3.2
45	2n	9	LYS	3.2
32	2a	1020	U	3.2
6	2G	35	GLU	3.2
47	1p	48	TRP	3.2
53	2y	13	THR	3.2
47	1p	49	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
51	1t	62	LEU	3.2
32	2a	1025	U	3.2
50	2s	57	HIS	3.2
41	1j	44	VAL	3.2
48	1q	27	PHE	3.2
34	2c	160	ALA	3.2
44	1m	90	LEU	3.2
51	2t	84	LEU	3.2
6	2G	75	LYS	3.2
31	29	15	LYS	3.2
51	1t	65	LYS	3.2
26	24	52	THR	3.2
1	1A	2152	G	3.2
40	2i	74	ILE	3.2
32	2a	1236	A	3.1
40	2i	27	THR	3.1
52	1u	17	THR	3.1
6	2G	73	ALA	3.1
7	2H	96	ALA	3.1
34	2c	71	ALA	3.1
41	2j	36	GLY	3.1
1	2A	1093	G	3.1
53	2y	19	HIS	3.1
41	2j	87	THR	3.1
1	1A	2176	A	3.1
1	2A	2178	C	3.1
12	2Q	121	ALA	3.1
35	2d	67	ILE	3.1
41	2j	29	ARG	3.1
41	2j	38	ILE	3.1
40	1i	19	LEU	3.1
48	2q	98	LEU	3.1
1	1A	2148	G	3.1
1	1A	2166	G	3.1
32	1a	1002	G	3.1
45	2n	22	THR	3.1
32	2a	1235	U	3.1
44	2m	68	GLY	3.1
7	2H	88	LEU	3.1
21	2Z	155	LEU	3.1
48	2q	65	ILE	3.1
44	1m	87	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	2A	1100	C	3.1
12	2Q	104	PHE	3.1
40	1i	111	ARG	3.1
1	1A	2157	G	3.1
7	2H	93	GLY	3.1
35	1d	167	GLY	3.1
32	1a	841	U	3.1
35	1d	73	ARG	3.1
51	1t	22	ARG	3.1
53	2y	95	ARG	3.1
22	20	76	GLY	3.1
14	2S	56	LEU	3.1
40	2i	49	PRO	3.1
48	1q	36	ILE	3.1
26	24	58	ARG	3.1
1	1A	2139	C	3.1
1	2A	1092	C	3.1
21	2Z	114	GLY	3.1
32	2a	949	A	3.1
34	2c	95	THR	3.1
53	2y	53	THR	3.1
21	1Z	192	ALA	3.1
53	2y	85	LEU	3.1
40	1i	125	TYR	3.1
45	2n	26	ARG	3.1
7	2H	24	VAL	3.1
1	2A	2158	A	3.1
32	2a	1363(A)	A	3.1
7	2H	10	PRO	3.1
40	1i	63	ILE	3.1
40	1i	105	ASP	3.1
3	1D	275	LYS	3.1
40	2i	87	GLN	3.1
45	2n	23	ARG	3.1
35	2d	6	GLY	3.0
1	2A	2187	G	3.0
6	2G	43	LEU	3.0
44	2m	65	LYS	3.0
52	2u	24	ARG	3.0
53	2y	91	LYS	3.0
1	2A	2163	C	3.0
6	2G	144	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	1A	2158	A	3.0
7	2H	111	HIS	3.0
45	1n	34	TYR	3.0
1	1A	2130	U	3.0
34	1c	168	ALA	3.0
41	2j	17	ASP	3.0
45	2n	31	ARG	3.0
12	2Q	114	ALA	3.0
51	1t	100	ILE	3.0
18	2W	112	GLY	3.0
32	2a	1019	C	3.0
34	2c	41	GLY	3.0
35	2d	4	TYR	3.0
51	1t	68	LYS	3.0
34	2c	177	THR	3.0
7	2H	76	VAL	3.0
52	1u	6	ARG	3.0
26	24	66	SER	3.0
33	2b	232	PRO	3.0
50	2s	2	PRO	3.0
7	2H	174	GLY	3.0
33	2b	127	ILE	3.0
1	1A	2187	G	3.0
7	2H	34	GLU	3.0
34	1c	201	TYR	3.0
34	2c	63	ASN	3.0
40	1i	104	ARG	3.0
51	1t	23	ARG	3.0
34	2c	195	VAL	3.0
34	2c	163	ALA	3.0
7	2H	36	PRO	3.0
34	2c	185	GLY	3.0
45	1n	14	PRO	3.0
35	2d	49	ARG	3.0
38	1g	32	ARG	3.0
51	1t	79	ARG	3.0
6	2G	41	GLN	3.0
1	1A	2136	C	3.0
32	2a	976	G	3.0
34	2c	17	ASP	3.0
14	2S	32	LEU	3.0
21	2Z	96	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
21	2Z	192	ALA	3.0
34	2c	199	LYS	3.0
32	2a	1148	U	3.0
44	2m	100	GLY	3.0
7	1H	2	SER	3.0
36	2e	16	THR	3.0
1	1A	2151	G	3.0
26	24	61	ARG	3.0
44	2m	4	ILE	3.0
50	2s	65	ASN	3.0
41	2j	54	PHE	3.0
44	2m	23	TYR	3.0
7	2H	37	VAL	3.0
44	1m	15	VAL	3.0
47	1p	37	GLY	3.0
52	1u	2	GLY	3.0
7	2H	168	PRO	3.0
32	2a	1362	C	2.9
1	2A	2166	G	2.9
7	2H	65	HIS	2.9
32	2a	1224	G	2.9
40	1i	37	PHE	2.9
33	1b	118	LEU	2.9
50	2s	68	GLY	2.9
44	2m	72	ALA	2.9
1	2A	2164	C	2.9
14	2S	58	LEU	2.9
40	2i	68	GLY	2.9
44	2m	103	THR	2.9
1	1A	2170	A	2.9
31	29	8	LYS	2.9
33	2b	165	VAL	2.9
34	2c	89	GLU	2.9
39	1h	134	ILE	2.9
1	1A	2109	U	2.9
1	1A	2111	C	2.9
40	1i	116	LYS	2.9
40	2i	86	VAL	2.9
1	1A	2123	G	2.9
7	2H	89	ILE	2.9
14	2S	12	PHE	2.9
26	14	46	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
26	24	59	PHE	2.9
40	2i	59	PHE	2.9
40	2i	104	ARG	2.9
44	1m	114	ARG	2.9
1	1A	1083	U	2.9
6	2G	94	LEU	2.9
7	2H	17	VAL	2.9
32	2a	979	C	2.9
32	2a	1039	C	2.9
51	1t	29	LYS	2.9
1	1A	2112	G	2.9
1	2A	2793	G	2.9
47	1p	25	ARG	2.9
51	1t	63	ILE	2.9
1	1A	1085	A	2.9
45	2n	51	GLY	2.9
34	2c	206	GLU	2.9
47	1p	39	TYR	2.9
7	2H	112	PRO	2.9
7	2H	175	LYS	2.9
32	2a	1018	C	2.9
41	2j	60	ARG	2.9
40	2i	37	PHE	2.9
1	1A	2125	G	2.9
1	1A	2181	G	2.9
6	2G	90	LEU	2.9
32	2a	80	G	2.9
41	1j	64	GLU	2.9
44	2m	81	LEU	2.9
26	24	28	LYS	2.9
32	2a	978	A	2.9
32	2a	1285	A	2.9
6	2G	15	VAL	2.9
47	1p	32	TYR	2.9
33	2b	130	ARG	2.9
41	2j	53	PRO	2.9
26	24	46	GLN	2.9
1	2A	1041	C	2.9
1	1A	1071	G	2.9
1	1A	2127	G	2.9
21	2Z	191	VAL	2.9
34	2c	3	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
45	1n	21	TYR	2.9
32	2a	975	A	2.8
41	2j	50	ILE	2.8
52	1u	13	ILE	2.8
33	2b	70	PHE	2.8
33	2b	152	PHE	2.8
40	1i	33	PHE	2.8
40	2i	103	THR	2.8
51	1t	17	ARG	2.8
44	2m	7	VAL	2.8
7	2H	46	GLU	2.8
26	24	54	GLY	2.8
47	1p	59	TRP	2.8
50	2s	70	LYS	2.8
1	2A	1062	G	2.8
32	1a	1024	G	2.8
1	2A	1057	A	2.8
1	2A	1070	A	2.8
51	1t	41	ILE	2.8
38	2g	33	ASP	2.8
42	1k	13	GLN	2.8
50	2s	28	LYS	2.8
35	2d	183	GLY	2.8
1	2A	2171	A	2.8
32	2a	1361	G	2.8
41	2j	85	LEU	2.8
44	2m	66	LEU	2.8
51	1t	45	GLN	2.8
35	1d	179	GLU	2.8
45	1n	13	THR	2.8
7	2H	107	VAL	2.8
41	2j	37	PRO	2.8
7	2H	51	ARG	2.8
3	1D	276	LYS	2.8
39	1h	133	LEU	2.8
45	2n	50	LYS	2.8
26	24	29	PRO	2.8
33	2b	48	MET	2.8
34	2c	61	ALA	2.8
1	1A	889	C	2.8
7	2H	23	ARG	2.8
22	20	74	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
39	1h	38	ILE	2.8
32	2a	1000	U	2.8
38	2g	25	ALA	2.8
41	2j	49	VAL	2.8
1	1A	2104	G	2.8
1	2A	2320	A	2.8
32	2a	998	G	2.8
40	1i	117	HIS	2.8
38	2g	85	TYR	2.8
51	1t	13	LEU	2.8
6	2G	65	GLY	2.8
41	2j	100	THR	2.8
1	1A	1082	U	2.8
7	2H	42	ARG	2.8
38	2g	36	LYS	2.8
40	1i	107	ARG	2.8
40	2i	111	ARG	2.8
41	1j	68	HIS	2.8
1	2A	2206	G	2.8
6	2G	52	ILE	2.8
40	1i	76	ALA	2.7
46	1o	83	GLU	2.7
32	1a	723	U	2.7
50	1s	4	SER	2.7
40	2i	60	ASP	2.7
7	2H	7	LEU	2.7
50	1s	74	PHE	2.7
6	2G	77	ILE	2.7
40	1i	10	ARG	2.7
44	2m	88	ARG	2.7
44	2m	93	ARG	2.7
32	2a	1279	A	2.7
32	2a	1260	C	2.7
47	1p	2	VAL	2.7
40	2i	54	ASP	2.7
35	1d	157	LEU	2.7
41	2j	93	GLY	2.7
51	2t	101	GLY	2.7
1	2A	6	A	2.7
1	2A	1077	A	2.7
1	2A	1096	A	2.7
6	2G	5	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
6	2G	57	ALA	2.7
41	2j	59	SER	2.7
42	1k	60	ALA	2.7
53	2y	94	ALA	2.7
40	2i	105	ASP	2.7
1	1A	2118	U	2.7
22	20	42	GLY	2.7
26	14	53	GLU	2.7
33	2b	118	LEU	2.7
34	2c	85	ARG	2.7
40	2i	40	LEU	2.7
48	1q	86	GLU	2.7
50	2s	36	ARG	2.7
52	2u	21	TYR	2.7
38	2g	27	ILE	2.7
7	2H	29	PRO	2.7
40	2i	123	PRO	2.7
40	1i	108	VAL	2.7
6	2G	86	MET	2.7
6	2G	137	GLU	2.7
36	2e	14	ARG	2.7
40	1i	80	GLY	2.7
1	2A	2122	U	2.7
1	2A	2180	U	2.7
32	2a	1042	G	2.7
7	2H	9	ILE	2.7
7	2H	121	ILE	2.7
33	2b	201	ILE	2.7
43	2l	13	LYS	2.7
50	1s	77	THR	2.7
33	2b	131	PRO	2.7
40	2i	15	ALA	2.7
51	1t	40	ALA	2.7
6	2G	92	VAL	2.7
38	1g	17	VAL	2.7
31	29	19	ARG	2.7
35	2d	3	ARG	2.7
41	2j	9	ARG	2.7
48	1q	91	ARG	2.7
44	1m	48	LEU	2.7
1	2A	1102	C	2.7
1	2A	1084	A	2.7

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Mol	Chain	Res	Type	RSRZ
1	2A	1060	U	2.7
32	1a	102	G	2.7
32	1a	1026	G	2.7
6	2G	151	ALA	2.7
7	2H	47	GLU	2.7
51	1t	61	SER	2.7
7	2H	54	ARG	2.7
46	1o	65	ARG	2.7
43	2l	88	GLY	2.7
6	2G	176	LEU	2.7
53	1y	24	LEU	2.7
34	2c	18	TRP	2.7
35	2d	20	TYR	2.7
7	2H	167	GLU	2.7
1	2A	1042	G	2.7
8	2I	3	VAL	2.7
32	2a	1355	G	2.7
8	2I	88	ILE	2.7
21	2Z	133	ILE	2.7
44	2m	25	ILE	2.7
47	2p	19	ILE	2.7
53	2y	56	THR	2.7
1	1A	2128	C	2.6
1	1A	2185	C	2.6
32	2a	1363	C	2.6
32	2a	1446	U	2.6
34	2c	60	ALA	2.6
32	2a	1288	A	2.6
14	2S	4	LEU	2.6
51	1t	84	LEU	2.6
45	2n	4	LYS	2.6
51	2t	42	GLN	2.6
40	2i	13	ALA	2.6
1	1A	1963	U	2.6
7	2H	43	VAL	2.6
7	2H	114	VAL	2.6
32	2a	1116	C	2.6
1	1A	2126	A	2.6
14	2S	20	ARG	2.6
22	20	11	ARG	2.6
33	1b	36	ARG	2.6
1	2A	2319	G	2.6

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Mol	Chain	Res	Type	RSRZ
2	2B	69	G	2.6
6	2G	161	THR	2.6
7	2H	161	GLY	2.6
32	1a	108	G	2.6
32	1a	146	G	2.6
38	1g	42	ILE	2.6
45	2n	32	SER	2.6
7	2H	156	ALA	2.6
40	2i	45	ALA	2.6
34	2c	64	VAL	2.6
38	1g	80	VAL	2.6
38	2g	37	ASN	2.6
47	1p	20	VAL	2.6
50	1s	58	VAL	2.6
34	2c	101	LEU	2.6
50	1s	20	LEU	2.6
1	1A	2138	C	2.6
39	2h	4	ASP	2.6
47	2p	9	PHE	2.6
7	2H	72	ILE	2.6
7	2H	92	ILE	2.6
7	2H	151	ILE	2.6
34	2c	39	ILE	2.6
53	2y	35	ILE	2.6
6	2G	32	PRO	2.6
53	2y	82	GLU	2.6
1	2A	1055	G	2.6
1	2A	2112	G	2.6
7	2H	141	VAL	2.6
8	1I	19	VAL	2.6
32	1a	1034	G	2.6
6	2G	175	LEU	2.6
35	2d	78	LEU	2.6
32	2a	1348	U	2.6
35	2d	75	PHE	2.6
21	2Z	142	SER	2.6
53	2y	92	GLY	2.6
7	2H	32	GLU	2.6
38	2g	7	ALA	2.6
51	2t	6	PRO	2.6
53	2y	37	PRO	2.6
32	1a	101	A	2.6

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Mol	Chain	Res	Type	RSRZ
44	2m	104	ARG	2.6
34	1c	89	GLU	2.6
39	2h	131	GLY	2.6
45	2n	58	LYS	2.6
46	2o	89	GLY	2.6
7	2H	126	PRO	2.6
35	2d	115	ARG	2.6
40	2i	93	ARG	2.6
7	2H	44	VAL	2.6
53	2y	18	GLN	2.6
32	1a	161	A	2.6
38	2g	101	LEU	2.6
40	2i	32	ASP	2.6
50	1s	71	LEU	2.6
26	24	17	GLY	2.6
36	2e	26	PHE	2.6
44	2m	24	GLY	2.6
31	29	18	ARG	2.6
43	1l	19	ARG	2.6
41	2j	91	PRO	2.6
34	2c	193	TYR	2.6
44	2m	106	ASN	2.6
32	1a	1369	C	2.6
40	2i	70	LYS	2.6
6	1G	49	ASP	2.6
41	2j	94	VAL	2.6
6	1G	82	LEU	2.6
39	1h	112	LEU	2.6
50	2s	5	LEU	2.6
22	20	8	GLY	2.6
1	1A	2171	A	2.6
32	2a	977	A	2.6
6	2G	112	PRO	2.5
1	2A	1115	G	2.5
7	2H	163	TYR	2.5
31	29	32	HIS	2.5
34	2c	58	GLU	2.5
43	2l	16	GLU	2.5
1	1A	2163	C	2.5
6	2G	80	PHE	2.5
21	2Z	4	ARG	2.5
14	2S	57	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
30	28	21	LYS	2.5
6	2G	108	ASN	2.5
6	2G	88	ILE	2.5
31	29	26	ILE	2.5
32	2a	1004	A	2.5
32	2a	1256	A	2.5
41	1j	17	ASP	2.5
6	2G	134	GLY	2.5
45	1n	38	GLY	2.5
32	1a	181	G	2.5
44	2m	111	LYS	2.5
1	1A	2188	C	2.5
32	1a	217	C	2.5
45	2n	27	CYS	2.5
26	24	7	PRO	2.5
51	1t	64	ASP	2.5
52	2u	8	THR	2.5
40	1i	114	TYR	2.5
40	2i	10	ARG	2.5
53	2y	89	GLN	2.5
1	2A	1063	G	2.5
1	2A	34	C	2.5
40	1i	119	ALA	2.5
43	1l	23	LYS	2.5
47	1p	4	ILE	2.5
29	17	47	ARG	2.5
32	1a	180	U	2.5
51	1t	75	ASN	2.5
51	2t	9	ASN	2.5
7	2H	30	LYS	2.5
22	20	55	ARG	2.5
1	2A	1044	G	2.5
1	2A	2183	C	2.5
41	2j	74	ILE	2.5
53	2y	59	GLY	2.5
7	2H	52	VAL	2.5
40	1i	26	VAL	2.5
41	2j	55	LYS	2.5
35	2d	16	GLY	2.5
43	2l	51	ALA	2.5
46	1o	89	GLY	2.5
32	2a	1017	G	2.5

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Mol	Chain	Res	Type	RSRZ
32	2a	1353	G	2.5
44	2m	99	ARG	2.5
40	2i	80	GLY	2.5
48	1q	33	GLY	2.5
31	29	28	GLU	2.5
40	1i	15	ALA	2.5
40	2i	117	HIS	2.5
41	2j	56	HIS	2.5
50	1s	75	ALA	2.5
50	2s	64	GLU	2.5
51	1t	33	ILE	2.5
33	2b	121	LEU	2.5
43	1l	91	LYS	2.5
45	1n	33	VAL	2.5
6	2G	25	TYR	2.5
1	1A	34	C	2.5
34	2c	186	PHE	2.5
44	2m	101	GLN	2.4
53	2y	76	GLU	2.4
6	2G	38	VAL	2.4
47	2p	48	TRP	2.4
44	1m	102	ARG	2.4
48	1q	25	ARG	2.4
53	1y	83	ARG	2.4
1	2A	2177	C	2.4
34	2c	158	GLY	2.4
22	20	75	LEU	2.4
26	24	33	VAL	2.4
33	2b	233	SER	2.4
44	1m	117	VAL	2.4
34	1c	63	ASN	2.4
35	2d	33	MET	2.4
40	2i	57	GLY	2.4
50	2s	72	GLY	2.4
6	2G	6	ALA	2.4
32	2a	1038	C	2.4
6	2G	82	LEU	2.4
35	2d	73	ARG	2.4
40	2i	16	ARG	2.4
43	2l	89	ARG	2.4
44	2m	108	ARG	2.4
51	2t	13	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
50	1s	38	SER	2.4
6	2G	109	VAL	2.4
7	2H	85	LYS	2.4
22	20	46	LYS	2.4
32	2a	1258	G	2.4
33	1b	228	GLY	2.4
35	2d	48	ALA	2.4
44	1m	108	ARG	2.4
21	2Z	5	LEU	2.4
51	1t	77	ALA	2.4
1	2A	1072	C	2.4
32	2a	1114	C	2.4
32	2a	1259	C	2.4
51	2t	100	ILE	2.4
52	2u	3	LYS	2.4
33	2b	81	VAL	2.4
48	2q	10	VAL	2.4
6	2G	178	PHE	2.4
32	1a	144	G	2.4
51	2t	83	ARG	2.4
34	2c	121	ALA	2.4
36	2e	17	ALA	2.4
32	1a	1035	A	2.4
1	1A	2180	U	2.4
6	2G	149	VAL	2.4
32	1a	103	C	2.4
23	21	26	ARG	2.4
45	1n	11	LYS	2.4
3	2D	2	ALA	2.4
8	2I	46	ALA	2.4
44	2m	60	VAL	2.4
1	2A	887	A	2.4
1	2A	2114	A	2.4
32	2a	1360	A	2.4
32	2a	1492	A	2.4
1	1A	2175	C	2.4
6	2G	72	ARG	2.4
7	2H	3	ARG	2.4
32	1a	219	C	2.4
32	2a	990	C	2.4
38	1g	13	GLN	2.4
40	2i	31	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
29	17	45	ALA	2.4
21	2Z	201	LYS	2.4
44	2m	13	LYS	2.4
7	2H	99	VAL	2.4
35	1d	50	ARG	2.4
41	2j	70	ARG	2.4
32	1a	1020	U	2.3
32	1a	1004	A	2.3
32	2a	1367	C	2.3
47	1p	58	TYR	2.3
19	2X	92	LEU	2.3
9	2N	81	GLY	2.3
14	2S	93	LYS	2.3
40	2i	112	LYS	2.3
41	2j	57	LYS	2.3
43	2l	46	LYS	2.3
9	2N	74	ARG	2.3
35	1d	70	ILE	2.3
1	1A	2110	G	2.3
32	2a	1138	G	2.3
6	2G	148	MET	2.3
43	1l	64	TYR	2.3
52	2u	5	ASP	2.3
7	2H	145	ALA	2.3
12	2Q	61	GLY	2.3
41	2j	35	SER	2.3
40	1i	83	ARG	2.3
40	1i	120	ARG	2.3
40	1i	121	ARG	2.3
6	2G	63	ILE	2.3
7	2H	173	PRO	2.3
26	14	51	ASP	2.3
35	2d	7	PRO	2.3
1	2A	1113	U	2.3
26	14	54	GLY	2.3
32	1a	1003	G	2.3
32	1a	1023	G	2.3
38	2g	8	GLU	2.3
42	2k	25	TYR	2.3
44	2m	75	ALA	2.3
44	2m	96	LEU	2.3
53	2y	81	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	1A	2135	A	2.3
32	2a	1447	A	2.3
37	1f	52	ILE	2.3
40	1i	118	LYS	2.3
45	1n	16	PHE	2.3
6	1G	48	GLU	2.3
6	2G	150	ASP	2.3
44	2m	69	GLU	2.3
33	1b	144	ARG	2.3
51	1t	53	LEU	2.3
47	1p	67	THR	2.3
1	2A	1105	U	2.3
1	2A	1074	G	2.3
1	1A	2103	C	2.3
32	2a	1045	C	2.3
38	2g	78	ARG	2.3
11	2P	109	GLY	2.3
40	1i	8	GLY	2.3
7	2H	80	SER	2.3
38	2g	28	ASN	2.3
41	2j	16	LEU	2.3
45	1n	39	LEU	2.3
51	1t	43	LEU	2.3
21	2Z	199	LYS	2.3
40	2i	11	LYS	2.3
47	1p	56	ALA	2.3
51	1t	38	LYS	2.3
1	2A	1101	U	2.3
32	1a	1000	U	2.3
50	1s	19	VAL	2.3
1	1A	1176	G	2.3
1	2A	1114	G	2.3
32	1a	145	G	2.3
32	1a	1187	G	2.3
32	2a	1024	G	2.3
40	2i	120	ARG	2.3
49	2r	87	ARG	2.3
41	2j	31	GLY	2.3
44	2m	26	GLY	2.3
36	2e	10	MET	2.3
40	1i	11	LYS	2.3
32	2a	958	A	2.3

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Mol	Chain	Res	Type	RSRZ
33	2b	44	LEU	2.3
38	2g	16	LEU	2.3
41	2j	69	ASN	2.3
7	2H	83	TYR	2.3
33	2b	231	GLU	2.3
41	2j	61	GLU	2.3
32	2a	991	U	2.3
39	1h	93	VAL	2.3
47	1p	51	VAL	2.3
6	2G	182	LYS	2.3
1	2A	1112	G	2.3
1	2A	2181	G	2.3
47	1p	41	PRO	2.3
26	24	1	MET	2.3
32	1a	194	C	2.3
36	1e	21	ALA	2.3
38	1g	85	TYR	2.3
32	2a	1250	A	2.3
32	2a	1319	A	2.3
6	2G	51	ARG	2.3
14	2S	17	ARG	2.3
31	29	17	ILE	2.3
9	2N	140	VAL	2.3
41	2j	77	PRO	2.2
50	2s	38	SER	2.2
51	1t	26	ASN	2.2
40	1i	7	THR	2.2
1	1A	2160	G	2.2
1	1A	2165	G	2.2
1	1A	2184	G	2.2
1	2A	2182	G	2.2
14	2S	11	LYS	2.2
32	1a	100	C	2.2
32	2a	1068	G	2.2
33	2b	132	LYS	2.2
40	2i	51	ARG	2.2
44	2m	94	ARG	2.2
2	2B	58	A	2.2
21	2Z	128	VAL	2.2
45	2n	28	GLY	2.2
50	1s	56	GLN	2.2
34	2c	178	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
26	24	62	ARG	2.2
33	2b	92	TYR	2.2
1	1A	2131	G	2.2
1	1A	2182	G	2.2
1	2A	1039	G	2.2
21	2Z	197	ILE	2.2
35	2d	56	VAL	2.2
26	24	8	LYS	2.2
48	1q	28	PRO	2.2
50	2s	32	LYS	2.2
51	1t	82	SER	2.2
32	1a	1005	A	2.2
34	2c	197	GLY	2.2
33	2b	164	VAL	2.2
41	1j	57	LYS	2.2
22	20	9	SER	2.2
30	28	62	LEU	2.2
40	1i	51	ARG	2.2
45	2n	19	ARG	2.2
44	1m	82	MET	2.2
32	1a	1183	A	2.2
45	1n	30	ALA	2.2
21	2Z	179	ASP	2.2
22	20	10	THR	2.2
6	2G	177	GLY	2.2
22	20	52	GLY	2.2
26	14	45	GLY	2.2
34	2c	13	GLY	2.2
8	1I	29	TYR	2.2
6	2G	28	VAL	2.2
12	2Q	132	VAL	2.2
7	2H	16	SER	2.2
40	1i	42	ARG	2.2
43	1l	89	ARG	2.2
47	1p	26	ARG	2.2
7	2H	87	LEU	2.2
1	1A	1104	C	2.2
32	2a	1320	C	2.2
44	1m	28	ALA	2.2
1	2A	1097	U	2.2
12	2Q	33	GLY	2.2
35	2d	61	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
42	2k	87	THR	2.2
1	1A	1095	A	2.2
1	2A	866	A	2.2
1	2A	2750	A	2.2
26	24	32	TYR	2.2
39	1h	58	TYR	2.2
41	1j	47	PHE	2.2
14	2S	82	ILE	2.2
21	2Z	171	ILE	2.2
33	1b	136	VAL	2.2
34	2c	30	ARG	2.2
48	1q	97	SER	2.2
7	2H	116	GLU	2.2
26	14	57	GLU	2.2
3	2D	167	GLY	2.2
32	2a	1008	C	2.2
32	2a	1223	C	2.2
32	2a	1254	C	2.2
45	1n	22	THR	2.2
14	2S	13	ARG	2.2
33	1b	175	ARG	2.2
44	2m	3	ARG	2.2
1	1A	2124	G	2.2
6	1G	146	TYR	2.2
32	2a	951	G	2.2
40	2i	23	ASN	2.2
53	1y	49	VAL	2.2
1	2A	890	A	2.2
34	1c	94	LEU	2.2
43	2l	28	LYS	2.2
6	2G	138	GLN	2.2
53	1y	82	GLU	2.2
34	2c	56	ASP	2.2
26	24	55	ARG	2.2
45	1n	29	ARG	2.2
14	2S	33	LYS	2.1
40	2i	25	LYS	2.1
12	2Q	34	LEU	2.1
1	2A	883	G	2.1
6	2G	49	ASP	2.1
32	2a	1368	G	2.1
32	2a	968	A	2.1

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Mol	Chain	Res	Type	RSRZ
40	1i	115	GLY	2.1
40	2i	55	ALA	2.1
6	2G	59	GLU	2.1
48	1q	66	SER	2.1
53	1y	58	ASN	2.1
32	2a	91	C	2.1
1	2A	271(K)	U	2.1
1	2A	958	U	2.1
6	2G	159	VAL	2.1
14	2S	14	VAL	2.1
43	2l	64	TYR	2.1
50	2s	58	VAL	2.1
7	2H	64	LEU	2.1
35	2d	162	LEU	2.1
6	1G	73	ALA	2.1
14	2S	86	ALA	2.1
29	27	1	MET	2.1
32	1a	184	G	2.1
32	2a	378	G	2.1
32	2a	1064	G	2.1
51	2t	26	ASN	2.1
3	1D	142	VAL	2.1
12	2Q	35	VAL	2.1
39	1h	53	VAL	2.1
1	2A	645	C	2.1
4	2E	52	LEU	2.1
34	2c	31	HIS	2.1
44	2m	92	HIS	2.1
38	2g	6	ARG	2.1
31	29	5	ALA	2.1
44	2m	82	MET	2.1
33	2b	181	PHE	2.1
50	2s	23	ASN	2.1
41	1j	59	SER	2.1
1	1A	1057	A	2.1
32	1a	262	A	2.1
25	23	17	LYS	2.1
30	28	38	GLY	2.1
34	1c	178	LEU	2.1
34	2c	40	ARG	2.1
38	2g	29	LYS	2.1
39	1h	86	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
45	1n	26	ARG	2.1
47	1p	38	TYR	2.1
50	1s	61	TYR	2.1
53	2y	43	LYS	2.1
32	1a	307	C	2.1
41	2j	97	GLU	2.1
40	1i	45	ALA	2.1
53	1y	94	ALA	2.1
38	2g	31	MET	2.1
51	1t	85	MET	2.1
7	2H	74	ASN	2.1
50	2s	78	ARG	2.1
6	2G	173	LEU	2.1
19	1X	95	LEU	2.1
19	2X	66	LEU	2.1
34	2c	57	ILE	2.1
34	2c	120	VAL	2.1
44	2m	98	VAL	2.1
47	2p	79	VAL	2.1
32	1a	1224	G	2.1
32	2a	963	G	2.1
32	2a	969	A	2.1
32	2a	1323	G	2.1
48	1q	95	TYR	2.1
1	2A	1066	U	2.1
21	2Z	188	ALA	2.1
32	2a	1012	U	2.1
38	2g	116	ALA	2.1
1	2A	1040	C	2.1
31	29	33	LYS	2.1
35	1d	61	LYS	2.1
44	1m	116	THR	2.1
7	2H	170	ARG	2.1
12	2Q	5	ARG	2.1
34	2c	164	ARG	2.1
48	2q	91	ARG	2.1
35	2d	23	GLY	2.1
14	2S	40	ILE	2.1
25	23	54	VAL	2.1
40	2i	47	LEU	2.1
44	2m	90	LEU	2.1
33	1b	214	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
51	1t	16	HIS	2.1
31	29	27	CYS	2.1
33	2b	95	GLN	2.1
1	1A	529	A	2.1
14	2S	51	ALA	2.1
32	1a	70	G	2.1
32	2a	532	A	2.1
32	2a	993	G	2.1
32	2a	1022	G	2.1
53	2y	83	ARG	2.1
1	2A	886	C	2.1
4	2E	115	GLY	2.1
34	2c	34	LEU	2.1
34	1c	39	ILE	2.1
38	2g	80	VAL	2.1
7	2H	62	LYS	2.1
33	1b	132	LYS	2.1
35	2d	166	LYS	2.1
26	24	18	CYS	2.1
7	2H	20	ALA	2.1
40	2i	52	ALA	2.1
49	1r	73	ALA	2.1
51	1t	32	ALA	2.1
21	2Z	82	ARG	2.1
45	1n	3	ARG	2.1
52	1u	22	ARG	2.1
38	2g	144	MET	2.1
1	1A	1097	U	2.0
32	1a	1025	U	2.0
32	2a	1280	A	2.1
33	2b	113	HIS	2.0
36	2e	105	VAL	2.0
44	1m	74	VAL	2.0
6	2G	110	ALA	2.0
34	2c	38	ARG	2.0
47	1p	57	ARG	2.0
33	1b	129	GLU	2.0
42	2k	117	ASN	2.0
30	28	17	THR	2.0
34	2c	194	GLY	2.0
8	2I	12	LEU	2.0
32	2a	950	U	2.0

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Mol	Chain	Res	Type	RSRZ
34	1c	204	LEU	2.0
1	1A	887	A	2.0
1	2A	2115	G	2.0
7	2H	144	VAL	2.0
34	2c	76	VAL	2.0
15	2T	110	ILE	2.0
34	1c	124	ILE	2.0
34	2c	174	PRO	2.0
36	2e	11	ILE	2.0
44	2m	113	PRO	2.0
31	29	22	ARG	2.0
32	2a	1218	C	2.0
40	1i	20	ARG	2.0
7	2H	150	ALA	2.0
40	1i	43	ALA	2.0
53	2y	79	ASN	2.0
41	2j	15	THR	2.0
43	1l	20	LYS	2.0
36	2e	84	PHE	2.0
41	1j	63	PHE	2.0
23	11	98	LEU	2.0
34	1c	12	LEU	2.0
38	2g	22	LEU	2.0
1	1A	272(A)	U	2.0
6	2G	95	ARG	2.0
21	1Z	203	GLU	2.0
32	1a	173	U	2.0
34	1c	179	ARG	2.0
41	1j	41	PRO	2.0
50	2s	43	GLU	2.0
52	1u	10	ARG	2.0
33	2b	223	ILE	2.0
34	1c	182	ILE	2.0
43	1l	7	ILE	2.0
22	20	78	TYR	2.0
32	1a	197	A	2.0
32	1a	218	C	2.0
32	1a	1019	C	2.0
32	2a	970	C	2.0
33	2b	123	ALA	2.0
34	2c	4	LYS	2.0
36	2e	133	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
53	1y	98	ALA	2.0
34	2c	154	SER	2.0
53	1y	72	THR	2.0
47	1p	80	PHE	2.0
21	2Z	80	ARG	2.0
35	2d	118	ARG	2.0
50	2s	37	ARG	2.0
7	2H	19	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
43	0TD	2l	92	10/11	0.86	0.22	65,71,73,93	0
1	PSU	2A	1911	20/21	0.88	0.14	69,77,90,92	0
32	5MC	2a	967	21/22	0.90	0.25	71,78,88,88	0
32	2MG	2a	1207	24/25	0.90	0.25	89,94,98,101	0
1	5MU	1A	1915	21/22	0.90	0.17	73,81,86,90	0
32	M2G	2a	966	25/26	0.91	0.19	65,72,87,92	0
1	PSU	1A	1917	20/21	0.91	0.15	70,75,86,86	0
1	5MU	2A	1915	21/22	0.91	0.12	80,89,96,109	0
1	PSU	2A	1917	20/21	0.91	0.14	78,83,98,100	0
43	0TD	1l	92	10/11	0.92	0.28	56,60,66,80	0
32	2MG	1a	1207	24/25	0.92	0.19	72,78,83,86	0
32	MA6	2a	1519	24/25	0.94	0.26	61,67,71,74	0
32	5MC	2a	1404	21/22	0.94	0.20	58,64,70,70	0
32	PSU	1a	516	20/21	0.95	0.15	63,68,74,75	0
32	5MC	2a	1400	21/22	0.95	0.30	72,76,80,83	0
32	4OC	2a	1402	22/23	0.95	0.20	61,69,73,74	0
32	PSU	2a	516	20/21	0.95	0.16	79,81,87,87	0
32	5MC	2a	1407	21/22	0.95	0.15	62,68,74,77	0
32	MA6	2a	1518	24/25	0.95	0.21	57,67,73,75	0
32	5MC	1a	967	21/22	0.95	0.22	66,72,80,82	0
1	PSU	1A	1911	20/21	0.95	0.15	63,70,72,72	0
32	M2G	1a	966	25/26	0.96	0.21	60,66,73,78	0
32	UR3	2a	1498	21/22	0.96	0.19	58,65,71,74	0
32	G7M	2a	527	24/25	0.96	0.19	68,73,75,77	0
32	5MC	1a	1404	21/22	0.96	0.21	51,54,60,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	OMC	2A	1920	21/22	0.96	0.16	63,73,78,82	0
32	G7M	1a	527	24/25	0.97	0.20	49,58,62,67	0
32	5MC	1a	1407	21/22	0.97	0.19	48,56,61,63	0
32	UR3	1a	1498	21/22	0.97	0.20	48,54,60,70	0
1	2MA	2A	2503	23/24	0.97	0.21	30,38,42,44	0
1	OMU	2A	2552	21/22	0.97	0.19	36,42,46,50	0
32	MA6	1a	1518	24/25	0.97	0.22	46,52,57,59	0
32	MA6	1a	1519	24/25	0.97	0.23	44,52,58,60	0
1	OMC	1A	1920	21/22	0.97	0.21	53,58,63,66	0
32	4OC	1a	1402	22/23	0.97	0.21	48,57,60,64	0
1	2MA	1A	2503	23/24	0.98	0.23	20,28,31,31	0
1	PSU	1A	2605	20/21	0.98	0.19	26,30,36,37	0
1	5MU	2A	1939	21/22	0.98	0.21	36,41,45,46	0
1	5MC	2A	1942	21/22	0.98	0.18	46,56,60,61	0
1	5MC	2A	1962	21/22	0.98	0.19	44,50,54,63	0
1	OMG	2A	2251	24/25	0.98	0.21	37,41,44,48	0
32	5MC	1a	1400	21/22	0.98	0.20	53,60,64,67	0
1	5MU	1A	1939	21/22	0.98	0.21	26,32,36,37	0
1	PSU	2A	2605	20/21	0.98	0.21	35,41,44,44	0
1	5MC	1A	1942	21/22	0.98	0.19	34,38,42,43	0
1	5MC	1A	1962	21/22	0.98	0.20	29,37,43,45	0
1	OMG	1A	2251	24/25	0.99	0.21	26,30,33,35	0
1	OMU	1A	2552	21/22	0.99	0.25	27,33,35,38	0

6.3 Carbohydrates (i)

There are no monosaccharides 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	1G	201	1/1	0.32	0.16	77,77,77,77	0
54	MG	2A	3380	1/1	0.37	0.34	59,59,59,59	0
54	MG	1A	3986	1/1	0.38	0.20	43,43,43,43	0
54	MG	2A	3204	1/1	0.39	0.29	68,68,68,68	0
54	MG	1a	1795	1/1	0.40	0.44	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3558	1/1	0.40	0.18	45,45,45,45	0
54	MG	1a	1743	1/1	0.43	0.22	87,87,87,87	0
54	MG	1A	3890	1/1	0.44	0.11	50,50,50,50	0
54	MG	2A	3409	1/1	0.45	0.29	84,84,84,84	0
54	MG	15	105	1/1	0.47	0.26	56,56,56,56	0
54	MG	2O	202	1/1	0.47	0.19	80,80,80,80	0
54	MG	2A	3644	1/1	0.49	0.14	62,62,62,62	0
54	MG	1a	1865	1/1	0.50	0.12	76,76,76,76	0
54	MG	2a	3016	1/1	0.50	0.24	89,89,89,89	0
54	MG	1g	201	1/1	0.51	0.21	67,67,67,67	0
54	MG	1a	1836	1/1	0.53	0.13	84,84,84,84	0
54	MG	2A	3345	1/1	0.53	0.23	80,80,80,80	0
54	MG	1A	3688	1/1	0.54	0.72	70,70,70,70	0
54	MG	1A	3838	1/1	0.54	0.11	60,60,60,60	0
54	MG	2A	3242	1/1	0.54	0.21	66,66,66,66	0
54	MG	2A	3451	1/1	0.54	0.12	70,70,70,70	0
54	MG	1A	3261	1/1	0.55	0.20	86,86,86,86	0
54	MG	2a	3158	1/1	0.55	0.10	68,68,68,68	0
54	MG	1A	3662	1/1	0.56	0.14	45,45,45,45	0
54	MG	1A	3872	1/1	0.56	0.21	75,75,75,75	0
54	MG	1E	306	1/1	0.56	0.45	70,70,70,70	0
54	MG	2F	303	1/1	0.57	0.30	59,59,59,59	0
54	MG	1A	3558	1/1	0.57	0.26	64,64,64,64	0
54	MG	1A	4040	1/1	0.57	0.21	63,63,63,63	0
54	MG	1A	3437	1/1	0.57	0.23	59,59,59,59	0
54	MG	2a	3191	1/1	0.57	0.14	88,88,88,88	0
54	MG	2B	215	1/1	0.58	0.11	75,75,75,75	0
54	MG	2a	3033	1/1	0.58	0.15	65,65,65,65	0
54	MG	1A	3703	1/1	0.58	0.41	59,59,59,59	0
54	MG	1A	3849	1/1	0.58	0.17	71,71,71,71	0
54	MG	1A	3364	1/1	0.59	0.26	48,48,48,48	0
54	MG	2A	3034	1/1	0.59	0.42	87,87,87,87	0
54	MG	2A	3190	1/1	0.59	0.48	75,75,75,75	0
54	MG	2A	3400	1/1	0.59	0.25	83,83,83,83	0
54	MG	1a	1675	1/1	0.59	0.24	84,84,84,84	0
54	MG	1a	1684	1/1	0.61	0.15	78,78,78,78	0
54	MG	2A	3579	1/1	0.61	0.17	62,62,62,62	0
54	MG	2G	202	1/1	0.61	0.16	80,80,80,80	0
54	MG	1a	1699	1/1	0.61	0.11	64,64,64,64	0
54	MG	1a	1689	1/1	0.62	0.12	70,70,70,70	0
54	MG	2A	3672	1/1	0.62	0.16	48,48,48,48	0
54	MG	1A	4017	1/1	0.62	0.21	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	3014	1/1	0.62	0.12	63,63,63,63	0
54	MG	2a	3194	1/1	0.62	0.11	86,86,86,86	0
54	MG	1A	3235	1/1	0.63	0.16	79,79,79,79	0
54	MG	1a	1860	1/1	0.63	0.27	79,79,79,79	0
54	MG	1a	1820	1/1	0.63	0.14	68,68,68,68	0
54	MG	2A	3580	1/1	0.63	0.12	54,54,54,54	0
54	MG	2A	3405	1/1	0.64	0.20	49,49,49,49	0
54	MG	2A	3616	1/1	0.64	0.10	58,58,58,58	0
54	MG	1A	3924	1/1	0.64	0.27	37,37,37,37	0
54	MG	2A	3442	1/1	0.64	0.18	69,69,69,69	0
54	MG	1A	3002	1/1	0.64	0.24	53,53,53,53	0
54	MG	1B	217	1/1	0.64	0.17	67,67,67,67	0
54	MG	1a	1802	1/1	0.64	0.15	90,90,90,90	0
54	MG	2A	3092	1/1	0.65	0.16	65,65,65,65	0
54	MG	2A	3124	1/1	0.65	0.17	76,76,76,76	0
54	MG	1A	3930	1/1	0.65	0.14	63,63,63,63	0
54	MG	1a	1821	1/1	0.65	0.29	78,78,78,78	0
54	MG	2A	3207	1/1	0.65	0.15	74,74,74,74	0
54	MG	2a	3055	1/1	0.65	0.10	74,74,74,74	0
54	MG	1a	1863	1/1	0.65	0.20	78,78,78,78	0
54	MG	2a	3187	1/1	0.65	0.15	74,74,74,74	0
54	MG	2A	3343	1/1	0.65	0.17	85,85,85,85	0
54	MG	2A	3474	1/1	0.65	0.31	58,58,58,58	0
54	MG	2a	3079	1/1	0.66	0.15	85,85,85,85	0
54	MG	2A	3175	1/1	0.66	0.32	75,75,75,75	0
54	MG	1a	1855	1/1	0.66	0.13	86,86,86,86	0
54	MG	2A	3098	1/1	0.66	0.25	67,67,67,67	0
54	MG	1A	3935	1/1	0.66	0.15	53,53,53,53	0
54	MG	18	101	1/1	0.67	0.29	77,77,77,77	0
54	MG	2A	3649	1/1	0.67	0.15	76,76,76,76	0
54	MG	1A	3860	1/1	0.67	0.11	85,85,85,85	0
54	MG	2A	3371	1/1	0.67	0.12	74,74,74,74	0
54	MG	1a	1768	1/1	0.67	0.13	74,74,74,74	0
54	MG	1A	3900	1/1	0.67	0.14	59,59,59,59	0
54	MG	1a	1859	1/1	0.67	0.18	78,78,78,78	0
54	MG	1A	3270	1/1	0.67	0.51	65,65,65,65	0
54	MG	1A	3359	1/1	0.68	0.16	41,41,41,41	0
54	MG	1a	1654	1/1	0.68	0.25	80,80,80,80	0
54	MG	1a	1655	1/1	0.68	0.16	76,76,76,76	0
54	MG	1A	3996	1/1	0.68	0.80	62,62,62,62	0
54	MG	1A	3581	1/1	0.68	0.27	53,53,53,53	0
54	MG	1a	1874	1/1	0.68	0.16	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3077	1/1	0.68	0.15	75,75,75,75	0
54	MG	11	104	1/1	0.68	0.14	55,55,55,55	0
54	MG	2a	3153	1/1	0.68	0.09	78,78,78,78	0
54	MG	2A	3657	1/1	0.68	0.25	45,45,45,45	0
54	MG	2A	3414	1/1	0.68	0.10	91,91,91,91	0
54	MG	2A	3235	1/1	0.68	0.26	83,83,83,83	0
54	MG	1A	3656	1/1	0.68	0.15	55,55,55,55	0
54	MG	2A	3693	1/1	0.69	0.30	60,60,60,60	0
54	MG	2A	3728	1/1	0.69	0.12	87,87,87,87	0
54	MG	2A	3729	1/1	0.69	0.22	82,82,82,82	0
54	MG	1A	3812	1/1	0.69	0.07	78,78,78,78	0
54	MG	1A	3435	1/1	0.69	0.19	39,39,39,39	0
54	MG	1A	3456	1/1	0.69	0.21	64,64,64,64	0
54	MG	1A	3962	1/1	0.69	0.19	53,53,53,53	0
54	MG	1a	1719	1/1	0.69	0.13	75,75,75,75	0
54	MG	2A	3208	1/1	0.69	0.33	77,77,77,77	0
54	MG	2A	3221	1/1	0.69	0.39	65,65,65,65	0
54	MG	1A	3555	1/1	0.69	0.18	44,44,44,44	0
54	MG	1a	1759	1/1	0.69	0.20	76,76,76,76	0
54	MG	1A	3741	1/1	0.69	0.12	51,51,51,51	0
54	MG	2a	3124	1/1	0.69	0.09	80,80,80,80	0
54	MG	2A	3628	1/1	0.69	0.23	90,90,90,90	0
54	MG	1a	1607	1/1	0.69	0.12	67,67,67,67	0
54	MG	1A	3777	1/1	0.69	0.19	38,38,38,38	0
54	MG	1a	1818	1/1	0.69	0.10	86,86,86,86	0
54	MG	1A	3786	1/1	0.69	0.09	51,51,51,51	0
54	MG	19	102	1/1	0.70	0.33	79,79,79,79	0
54	MG	2A	3016	1/1	0.70	0.18	74,74,74,74	0
54	MG	2A	3384	1/1	0.70	0.21	60,60,60,60	0
54	MG	2A	3596	1/1	0.70	0.17	49,49,49,49	0
54	MG	1a	1659	1/1	0.70	0.12	64,64,64,64	0
54	MG	2a	3025	1/1	0.70	0.20	70,70,70,70	0
54	MG	1A	3579	1/1	0.70	0.09	62,62,62,62	0
54	MG	2a	3041	1/1	0.70	0.12	86,86,86,86	0
54	MG	2a	3052	1/1	0.70	0.14	87,87,87,87	0
54	MG	1a	1641	1/1	0.70	0.31	81,81,81,81	0
54	MG	1A	3833	1/1	0.70	0.17	63,63,63,63	0
54	MG	2A	3138	1/1	0.70	0.28	62,62,62,62	0
54	MG	1a	1781	1/1	0.70	0.09	90,90,90,90	0
54	MG	2A	3684	1/1	0.70	0.18	51,51,51,51	0
54	MG	2A	3185	1/1	0.70	0.13	86,86,86,86	0
54	MG	2A	3499	1/1	0.70	0.08	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3509	1/1	0.70	0.19	65,65,65,65	0
54	MG	2A	3557	1/1	0.70	0.24	43,43,43,43	0
54	MG	2A	3109	1/1	0.71	0.15	73,73,73,73	0
54	MG	2A	3301	1/1	0.71	0.21	60,60,60,60	0
54	MG	1A	3888	1/1	0.71	0.14	38,38,38,38	0
54	MG	1A	3624	1/1	0.71	0.25	34,34,34,34	0
54	MG	2A	3426	1/1	0.71	0.36	59,59,59,59	0
54	MG	2A	3441	1/1	0.71	0.20	67,67,67,67	0
54	MG	2A	3736	1/1	0.71	0.34	86,86,86,86	0
54	MG	2A	3593	1/1	0.71	0.11	72,72,72,72	0
54	MG	1A	3790	1/1	0.71	0.23	61,61,61,61	0
54	MG	2a	3157	1/1	0.71	0.25	93,93,93,93	0
54	MG	1i	201	1/1	0.71	0.18	77,77,77,77	0
54	MG	2A	3460	1/1	0.71	0.15	64,64,64,64	0
54	MG	2A	3189	1/1	0.71	0.30	66,66,66,66	0
54	MG	2A	3477	1/1	0.71	0.10	75,75,75,75	0
54	MG	2A	3479	1/1	0.72	0.18	42,42,42,42	0
54	MG	1B	221	1/1	0.72	0.19	66,66,66,66	0
54	MG	2A	3054	1/1	0.72	0.11	76,76,76,76	0
54	MG	1A	3157	1/1	0.72	0.23	73,73,73,73	0
54	MG	1A	3260	1/1	0.72	0.16	62,62,62,62	0
54	MG	1A	3753	1/1	0.72	0.24	27,27,27,27	0
54	MG	1A	4047	1/1	0.72	0.32	55,55,55,55	0
54	MG	2a	3163	1/1	0.72	0.07	71,71,71,71	0
54	MG	2A	3218	1/1	0.72	0.26	72,72,72,72	0
54	MG	1A	3641	1/1	0.72	0.73	48,48,48,48	0
54	MG	2A	3031	1/1	0.72	0.13	77,77,77,77	0
54	MG	2A	3742	1/1	0.73	0.18	50,50,50,50	0
54	MG	2B	201	1/1	0.73	0.22	85,85,85,85	0
54	MG	1A	3882	1/1	0.73	0.16	40,40,40,40	0
54	MG	1A	3699	1/1	0.73	0.18	73,73,73,73	0
54	MG	1A	3796	1/1	0.73	0.19	74,74,74,74	0
54	MG	1A	3891	1/1	0.73	0.35	60,60,60,60	0
54	MG	1A	3804	1/1	0.73	0.16	57,57,57,57	0
54	MG	1A	3906	1/1	0.73	0.08	64,64,64,64	0
54	MG	1A	3398	1/1	0.73	0.22	34,34,34,34	0
54	MG	1A	3708	1/1	0.73	0.10	37,37,37,37	0
54	MG	2A	3422	1/1	0.73	0.12	61,61,61,61	0
54	MG	1A	3424	1/1	0.73	0.19	69,69,69,69	0
54	MG	2a	3054	1/1	0.73	0.15	83,83,83,83	0
54	MG	1A	3956	1/1	0.73	0.14	67,67,67,67	0
54	MG	1A	3489	1/1	0.73	0.17	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	1a	1604	1/1	0.73	0.18	76,76,76,76	0
54	MG	2A	3679	1/1	0.73	0.12	48,48,48,48	0
54	MG	2a	3149	1/1	0.73	0.11	71,71,71,71	0
54	MG	2A	3682	1/1	0.73	0.15	74,74,74,74	0
54	MG	1A	3670	1/1	0.73	0.40	37,37,37,37	0
54	MG	1a	1631	1/1	0.73	0.22	74,74,74,74	0
54	MG	2A	3707	1/1	0.73	0.73	56,56,56,56	0
54	MG	2a	3164	1/1	0.73	0.11	69,69,69,69	0
54	MG	2a	3185	1/1	0.73	0.14	77,77,77,77	0
54	MG	2A	3046	1/1	0.73	0.15	65,65,65,65	0
54	MG	1a	1813	1/1	0.73	0.20	69,69,69,69	0
54	MG	1A	3311	1/1	0.73	0.16	55,55,55,55	0
54	MG	2a	3074	1/1	0.74	0.15	70,70,70,70	0
54	MG	1A	3704	1/1	0.74	0.44	53,53,53,53	0
54	MG	2A	3042	1/1	0.74	0.52	81,81,81,81	0
54	MG	2a	3096	1/1	0.74	0.15	65,65,65,65	0
54	MG	1A	3778	1/1	0.74	0.26	28,28,28,28	0
54	MG	1A	3357	1/1	0.74	0.17	49,49,49,49	0
54	MG	2A	3071	1/1	0.74	0.26	50,50,50,50	0
54	MG	1A	3719	1/1	0.74	0.16	74,74,74,74	0
54	MG	1A	3380	1/1	0.74	0.12	63,63,63,63	0
54	MG	1A	3964	1/1	0.74	0.18	66,66,66,66	0
54	MG	2A	3716	1/1	0.74	0.16	40,40,40,40	0
54	MG	2a	3181	1/1	0.74	0.14	78,78,78,78	0
54	MG	2A	3610	1/1	0.74	0.15	82,82,82,82	0
54	MG	1a	1679	1/1	0.74	0.11	72,72,72,72	0
54	MG	1A	3383	1/1	0.74	0.17	54,54,54,54	0
54	MG	2A	3486	1/1	0.74	0.21	70,70,70,70	0
54	MG	1A	3792	1/1	0.75	0.21	35,35,35,35	0
54	MG	2A	3630	1/1	0.75	0.11	61,61,61,61	0
54	MG	2A	3227	1/1	0.75	0.24	65,65,65,65	0
54	MG	1a	1805	1/1	0.75	0.12	70,70,70,70	0
54	MG	1E	303	1/1	0.75	0.19	29,29,29,29	0
54	MG	2A	3256	1/1	0.75	0.18	57,57,57,57	0
54	MG	1A	3202	1/1	0.75	0.19	66,66,66,66	0
54	MG	1A	4022	1/1	0.75	0.14	54,54,54,54	0
54	MG	2a	3064	1/1	0.75	0.28	78,78,78,78	0
54	MG	2A	3344	1/1	0.75	0.19	40,40,40,40	0
54	MG	2A	3167	1/1	0.75	0.13	53,53,53,53	0
54	MG	2A	3695	1/1	0.75	0.17	53,53,53,53	0
54	MG	2A	3502	1/1	0.75	0.21	69,69,69,69	0
54	MG	1N	205	1/1	0.75	0.21	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	3884	1/1	0.75	0.24	65,65,65,65	0
54	MG	1A	3634	1/1	0.75	0.24	35,35,35,35	0
54	MG	2A	3567	1/1	0.75	0.20	54,54,54,54	0
54	MG	1B	205	1/1	0.75	0.19	59,59,59,59	0
54	MG	2A	3048	1/1	0.75	0.28	55,55,55,55	0
54	MG	2A	3206	1/1	0.75	0.60	55,55,55,55	0
54	MG	1A	3677	1/1	0.75	0.15	67,67,67,67	0
54	MG	1a	1800	1/1	0.75	0.15	71,71,71,71	0
54	MG	2A	3089	1/1	0.75	0.11	70,70,70,70	0
54	MG	28	102	1/1	0.75	0.19	60,60,60,60	0
54	MG	2a	3009	1/1	0.75	0.20	70,70,70,70	0
54	MG	1A	3463	1/1	0.76	0.20	27,27,27,27	0
54	MG	1A	3366	1/1	0.76	0.15	54,54,54,54	0
54	MG	2A	3264	1/1	0.76	0.27	73,73,73,73	0
54	MG	2A	3599	1/1	0.76	0.09	56,56,56,56	0
54	MG	2A	3299	1/1	0.76	0.12	70,70,70,70	0
54	MG	1A	3282	1/1	0.76	0.11	84,84,84,84	0
54	MG	1A	3950	1/1	0.76	0.25	51,51,51,51	0
54	MG	1a	1775	1/1	0.76	0.14	86,86,86,86	0
54	MG	2a	3131	1/1	0.76	0.13	53,53,53,53	0
54	MG	2a	3136	1/1	0.76	0.08	75,75,75,75	0
54	MG	1A	3870	1/1	0.76	0.14	46,46,46,46	0
54	MG	1a	1661	1/1	0.76	0.22	72,72,72,72	0
54	MG	1A	3310	1/1	0.76	0.41	64,64,64,64	0
54	MG	1a	1870	1/1	0.76	0.12	72,72,72,72	0
54	MG	2a	3010	1/1	0.76	0.12	68,68,68,68	0
54	MG	2A	3507	1/1	0.76	0.26	42,42,42,42	0
54	MG	2A	3209	1/1	0.76	0.25	58,58,58,58	0
54	MG	1A	3904	1/1	0.76	0.10	69,69,69,69	0
54	MG	1A	3208	1/1	0.76	0.13	73,73,73,73	0
54	MG	1A	3994	1/1	0.76	0.24	49,49,49,49	0
54	MG	1a	1630	1/1	0.76	0.22	68,68,68,68	0
54	MG	2A	3329	1/1	0.77	0.21	51,51,51,51	0
54	MG	2A	3561	1/1	0.77	0.32	54,54,54,54	0
54	MG	2A	3152	1/1	0.77	0.30	52,52,52,52	0
54	MG	1A	3767	1/1	0.77	0.19	67,67,67,67	0
54	MG	2a	3007	1/1	0.77	0.09	71,71,71,71	0
54	MG	1A	3837	1/1	0.77	0.13	44,44,44,44	0
54	MG	1A	3241	1/1	0.77	0.17	48,48,48,48	0
54	MG	1y	204	1/1	0.77	0.21	86,86,86,86	0
54	MG	1A	3392	1/1	0.77	0.18	37,37,37,37	0
54	MG	2A	3202	1/1	0.77	0.45	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	1667	1/1	0.77	0.09	64,64,64,64	0
54	MG	2A	3622	1/1	0.77	0.19	66,66,66,66	0
54	MG	2A	3033	1/1	0.77	0.20	53,53,53,53	0
54	MG	1a	1674	1/1	0.77	0.34	76,76,76,76	0
54	MG	15	104	1/1	0.77	0.38	31,31,31,31	0
54	MG	1a	1676	1/1	0.77	0.11	85,85,85,85	0
54	MG	2A	3215	1/1	0.77	0.19	63,63,63,63	0
54	MG	1A	3297	1/1	0.77	0.25	53,53,53,53	0
54	MG	2A	3449	1/1	0.77	0.18	58,58,58,58	0
54	MG	1A	3648	1/1	0.77	0.23	57,57,57,57	0
54	MG	1A	3567	1/1	0.77	0.17	64,64,64,64	0
54	MG	1A	3874	1/1	0.77	0.16	53,53,53,53	0
54	MG	1a	1711	1/1	0.77	0.40	74,74,74,74	0
54	MG	2A	3245	1/1	0.77	0.27	62,62,62,62	0
54	MG	1A	3940	1/1	0.77	0.27	54,54,54,54	0
54	MG	2A	3725	1/1	0.77	0.10	75,75,75,75	0
54	MG	1A	3103	1/1	0.77	0.19	45,45,45,45	0
54	MG	2A	3286	1/1	0.77	0.22	52,52,52,52	0
54	MG	1A	3464	1/1	0.77	0.08	46,46,46,46	0
54	MG	2A	3739	1/1	0.77	0.12	60,60,60,60	0
54	MG	1A	3611	1/1	0.77	0.12	72,72,72,72	0
54	MG	2A	3540	1/1	0.77	0.20	85,85,85,85	0
54	MG	2A	3328	1/1	0.77	0.10	50,50,50,50	0
54	MG	2D	311	1/1	0.77	0.40	65,65,65,65	0
54	MG	2r	101	1/1	0.77	0.20	68,68,68,68	0
57	ARG	1F	320	12/12	0.77	0.17	58,76,81,84	0
54	MG	1A	3426	1/1	0.78	0.22	40,40,40,40	0
54	MG	1A	4051	1/1	0.78	0.58	49,49,49,49	0
54	MG	1A	4057	1/1	0.78	0.20	44,44,44,44	0
54	MG	2A	3676	1/1	0.78	0.10	55,55,55,55	0
54	MG	1A	3478	1/1	0.78	0.23	32,32,32,32	0
54	MG	1B	210	1/1	0.78	0.24	84,84,84,84	0
54	MG	1A	3591	1/1	0.78	0.25	53,53,53,53	0
54	MG	2A	3080	1/1	0.78	0.42	68,68,68,68	0
54	MG	2A	3521	1/1	0.78	0.11	74,74,74,74	0
54	MG	2A	3210	1/1	0.78	0.24	62,62,62,62	0
54	MG	2A	3708	1/1	0.78	0.09	74,74,74,74	0
54	MG	1A	3389	1/1	0.78	0.20	33,33,33,33	0
54	MG	2a	3080	1/1	0.78	0.07	75,75,75,75	0
54	MG	2a	3082	1/1	0.78	0.08	80,80,80,80	0
54	MG	1A	3518	1/1	0.78	0.16	60,60,60,60	0
54	MG	2a	3102	1/1	0.78	0.27	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	3920	1/1	0.78	0.09	53,53,53,53	0
54	MG	1A	3213	1/1	0.78	0.14	73,73,73,73	0
54	MG	2A	3576	1/1	0.78	0.14	66,66,66,66	0
54	MG	2A	3410	1/1	0.78	0.15	71,71,71,71	0
54	MG	1d	304	1/1	0.78	0.23	65,65,65,65	0
54	MG	2A	3417	1/1	0.78	0.35	68,68,68,68	0
54	MG	1A	3113	1/1	0.78	0.22	45,45,45,45	0
54	MG	10	105	1/1	0.78	0.19	57,57,57,57	0
54	MG	1A	3329	1/1	0.78	0.24	31,31,31,31	0
54	MG	2A	3613	1/1	0.78	0.18	61,61,61,61	0
54	MG	14	101	1/1	0.78	0.10	81,81,81,81	0
54	MG	2A	3271	1/1	0.78	0.09	77,77,77,77	0
54	MG	2a	3003	1/1	0.78	0.32	70,70,70,70	0
54	MG	2A	3277	1/1	0.78	0.19	34,34,34,34	0
54	MG	1A	4036	1/1	0.78	0.14	65,65,65,65	0
54	MG	1A	3889	1/1	0.78	0.18	45,45,45,45	0
54	MG	1A	3947	1/1	0.79	0.21	52,52,52,52	0
54	MG	2A	3524	1/1	0.79	0.52	85,85,85,85	0
54	MG	1A	3430	1/1	0.79	0.20	29,29,29,29	0
54	MG	1A	3622	1/1	0.79	0.12	69,69,69,69	0
54	MG	1A	3576	1/1	0.79	0.26	52,52,52,52	0
54	MG	1A	3672	1/1	0.79	0.09	50,50,50,50	0
54	MG	1B	207	1/1	0.79	0.42	61,61,61,61	0
54	MG	2a	3069	1/1	0.79	0.09	68,68,68,68	0
54	MG	2A	3162	1/1	0.79	0.51	68,68,68,68	0
54	MG	2A	3421	1/1	0.79	0.17	69,69,69,69	0
54	MG	2A	3009	1/1	0.79	0.26	56,56,56,56	0
54	MG	2A	3270	1/1	0.79	0.27	83,83,83,83	0
54	MG	2A	3730	1/1	0.79	0.18	74,74,74,74	0
54	MG	1A	3975	1/1	0.79	0.16	56,56,56,56	0
54	MG	1A	3722	1/1	0.79	0.14	40,40,40,40	0
54	MG	2a	3105	1/1	0.79	0.20	72,72,72,72	0
54	MG	2A	3602	1/1	0.79	0.21	48,48,48,48	0
54	MG	1B	218	1/1	0.79	0.15	59,59,59,59	0
54	MG	1a	1623	1/1	0.79	0.11	58,58,58,58	0
54	MG	1A	3095	1/1	0.79	0.20	51,51,51,51	0
54	MG	2E	305	1/1	0.79	0.07	57,57,57,57	0
54	MG	2A	3045	1/1	0.79	0.20	67,67,67,67	0
54	MG	1A	3805	1/1	0.79	0.12	44,44,44,44	0
54	MG	1a	1730	1/1	0.79	0.26	75,75,75,75	0
54	MG	1A	3680	1/1	0.79	0.09	57,57,57,57	0
54	MG	2A	3645	1/1	0.79	0.08	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	3404	1/1	0.79	0.19	30,30,30,30	0
54	MG	2a	3008	1/1	0.79	0.09	75,75,75,75	0
54	MG	2A	3653	1/1	0.79	0.10	57,57,57,57	0
54	MG	2A	3359	1/1	0.79	0.12	60,60,60,60	0
54	MG	1A	3449	1/1	0.79	0.10	63,63,63,63	0
54	MG	1a	1866	1/1	0.79	0.38	80,80,80,80	0
54	MG	1A	3501	1/1	0.80	0.09	67,67,67,67	0
54	MG	2A	3501	1/1	0.80	0.10	85,85,85,85	0
54	MG	2A	3056	1/1	0.80	0.26	59,59,59,59	0
54	MG	2A	3250	1/1	0.80	0.18	73,73,73,73	0
54	MG	2A	3252	1/1	0.80	0.14	65,65,65,65	0
54	MG	1A	3376	1/1	0.80	0.14	43,43,43,43	0
54	MG	2A	3074	1/1	0.80	0.34	58,58,58,58	0
54	MG	1a	1857	1/1	0.80	0.12	81,81,81,81	0
54	MG	1a	1709	1/1	0.80	0.10	56,56,56,56	0
54	MG	2A	3275	1/1	0.80	0.19	59,59,59,59	0
54	MG	1B	220	1/1	0.80	0.25	50,50,50,50	0
54	MG	2A	3097	1/1	0.80	0.16	54,54,54,54	0
54	MG	1a	1861	1/1	0.80	0.10	71,71,71,71	0
54	MG	2A	3578	1/1	0.80	0.14	50,50,50,50	0
54	MG	2A	3300	1/1	0.80	0.18	71,71,71,71	0
54	MG	2A	3100	1/1	0.80	0.18	63,63,63,63	0
54	MG	2A	3589	1/1	0.80	0.12	66,66,66,66	0
54	MG	1A	3537	1/1	0.80	0.16	51,51,51,51	0
54	MG	2A	3110	1/1	0.80	0.36	56,56,56,56	0
54	MG	2A	3116	1/1	0.80	0.08	82,82,82,82	0
54	MG	1A	4010	1/1	0.80	0.10	54,54,54,54	0
54	MG	2a	3050	1/1	0.80	0.19	69,69,69,69	0
54	MG	1a	1741	1/1	0.80	0.23	68,68,68,68	0
54	MG	1a	1632	1/1	0.80	0.12	42,42,42,42	0
54	MG	2A	3614	1/1	0.80	0.06	71,71,71,71	0
54	MG	1A	3584	1/1	0.80	0.26	53,53,53,53	0
54	MG	2A	3618	1/1	0.80	0.09	88,88,88,88	0
54	MG	2A	3163	1/1	0.80	0.08	63,63,63,63	0
54	MG	1A	3758	1/1	0.80	0.15	52,52,52,52	0
54	MG	1d	305	1/1	0.80	0.25	94,94,94,94	0
54	MG	1A	3082	1/1	0.80	0.19	57,57,57,57	0
54	MG	1g	202	1/1	0.80	0.15	73,73,73,73	0
54	MG	1A	3483	1/1	0.80	0.20	31,31,31,31	0
54	MG	2A	3192	1/1	0.80	0.17	65,65,65,65	0
54	MG	2A	3656	1/1	0.80	0.27	33,33,33,33	0
54	MG	1n	101	1/1	0.80	0.19	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3125	1/1	0.80	0.10	82,82,82,82	0
54	MG	1a	1785	1/1	0.80	0.13	79,79,79,79	0
54	MG	2A	3675	1/1	0.80	0.12	60,60,60,60	0
54	MG	1A	3664	1/1	0.80	0.38	64,64,64,64	0
54	MG	2A	3012	1/1	0.80	0.32	68,68,68,68	0
54	MG	2a	3154	1/1	0.80	0.15	67,67,67,67	0
54	MG	1a	1796	1/1	0.80	0.08	86,86,86,86	0
54	MG	1A	3952	1/1	0.80	0.11	68,68,68,68	0
54	MG	1A	3144	1/1	0.80	0.28	69,69,69,69	0
54	MG	1A	3788	1/1	0.80	0.20	66,66,66,66	0
54	MG	15	107	1/1	0.80	0.21	77,77,77,77	0
54	MG	2A	3461	1/1	0.80	0.10	72,72,72,72	0
54	MG	2A	3468	1/1	0.80	0.23	69,69,69,69	0
54	MG	2A	3219	1/1	0.80	0.40	51,51,51,51	0
54	MG	1a	1677	1/1	0.80	0.55	63,63,63,63	0
54	MG	2f	202	1/1	0.80	0.14	69,69,69,69	0
54	MG	1A	3857	1/1	0.80	0.11	62,62,62,62	0
56	MPD	2B	219	8/8	0.80	0.30	66,74,79,84	0
54	MG	1A	3859	1/1	0.80	0.25	34,34,34,34	0
58	ZN	14	102	1/1	0.80	0.16	144,144,144,144	0
54	MG	1A	4004	1/1	0.81	0.15	86,86,86,86	0
54	MG	2A	3508	1/1	0.81	0.09	67,67,67,67	0
54	MG	1A	3251	1/1	0.81	0.14	76,76,76,76	0
54	MG	1A	3893	1/1	0.81	0.12	60,60,60,60	0
54	MG	2B	208	1/1	0.81	0.21	66,66,66,66	0
54	MG	1A	3271	1/1	0.81	0.12	48,48,48,48	0
54	MG	2A	3526	1/1	0.81	0.10	58,58,58,58	0
54	MG	1A	3370	1/1	0.81	0.14	47,47,47,47	0
54	MG	1A	3829	1/1	0.81	0.60	45,45,45,45	0
54	MG	1a	1811	1/1	0.81	0.15	71,71,71,71	0
54	MG	1A	3918	1/1	0.81	0.12	51,51,51,51	0
54	MG	1A	3560	1/1	0.81	0.15	42,42,42,42	0
54	MG	2a	3002	1/1	0.81	0.09	81,81,81,81	0
54	MG	1A	3923	1/1	0.81	0.06	57,57,57,57	0
54	MG	1a	1657	1/1	0.81	0.30	77,77,77,77	0
54	MG	1A	3649	1/1	0.81	0.41	40,40,40,40	0
54	MG	1A	3281	1/1	0.81	0.08	77,77,77,77	0
54	MG	2A	3582	1/1	0.81	0.12	60,60,60,60	0
54	MG	1A	3379	1/1	0.81	0.10	74,74,74,74	0
54	MG	1a	1671	1/1	0.81	0.37	73,73,73,73	0
54	MG	1A	3331	1/1	0.81	0.14	30,30,30,30	0
54	MG	2A	3132	1/1	0.81	0.21	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	3040	1/1	0.81	0.16	78,78,78,78	0
54	MG	1A	3941	1/1	0.81	0.08	50,50,50,50	0
54	MG	2a	3048	1/1	0.81	0.14	74,74,74,74	0
54	MG	2A	3147	1/1	0.81	0.11	79,79,79,79	0
54	MG	2A	3367	1/1	0.81	0.12	66,66,66,66	0
54	MG	1A	3760	1/1	0.81	0.21	63,63,63,63	0
54	MG	1A	3666	1/1	0.81	0.24	48,48,48,48	0
54	MG	1A	3951	1/1	0.81	0.28	68,68,68,68	0
54	MG	1A	3668	1/1	0.81	0.13	47,47,47,47	0
54	MG	2a	3072	1/1	0.81	0.30	82,82,82,82	0
54	MG	2A	3623	1/1	0.81	0.28	62,62,62,62	0
54	MG	2A	3174	1/1	0.81	0.14	70,70,70,70	0
54	MG	1A	3093	1/1	0.81	0.31	64,64,64,64	0
54	MG	2A	3632	1/1	0.81	0.25	86,86,86,86	0
54	MG	2A	3642	1/1	0.81	0.11	80,80,80,80	0
54	MG	1a	1876	1/1	0.81	0.10	74,74,74,74	0
54	MG	2a	3098	1/1	0.81	0.11	85,85,85,85	0
54	MG	1d	303	1/1	0.81	0.34	74,74,74,74	0
54	MG	2a	3103	1/1	0.81	0.23	70,70,70,70	0
54	MG	2A	3647	1/1	0.81	0.18	53,53,53,53	0
54	MG	1a	1694	1/1	0.81	0.25	69,69,69,69	0
54	MG	1A	3782	1/1	0.81	0.29	45,45,45,45	0
54	MG	2A	3194	1/1	0.81	0.15	47,47,47,47	0
54	MG	1T	201	1/1	0.81	0.14	52,52,52,52	0
54	MG	2A	3431	1/1	0.81	0.12	52,52,52,52	0
54	MG	1A	3963	1/1	0.81	0.16	66,66,66,66	0
54	MG	1A	3217	1/1	0.81	0.51	42,42,42,42	0
54	MG	1A	3973	1/1	0.81	0.12	44,44,44,44	0
54	MG	1A	3448	1/1	0.81	0.18	49,49,49,49	0
54	MG	1A	3593	1/1	0.81	0.19	66,66,66,66	0
54	MG	1a	1749	1/1	0.81	0.11	61,61,61,61	0
54	MG	1A	3531	1/1	0.81	0.16	68,68,68,68	0
54	MG	1a	1761	1/1	0.81	0.21	70,70,70,70	0
54	MG	1A	3534	1/1	0.81	0.17	55,55,55,55	0
54	MG	2A	3715	1/1	0.81	0.13	67,67,67,67	0
54	MG	1A	4000	1/1	0.81	0.19	84,84,84,84	0
54	MG	2A	3722	1/1	0.81	0.17	48,48,48,48	0
54	MG	1a	1603	1/1	0.81	0.14	72,72,72,72	0
54	MG	2A	3043	1/1	0.81	0.24	56,56,56,56	0
54	MG	1a	1782	1/1	0.81	0.34	70,70,70,70	0
54	MG	2A	3243	1/1	0.81	0.27	44,44,44,44	0
54	MG	1A	3303	1/1	0.82	0.37	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	1a	1783	1/1	0.82	0.10	80,80,80,80	0
54	MG	2A	3453	1/1	0.82	0.14	74,74,74,74	0
54	MG	1A	3125	1/1	0.82	0.66	46,46,46,46	0
54	MG	2A	3122	1/1	0.82	0.61	45,45,45,45	0
54	MG	2A	3643	1/1	0.82	0.11	56,56,56,56	0
54	MG	1a	1789	1/1	0.82	0.18	66,66,66,66	0
54	MG	1A	3903	1/1	0.82	0.12	42,42,42,42	0
54	MG	1B	202	1/1	0.82	0.15	74,74,74,74	0
54	MG	1A	3755	1/1	0.82	0.14	62,62,62,62	0
54	MG	2A	3002	1/1	0.82	0.14	50,50,50,50	0
54	MG	2A	3488	1/1	0.82	0.10	73,73,73,73	0
54	MG	2A	3276	1/1	0.82	0.08	87,87,87,87	0
54	MG	2A	3669	1/1	0.82	0.18	60,60,60,60	0
54	MG	1A	3868	1/1	0.82	0.11	65,65,65,65	0
54	MG	1A	3911	1/1	0.82	0.20	39,39,39,39	0
54	MG	1A	3869	1/1	0.82	0.18	39,39,39,39	0
54	MG	2a	3070	1/1	0.82	0.20	54,54,54,54	0
54	MG	2A	3023	1/1	0.82	0.19	69,69,69,69	0
54	MG	2A	3681	1/1	0.82	0.24	78,78,78,78	0
54	MG	2A	3024	1/1	0.82	0.21	67,67,67,67	0
54	MG	1A	3600	1/1	0.82	0.09	44,44,44,44	0
54	MG	1a	1700	1/1	0.82	0.16	64,64,64,64	0
54	MG	2A	3333	1/1	0.82	0.23	62,62,62,62	0
54	MG	1A	3606	1/1	0.82	0.40	50,50,50,50	0
54	MG	1A	3122	1/1	0.82	0.08	67,67,67,67	0
54	MG	2A	3193	1/1	0.82	0.21	68,68,68,68	0
54	MG	1a	1712	1/1	0.82	0.12	64,64,64,64	0
54	MG	2A	3196	1/1	0.82	0.28	63,63,63,63	0
54	MG	2A	3723	1/1	0.82	0.27	67,67,67,67	0
54	MG	2A	3574	1/1	0.82	0.26	60,60,60,60	0
54	MG	1a	1840	1/1	0.82	0.08	64,64,64,64	0
54	MG	2A	3203	1/1	0.82	0.23	56,56,56,56	0
54	MG	1D	318	1/1	0.82	0.19	59,59,59,59	0
54	MG	2A	3391	1/1	0.82	0.15	75,75,75,75	0
54	MG	1A	3880	1/1	0.82	0.22	57,57,57,57	0
54	MG	1a	1740	1/1	0.82	0.12	65,65,65,65	0
54	MG	1A	3312	1/1	0.82	0.17	47,47,47,47	0
54	MG	2A	3059	1/1	0.82	0.20	73,73,73,73	0
54	MG	2B	209	1/1	0.82	0.15	70,70,70,70	0
54	MG	2a	3174	1/1	0.82	0.09	86,86,86,86	0
54	MG	1F	312	1/1	0.82	0.19	39,39,39,39	0
54	MG	1F	318	1/1	0.82	0.07	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	1754	1/1	0.82	0.10	90,90,90,90	0
54	MG	1A	3420	1/1	0.82	0.25	29,29,29,29	0
54	MG	1A	3543	1/1	0.82	0.20	65,65,65,65	0
54	MG	2d	301	1/1	0.82	0.13	67,67,67,67	0
54	MG	1A	3155	1/1	0.82	0.28	42,42,42,42	0
54	MG	1A	3848	1/1	0.82	0.20	53,53,53,53	0
54	MG	2A	3619	1/1	0.82	0.73	53,53,53,53	0
54	MG	1A	3733	1/1	0.82	0.19	42,42,42,42	0
54	MG	2a	3004	1/1	0.82	0.15	73,73,73,73	0
54	MG	1A	3467	1/1	0.83	0.16	49,49,49,49	0
54	MG	1a	1867	1/1	0.83	0.12	73,73,73,73	0
54	MG	2A	3137	1/1	0.83	0.23	51,51,51,51	0
54	MG	2A	3330	1/1	0.83	0.17	35,35,35,35	0
54	MG	1A	3187	1/1	0.83	0.21	59,59,59,59	0
54	MG	1A	3074	1/1	0.83	0.53	53,53,53,53	0
54	MG	2A	3149	1/1	0.83	0.16	40,40,40,40	0
54	MG	1A	4014	1/1	0.83	0.11	67,67,67,67	0
54	MG	1A	3922	1/1	0.83	0.12	52,52,52,52	0
54	MG	2A	3604	1/1	0.83	0.27	46,46,46,46	0
54	MG	2A	3363	1/1	0.83	0.14	71,71,71,71	0
54	MG	1A	3617	1/1	0.83	0.13	48,48,48,48	0
54	MG	1A	3079	1/1	0.83	0.83	45,45,45,45	0
54	MG	1A	3925	1/1	0.83	0.12	54,54,54,54	0
54	MG	1a	1605	1/1	0.83	0.14	67,67,67,67	0
54	MG	2A	3179	1/1	0.83	0.19	52,52,52,52	0
54	MG	2a	3034	1/1	0.83	0.17	73,73,73,73	0
54	MG	2a	3038	1/1	0.83	0.15	89,89,89,89	0
54	MG	1A	3011	1/1	0.83	0.20	66,66,66,66	0
54	MG	2A	3402	1/1	0.83	0.16	45,45,45,45	0
54	MG	2A	3627	1/1	0.83	0.07	71,71,71,71	0
54	MG	2A	3404	1/1	0.83	0.68	70,70,70,70	0
54	MG	2A	3629	1/1	0.83	0.13	73,73,73,73	0
54	MG	1A	3034	1/1	0.83	0.26	63,63,63,63	0
54	MG	1A	3578	1/1	0.83	0.16	72,72,72,72	0
54	MG	2A	3001	1/1	0.83	0.20	70,70,70,70	0
54	MG	1A	3520	1/1	0.83	0.12	61,61,61,61	0
54	MG	1a	1777	1/1	0.83	0.10	82,82,82,82	0
54	MG	1A	3313	1/1	0.83	0.65	52,52,52,52	0
54	MG	1a	1639	1/1	0.83	0.12	68,68,68,68	0
54	MG	1A	3036	1/1	0.83	0.25	62,62,62,62	0
54	MG	1a	1647	1/1	0.83	0.15	51,51,51,51	0
54	MG	2A	3437	1/1	0.83	0.21	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3587	1/1	0.83	0.16	64,64,64,64	0
54	MG	1a	1793	1/1	0.83	0.08	74,74,74,74	0
54	MG	1A	3886	1/1	0.83	0.13	31,31,31,31	0
54	MG	2a	3099	1/1	0.83	0.23	74,74,74,74	0
54	MG	1A	3738	1/1	0.83	0.10	54,54,54,54	0
54	MG	1a	1799	1/1	0.83	0.15	67,67,67,67	0
54	MG	1A	3817	1/1	0.83	0.18	41,41,41,41	0
54	MG	1A	3536	1/1	0.83	0.28	44,44,44,44	0
54	MG	1D	313	1/1	0.83	0.40	66,66,66,66	0
54	MG	2A	3049	1/1	0.83	0.13	47,47,47,47	0
54	MG	1A	3046	1/1	0.83	0.36	42,42,42,42	0
54	MG	2a	3139	1/1	0.83	0.08	73,73,73,73	0
54	MG	2A	3230	1/1	0.83	0.18	68,68,68,68	0
54	MG	1a	1673	1/1	0.83	0.20	63,63,63,63	0
54	MG	1A	3835	1/1	0.83	0.19	63,63,63,63	0
54	MG	2A	3060	1/1	0.83	0.20	44,44,44,44	0
54	MG	1A	3974	1/1	0.83	0.09	64,64,64,64	0
54	MG	2A	3249	1/1	0.83	0.13	68,68,68,68	0
54	MG	1A	3836	1/1	0.83	0.16	53,53,53,53	0
54	MG	1a	1825	1/1	0.83	0.16	51,51,51,51	0
54	MG	2a	3180	1/1	0.83	0.18	76,76,76,76	0
54	MG	1A	3979	1/1	0.83	0.16	50,50,50,50	0
54	MG	1A	3754	1/1	0.83	0.15	48,48,48,48	0
54	MG	2A	3093	1/1	0.83	0.13	76,76,76,76	0
54	MG	1A	3987	1/1	0.83	0.16	53,53,53,53	0
54	MG	1a	1687	1/1	0.83	0.23	59,59,59,59	0
54	MG	1P	206	1/1	0.83	0.25	48,48,48,48	0
54	MG	1A	3990	1/1	0.83	0.21	61,61,61,61	0
54	MG	1Z	301	1/1	0.83	0.19	69,69,69,69	0
56	MPD	1O	202	8/8	0.83	0.29	67,75,81,81	0
54	MG	2A	3290	1/1	0.83	0.13	62,62,62,62	0
54	MG	1A	3667	1/1	0.83	0.21	31,31,31,31	0
54	MG	1A	3599	1/1	0.83	0.13	47,47,47,47	0
54	MG	2A	3010	1/1	0.84	0.12	73,73,73,73	0
54	MG	1a	1837	1/1	0.84	0.10	89,89,89,89	0
54	MG	2A	3490	1/1	0.84	0.33	65,65,65,65	0
54	MG	1a	1765	1/1	0.84	0.09	81,81,81,81	0
54	MG	1P	203	1/1	0.84	0.19	39,39,39,39	0
54	MG	2a	3020	1/1	0.84	0.31	63,63,63,63	0
54	MG	2A	3346	1/1	0.84	0.24	42,42,42,42	0
54	MG	2a	3030	1/1	0.84	0.17	73,73,73,73	0
54	MG	2A	3354	1/1	0.84	0.12	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3650	1/1	0.84	0.15	57,57,57,57	0
54	MG	1a	1681	1/1	0.84	0.07	59,59,59,59	0
54	MG	1A	3277	1/1	0.84	0.85	36,36,36,36	0
54	MG	1A	3993	1/1	0.84	0.67	52,52,52,52	0
54	MG	2A	3663	1/1	0.84	0.48	85,85,85,85	0
54	MG	1A	3485	1/1	0.84	0.21	46,46,46,46	0
54	MG	2a	3051	1/1	0.84	0.13	77,77,77,77	0
54	MG	2A	3670	1/1	0.84	0.13	71,71,71,71	0
54	MG	2A	3379	1/1	0.84	0.23	58,58,58,58	0
54	MG	2A	3537	1/1	0.84	0.10	63,63,63,63	0
54	MG	2A	3038	1/1	0.84	0.19	67,67,67,67	0
54	MG	2A	3547	1/1	0.84	0.12	38,38,38,38	0
54	MG	2A	3548	1/1	0.84	0.15	72,72,72,72	0
54	MG	2A	3554	1/1	0.84	0.49	77,77,77,77	0
54	MG	2A	3381	1/1	0.84	0.17	47,47,47,47	0
54	MG	2A	3688	1/1	0.84	0.13	75,75,75,75	0
54	MG	1a	1690	1/1	0.84	0.17	73,73,73,73	0
54	MG	2A	3694	1/1	0.84	0.14	69,69,69,69	0
54	MG	1a	1691	1/1	0.84	0.22	59,59,59,59	0
54	MG	2A	3562	1/1	0.84	0.16	62,62,62,62	0
54	MG	10	102	1/1	0.84	0.83	56,56,56,56	0
54	MG	1A	3958	1/1	0.84	0.26	54,54,54,54	0
54	MG	1a	1650	1/1	0.84	0.14	69,69,69,69	0
54	MG	1A	3487	1/1	0.84	0.24	34,34,34,34	0
54	MG	1A	3316	1/1	0.84	0.58	53,53,53,53	0
54	MG	2a	3120	1/1	0.84	0.10	55,55,55,55	0
54	MG	2A	3253	1/1	0.84	0.31	72,72,72,72	0
54	MG	1A	4008	1/1	0.84	0.17	49,49,49,49	0
54	MG	1A	3497	1/1	0.84	0.17	48,48,48,48	0
54	MG	2A	3188	1/1	0.84	0.17	54,54,54,54	0
54	MG	2A	3735	1/1	0.84	0.12	77,77,77,77	0
54	MG	2a	3142	1/1	0.84	0.11	66,66,66,66	0
54	MG	1A	3071	1/1	0.84	0.61	49,49,49,49	0
54	MG	2A	3273	1/1	0.84	0.23	61,61,61,61	0
54	MG	2A	3600	1/1	0.84	0.19	44,44,44,44	0
54	MG	1A	3092	1/1	0.84	0.20	62,62,62,62	0
54	MG	2B	202	1/1	0.84	0.11	82,82,82,82	0
54	MG	2A	3436	1/1	0.84	0.11	49,49,49,49	0
54	MG	2A	3072	1/1	0.84	0.21	70,70,70,70	0
54	MG	2a	3169	1/1	0.84	0.06	73,73,73,73	0
54	MG	1A	3142	1/1	0.84	0.18	58,58,58,58	0
54	MG	2a	3176	1/1	0.84	0.18	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	2D	306	1/1	0.84	0.43	47,47,47,47	0
54	MG	1a	1816	1/1	0.84	0.08	65,65,65,65	0
54	MG	2E	304	1/1	0.84	0.19	41,41,41,41	0
54	MG	2A	3195	1/1	0.84	0.14	67,67,67,67	0
54	MG	1A	3605	1/1	0.84	0.16	42,42,42,42	0
54	MG	2a	3193	1/1	0.84	0.20	76,76,76,76	0
54	MG	1A	3984	1/1	0.84	0.11	65,65,65,65	0
54	MG	2O	201	1/1	0.84	0.22	65,65,65,65	0
54	MG	2f	201	1/1	0.84	0.18	56,56,56,56	0
54	MG	1A	3985	1/1	0.84	0.08	54,54,54,54	0
54	MG	2A	3310	1/1	0.84	0.12	67,67,67,67	0
54	MG	2A	3322	1/1	0.84	0.16	55,55,55,55	0
54	MG	1A	3522	1/1	0.84	0.14	58,58,58,58	0
54	MG	2A	3003	1/1	0.84	0.20	66,66,66,66	0
54	MG	1A	3480	1/1	0.84	0.23	25,25,25,25	0
58	ZN	24	501	1/1	0.84	0.27	157,157,157,157	0
54	MG	1A	4054	1/1	0.85	0.23	64,64,64,64	0
54	MG	1A	3481	1/1	0.85	0.20	40,40,40,40	0
54	MG	1a	1615	1/1	0.85	0.12	57,57,57,57	0
54	MG	1a	1621	1/1	0.85	0.15	58,58,58,58	0
54	MG	1A	3959	1/1	0.85	0.21	59,59,59,59	0
54	MG	1h	201	1/1	0.85	0.17	59,59,59,59	0
54	MG	1A	3960	1/1	0.85	0.10	65,65,65,65	0
54	MG	1B	206	1/1	0.85	0.29	64,64,64,64	0
54	MG	1a	1763	1/1	0.85	0.27	68,68,68,68	0
54	MG	1A	3482	1/1	0.85	0.16	26,26,26,26	0
54	MG	1a	1636	1/1	0.85	0.10	40,40,40,40	0
54	MG	2A	3611	1/1	0.85	0.30	37,37,37,37	0
54	MG	1a	1638	1/1	0.85	0.14	80,80,80,80	0
54	MG	2a	3015	1/1	0.85	0.13	53,53,53,53	0
54	MG	1A	3340	1/1	0.85	0.14	65,65,65,65	0
54	MG	1A	3269	1/1	0.85	0.24	59,59,59,59	0
54	MG	1A	3186	1/1	0.85	0.19	60,60,60,60	0
54	MG	1A	3061	1/1	0.85	0.12	55,55,55,55	0
54	MG	2A	3017	1/1	0.85	0.39	61,61,61,61	0
54	MG	1A	3189	1/1	0.85	0.26	68,68,68,68	0
54	MG	1A	3905	1/1	0.85	0.23	75,75,75,75	0
54	MG	2A	3025	1/1	0.85	0.11	52,52,52,52	0
54	MG	1A	3983	1/1	0.85	0.18	81,81,81,81	0
54	MG	2a	3043	1/1	0.85	0.36	63,63,63,63	0
54	MG	2a	3044	1/1	0.85	0.17	60,60,60,60	0
54	MG	1A	3565	1/1	0.85	0.21	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	3910	1/1	0.85	0.20	27,27,27,27	0
54	MG	2A	3634	1/1	0.85	0.14	62,62,62,62	0
54	MG	2A	3212	1/1	0.85	0.24	67,67,67,67	0
54	MG	2A	3429	1/1	0.85	0.24	43,43,43,43	0
54	MG	1E	307	1/1	0.85	0.23	34,34,34,34	0
54	MG	1A	3771	1/1	0.85	0.16	54,54,54,54	0
54	MG	1F	315	1/1	0.85	0.14	47,47,47,47	0
54	MG	2A	3220	1/1	0.85	0.40	61,61,61,61	0
54	MG	1A	3410	1/1	0.85	0.18	32,32,32,32	0
54	MG	1A	3693	1/1	0.85	0.14	69,69,69,69	0
54	MG	1H	203	1/1	0.85	0.12	66,66,66,66	0
54	MG	1A	3781	1/1	0.85	0.20	33,33,33,33	0
54	MG	1A	3505	1/1	0.85	0.14	63,63,63,63	0
54	MG	1A	3700	1/1	0.85	0.15	49,49,49,49	0
54	MG	2a	3090	1/1	0.85	0.24	58,58,58,58	0
54	MG	2A	3462	1/1	0.85	0.18	56,56,56,56	0
54	MG	1a	1683	1/1	0.85	0.14	78,78,78,78	0
54	MG	2A	3471	1/1	0.85	0.16	55,55,55,55	0
54	MG	1A	3508	1/1	0.85	0.11	47,47,47,47	0
54	MG	1a	1834	1/1	0.85	0.16	51,51,51,51	0
54	MG	1a	1686	1/1	0.85	0.14	66,66,66,66	0
54	MG	2A	3482	1/1	0.85	0.11	64,64,64,64	0
54	MG	2a	3123	1/1	0.85	0.08	64,64,64,64	0
54	MG	2A	3483	1/1	0.85	0.18	61,61,61,61	0
54	MG	2A	3485	1/1	0.85	0.11	42,42,42,42	0
54	MG	2A	3691	1/1	0.85	0.16	51,51,51,51	0
54	MG	1A	3278	1/1	0.85	0.57	56,56,56,56	0
54	MG	1A	3039	1/1	0.85	0.24	57,57,57,57	0
54	MG	1a	1846	1/1	0.85	0.36	80,80,80,80	0
54	MG	2A	3699	1/1	0.85	0.09	66,66,66,66	0
54	MG	1a	1847	1/1	0.85	0.12	73,73,73,73	0
54	MG	1a	1853	1/1	0.85	0.22	66,66,66,66	0
54	MG	2A	3710	1/1	0.85	0.16	63,63,63,63	0
54	MG	1A	3710	1/1	0.85	0.13	52,52,52,52	0
54	MG	1A	3799	1/1	0.85	0.24	70,70,70,70	0
54	MG	2A	3719	1/1	0.85	0.14	66,66,66,66	0
54	MG	1A	3945	1/1	0.85	0.10	42,42,42,42	0
54	MG	2a	3173	1/1	0.85	0.16	83,83,83,83	0
54	MG	1A	3883	1/1	0.85	0.20	28,28,28,28	0
54	MG	1A	4026	1/1	0.85	0.16	56,56,56,56	0
54	MG	1a	1862	1/1	0.85	0.08	65,65,65,65	0
54	MG	2A	3294	1/1	0.85	0.12	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	3298	1/1	0.85	0.07	64,64,64,64	0
54	MG	2A	3538	1/1	0.85	0.19	58,58,58,58	0
54	MG	2A	3121	1/1	0.85	0.28	72,72,72,72	0
54	MG	1A	3033	1/1	0.85	0.17	48,48,48,48	0
54	MG	1A	3139	1/1	0.85	0.22	67,67,67,67	0
54	MG	1A	3887	1/1	0.85	0.07	68,68,68,68	0
54	MG	2A	3311	1/1	0.85	0.18	56,56,56,56	0
54	MG	1a	1713	1/1	0.85	0.09	94,94,94,94	0
54	MG	1A	4049	1/1	0.85	0.14	62,62,62,62	0
54	MG	1a	1723	1/1	0.85	0.06	60,60,60,60	0
56	MPD	2A	3743	8/8	0.85	0.36	46,57,62,63	0
54	MG	1A	3588	1/1	0.85	0.10	45,45,45,45	0
54	MG	1b	301	1/1	0.85	0.12	80,80,80,80	0
54	MG	2A	3342	1/1	0.85	0.21	40,40,40,40	0
54	MG	2A	3159	1/1	0.85	0.29	71,71,71,71	0
54	MG	1A	3892	1/1	0.86	0.12	59,59,59,59	0
54	MG	2A	3123	1/1	0.86	0.37	42,42,42,42	0
54	MG	1A	3101	1/1	0.86	0.48	43,43,43,43	0
54	MG	1A	3620	1/1	0.86	0.29	45,45,45,45	0
54	MG	2F	302	1/1	0.86	0.17	44,44,44,44	0
54	MG	2A	3570	1/1	0.86	0.17	56,56,56,56	0
54	MG	1A	3842	1/1	0.86	0.09	33,33,33,33	0
54	MG	2G	203	1/1	0.86	0.10	78,78,78,78	0
54	MG	2A	3339	1/1	0.86	0.17	37,37,37,37	0
54	MG	1A	3965	1/1	0.86	0.12	59,59,59,59	0
54	MG	1A	3845	1/1	0.86	0.51	60,60,60,60	0
54	MG	1a	1725	1/1	0.86	0.08	62,62,62,62	0
54	MG	1A	3406	1/1	0.86	0.15	28,28,28,28	0
54	MG	2A	3153	1/1	0.86	0.20	71,71,71,71	0
54	MG	1a	1612	1/1	0.86	0.12	84,84,84,84	0
54	MG	1d	301	1/1	0.86	0.22	75,75,75,75	0
54	MG	1B	209	1/1	0.86	0.13	62,62,62,62	0
54	MG	1A	3572	1/1	0.86	0.17	25,25,25,25	0
54	MG	1A	3908	1/1	0.86	0.41	40,40,40,40	0
54	MG	1a	1752	1/1	0.86	0.08	75,75,75,75	0
54	MG	1a	1624	1/1	0.86	0.11	59,59,59,59	0
54	MG	1A	3854	1/1	0.86	0.14	48,48,48,48	0
54	MG	1A	3856	1/1	0.86	0.10	47,47,47,47	0
54	MG	1a	1762	1/1	0.86	0.12	57,57,57,57	0
54	MG	2A	3392	1/1	0.86	0.31	62,62,62,62	0
54	MG	1y	201	1/1	0.86	0.30	76,76,76,76	0
54	MG	1A	3628	1/1	0.86	0.23	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3220	1/1	0.86	0.14	41,41,41,41	0
54	MG	1D	317	1/1	0.86	0.34	52,52,52,52	0
54	MG	2A	3624	1/1	0.86	0.17	76,76,76,76	0
54	MG	1A	3510	1/1	0.86	0.15	73,73,73,73	0
54	MG	2A	3005	1/1	0.86	0.21	59,59,59,59	0
54	MG	1A	3517	1/1	0.86	0.11	44,44,44,44	0
54	MG	1a	1778	1/1	0.86	0.16	76,76,76,76	0
54	MG	1a	1779	1/1	0.86	0.16	55,55,55,55	0
54	MG	1A	3412	1/1	0.86	0.15	25,25,25,25	0
54	MG	2A	3641	1/1	0.86	0.10	63,63,63,63	0
54	MG	1A	3417	1/1	0.86	0.17	36,36,36,36	0
54	MG	1A	3321	1/1	0.86	0.43	55,55,55,55	0
54	MG	1F	314	1/1	0.86	0.70	43,43,43,43	0
54	MG	2A	3432	1/1	0.86	0.13	78,78,78,78	0
54	MG	1A	3800	1/1	0.86	0.07	82,82,82,82	0
54	MG	1A	4002	1/1	0.86	0.25	56,56,56,56	0
54	MG	2a	3078	1/1	0.86	0.18	70,70,70,70	0
54	MG	2A	3438	1/1	0.86	0.14	54,54,54,54	0
54	MG	1A	3938	1/1	0.86	0.13	59,59,59,59	0
54	MG	1a	1665	1/1	0.86	0.13	77,77,77,77	0
54	MG	2A	3447	1/1	0.86	0.14	44,44,44,44	0
54	MG	2a	3094	1/1	0.86	0.09	62,62,62,62	0
54	MG	2A	3448	1/1	0.86	0.12	56,56,56,56	0
54	MG	1G	202	1/1	0.86	0.17	71,71,71,71	0
54	MG	1a	1669	1/1	0.86	0.10	66,66,66,66	0
54	MG	1A	3191	1/1	0.86	0.25	38,38,38,38	0
54	MG	2A	3224	1/1	0.86	0.22	56,56,56,56	0
54	MG	2a	3104	1/1	0.86	0.10	81,81,81,81	0
54	MG	1a	1672	1/1	0.86	0.16	48,48,48,48	0
54	MG	2a	3112	1/1	0.86	0.16	55,55,55,55	0
54	MG	2a	3113	1/1	0.86	0.14	69,69,69,69	0
54	MG	1a	1808	1/1	0.86	0.14	92,92,92,92	0
54	MG	2a	3122	1/1	0.86	0.16	78,78,78,78	0
54	MG	1N	203	1/1	0.86	0.18	63,63,63,63	0
54	MG	1A	3299	1/1	0.86	0.20	67,67,67,67	0
54	MG	2A	3683	1/1	0.86	0.14	78,78,78,78	0
54	MG	2A	3053	1/1	0.86	0.08	77,77,77,77	0
54	MG	2A	3686	1/1	0.86	0.18	67,67,67,67	0
54	MG	1O	201	1/1	0.86	0.22	59,59,59,59	0
54	MG	2A	3478	1/1	0.86	0.24	34,34,34,34	0
54	MG	2A	3247	1/1	0.86	0.19	60,60,60,60	0
54	MG	1A	3182	1/1	0.86	0.09	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	1A	3274	1/1	0.86	0.52	63,63,63,63	0
54	MG	2A	3698	1/1	0.86	0.22	62,62,62,62	0
54	MG	1Q	205	1/1	0.86	0.21	54,54,54,54	0
54	MG	2A	3062	1/1	0.86	0.15	61,61,61,61	0
54	MG	2A	3064	1/1	0.86	0.17	55,55,55,55	0
54	MG	1R	202	1/1	0.86	0.23	50,50,50,50	0
54	MG	2A	3269	1/1	0.86	0.11	66,66,66,66	0
54	MG	1a	1832	1/1	0.86	0.08	75,75,75,75	0
54	MG	1R	206	1/1	0.86	0.28	58,58,58,58	0
54	MG	1A	3821	1/1	0.86	0.15	77,77,77,77	0
54	MG	2A	3086	1/1	0.86	0.21	80,80,80,80	0
54	MG	2a	3182	1/1	0.86	0.14	66,66,66,66	0
54	MG	1V	206	1/1	0.86	0.40	59,59,59,59	0
54	MG	1A	3486	1/1	0.86	0.22	32,32,32,32	0
54	MG	1A	4033	1/1	0.86	0.23	75,75,75,75	0
54	MG	2A	3525	1/1	0.86	0.12	63,63,63,63	0
54	MG	1A	3050	1/1	0.86	0.53	32,32,32,32	0
54	MG	1A	3834	1/1	0.86	0.11	59,59,59,59	0
54	MG	2A	3737	1/1	0.86	0.15	72,72,72,72	0
54	MG	1A	4046	1/1	0.86	0.18	69,69,69,69	0
54	MG	1a	1696	1/1	0.86	0.17	66,66,66,66	0
54	MG	1A	3140	1/1	0.86	0.17	41,41,41,41	0
56	MPD	1a	1878	8/8	0.86	0.19	55,70,73,73	0
54	MG	2A	3113	1/1	0.86	0.13	76,76,76,76	0
54	MG	2B	207	1/1	0.86	0.09	81,81,81,81	0
54	MG	2A	3552	1/1	0.86	0.06	80,80,80,80	0
54	MG	1A	3402	1/1	0.86	0.23	29,29,29,29	0
54	MG	1a	1703	1/1	0.86	0.15	39,39,39,39	0
54	MG	2A	3272	1/1	0.87	0.15	76,76,76,76	0
54	MG	1A	3472	1/1	0.87	0.14	57,57,57,57	0
54	MG	2A	3146	1/1	0.87	0.32	56,56,56,56	0
54	MG	2a	3021	1/1	0.87	0.29	71,71,71,71	0
54	MG	1A	3118	1/1	0.87	0.27	41,41,41,41	0
54	MG	1A	3650	1/1	0.87	0.18	53,53,53,53	0
54	MG	2A	3465	1/1	0.87	0.19	60,60,60,60	0
54	MG	2A	3280	1/1	0.87	0.17	53,53,53,53	0
54	MG	2A	3470	1/1	0.87	0.18	84,84,84,84	0
54	MG	1A	3927	1/1	0.87	0.06	56,56,56,56	0
54	MG	1A	3991	1/1	0.87	0.09	50,50,50,50	0
54	MG	1A	3727	1/1	0.87	0.04	71,71,71,71	0
54	MG	1A	3374	1/1	0.87	0.14	67,67,67,67	0
54	MG	2A	3030	1/1	0.87	0.16	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	2A	3166	1/1	0.87	0.10	61,61,61,61	0
54	MG	2A	3660	1/1	0.87	0.16	31,31,31,31	0
54	MG	1A	3995	1/1	0.87	0.26	46,46,46,46	0
54	MG	2A	3173	1/1	0.87	0.34	62,62,62,62	0
54	MG	2A	3032	1/1	0.87	0.37	58,58,58,58	0
54	MG	2a	3062	1/1	0.87	0.23	85,85,85,85	0
54	MG	1a	1715	1/1	0.87	0.59	86,86,86,86	0
54	MG	1A	3937	1/1	0.87	0.10	46,46,46,46	0
54	MG	1A	3244	1/1	0.87	0.79	45,45,45,45	0
54	MG	2A	3677	1/1	0.87	0.07	74,74,74,74	0
54	MG	2A	3187	1/1	0.87	0.21	58,58,58,58	0
54	MG	1A	3060	1/1	0.87	0.09	62,62,62,62	0
54	MG	1A	4003	1/1	0.87	0.33	62,62,62,62	0
54	MG	1A	3825	1/1	0.87	0.55	45,45,45,45	0
54	MG	1A	3054	1/1	0.87	0.14	58,58,58,58	0
54	MG	2A	3511	1/1	0.87	0.13	66,66,66,66	0
54	MG	2A	3512	1/1	0.87	0.35	45,45,45,45	0
54	MG	1A	3285	1/1	0.87	0.20	64,64,64,64	0
54	MG	1A	4013	1/1	0.87	0.23	47,47,47,47	0
54	MG	2A	3051	1/1	0.87	0.18	62,62,62,62	0
54	MG	2A	3347	1/1	0.87	0.18	48,48,48,48	0
54	MG	2A	3533	1/1	0.87	0.15	57,57,57,57	0
54	MG	1a	1750	1/1	0.87	0.17	60,60,60,60	0
54	MG	1A	3949	1/1	0.87	0.14	60,60,60,60	0
54	MG	2A	3360	1/1	0.87	0.23	50,50,50,50	0
54	MG	2A	3055	1/1	0.87	0.18	43,43,43,43	0
54	MG	2A	3364	1/1	0.87	0.12	84,84,84,84	0
54	MG	2A	3551	1/1	0.87	0.18	53,53,53,53	0
54	MG	1A	3386	1/1	0.87	0.12	67,67,67,67	0
54	MG	2A	3057	1/1	0.87	0.28	58,58,58,58	0
54	MG	2A	3377	1/1	0.87	0.12	58,58,58,58	0
54	MG	1A	3603	1/1	0.87	0.24	45,45,45,45	0
54	MG	2A	3560	1/1	0.87	0.13	44,44,44,44	0
54	MG	1A	4024	1/1	0.87	0.11	65,65,65,65	0
54	MG	1A	3330	1/1	0.87	0.09	65,65,65,65	0
54	MG	1A	3954	1/1	0.87	0.10	31,31,31,31	0
54	MG	2a	3143	1/1	0.87	0.18	55,55,55,55	0
54	MG	2a	3145	1/1	0.87	0.10	82,82,82,82	0
54	MG	1A	3676	1/1	0.87	0.10	44,44,44,44	0
54	MG	1R	204	1/1	0.87	0.21	52,52,52,52	0
54	MG	2A	3395	1/1	0.87	0.09	61,61,61,61	0
54	MG	1a	1875	1/1	0.87	0.09	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3216	1/1	0.87	0.79	50,50,50,50	0
54	MG	2a	3161	1/1	0.87	0.11	64,64,64,64	0
54	MG	1A	3678	1/1	0.87	0.24	42,42,42,42	0
54	MG	1A	3163	1/1	0.87	0.21	44,44,44,44	0
54	MG	1A	3779	1/1	0.87	0.15	51,51,51,51	0
54	MG	1A	3450	1/1	0.87	0.16	74,74,74,74	0
54	MG	10	103	1/1	0.87	0.14	52,52,52,52	0
54	MG	2A	3415	1/1	0.87	0.19	47,47,47,47	0
54	MG	1A	4053	1/1	0.87	0.23	53,53,53,53	0
54	MG	1A	3172	1/1	0.87	0.11	67,67,67,67	0
54	MG	2A	3107	1/1	0.87	0.17	58,58,58,58	0
54	MG	2A	3606	1/1	0.87	0.34	62,62,62,62	0
54	MG	2A	3608	1/1	0.87	0.12	84,84,84,84	0
54	MG	13	103	1/1	0.87	0.11	69,69,69,69	0
54	MG	1A	3784	1/1	0.87	0.15	49,49,49,49	0
54	MG	1A	3308	1/1	0.87	0.69	49,49,49,49	0
54	MG	2A	3115	1/1	0.87	0.37	56,56,56,56	0
54	MG	25	101	1/1	0.87	0.17	70,70,70,70	0
54	MG	2A	3433	1/1	0.87	0.23	62,62,62,62	0
54	MG	1A	3575	1/1	0.87	0.19	47,47,47,47	0
54	MG	1A	3916	1/1	0.87	0.15	39,39,39,39	0
54	MG	1a	1688	1/1	0.87	0.14	77,77,77,77	0
54	MG	2A	3260	1/1	0.87	0.19	31,31,31,31	0
54	MG	1A	3228	1/1	0.87	0.77	44,44,44,44	0
54	MG	1A	3982	1/1	0.87	0.26	51,51,51,51	0
54	MG	1A	3511	1/1	0.87	0.23	54,54,54,54	0
58	ZN	2Y	202	1/1	0.87	0.14	97,97,97,97	0
54	MG	1A	3194	1/1	0.87	0.33	54,54,54,54	0
54	MG	1a	1602	1/1	0.88	0.12	78,78,78,78	0
54	MG	1a	1708	1/1	0.88	0.11	72,72,72,72	0
54	MG	1A	3238	1/1	0.88	0.62	42,42,42,42	0
54	MG	1A	3861	1/1	0.88	0.09	34,34,34,34	0
54	MG	1A	3863	1/1	0.88	0.12	53,53,53,53	0
54	MG	1B	219	1/1	0.88	0.16	35,35,35,35	0
54	MG	2A	3061	1/1	0.88	0.73	61,61,61,61	0
54	MG	1A	3193	1/1	0.88	0.23	64,64,64,64	0
54	MG	1A	3367	1/1	0.88	0.21	26,26,26,26	0
54	MG	2a	3012	1/1	0.88	0.24	68,68,68,68	0
54	MG	1D	309	1/1	0.88	0.67	57,57,57,57	0
54	MG	1A	3580	1/1	0.88	0.18	24,24,24,24	0
54	MG	1A	3325	1/1	0.88	0.18	39,39,39,39	0
54	MG	2a	3019	1/1	0.88	0.24	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1731	1/1	0.88	0.15	59,59,59,59	0
54	MG	2A	3081	1/1	0.88	0.39	48,48,48,48	0
54	MG	2a	3022	1/1	0.88	0.10	77,77,77,77	0
54	MG	1a	1736	1/1	0.88	0.07	67,67,67,67	0
54	MG	1A	3627	1/1	0.88	0.21	39,39,39,39	0
54	MG	1A	3875	1/1	0.88	0.17	69,69,69,69	0
54	MG	2A	3444	1/1	0.88	0.21	66,66,66,66	0
54	MG	2a	3037	1/1	0.88	0.08	74,74,74,74	0
54	MG	2A	3446	1/1	0.88	0.12	64,64,64,64	0
54	MG	1a	1868	1/1	0.88	0.14	65,65,65,65	0
54	MG	1A	3819	1/1	0.88	0.16	48,48,48,48	0
54	MG	2a	3042	1/1	0.88	0.24	74,74,74,74	0
54	MG	1a	1745	1/1	0.88	0.10	57,57,57,57	0
54	MG	2A	3640	1/1	0.88	0.09	74,74,74,74	0
54	MG	2A	3099	1/1	0.88	0.14	65,65,65,65	0
54	MG	2A	3452	1/1	0.88	0.19	38,38,38,38	0
54	MG	1a	1635	1/1	0.88	0.17	65,65,65,65	0
54	MG	2A	3265	1/1	0.88	0.16	32,32,32,32	0
54	MG	1A	3088	1/1	0.88	0.36	40,40,40,40	0
54	MG	1A	3944	1/1	0.88	0.11	64,64,64,64	0
54	MG	2a	3061	1/1	0.88	0.15	68,68,68,68	0
54	MG	1A	3201	1/1	0.88	0.75	49,49,49,49	0
54	MG	1A	3765	1/1	0.88	0.21	47,47,47,47	0
54	MG	2A	3651	1/1	0.88	0.17	57,57,57,57	0
54	MG	1A	4009	1/1	0.88	0.22	64,64,64,64	0
54	MG	1A	3830	1/1	0.88	0.20	36,36,36,36	0
54	MG	2A	3118	1/1	0.88	0.43	45,45,45,45	0
54	MG	2A	3119	1/1	0.88	0.13	38,38,38,38	0
54	MG	1e	201	1/1	0.88	0.34	59,59,59,59	0
54	MG	2A	3284	1/1	0.88	0.21	44,44,44,44	0
54	MG	1A	3683	1/1	0.88	0.14	68,68,68,68	0
54	MG	1A	3416	1/1	0.88	0.30	68,68,68,68	0
54	MG	1a	1656	1/1	0.88	0.46	50,50,50,50	0
54	MG	2a	3092	1/1	0.88	0.12	80,80,80,80	0
54	MG	1h	202	1/1	0.88	0.18	64,64,64,64	0
54	MG	2A	3136	1/1	0.88	0.19	62,62,62,62	0
54	MG	2a	3097	1/1	0.88	0.08	86,86,86,86	0
54	MG	1A	3646	1/1	0.88	0.10	78,78,78,78	0
54	MG	1A	3055	1/1	0.88	0.14	51,51,51,51	0
54	MG	1n	103	1/1	0.88	0.13	73,73,73,73	0
54	MG	1A	3335	1/1	0.88	0.16	32,32,32,32	0
54	MG	2A	3504	1/1	0.88	0.12	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	2A	3321	1/1	0.88	0.14	48,48,48,48	0
54	MG	2a	3110	1/1	0.88	0.17	77,77,77,77	0
54	MG	1A	3204	1/1	0.88	0.63	50,50,50,50	0
54	MG	1P	205	1/1	0.88	0.16	74,74,74,74	0
54	MG	2a	3119	1/1	0.88	0.19	86,86,86,86	0
54	MG	1A	4027	1/1	0.88	0.14	59,59,59,59	0
54	MG	1Q	204	1/1	0.88	0.29	48,48,48,48	0
54	MG	2A	3517	1/1	0.88	0.09	70,70,70,70	0
54	MG	2A	3696	1/1	0.88	0.14	63,63,63,63	0
54	MG	1A	4029	1/1	0.88	0.12	46,46,46,46	0
54	MG	2a	3130	1/1	0.88	0.08	70,70,70,70	0
54	MG	2A	3522	1/1	0.88	0.17	64,64,64,64	0
54	MG	2A	3523	1/1	0.88	0.20	51,51,51,51	0
54	MG	2A	3336	1/1	0.88	0.14	49,49,49,49	0
54	MG	1A	3654	1/1	0.88	0.13	69,69,69,69	0
54	MG	1a	1790	1/1	0.88	0.09	74,74,74,74	0
54	MG	2A	3529	1/1	0.88	0.13	49,49,49,49	0
54	MG	1A	4034	1/1	0.88	0.60	59,59,59,59	0
54	MG	2A	3720	1/1	0.88	0.18	57,57,57,57	0
54	MG	2A	3170	1/1	0.88	0.28	67,67,67,67	0
54	MG	1A	3843	1/1	0.88	0.19	43,43,43,43	0
54	MG	2A	3724	1/1	0.88	0.20	71,71,71,71	0
54	MG	1A	4038	1/1	0.88	0.16	60,60,60,60	0
54	MG	2A	3727	1/1	0.88	0.14	62,62,62,62	0
54	MG	1A	3655	1/1	0.88	0.11	39,39,39,39	0
54	MG	1W	202	1/1	0.88	0.29	54,54,54,54	0
54	MG	1a	1801	1/1	0.88	0.15	71,71,71,71	0
54	MG	1A	3846	1/1	0.88	0.12	55,55,55,55	0
54	MG	2A	3553	1/1	0.88	0.09	75,75,75,75	0
54	MG	2a	3177	1/1	0.88	0.11	72,72,72,72	0
54	MG	2a	3178	1/1	0.88	0.09	58,58,58,58	0
54	MG	1a	1804	1/1	0.88	0.09	71,71,71,71	0
54	MG	1A	3785	1/1	0.88	0.13	41,41,41,41	0
54	MG	1A	3709	1/1	0.88	0.35	66,66,66,66	0
54	MG	1A	3852	1/1	0.88	0.18	43,43,43,43	0
54	MG	1A	3344	1/1	0.88	0.19	32,32,32,32	0
54	MG	2A	3039	1/1	0.88	0.15	57,57,57,57	0
54	MG	11	105	1/1	0.88	0.12	44,44,44,44	0
54	MG	1A	3855	1/1	0.88	0.27	50,50,50,50	0
54	MG	2A	3198	1/1	0.88	0.11	77,77,77,77	0
54	MG	2A	3389	1/1	0.88	0.18	40,40,40,40	0
54	MG	1A	3976	1/1	0.88	0.18	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	2j	201	1/1	0.88	0.16	82,82,82,82	0
54	MG	1A	3913	1/1	0.88	0.19	29,29,29,29	0
56	MPD	1A	4058	8/8	0.88	0.16	51,55,64,66	0
54	MG	1A	3981	1/1	0.88	0.13	60,60,60,60	0
54	MG	1A	3265	1/1	0.88	0.28	62,62,62,62	0
54	MG	1A	3150	1/1	0.88	1.18	45,45,45,45	0
56	MPD	2A	3744	8/8	0.88	0.22	63,68,74,74	0
54	MG	2A	3590	1/1	0.88	0.17	41,41,41,41	0
54	MG	2A	3052	1/1	0.88	0.17	72,72,72,72	0
54	MG	1A	3519	1/1	0.88	0.17	27,27,27,27	0
54	MG	2A	3598	1/1	0.88	0.35	62,62,62,62	0
54	MG	2Y	201	1/1	0.88	0.29	60,60,60,60	0
54	MG	2A	3594	1/1	0.89	0.23	58,58,58,58	0
54	MG	1A	3618	1/1	0.89	0.20	36,36,36,36	0
54	MG	1A	4035	1/1	0.89	0.12	62,62,62,62	0
54	MG	2a	3005	1/1	0.89	0.14	54,54,54,54	0
54	MG	1A	3324	1/1	0.89	0.16	33,33,33,33	0
54	MG	1A	4037	1/1	0.89	0.17	71,71,71,71	0
54	MG	1A	3697	1/1	0.89	0.08	61,61,61,61	0
54	MG	2A	3050	1/1	0.89	0.12	42,42,42,42	0
54	MG	1A	3290	1/1	0.89	0.16	56,56,56,56	0
54	MG	1A	4041	1/1	0.89	0.56	45,45,45,45	0
54	MG	1A	3428	1/1	0.89	0.34	47,47,47,47	0
54	MG	1a	1833	1/1	0.89	0.24	72,72,72,72	0
54	MG	2A	3425	1/1	0.89	0.26	70,70,70,70	0
54	MG	1A	3702	1/1	0.89	0.34	43,43,43,43	0
54	MG	1A	3808	1/1	0.89	0.17	62,62,62,62	0
54	MG	1A	3625	1/1	0.89	0.23	30,30,30,30	0
54	MG	1A	3813	1/1	0.89	0.32	38,38,38,38	0
54	MG	2A	3621	1/1	0.89	0.27	64,64,64,64	0
54	MG	1A	3292	1/1	0.89	0.13	51,51,51,51	0
54	MG	1A	3969	1/1	0.89	0.26	60,60,60,60	0
54	MG	1a	1849	1/1	0.89	0.09	72,72,72,72	0
54	MG	1a	1705	1/1	0.89	0.16	78,78,78,78	0
54	MG	1a	1854	1/1	0.89	0.09	62,62,62,62	0
54	MG	1A	3022	1/1	0.89	0.22	45,45,45,45	0
54	MG	1a	1856	1/1	0.89	0.18	63,63,63,63	0
54	MG	1A	3630	1/1	0.89	0.18	27,27,27,27	0
54	MG	1A	3492	1/1	0.89	0.16	24,24,24,24	0
54	MG	2a	3046	1/1	0.89	0.20	61,61,61,61	0
54	MG	2A	3637	1/1	0.89	0.07	64,64,64,64	0
54	MG	2A	3085	1/1	0.89	0.25	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3895	1/1	0.89	0.47	39,39,39,39	0
54	MG	1B	208	1/1	0.89	0.14	45,45,45,45	0
54	MG	1A	3713	1/1	0.89	0.19	54,54,54,54	0
54	MG	1A	3718	1/1	0.89	0.39	53,53,53,53	0
54	MG	2a	3056	1/1	0.89	0.07	76,76,76,76	0
54	MG	1A	3832	1/1	0.89	0.17	52,52,52,52	0
54	MG	1A	3145	1/1	0.89	0.25	56,56,56,56	0
54	MG	2a	3063	1/1	0.89	0.12	68,68,68,68	0
54	MG	1A	3642	1/1	0.89	0.74	67,67,67,67	0
54	MG	1a	1619	1/1	0.89	0.15	47,47,47,47	0
54	MG	2A	3106	1/1	0.89	0.23	54,54,54,54	0
54	MG	1a	1735	1/1	0.89	0.17	70,70,70,70	0
54	MG	2A	3274	1/1	0.89	0.13	43,43,43,43	0
54	MG	1A	3273	1/1	0.89	0.15	39,39,39,39	0
54	MG	1A	3730	1/1	0.89	0.18	67,67,67,67	0
54	MG	1B	224	1/1	0.89	0.17	72,72,72,72	0
54	MG	1a	1626	1/1	0.89	0.12	64,64,64,64	0
54	MG	1A	3305	1/1	0.89	0.25	48,48,48,48	0
54	MG	2a	3087	1/1	0.89	0.11	53,53,53,53	0
54	MG	2a	3089	1/1	0.89	0.06	60,60,60,60	0
54	MG	1A	3735	1/1	0.89	0.19	63,63,63,63	0
54	MG	2A	3674	1/1	0.89	0.13	72,72,72,72	0
54	MG	1A	3914	1/1	0.89	0.14	38,38,38,38	0
54	MG	2A	3293	1/1	0.89	0.11	39,39,39,39	0
54	MG	1A	3506	1/1	0.89	0.09	53,53,53,53	0
54	MG	1A	3395	1/1	0.89	0.15	37,37,37,37	0
54	MG	2A	3491	1/1	0.89	0.18	42,42,42,42	0
54	MG	1A	3343	1/1	0.89	0.12	43,43,43,43	0
54	MG	1a	1760	1/1	0.89	0.08	68,68,68,68	0
54	MG	1A	3458	1/1	0.89	0.11	55,55,55,55	0
54	MG	2A	3308	1/1	0.89	0.11	67,67,67,67	0
54	MG	2a	3107	1/1	0.89	0.39	75,75,75,75	0
54	MG	1F	307	1/1	0.89	0.13	37,37,37,37	0
54	MG	1a	1645	1/1	0.89	0.18	74,74,74,74	0
54	MG	1l	202	1/1	0.89	0.07	83,83,83,83	0
54	MG	1A	3999	1/1	0.89	0.11	62,62,62,62	0
54	MG	1a	1766	1/1	0.89	0.15	84,84,84,84	0
54	MG	1t	201	1/1	0.89	0.42	74,74,74,74	0
54	MG	2A	3518	1/1	0.89	0.06	61,61,61,61	0
54	MG	1A	3585	1/1	0.89	0.41	45,45,45,45	0
54	MG	2A	3701	1/1	0.89	0.16	65,65,65,65	0
54	MG	2a	3127	1/1	0.89	0.12	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	1652	1/1	0.89	0.20	60,60,60,60	0
54	MG	1A	3660	1/1	0.89	0.36	53,53,53,53	0
54	MG	1A	3516	1/1	0.89	0.19	29,29,29,29	0
54	MG	2A	3341	1/1	0.89	0.15	53,53,53,53	0
54	MG	1A	3181	1/1	0.89	0.18	58,58,58,58	0
54	MG	1a	1780	1/1	0.89	0.08	85,85,85,85	0
54	MG	2A	3530	1/1	0.89	0.17	44,44,44,44	0
54	MG	2a	3148	1/1	0.89	0.17	67,67,67,67	0
54	MG	1A	3027	1/1	0.89	0.14	65,65,65,65	0
54	MG	1H	201	1/1	0.89	0.23	66,66,66,66	0
54	MG	1a	1660	1/1	0.89	0.08	71,71,71,71	0
54	MG	2a	3156	1/1	0.89	0.14	73,73,73,73	0
54	MG	2A	3539	1/1	0.89	0.10	56,56,56,56	0
54	MG	1H	202	1/1	0.89	0.29	59,59,59,59	0
54	MG	2a	3160	1/1	0.89	0.12	82,82,82,82	0
54	MG	2A	3545	1/1	0.89	0.16	77,77,77,77	0
54	MG	1A	3466	1/1	0.89	0.11	57,57,57,57	0
54	MG	2A	3356	1/1	0.89	0.11	72,72,72,72	0
54	MG	2A	3550	1/1	0.89	0.16	55,55,55,55	0
54	MG	2A	3178	1/1	0.89	0.10	61,61,61,61	0
54	MG	1A	3594	1/1	0.89	0.14	75,75,75,75	0
54	MG	2A	3362	1/1	0.89	0.28	62,62,62,62	0
54	MG	2A	3181	1/1	0.89	0.32	58,58,58,58	0
54	MG	2A	3556	1/1	0.89	0.10	65,65,65,65	0
54	MG	2A	3183	1/1	0.89	0.14	61,61,61,61	0
54	MG	2A	3366	1/1	0.89	0.20	43,43,43,43	0
54	MG	1A	3100	1/1	0.89	0.58	38,38,38,38	0
54	MG	1A	3671	1/1	0.89	0.06	65,65,65,65	0
54	MG	2A	3028	1/1	0.89	0.17	61,61,61,61	0
54	MG	2D	304	1/1	0.89	0.65	52,52,52,52	0
54	MG	2a	3192	1/1	0.89	0.14	82,82,82,82	0
54	MG	1A	3279	1/1	0.89	0.18	51,51,51,51	0
54	MG	1A	3673	1/1	0.89	0.14	65,65,65,65	0
54	MG	2A	3573	1/1	0.89	0.10	58,58,58,58	0
54	MG	1A	3476	1/1	0.89	0.22	51,51,51,51	0
54	MG	2A	3383	1/1	0.89	0.27	52,52,52,52	0
54	MG	1A	3014	1/1	0.89	0.27	65,65,65,65	0
54	MG	2p	101	1/1	0.89	0.23	67,67,67,67	0
54	MG	2A	3386	1/1	0.89	0.17	40,40,40,40	0
54	MG	2t	201	1/1	0.89	0.11	54,54,54,54	0
54	MG	1A	3267	1/1	0.89	1.00	55,55,55,55	0
54	MG	2A	3036	1/1	0.89	0.12	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3584	1/1	0.89	0.17	69,69,69,69	0
54	MG	2Q	202	1/1	0.89	0.15	66,66,66,66	0
54	MG	2T	201	1/1	0.89	0.20	68,68,68,68	0
54	MG	2W	203	1/1	0.89	0.26	64,64,64,64	0
54	MG	1A	3320	1/1	0.89	0.12	77,77,77,77	0
54	MG	20	102	1/1	0.89	0.08	71,71,71,71	0
54	MG	1A	3159	1/1	0.89	0.21	38,38,38,38	0
54	MG	1a	1680	1/1	0.89	0.12	75,75,75,75	0
54	MG	1A	3504	1/1	0.90	0.19	61,61,61,61	0
54	MG	1a	1611	1/1	0.90	0.18	69,69,69,69	0
54	MG	1A	3010	1/1	0.90	0.14	58,58,58,58	0
54	MG	2A	3083	1/1	0.90	0.34	48,48,48,48	0
54	MG	2a	3018	1/1	0.90	0.15	57,57,57,57	0
54	MG	1A	3827	1/1	0.90	0.30	59,59,59,59	0
54	MG	1a	1728	1/1	0.90	0.14	56,56,56,56	0
54	MG	1a	1618	1/1	0.90	0.11	65,65,65,65	0
54	MG	1A	3152	1/1	0.90	0.32	33,33,33,33	0
54	MG	1A	3440	1/1	0.90	0.09	72,72,72,72	0
54	MG	2A	3262	1/1	0.90	0.88	52,52,52,52	0
54	MG	2A	3263	1/1	0.90	0.15	52,52,52,52	0
54	MG	2A	3094	1/1	0.90	0.10	55,55,55,55	0
54	MG	2a	3035	1/1	0.90	0.22	72,72,72,72	0
54	MG	1A	3319	1/1	0.90	0.19	60,60,60,60	0
54	MG	1B	226	1/1	0.90	0.16	73,73,73,73	0
54	MG	1a	1869	1/1	0.90	0.15	66,66,66,66	0
54	MG	1A	3098	1/1	0.90	0.38	59,59,59,59	0
54	MG	2A	3102	1/1	0.90	0.12	56,56,56,56	0
54	MG	1A	3907	1/1	0.90	0.10	53,53,53,53	0
54	MG	1A	3052	1/1	0.90	0.11	44,44,44,44	0
54	MG	1a	1747	1/1	0.90	0.08	54,54,54,54	0
54	MG	1A	3384	1/1	0.90	0.14	53,53,53,53	0
54	MG	2a	3049	1/1	0.90	0.25	84,84,84,84	0
54	MG	1A	3747	1/1	0.90	0.09	65,65,65,65	0
54	MG	1A	3752	1/1	0.90	0.23	39,39,39,39	0
54	MG	1A	3044	1/1	0.90	0.15	31,31,31,31	0
54	MG	1a	1756	1/1	0.90	0.43	66,66,66,66	0
54	MG	1a	1757	1/1	0.90	0.17	56,56,56,56	0
54	MG	1E	309	1/1	0.90	0.43	58,58,58,58	0
54	MG	2a	3057	1/1	0.90	0.11	88,88,88,88	0
54	MG	2a	3059	1/1	0.90	0.33	75,75,75,75	0
54	MG	1A	3839	1/1	0.90	0.18	39,39,39,39	0
54	MG	2A	3662	1/1	0.90	0.09	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	3598	1/1	0.90	0.14	68,68,68,68	0
54	MG	2A	3666	1/1	0.90	0.11	62,62,62,62	0
54	MG	1A	4001	1/1	0.90	0.14	81,81,81,81	0
54	MG	2A	3494	1/1	0.90	0.12	53,53,53,53	0
54	MG	2A	3496	1/1	0.90	0.23	72,72,72,72	0
54	MG	2a	3073	1/1	0.90	0.14	75,75,75,75	0
54	MG	1A	3243	1/1	0.90	0.10	46,46,46,46	0
54	MG	2a	3075	1/1	0.90	0.11	70,70,70,70	0
54	MG	1A	3161	1/1	0.90	0.14	43,43,43,43	0
54	MG	1m	201	1/1	0.90	0.10	79,79,79,79	0
54	MG	1A	3283	1/1	0.90	0.12	49,49,49,49	0
54	MG	1A	3249	1/1	0.90	0.21	56,56,56,56	0
54	MG	1A	3766	1/1	0.90	0.14	31,31,31,31	0
54	MG	2a	3083	1/1	0.90	0.32	82,82,82,82	0
54	MG	2A	3148	1/1	0.90	0.09	66,66,66,66	0
54	MG	1A	3851	1/1	0.90	0.12	54,54,54,54	0
54	MG	1y	202	1/1	0.90	0.29	71,71,71,71	0
54	MG	2A	3513	1/1	0.90	0.18	56,56,56,56	0
54	MG	1A	4011	1/1	0.90	0.19	53,53,53,53	0
54	MG	2a	3095	1/1	0.90	0.17	58,58,58,58	0
54	MG	1A	3250	1/1	0.90	0.18	64,64,64,64	0
54	MG	2A	3692	1/1	0.90	0.15	44,44,44,44	0
54	MG	2A	3519	1/1	0.90	0.22	72,72,72,72	0
54	MG	1A	3195	1/1	0.90	0.11	52,52,52,52	0
54	MG	1a	1662	1/1	0.90	0.13	67,67,67,67	0
54	MG	1A	4016	1/1	0.90	0.15	63,63,63,63	0
54	MG	1A	3342	1/1	0.90	0.12	48,48,48,48	0
54	MG	1a	1668	1/1	0.90	0.11	60,60,60,60	0
54	MG	2a	3106	1/1	0.90	0.11	66,66,66,66	0
54	MG	2A	3700	1/1	0.90	0.09	61,61,61,61	0
54	MG	2a	3108	1/1	0.90	0.18	71,71,71,71	0
54	MG	1A	3679	1/1	0.90	0.15	70,70,70,70	0
54	MG	2A	3705	1/1	0.90	0.44	51,51,51,51	0
54	MG	1A	3541	1/1	0.90	0.17	63,63,63,63	0
54	MG	2a	3116	1/1	0.90	0.12	58,58,58,58	0
54	MG	1A	3681	1/1	0.90	0.26	56,56,56,56	0
54	MG	2A	3176	1/1	0.90	0.20	65,65,65,65	0
54	MG	2A	3714	1/1	0.90	0.26	65,65,65,65	0
54	MG	2A	3534	1/1	0.90	0.07	69,69,69,69	0
54	MG	1A	3619	1/1	0.90	0.14	44,44,44,44	0
54	MG	1A	3102	1/1	0.90	0.24	36,36,36,36	0
54	MG	1A	3550	1/1	0.90	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	3026	1/1	0.90	0.22	58,58,58,58	0
54	MG	2A	3544	1/1	0.90	0.14	60,60,60,60	0
54	MG	2a	3134	1/1	0.90	0.39	69,69,69,69	0
54	MG	1A	3948	1/1	0.90	0.24	62,62,62,62	0
54	MG	1A	3694	1/1	0.90	0.15	71,71,71,71	0
54	MG	2a	3141	1/1	0.90	0.13	64,64,64,64	0
54	MG	1T	202	1/1	0.90	0.13	65,65,65,65	0
54	MG	1T	203	1/1	0.90	0.07	65,65,65,65	0
54	MG	1A	3170	1/1	0.90	0.23	54,54,54,54	0
54	MG	1a	1682	1/1	0.90	0.11	59,59,59,59	0
54	MG	2A	3373	1/1	0.90	0.14	62,62,62,62	0
54	MG	1A	3413	1/1	0.90	0.10	42,42,42,42	0
54	MG	2A	3555	1/1	0.90	0.12	72,72,72,72	0
54	MG	2a	3155	1/1	0.90	0.14	54,54,54,54	0
54	MG	2A	3738	1/1	0.90	0.06	81,81,81,81	0
54	MG	1A	3038	1/1	0.90	0.19	49,49,49,49	0
54	MG	1a	1815	1/1	0.90	0.12	67,67,67,67	0
54	MG	1a	1685	1/1	0.90	0.12	59,59,59,59	0
54	MG	2A	3382	1/1	0.90	0.17	53,53,53,53	0
54	MG	2a	3162	1/1	0.90	0.10	79,79,79,79	0
54	MG	1a	1817	1/1	0.90	0.11	76,76,76,76	0
54	MG	2A	3201	1/1	0.90	0.11	56,56,56,56	0
54	MG	2a	3168	1/1	0.90	0.07	71,71,71,71	0
54	MG	2A	3563	1/1	0.90	0.16	38,38,38,38	0
54	MG	2B	210	1/1	0.90	0.11	82,82,82,82	0
54	MG	2A	3385	1/1	0.90	0.14	65,65,65,65	0
54	MG	2B	217	1/1	0.90	0.16	83,83,83,83	0
54	MG	1A	3561	1/1	0.90	0.14	54,54,54,54	0
54	MG	2A	3388	1/1	0.90	0.33	72,72,72,72	0
54	MG	2D	309	1/1	0.90	0.31	42,42,42,42	0
54	MG	1A	3173	1/1	0.90	0.54	46,46,46,46	0
54	MG	1A	3957	1/1	0.90	0.14	55,55,55,55	0
54	MG	1A	3878	1/1	0.90	0.22	40,40,40,40	0
54	MG	2a	3186	1/1	0.90	0.17	78,78,78,78	0
54	MG	1a	1826	1/1	0.90	0.09	82,82,82,82	0
54	MG	1A	3268	1/1	0.90	0.14	35,35,35,35	0
54	MG	2A	3401	1/1	0.90	0.13	50,50,50,50	0
54	MG	1A	3801	1/1	0.90	0.14	49,49,49,49	0
54	MG	2A	3588	1/1	0.90	0.15	38,38,38,38	0
54	MG	1A	3178	1/1	0.90	0.52	52,52,52,52	0
54	MG	2A	3211	1/1	0.90	0.26	64,64,64,64	0
54	MG	1a	1835	1/1	0.90	0.17	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	2A	3214	1/1	0.90	0.20	49,49,49,49	0
54	MG	2o	101	1/1	0.90	0.18	69,69,69,69	0
54	MG	1A	3108	1/1	0.90	0.12	42,42,42,42	0
54	MG	1A	3885	1/1	0.90	0.15	44,44,44,44	0
54	MG	1A	3369	1/1	0.90	0.22	65,65,65,65	0
54	MG	1A	3811	1/1	0.90	0.45	47,47,47,47	0
54	MG	18	103	1/1	0.90	0.38	42,42,42,42	0
54	MG	1A	3078	1/1	0.90	0.19	52,52,52,52	0
54	MG	2A	3226	1/1	0.90	0.81	57,57,57,57	0
54	MG	1A	3715	1/1	0.90	0.13	28,28,28,28	0
54	MG	2a	3006	1/1	0.90	0.22	58,58,58,58	0
54	MG	1A	3716	1/1	0.90	0.21	29,29,29,29	0
54	MG	2A	3231	1/1	0.90	0.40	41,41,41,41	0
54	MG	1A	3434	1/1	0.90	0.22	65,65,65,65	0
54	MG	1A	3820	1/1	0.90	0.10	53,53,53,53	0
54	MG	2A	3216	1/1	0.91	0.20	67,67,67,67	0
54	MG	2A	3423	1/1	0.91	0.20	66,66,66,66	0
54	MG	1A	3864	1/1	0.91	0.12	51,51,51,51	0
54	MG	1a	1845	1/1	0.91	0.17	60,60,60,60	0
54	MG	2A	3428	1/1	0.91	0.12	62,62,62,62	0
54	MG	1A	3867	1/1	0.91	0.32	45,45,45,45	0
54	MG	1A	3459	1/1	0.91	0.18	52,52,52,52	0
54	MG	1A	3787	1/1	0.91	0.14	50,50,50,50	0
54	MG	1A	3275	1/1	0.91	0.17	33,33,33,33	0
54	MG	1A	3164	1/1	0.91	0.13	51,51,51,51	0
54	MG	2A	3228	1/1	0.91	0.11	71,71,71,71	0
54	MG	2A	3229	1/1	0.91	0.16	67,67,67,67	0
54	MG	15	106	1/1	0.91	0.14	50,50,50,50	0
54	MG	1A	4052	1/1	0.91	0.25	64,64,64,64	0
54	MG	1A	3242	1/1	0.91	0.69	43,43,43,43	0
54	MG	2A	3240	1/1	0.91	0.61	43,43,43,43	0
54	MG	2A	3076	1/1	0.91	0.13	54,54,54,54	0
54	MG	1A	3795	1/1	0.91	0.26	70,70,70,70	0
54	MG	1A	3105	1/1	0.91	0.40	70,70,70,70	0
54	MG	2a	3045	1/1	0.91	0.36	84,84,84,84	0
54	MG	1A	3469	1/1	0.91	0.17	57,57,57,57	0
54	MG	1A	3471	1/1	0.91	0.19	58,58,58,58	0
54	MG	1A	3551	1/1	0.91	0.26	46,46,46,46	0
54	MG	1A	3803	1/1	0.91	0.33	63,63,63,63	0
54	MG	2A	3090	1/1	0.91	0.22	72,72,72,72	0
54	MG	2A	3091	1/1	0.91	0.09	68,68,68,68	0
54	MG	2A	3464	1/1	0.91	0.07	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3632	1/1	0.91	0.19	50,50,50,50	0
54	MG	2A	3654	1/1	0.91	0.05	85,85,85,85	0
54	MG	2A	3467	1/1	0.91	0.17	34,34,34,34	0
54	MG	2A	3261	1/1	0.91	0.30	62,62,62,62	0
54	MG	2a	3060	1/1	0.91	0.35	67,67,67,67	0
54	MG	1A	3280	1/1	0.91	0.81	52,52,52,52	0
54	MG	1A	3807	1/1	0.91	0.12	57,57,57,57	0
54	MG	2A	3096	1/1	0.91	0.15	48,48,48,48	0
54	MG	2A	3664	1/1	0.91	0.07	62,62,62,62	0
54	MG	1B	215	1/1	0.91	0.34	56,56,56,56	0
54	MG	2A	3266	1/1	0.91	0.07	74,74,74,74	0
54	MG	1a	1617	1/1	0.91	0.10	67,67,67,67	0
54	MG	1a	1871	1/1	0.91	0.10	78,78,78,78	0
54	MG	1A	3196	1/1	0.91	0.24	67,67,67,67	0
54	MG	1A	3977	1/1	0.91	0.13	27,27,27,27	0
54	MG	2a	3076	1/1	0.91	0.18	72,72,72,72	0
54	MG	1A	3049	1/1	0.91	0.32	40,40,40,40	0
54	MG	2A	3487	1/1	0.91	0.15	52,52,52,52	0
54	MG	2A	3678	1/1	0.91	0.12	62,62,62,62	0
54	MG	1A	3097	1/1	0.91	0.31	36,36,36,36	0
54	MG	1A	3332	1/1	0.91	0.15	29,29,29,29	0
54	MG	1d	302	1/1	0.91	0.23	65,65,65,65	0
54	MG	1A	3284	1/1	0.91	0.09	77,77,77,77	0
54	MG	1B	225	1/1	0.91	0.15	44,44,44,44	0
54	MG	1A	3149	1/1	0.91	0.49	50,50,50,50	0
54	MG	1B	228	1/1	0.91	0.16	68,68,68,68	0
54	MG	2A	3690	1/1	0.91	0.15	56,56,56,56	0
54	MG	1A	3725	1/1	0.91	0.14	36,36,36,36	0
54	MG	2A	3292	1/1	0.91	0.07	59,59,59,59	0
54	MG	1D	311	1/1	0.91	0.19	49,49,49,49	0
54	MG	1A	3899	1/1	0.91	0.20	41,41,41,41	0
54	MG	1D	315	1/1	0.91	0.07	73,73,73,73	0
54	MG	2A	3510	1/1	0.91	0.17	38,38,38,38	0
54	MG	1A	3484	1/1	0.91	0.23	30,30,30,30	0
54	MG	2A	3125	1/1	0.91	0.14	66,66,66,66	0
54	MG	1a	1642	1/1	0.91	0.11	68,68,68,68	0
54	MG	2A	3307	1/1	0.91	0.23	45,45,45,45	0
54	MG	2A	3134	1/1	0.91	0.19	70,70,70,70	0
54	MG	2A	3706	1/1	0.91	0.18	65,65,65,65	0
54	MG	1A	3824	1/1	0.91	0.31	41,41,41,41	0
54	MG	1A	3729	1/1	0.91	0.14	52,52,52,52	0
54	MG	2A	3313	1/1	0.91	0.21	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	2A	3711	1/1	0.91	0.16	74,74,74,74	0
54	MG	2A	3319	1/1	0.91	0.13	53,53,53,53	0
54	MG	2A	3320	1/1	0.91	0.17	69,69,69,69	0
54	MG	1A	3253	1/1	0.91	0.14	46,46,46,46	0
54	MG	2A	3143	1/1	0.91	0.27	42,42,42,42	0
54	MG	2A	3528	1/1	0.91	0.14	42,42,42,42	0
54	MG	2A	3144	1/1	0.91	0.21	54,54,54,54	0
54	MG	1A	3059	1/1	0.91	0.18	37,37,37,37	0
54	MG	1A	3295	1/1	0.91	0.47	41,41,41,41	0
54	MG	1A	3355	1/1	0.91	0.12	38,38,38,38	0
54	MG	1y	203	1/1	0.91	0.26	80,80,80,80	0
54	MG	2A	3150	1/1	0.91	0.09	68,68,68,68	0
54	MG	2A	3151	1/1	0.91	0.21	67,67,67,67	0
54	MG	1A	3209	1/1	0.91	0.58	43,43,43,43	0
54	MG	2A	3734	1/1	0.91	0.19	51,51,51,51	0
54	MG	1A	3665	1/1	0.91	0.16	22,22,22,22	0
54	MG	2a	3144	1/1	0.91	0.30	47,47,47,47	0
54	MG	1A	3748	1/1	0.91	0.33	67,67,67,67	0
54	MG	2A	3160	1/1	0.91	0.26	75,75,75,75	0
54	MG	1A	3750	1/1	0.91	0.18	46,46,46,46	0
54	MG	2a	3152	1/1	0.91	0.10	57,57,57,57	0
54	MG	2A	3004	1/1	0.91	0.14	45,45,45,45	0
54	MG	1A	3495	1/1	0.91	0.14	31,31,31,31	0
54	MG	2A	3008	1/1	0.91	0.25	53,53,53,53	0
54	MG	1A	3422	1/1	0.91	0.23	62,62,62,62	0
54	MG	1a	1664	1/1	0.91	0.14	83,83,83,83	0
54	MG	1a	1792	1/1	0.91	0.16	66,66,66,66	0
54	MG	1A	4005	1/1	0.91	0.46	38,38,38,38	0
54	MG	1A	4007	1/1	0.91	0.33	42,42,42,42	0
54	MG	2B	213	1/1	0.91	0.11	78,78,78,78	0
54	MG	2A	3177	1/1	0.91	0.25	71,71,71,71	0
54	MG	2A	3018	1/1	0.91	0.78	54,54,54,54	0
54	MG	2A	3019	1/1	0.91	0.96	51,51,51,51	0
54	MG	2D	305	1/1	0.91	1.05	48,48,48,48	0
54	MG	2a	3171	1/1	0.91	0.14	61,61,61,61	0
54	MG	2A	3022	1/1	0.91	0.44	51,51,51,51	0
54	MG	1A	3499	1/1	0.91	0.18	51,51,51,51	0
54	MG	2A	3564	1/1	0.91	0.12	61,61,61,61	0
54	MG	1A	3840	1/1	0.91	0.10	59,59,59,59	0
54	MG	1A	3030	1/1	0.91	0.13	35,35,35,35	0
54	MG	1A	3362	1/1	0.91	0.19	70,70,70,70	0
54	MG	1A	3266	1/1	0.91	0.34	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3185	1/1	0.91	0.37	50,50,50,50	0
54	MG	2A	3577	1/1	0.91	0.22	59,59,59,59	0
54	MG	1A	3929	1/1	0.91	0.12	58,58,58,58	0
54	MG	1A	3123	1/1	0.91	0.13	35,35,35,35	0
54	MG	1A	3309	1/1	0.91	0.42	41,41,41,41	0
54	MG	2R	203	1/1	0.91	0.18	60,60,60,60	0
54	MG	1A	4023	1/1	0.91	0.16	28,28,28,28	0
54	MG	1A	3769	1/1	0.91	0.09	29,29,29,29	0
54	MG	1A	3124	1/1	0.91	0.11	39,39,39,39	0
54	MG	1A	3775	1/1	0.91	0.17	34,34,34,34	0
54	MG	20	103	1/1	0.91	0.26	72,72,72,72	0
54	MG	21	101	1/1	0.91	0.21	84,84,84,84	0
54	MG	23	101	1/1	0.91	0.38	59,59,59,59	0
54	MG	1A	3371	1/1	0.91	0.17	34,34,34,34	0
54	MG	2A	3398	1/1	0.91	0.24	66,66,66,66	0
54	MG	1A	4032	1/1	0.91	0.23	59,59,59,59	0
54	MG	1U	203	1/1	0.91	0.48	40,40,40,40	0
54	MG	1a	1822	1/1	0.91	0.10	71,71,71,71	0
54	MG	1A	3075	1/1	0.91	0.50	45,45,45,45	0
54	MG	1A	3076	1/1	0.91	0.51	44,44,44,44	0
54	MG	1A	3378	1/1	0.91	0.10	46,46,46,46	0
54	MG	1A	3684	1/1	0.91	0.07	61,61,61,61	0
57	ARG	1B	230	12/12	0.91	0.22	37,56,63,63	0
54	MG	1A	3237	1/1	0.91	0.26	58,58,58,58	0
54	MG	10	104	1/1	0.91	0.07	50,50,50,50	0
54	MG	1A	3077	1/1	0.91	0.29	35,35,35,35	0
54	MG	10	106	1/1	0.91	0.13	60,60,60,60	0
54	MG	1A	3602	1/1	0.92	0.19	53,53,53,53	0
54	MG	2A	3014	1/1	0.92	0.15	49,49,49,49	0
54	MG	1B	216	1/1	0.92	0.14	69,69,69,69	0
54	MG	1A	3147	1/1	0.92	0.30	45,45,45,45	0
54	MG	2A	3655	1/1	0.92	0.15	49,49,49,49	0
54	MG	2A	3306	1/1	0.92	0.28	60,60,60,60	0
54	MG	1A	3604	1/1	0.92	0.17	43,43,43,43	0
54	MG	2A	3658	1/1	0.92	0.13	42,42,42,42	0
54	MG	1A	3739	1/1	0.92	0.28	52,52,52,52	0
54	MG	1A	3546	1/1	0.92	0.13	35,35,35,35	0
54	MG	1A	3494	1/1	0.92	0.09	67,67,67,67	0
54	MG	1A	3158	1/1	0.92	0.24	64,64,64,64	0
54	MG	2A	3316	1/1	0.92	0.21	53,53,53,53	0
54	MG	2A	3318	1/1	0.92	0.20	40,40,40,40	0
54	MG	1a	1814	1/1	0.92	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	2A	3169	1/1	0.92	0.08	45,45,45,45	0
54	MG	1A	3615	1/1	0.92	0.34	38,38,38,38	0
54	MG	1A	3070	1/1	0.92	0.16	44,44,44,44	0
54	MG	2A	3324	1/1	0.92	0.19	35,35,35,35	0
54	MG	1A	3823	1/1	0.92	0.46	42,42,42,42	0
54	MG	1A	3177	1/1	0.92	0.22	53,53,53,53	0
54	MG	1A	3465	1/1	0.92	0.24	73,73,73,73	0
54	MG	1a	1601	1/1	0.92	0.07	78,78,78,78	0
54	MG	2A	3334	1/1	0.92	0.21	37,37,37,37	0
54	MG	2A	3514	1/1	0.92	0.17	62,62,62,62	0
54	MG	2A	3516	1/1	0.92	0.11	67,67,67,67	0
54	MG	1D	312	1/1	0.92	0.44	44,44,44,44	0
54	MG	1A	3288	1/1	0.92	0.37	46,46,46,46	0
54	MG	2a	3071	1/1	0.92	0.14	69,69,69,69	0
54	MG	2A	3037	1/1	0.92	0.18	52,52,52,52	0
54	MG	2A	3520	1/1	0.92	0.11	62,62,62,62	0
54	MG	1A	3682	1/1	0.92	0.14	56,56,56,56	0
54	MG	1a	1827	1/1	0.92	0.47	86,86,86,86	0
54	MG	1a	1830	1/1	0.92	0.17	64,64,64,64	0
54	MG	1A	3564	1/1	0.92	0.22	44,44,44,44	0
54	MG	1A	3831	1/1	0.92	0.14	26,26,26,26	0
54	MG	1A	3230	1/1	0.92	0.76	47,47,47,47	0
54	MG	2A	3349	1/1	0.92	0.16	34,34,34,34	0
54	MG	2a	3081	1/1	0.92	0.12	74,74,74,74	0
54	MG	2A	3351	1/1	0.92	0.19	61,61,61,61	0
54	MG	1E	304	1/1	0.92	0.07	52,52,52,52	0
54	MG	2A	3532	1/1	0.92	0.09	54,54,54,54	0
54	MG	1a	1710	1/1	0.92	0.07	67,67,67,67	0
54	MG	2A	3358	1/1	0.92	0.17	42,42,42,42	0
54	MG	2A	3535	1/1	0.92	0.11	67,67,67,67	0
54	MG	1A	3686	1/1	0.92	0.11	77,77,77,77	0
54	MG	1A	3346	1/1	0.92	0.11	40,40,40,40	0
54	MG	1a	1842	1/1	0.92	0.15	67,67,67,67	0
54	MG	1a	1844	1/1	0.92	0.24	65,65,65,65	0
54	MG	2A	3542	1/1	0.92	0.15	69,69,69,69	0
54	MG	1A	3382	1/1	0.92	0.10	50,50,50,50	0
54	MG	1A	3573	1/1	0.92	0.16	48,48,48,48	0
54	MG	1a	1620	1/1	0.92	0.10	64,64,64,64	0
54	MG	1a	1720	1/1	0.92	0.20	70,70,70,70	0
54	MG	2A	3205	1/1	0.92	0.23	63,63,63,63	0
54	MG	2A	3375	1/1	0.92	0.22	40,40,40,40	0
54	MG	2A	3058	1/1	0.92	0.12	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	1a	1722	1/1	0.92	0.11	61,61,61,61	0
54	MG	1A	3354	1/1	0.92	0.18	60,60,60,60	0
54	MG	1F	313	1/1	0.92	0.40	48,48,48,48	0
54	MG	2A	3731	1/1	0.92	0.19	72,72,72,72	0
54	MG	2a	3115	1/1	0.92	0.08	69,69,69,69	0
54	MG	1A	4030	1/1	0.92	0.23	75,75,75,75	0
54	MG	2A	3063	1/1	0.92	0.14	48,48,48,48	0
54	MG	1a	1625	1/1	0.92	0.11	55,55,55,55	0
54	MG	1A	4031	1/1	0.92	0.05	66,66,66,66	0
54	MG	1a	1629	1/1	0.92	0.12	51,51,51,51	0
54	MG	1A	3898	1/1	0.92	0.12	42,42,42,42	0
54	MG	1A	3474	1/1	0.92	0.05	45,45,45,45	0
54	MG	1A	3577	1/1	0.92	0.10	46,46,46,46	0
54	MG	1a	1742	1/1	0.92	0.19	80,80,80,80	0
54	MG	2B	203	1/1	0.92	0.16	70,70,70,70	0
54	MG	2A	3568	1/1	0.92	0.16	51,51,51,51	0
54	MG	1A	3514	1/1	0.92	0.22	27,27,27,27	0
54	MG	2a	3138	1/1	0.92	0.18	70,70,70,70	0
54	MG	2A	3084	1/1	0.92	0.21	42,42,42,42	0
54	MG	2a	3140	1/1	0.92	0.20	72,72,72,72	0
54	MG	1A	3427	1/1	0.92	0.26	59,59,59,59	0
54	MG	2B	212	1/1	0.92	0.09	72,72,72,72	0
54	MG	1A	3232	1/1	0.92	0.33	41,41,41,41	0
54	MG	1A	3705	1/1	0.92	0.27	43,43,43,43	0
54	MG	1A	4039	1/1	0.92	0.13	63,63,63,63	0
54	MG	2B	218	1/1	0.92	0.12	55,55,55,55	0
54	MG	1A	3647	1/1	0.92	0.29	68,68,68,68	0
54	MG	1a	1753	1/1	0.92	0.08	59,59,59,59	0
54	MG	1A	3256	1/1	0.92	0.25	44,44,44,44	0
54	MG	2A	3583	1/1	0.92	0.08	71,71,71,71	0
54	MG	1a	1646	1/1	0.92	0.23	58,58,58,58	0
54	MG	2D	312	1/1	0.92	0.22	56,56,56,56	0
54	MG	2E	302	1/1	0.92	0.81	52,52,52,52	0
54	MG	2A	3241	1/1	0.92	0.21	54,54,54,54	0
54	MG	1A	3909	1/1	0.92	0.12	19,19,19,19	0
54	MG	2A	3419	1/1	0.92	0.15	55,55,55,55	0
54	MG	1A	3190	1/1	0.92	0.31	72,72,72,72	0
54	MG	2A	3244	1/1	0.92	0.14	63,63,63,63	0
54	MG	1Q	203	1/1	0.92	0.16	56,56,56,56	0
54	MG	1A	3712	1/1	0.92	0.21	66,66,66,66	0
54	MG	1A	3298	1/1	0.92	0.41	60,60,60,60	0
54	MG	1A	3205	1/1	0.92	0.52	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	3251	1/1	0.92	0.36	63,63,63,63	0
54	MG	1a	1764	1/1	0.92	0.09	82,82,82,82	0
54	MG	1f	201	1/1	0.92	0.23	71,71,71,71	0
54	MG	1f	202	1/1	0.92	0.18	49,49,49,49	0
54	MG	1A	3365	1/1	0.92	0.12	24,24,24,24	0
54	MG	1a	1658	1/1	0.92	0.22	72,72,72,72	0
54	MG	1A	3532	1/1	0.92	0.18	55,55,55,55	0
54	MG	2A	3440	1/1	0.92	0.18	68,68,68,68	0
54	MG	23	102	1/1	0.92	0.17	48,48,48,48	0
54	MG	1A	3592	1/1	0.92	0.21	54,54,54,54	0
54	MG	1A	3988	1/1	0.92	0.09	75,75,75,75	0
54	MG	1B	204	1/1	0.92	0.14	52,52,52,52	0
54	MG	1a	1663	1/1	0.92	0.13	69,69,69,69	0
54	MG	2A	3267	1/1	0.92	0.39	52,52,52,52	0
54	MG	1U	201	1/1	0.92	0.28	41,41,41,41	0
54	MG	2a	3195	1/1	0.92	0.10	81,81,81,81	0
54	MG	1U	202	1/1	0.92	0.19	33,33,33,33	0
54	MG	1A	3533	1/1	0.92	0.10	28,28,28,28	0
54	MG	1U	205	1/1	0.92	0.56	33,33,33,33	0
54	MG	1V	204	1/1	0.92	0.27	54,54,54,54	0
54	MG	1a	1786	1/1	0.92	0.08	60,60,60,60	0
54	MG	1a	1788	1/1	0.92	0.06	73,73,73,73	0
54	MG	1V	205	1/1	0.92	0.14	63,63,63,63	0
54	MG	1A	3029	1/1	0.92	0.18	40,40,40,40	0
55	CPF	1A	4056	24/24	0.92	0.28	34,46,55,61	0
54	MG	2A	3638	1/1	0.92	0.18	40,40,40,40	0
54	MG	2A	3142	1/1	0.92	0.48	68,68,68,68	0
54	MG	1a	1791	1/1	0.92	0.29	75,75,75,75	0
54	MG	1A	3067	1/1	0.92	0.14	53,53,53,53	0
54	MG	1A	3069	1/1	0.92	0.21	35,35,35,35	0
54	MG	1A	3409	1/1	0.92	0.17	59,59,59,59	0
54	MG	2a	3024	1/1	0.92	0.13	65,65,65,65	0
54	MG	1A	3928	1/1	0.92	0.14	56,56,56,56	0
54	MG	1B	211	1/1	0.92	0.12	61,61,61,61	0
54	MG	2a	3031	1/1	0.92	0.23	80,80,80,80	0
54	MG	2A	3297	1/1	0.92	0.14	49,49,49,49	0
58	ZN	29	501	1/1	0.92	0.09	76,76,76,76	0
54	MG	1A	3236	1/1	0.93	0.26	64,64,64,64	0
54	MG	2Q	201	1/1	0.93	0.10	64,64,64,64	0
54	MG	1A	3926	1/1	0.93	0.08	66,66,66,66	0
54	MG	1A	3500	1/1	0.93	0.15	24,24,24,24	0
54	MG	1A	3136	1/1	0.93	0.11	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	2T	203	1/1	0.93	0.17	63,63,63,63	0
54	MG	2W	202	1/1	0.93	0.26	52,52,52,52	0
54	MG	1a	1724	1/1	0.93	0.12	67,67,67,67	0
54	MG	1A	3610	1/1	0.93	0.69	41,41,41,41	0
54	MG	2A	3355	1/1	0.93	0.19	53,53,53,53	0
54	MG	1a	1727	1/1	0.93	0.16	46,46,46,46	0
54	MG	1A	3023	1/1	0.93	0.21	30,30,30,30	0
54	MG	1A	3933	1/1	0.93	0.15	36,36,36,36	0
54	MG	13	104	1/1	0.93	0.21	48,48,48,48	0
54	MG	2A	3361	1/1	0.93	0.14	63,63,63,63	0
54	MG	1a	1734	1/1	0.93	0.18	69,69,69,69	0
54	MG	1l	201	1/1	0.93	0.27	65,65,65,65	0
54	MG	1A	3240	1/1	0.93	0.26	64,64,64,64	0
54	MG	2A	3171	1/1	0.93	0.15	51,51,51,51	0
54	MG	1A	3089	1/1	0.93	0.13	42,42,42,42	0
54	MG	2A	3368	1/1	0.93	0.32	79,79,79,79	0
54	MG	1A	4043	1/1	0.93	0.15	62,62,62,62	0
54	MG	1A	4044	1/1	0.93	0.83	46,46,46,46	0
54	MG	1A	4045	1/1	0.93	0.12	64,64,64,64	0
54	MG	17	104	1/1	0.93	0.33	38,38,38,38	0
54	MG	1A	3167	1/1	0.93	0.23	51,51,51,51	0
54	MG	18	102	1/1	0.93	0.30	45,45,45,45	0
54	MG	2A	3591	1/1	0.93	0.17	49,49,49,49	0
54	MG	1A	3037	1/1	0.93	0.15	53,53,53,53	0
54	MG	2A	3182	1/1	0.93	0.29	60,60,60,60	0
54	MG	2A	3595	1/1	0.93	0.13	65,65,65,65	0
54	MG	1A	3421	1/1	0.93	0.21	29,29,29,29	0
54	MG	1a	1751	1/1	0.93	0.12	64,64,64,64	0
54	MG	1A	4050	1/1	0.93	0.10	76,76,76,76	0
54	MG	1A	3942	1/1	0.93	0.10	48,48,48,48	0
54	MG	2A	3387	1/1	0.93	0.15	72,72,72,72	0
54	MG	1A	3345	1/1	0.93	0.20	50,50,50,50	0
54	MG	1A	3064	1/1	0.93	0.50	43,43,43,43	0
54	MG	1A	3425	1/1	0.93	0.25	32,32,32,32	0
54	MG	1A	3347	1/1	0.93	0.15	55,55,55,55	0
54	MG	2A	3393	1/1	0.93	0.16	34,34,34,34	0
54	MG	1B	201	1/1	0.93	0.26	54,54,54,54	0
54	MG	2A	3396	1/1	0.93	0.17	37,37,37,37	0
54	MG	2A	3615	1/1	0.93	0.11	71,71,71,71	0
54	MG	2A	3397	1/1	0.93	0.17	57,57,57,57	0
54	MG	1A	3737	1/1	0.93	0.39	41,41,41,41	0
54	MG	1a	1614	1/1	0.93	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	3620	1/1	0.93	0.11	58,58,58,58	0
54	MG	1B	203	1/1	0.93	0.45	69,69,69,69	0
54	MG	1a	1616	1/1	0.93	0.11	73,73,73,73	0
54	MG	1A	3348	1/1	0.93	0.17	56,56,56,56	0
54	MG	1A	3629	1/1	0.93	0.23	60,60,60,60	0
54	MG	2A	3406	1/1	0.93	0.27	66,66,66,66	0
54	MG	1A	3353	1/1	0.93	0.13	47,47,47,47	0
54	MG	1a	1772	1/1	0.93	0.24	71,71,71,71	0
54	MG	2a	3053	1/1	0.93	0.09	64,64,64,64	0
54	MG	2A	3412	1/1	0.93	0.14	50,50,50,50	0
54	MG	1A	3289	1/1	0.93	0.27	58,58,58,58	0
54	MG	2A	3633	1/1	0.93	0.17	61,61,61,61	0
54	MG	1A	3528	1/1	0.93	0.10	52,52,52,52	0
54	MG	2A	3027	1/1	0.93	0.13	39,39,39,39	0
54	MG	1A	3433	1/1	0.93	0.13	40,40,40,40	0
54	MG	2A	3420	1/1	0.93	0.28	76,76,76,76	0
54	MG	1A	3246	1/1	0.93	0.80	48,48,48,48	0
54	MG	1A	3109	1/1	0.93	0.36	38,38,38,38	0
54	MG	1B	212	1/1	0.93	0.21	47,47,47,47	0
54	MG	2a	3067	1/1	0.93	0.07	66,66,66,66	0
54	MG	2a	3068	1/1	0.93	0.11	72,72,72,72	0
54	MG	1a	1627	1/1	0.93	0.11	52,52,52,52	0
54	MG	1A	3294	1/1	0.93	0.09	57,57,57,57	0
54	MG	1A	3961	1/1	0.93	0.10	69,69,69,69	0
54	MG	2A	3217	1/1	0.93	0.07	51,51,51,51	0
54	MG	2A	3430	1/1	0.93	0.12	60,60,60,60	0
54	MG	1A	3439	1/1	0.93	0.18	56,56,56,56	0
54	MG	1a	1787	1/1	0.93	0.12	72,72,72,72	0
54	MG	1A	3111	1/1	0.93	0.39	39,39,39,39	0
54	MG	1A	3441	1/1	0.93	0.28	71,71,71,71	0
54	MG	1A	3761	1/1	0.93	0.13	51,51,51,51	0
54	MG	1A	3967	1/1	0.93	0.46	75,75,75,75	0
54	MG	1B	223	1/1	0.93	0.07	58,58,58,58	0
54	MG	2A	3659	1/1	0.93	0.14	34,34,34,34	0
54	MG	1a	1640	1/1	0.93	0.10	83,83,83,83	0
54	MG	1A	3968	1/1	0.93	0.22	51,51,51,51	0
54	MG	1A	3764	1/1	0.93	0.43	59,59,59,59	0
54	MG	2A	3445	1/1	0.93	0.15	66,66,66,66	0
54	MG	1A	3970	1/1	0.93	0.09	70,70,70,70	0
54	MG	2A	3667	1/1	0.93	0.17	62,62,62,62	0
54	MG	1A	3443	1/1	0.93	0.18	62,62,62,62	0
54	MG	2A	3239	1/1	0.93	1.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3671	1/1	0.93	0.16	64,64,64,64	0
54	MG	1A	3445	1/1	0.93	0.14	43,43,43,43	0
54	MG	1A	3549	1/1	0.93	0.12	51,51,51,51	0
54	MG	1a	1651	1/1	0.93	0.12	46,46,46,46	0
54	MG	2a	3100	1/1	0.93	0.14	60,60,60,60	0
54	MG	1A	3094	1/1	0.93	0.25	38,38,38,38	0
54	MG	1A	3871	1/1	0.93	0.15	46,46,46,46	0
54	MG	1a	1810	1/1	0.93	0.09	76,76,76,76	0
54	MG	1A	3206	1/1	0.93	0.49	47,47,47,47	0
54	MG	2A	3680	1/1	0.93	0.09	42,42,42,42	0
54	MG	1A	3554	1/1	0.93	0.35	44,44,44,44	0
54	MG	1A	3255	1/1	0.93	0.60	47,47,47,47	0
54	MG	2a	3109	1/1	0.93	0.11	78,78,78,78	0
54	MG	1A	3877	1/1	0.93	0.13	46,46,46,46	0
54	MG	1A	3302	1/1	0.93	0.32	47,47,47,47	0
54	MG	2A	3469	1/1	0.93	0.14	64,64,64,64	0
54	MG	2A	3687	1/1	0.93	0.12	62,62,62,62	0
54	MG	1A	3180	1/1	0.93	0.16	57,57,57,57	0
54	MG	2A	3066	1/1	0.93	0.14	61,61,61,61	0
54	MG	2A	3067	1/1	0.93	0.37	58,58,58,58	0
54	MG	1A	3304	1/1	0.93	0.36	39,39,39,39	0
54	MG	1A	3669	1/1	0.93	0.11	65,65,65,65	0
54	MG	1F	306	1/1	0.93	0.36	38,38,38,38	0
54	MG	2A	3481	1/1	0.93	0.12	57,57,57,57	0
54	MG	2a	3126	1/1	0.93	0.18	75,75,75,75	0
54	MG	1A	3258	1/1	0.93	0.34	38,38,38,38	0
54	MG	1F	310	1/1	0.93	0.29	54,54,54,54	0
54	MG	1a	1666	1/1	0.93	0.29	63,63,63,63	0
54	MG	2A	3082	1/1	0.93	0.94	49,49,49,49	0
54	MG	1A	3372	1/1	0.93	0.15	34,34,34,34	0
54	MG	2a	3137	1/1	0.93	0.23	68,68,68,68	0
54	MG	1A	3008	1/1	0.93	0.11	45,45,45,45	0
54	MG	1A	3057	1/1	0.93	0.14	35,35,35,35	0
54	MG	1A	3214	1/1	0.93	0.15	58,58,58,58	0
54	MG	2A	3493	1/1	0.93	0.12	73,73,73,73	0
54	MG	2A	3087	1/1	0.93	0.21	49,49,49,49	0
54	MG	1A	3184	1/1	0.93	0.44	46,46,46,46	0
54	MG	1A	3154	1/1	0.93	0.62	38,38,38,38	0
54	MG	1A	3997	1/1	0.93	0.38	43,43,43,43	0
54	MG	1A	3794	1/1	0.93	0.13	39,39,39,39	0
54	MG	2A	3717	1/1	0.93	0.18	64,64,64,64	0
54	MG	2a	3151	1/1	0.93	0.29	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	3503	1/1	0.93	0.15	73,73,73,73	0
54	MG	1A	3381	1/1	0.93	0.21	41,41,41,41	0
54	MG	2A	3721	1/1	0.93	0.24	68,68,68,68	0
54	MG	1A	3218	1/1	0.93	0.13	43,43,43,43	0
54	MG	1a	1678	1/1	0.93	0.21	65,65,65,65	0
54	MG	1A	3314	1/1	0.93	0.60	39,39,39,39	0
54	MG	1A	3219	1/1	0.93	0.18	37,37,37,37	0
54	MG	1A	3385	1/1	0.93	0.10	58,58,58,58	0
54	MG	1A	3317	1/1	0.93	0.74	54,54,54,54	0
54	MG	2A	3296	1/1	0.93	0.21	39,39,39,39	0
54	MG	1a	1850	1/1	0.93	0.09	66,66,66,66	0
54	MG	1A	3685	1/1	0.93	0.09	70,70,70,70	0
54	MG	1A	3058	1/1	0.93	0.28	45,45,45,45	0
54	MG	1A	3391	1/1	0.93	0.14	30,30,30,30	0
54	MG	1A	3221	1/1	0.93	0.58	41,41,41,41	0
54	MG	2A	3304	1/1	0.93	0.13	77,77,77,77	0
54	MG	2A	3112	1/1	0.93	0.15	58,58,58,58	0
54	MG	1A	3810	1/1	0.93	0.16	64,64,64,64	0
54	MG	1A	3223	1/1	0.93	0.32	41,41,41,41	0
54	MG	1A	3081	1/1	0.93	0.60	47,47,47,47	0
54	MG	1A	4015	1/1	0.93	0.55	48,48,48,48	0
54	MG	1A	3399	1/1	0.93	0.16	40,40,40,40	0
54	MG	2B	204	1/1	0.93	0.08	75,75,75,75	0
54	MG	2B	206	1/1	0.93	0.12	69,69,69,69	0
54	MG	1A	3814	1/1	0.93	0.11	44,44,44,44	0
54	MG	1a	1864	1/1	0.93	0.10	62,62,62,62	0
54	MG	1A	4018	1/1	0.93	0.21	50,50,50,50	0
54	MG	1A	4020	1/1	0.93	0.19	61,61,61,61	0
54	MG	2B	211	1/1	0.93	0.15	63,63,63,63	0
54	MG	1A	3401	1/1	0.93	0.17	26,26,26,26	0
54	MG	1a	1701	1/1	0.93	0.22	66,66,66,66	0
54	MG	1A	3595	1/1	0.93	0.14	60,60,60,60	0
54	MG	2B	216	1/1	0.93	0.18	69,69,69,69	0
54	MG	2A	3325	1/1	0.93	0.22	34,34,34,34	0
54	MG	1A	3188	1/1	0.93	0.19	68,68,68,68	0
54	MG	1V	201	1/1	0.93	0.67	38,38,38,38	0
54	MG	1a	1872	1/1	0.93	0.07	65,65,65,65	0
54	MG	2A	3332	1/1	0.93	0.35	67,67,67,67	0
54	MG	2A	3140	1/1	0.93	0.28	54,54,54,54	0
54	MG	2D	310	1/1	0.93	0.24	31,31,31,31	0
54	MG	2A	3141	1/1	0.93	0.12	61,61,61,61	0
54	MG	2A	3546	1/1	0.93	0.15	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	3917	1/1	0.93	0.23	29,29,29,29	0
54	MG	2A	3338	1/1	0.93	0.20	41,41,41,41	0
54	MG	1A	3035	1/1	0.93	0.14	53,53,53,53	0
54	MG	2F	301	1/1	0.93	0.73	48,48,48,48	0
54	MG	2A	3340	1/1	0.93	0.17	79,79,79,79	0
54	MG	1A	3128	1/1	0.93	0.12	44,44,44,44	0
54	MG	1A	3706	1/1	0.93	0.20	53,53,53,53	0
54	MG	1A	3407	1/1	0.93	0.16	26,26,26,26	0
54	MG	2N	201	1/1	0.93	0.11	77,77,77,77	0
54	MG	1A	3498	1/1	0.93	0.19	58,58,58,58	0
58	ZN	2n	102	1/1	0.93	0.06	102,102,102,102	0
54	MG	1P	201	1/1	0.94	0.55	38,38,38,38	0
54	MG	1P	202	1/1	0.94	0.28	38,38,38,38	0
54	MG	2A	3105	1/1	0.94	0.39	55,55,55,55	0
54	MG	1A	3068	1/1	0.94	0.13	31,31,31,31	0
54	MG	2A	3536	1/1	0.94	0.09	65,65,65,65	0
54	MG	2E	306	1/1	0.94	0.18	32,32,32,32	0
54	MG	2A	3314	1/1	0.94	0.17	49,49,49,49	0
54	MG	1A	3423	1/1	0.94	0.17	32,32,32,32	0
54	MG	2A	3108	1/1	0.94	0.10	57,57,57,57	0
54	MG	2G	201	1/1	0.94	0.45	84,84,84,84	0
54	MG	1A	3570	1/1	0.94	0.17	57,57,57,57	0
54	MG	1A	4012	1/1	0.94	0.12	69,69,69,69	0
54	MG	2A	3111	1/1	0.94	0.18	51,51,51,51	0
54	MG	1A	3183	1/1	0.94	0.30	34,34,34,34	0
54	MG	1A	3488	1/1	0.94	0.21	33,33,33,33	0
54	MG	1A	3574	1/1	0.94	0.17	65,65,65,65	0
54	MG	1A	3126	1/1	0.94	0.33	40,40,40,40	0
54	MG	1A	3012	1/1	0.94	0.16	44,44,44,44	0
54	MG	1A	3493	1/1	0.94	0.10	40,40,40,40	0
54	MG	1A	4019	1/1	0.94	0.28	39,39,39,39	0
54	MG	1A	3798	1/1	0.94	0.18	65,65,65,65	0
54	MG	1T	204	1/1	0.94	0.12	81,81,81,81	0
54	MG	2X	101	1/1	0.94	0.15	58,58,58,58	0
54	MG	1A	3131	1/1	0.94	0.31	59,59,59,59	0
54	MG	20	101	1/1	0.94	0.29	65,65,65,65	0
54	MG	2A	3337	1/1	0.94	0.06	67,67,67,67	0
54	MG	1A	3327	1/1	0.94	0.23	56,56,56,56	0
54	MG	2A	3127	1/1	0.94	0.13	65,65,65,65	0
54	MG	1A	3496	1/1	0.94	0.16	28,28,28,28	0
54	MG	2A	3133	1/1	0.94	0.09	51,51,51,51	0
54	MG	1A	3009	1/1	0.94	0.23	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	28	101	1/1	0.94	0.14	58,58,58,58	0
54	MG	1U	207	1/1	0.94	0.34	40,40,40,40	0
54	MG	1A	3080	1/1	0.94	0.77	46,46,46,46	0
54	MG	1A	3096	1/1	0.94	0.58	49,49,49,49	0
54	MG	1A	3586	1/1	0.94	0.37	58,58,58,58	0
54	MG	1A	3165	1/1	0.94	0.15	40,40,40,40	0
54	MG	2A	3571	1/1	0.94	0.13	53,53,53,53	0
54	MG	2A	3348	1/1	0.94	0.11	38,38,38,38	0
54	MG	1A	3048	1/1	0.94	0.41	47,47,47,47	0
54	MG	1A	3689	1/1	0.94	0.33	47,47,47,47	0
54	MG	2A	3352	1/1	0.94	0.22	65,65,65,65	0
54	MG	1a	1873	1/1	0.94	0.10	61,61,61,61	0
54	MG	1A	3691	1/1	0.94	0.08	36,36,36,36	0
54	MG	1A	3502	1/1	0.94	0.14	41,41,41,41	0
54	MG	1A	3336	1/1	0.94	0.16	33,33,33,33	0
54	MG	1a	1877	1/1	0.94	0.10	69,69,69,69	0
54	MG	1A	3815	1/1	0.94	0.18	42,42,42,42	0
54	MG	2A	3586	1/1	0.94	0.14	73,73,73,73	0
54	MG	1A	3696	1/1	0.94	0.26	56,56,56,56	0
54	MG	10	107	1/1	0.94	0.11	73,73,73,73	0
54	MG	11	101	1/1	0.94	0.39	45,45,45,45	0
54	MG	2A	3157	1/1	0.94	0.41	54,54,54,54	0
54	MG	2a	3027	1/1	0.94	0.13	74,74,74,74	0
54	MG	2A	3592	1/1	0.94	0.09	42,42,42,42	0
54	MG	11	103	1/1	0.94	0.17	55,55,55,55	0
54	MG	1A	3264	1/1	0.94	0.49	30,30,30,30	0
54	MG	1A	3192	1/1	0.94	0.32	45,45,45,45	0
54	MG	2A	3369	1/1	0.94	0.15	51,51,51,51	0
54	MG	1e	202	1/1	0.94	0.12	68,68,68,68	0
54	MG	2A	3164	1/1	0.94	0.52	55,55,55,55	0
54	MG	2a	3039	1/1	0.94	0.20	70,70,70,70	0
54	MG	2A	3374	1/1	0.94	0.14	54,54,54,54	0
54	MG	13	102	1/1	0.94	0.21	46,46,46,46	0
54	MG	2A	3376	1/1	0.94	0.17	37,37,37,37	0
54	MG	1A	3225	1/1	0.94	0.12	59,59,59,59	0
54	MG	2A	3607	1/1	0.94	0.13	54,54,54,54	0
54	MG	2A	3378	1/1	0.94	0.31	74,74,74,74	0
54	MG	1A	3822	1/1	0.94	0.17	31,31,31,31	0
54	MG	1A	3597	1/1	0.94	0.18	52,52,52,52	0
54	MG	1A	3936	1/1	0.94	0.20	47,47,47,47	0
54	MG	1a	1732	1/1	0.94	0.10	56,56,56,56	0
54	MG	1A	3509	1/1	0.94	0.17	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	1A	3444	1/1	0.94	0.12	50,50,50,50	0
54	MG	2A	3617	1/1	0.94	0.14	68,68,68,68	0
54	MG	1A	3826	1/1	0.94	0.37	35,35,35,35	0
54	MG	1a	1739	1/1	0.94	0.11	66,66,66,66	0
54	MG	15	108	1/1	0.94	0.57	42,42,42,42	0
54	MG	1n	102	1/1	0.94	0.17	67,67,67,67	0
54	MG	2a	3058	1/1	0.94	0.12	77,77,77,77	0
54	MG	2A	3180	1/1	0.94	0.07	69,69,69,69	0
54	MG	17	101	1/1	0.94	0.21	38,38,38,38	0
54	MG	1o	3100	1/1	0.94	0.20	50,50,50,50	0
54	MG	2A	3625	1/1	0.94	0.10	74,74,74,74	0
54	MG	17	102	1/1	0.94	0.23	43,43,43,43	0
54	MG	2A	3394	1/1	0.94	0.17	64,64,64,64	0
54	MG	2a	3066	1/1	0.94	0.22	63,63,63,63	0
54	MG	1A	3300	1/1	0.94	0.50	68,68,68,68	0
54	MG	17	106	1/1	0.94	0.36	59,59,59,59	0
54	MG	2A	3631	1/1	0.94	0.07	71,71,71,71	0
54	MG	1A	3512	1/1	0.94	0.13	60,60,60,60	0
54	MG	1a	1748	1/1	0.94	0.17	67,67,67,67	0
54	MG	1A	3117	1/1	0.94	0.17	41,41,41,41	0
54	MG	2A	3636	1/1	0.94	0.14	58,58,58,58	0
54	MG	1A	3015	1/1	0.94	0.17	35,35,35,35	0
54	MG	1A	3946	1/1	0.94	0.18	31,31,31,31	0
54	MG	1A	3393	1/1	0.94	0.16	44,44,44,44	0
54	MG	1A	3453	1/1	0.94	0.11	55,55,55,55	0
54	MG	2A	3006	1/1	0.94	0.14	54,54,54,54	0
54	MG	2A	3407	1/1	0.94	0.12	70,70,70,70	0
54	MG	1A	3394	1/1	0.94	0.16	37,37,37,37	0
54	MG	1a	1755	1/1	0.94	0.09	74,74,74,74	0
54	MG	1A	3120	1/1	0.94	0.13	52,52,52,52	0
54	MG	2A	3011	1/1	0.94	0.22	41,41,41,41	0
54	MG	2a	3084	1/1	0.94	0.16	41,41,41,41	0
54	MG	2a	3085	1/1	0.94	0.09	68,68,68,68	0
54	MG	1A	3521	1/1	0.94	0.09	64,64,64,64	0
54	MG	2A	3416	1/1	0.94	0.16	58,58,58,58	0
54	MG	2A	3652	1/1	0.94	0.17	59,59,59,59	0
54	MG	1a	1758	1/1	0.94	0.10	66,66,66,66	0
54	MG	1A	3616	1/1	0.94	0.38	38,38,38,38	0
54	MG	1a	1608	1/1	0.94	0.24	67,67,67,67	0
54	MG	1A	3175	1/1	0.94	0.45	36,36,36,36	0
54	MG	1A	3523	1/1	0.94	0.12	24,24,24,24	0
54	MG	2A	3020	1/1	0.94	0.50	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	1a	1613	1/1	0.94	0.15	31,31,31,31	0
54	MG	1A	3525	1/1	0.94	0.16	63,63,63,63	0
54	MG	2A	3661	1/1	0.94	0.07	80,80,80,80	0
54	MG	1A	3726	1/1	0.94	0.16	52,52,52,52	0
54	MG	1A	3527	1/1	0.94	0.18	60,60,60,60	0
54	MG	1a	1767	1/1	0.94	0.09	79,79,79,79	0
54	MG	1A	3462	1/1	0.94	0.23	43,43,43,43	0
54	MG	1a	1769	1/1	0.94	0.10	67,67,67,67	0
54	MG	1a	1770	1/1	0.94	0.09	68,68,68,68	0
54	MG	1a	1771	1/1	0.94	0.12	77,77,77,77	0
54	MG	1A	3351	1/1	0.94	0.16	52,52,52,52	0
54	MG	2A	3222	1/1	0.94	0.25	52,52,52,52	0
54	MG	2A	3439	1/1	0.94	0.17	52,52,52,52	0
54	MG	1B	213	1/1	0.94	0.20	39,39,39,39	0
54	MG	1a	1776	1/1	0.94	0.15	71,71,71,71	0
54	MG	2a	3118	1/1	0.94	0.06	56,56,56,56	0
54	MG	1B	214	1/1	0.94	0.14	49,49,49,49	0
54	MG	1A	3731	1/1	0.94	0.18	36,36,36,36	0
54	MG	1a	1622	1/1	0.94	0.10	48,48,48,48	0
54	MG	1A	3352	1/1	0.94	0.14	29,29,29,29	0
54	MG	1A	3197	1/1	0.94	0.11	56,56,56,56	0
54	MG	2A	3232	1/1	0.94	0.16	59,59,59,59	0
54	MG	2A	3233	1/1	0.94	0.23	72,72,72,72	0
54	MG	1A	3736	1/1	0.94	0.09	46,46,46,46	0
54	MG	2a	3128	1/1	0.94	0.10	71,71,71,71	0
54	MG	1A	3853	1/1	0.94	0.17	50,50,50,50	0
54	MG	1A	3403	1/1	0.94	0.23	23,23,23,23	0
54	MG	2a	3132	1/1	0.94	0.16	52,52,52,52	0
54	MG	2a	3133	1/1	0.94	0.10	76,76,76,76	0
54	MG	2A	3455	1/1	0.94	0.24	42,42,42,42	0
54	MG	2A	3458	1/1	0.94	0.23	64,64,64,64	0
54	MG	2A	3459	1/1	0.94	0.14	73,73,73,73	0
54	MG	2A	3047	1/1	0.94	0.13	59,59,59,59	0
54	MG	1A	3535	1/1	0.94	0.08	56,56,56,56	0
54	MG	1A	3199	1/1	0.94	0.26	48,48,48,48	0
54	MG	1A	3631	1/1	0.94	0.13	59,59,59,59	0
54	MG	1A	3468	1/1	0.94	0.10	60,60,60,60	0
54	MG	2A	3466	1/1	0.94	0.08	73,73,73,73	0
54	MG	2A	3246	1/1	0.94	0.36	60,60,60,60	0
54	MG	1A	3540	1/1	0.94	0.21	57,57,57,57	0
54	MG	2a	3146	1/1	0.94	0.10	70,70,70,70	0
54	MG	1A	3749	1/1	0.94	0.20	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	1A	3638	1/1	0.94	0.09	58,58,58,58	0
54	MG	2a	3150	1/1	0.94	0.12	78,78,78,78	0
54	MG	1A	3176	1/1	0.94	0.62	46,46,46,46	0
54	MG	1A	3980	1/1	0.94	0.16	57,57,57,57	0
54	MG	2A	3476	1/1	0.94	0.17	61,61,61,61	0
54	MG	1A	3866	1/1	0.94	0.16	46,46,46,46	0
54	MG	2A	3254	1/1	0.94	0.38	46,46,46,46	0
54	MG	2A	3255	1/1	0.94	0.20	51,51,51,51	0
54	MG	2A	3480	1/1	0.94	0.22	61,61,61,61	0
54	MG	1D	314	1/1	0.94	0.15	60,60,60,60	0
54	MG	2a	3159	1/1	0.94	0.16	59,59,59,59	0
54	MG	2A	3257	1/1	0.94	0.17	21,21,21,21	0
54	MG	2A	3718	1/1	0.94	0.18	51,51,51,51	0
54	MG	2A	3258	1/1	0.94	0.69	44,44,44,44	0
54	MG	1a	1644	1/1	0.94	0.20	61,61,61,61	0
54	MG	1A	3542	1/1	0.94	0.31	35,35,35,35	0
54	MG	2a	3165	1/1	0.94	0.11	79,79,79,79	0
54	MG	1D	316	1/1	0.94	0.13	53,53,53,53	0
54	MG	1A	3643	1/1	0.94	0.31	38,38,38,38	0
54	MG	2A	3489	1/1	0.94	0.20	72,72,72,72	0
54	MG	2a	3172	1/1	0.94	0.15	78,78,78,78	0
54	MG	1a	1649	1/1	0.94	0.19	63,63,63,63	0
54	MG	1A	3644	1/1	0.94	0.17	49,49,49,49	0
54	MG	2A	3065	1/1	0.94	0.29	51,51,51,51	0
54	MG	1A	3756	1/1	0.94	0.31	67,67,67,67	0
54	MG	1A	3645	1/1	0.94	0.45	49,49,49,49	0
54	MG	2a	3179	1/1	0.94	0.20	69,69,69,69	0
54	MG	2A	3497	1/1	0.94	0.14	45,45,45,45	0
54	MG	2A	3732	1/1	0.94	0.16	74,74,74,74	0
54	MG	1A	3121	1/1	0.94	0.22	49,49,49,49	0
54	MG	1A	3358	1/1	0.94	0.18	34,34,34,34	0
54	MG	1A	3203	1/1	0.94	0.38	40,40,40,40	0
54	MG	1F	303	1/1	0.94	0.21	34,34,34,34	0
54	MG	2A	3079	1/1	0.94	0.13	61,61,61,61	0
54	MG	1A	3360	1/1	0.94	0.09	26,26,26,26	0
54	MG	1A	3992	1/1	0.94	0.11	19,19,19,19	0
54	MG	1A	3477	1/1	0.94	0.24	52,52,52,52	0
54	MG	2A	3279	1/1	0.94	0.16	32,32,32,32	0
54	MG	1A	3087	1/1	0.94	0.33	39,39,39,39	0
54	MG	2e	201	1/1	0.94	0.22	65,65,65,65	0
54	MG	2A	3283	1/1	0.94	0.24	33,33,33,33	0
54	MG	2B	205	1/1	0.94	0.14	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	3415	1/1	0.94	0.15	31,31,31,31	0
54	MG	2k	201	1/1	0.94	0.18	57,57,57,57	0
54	MG	1A	3770	1/1	0.94	0.19	62,62,62,62	0
54	MG	2A	3515	1/1	0.94	0.17	75,75,75,75	0
54	MG	1A	3556	1/1	0.94	0.07	64,64,64,64	0
54	MG	1A	3772	1/1	0.94	0.14	34,34,34,34	0
54	MG	2A	3088	1/1	0.94	0.68	57,57,57,57	0
54	MG	1a	1828	1/1	0.94	0.25	84,84,84,84	0
54	MG	1a	1829	1/1	0.94	0.23	83,83,83,83	0
54	MG	1A	3658	1/1	0.94	0.12	54,54,54,54	0
54	MG	1A	3065	1/1	0.94	0.39	35,35,35,35	0
54	MG	1A	3559	1/1	0.94	0.13	52,52,52,52	0
54	MG	1A	3315	1/1	0.94	0.28	55,55,55,55	0
54	MG	1A	3020	1/1	0.94	0.59	41,41,41,41	0
54	MG	1A	3562	1/1	0.94	0.17	71,71,71,71	0
54	MG	2A	3305	1/1	0.94	0.15	69,69,69,69	0
58	ZN	15	109	1/1	0.94	0.15	61,61,61,61	0
54	MG	2D	307	1/1	0.94	0.58	51,51,51,51	0
54	MG	2D	308	1/1	0.94	0.13	77,77,77,77	0
54	MG	1A	3783	1/1	0.94	0.23	43,43,43,43	0
54	MG	1A	3245	1/1	0.94	0.35	39,39,39,39	0
54	MG	2A	3238	1/1	0.95	0.13	61,61,61,61	0
54	MG	2A	3612	1/1	0.95	0.22	57,57,57,57	0
54	MG	1A	3757	1/1	0.95	0.14	46,46,46,46	0
54	MG	2A	3075	1/1	0.95	0.24	58,58,58,58	0
54	MG	1A	3408	1/1	0.95	0.22	57,57,57,57	0
54	MG	2A	3077	1/1	0.95	0.38	61,61,61,61	0
54	MG	1A	3759	1/1	0.95	0.15	48,48,48,48	0
54	MG	1A	3051	1/1	0.95	0.68	36,36,36,36	0
54	MG	1A	3091	1/1	0.95	0.13	24,24,24,24	0
54	MG	1A	3411	1/1	0.95	0.40	73,73,73,73	0
54	MG	1A	3026	1/1	0.95	0.38	32,32,32,32	0
54	MG	2A	3248	1/1	0.95	0.10	57,57,57,57	0
54	MG	1A	3589	1/1	0.95	0.10	69,69,69,69	0
54	MG	1A	3107	1/1	0.95	0.46	42,42,42,42	0
54	MG	1A	3675	1/1	0.95	0.42	55,55,55,55	0
54	MG	2a	3023	1/1	0.95	0.21	62,62,62,62	0
54	MG	2A	3434	1/1	0.95	0.07	63,63,63,63	0
54	MG	1A	3333	1/1	0.95	0.23	52,52,52,52	0
54	MG	1A	3373	1/1	0.95	0.21	36,36,36,36	0
54	MG	1A	3524	1/1	0.95	0.33	51,51,51,51	0
54	MG	1A	3774	1/1	0.95	0.14	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	3972	1/1	0.95	0.11	33,33,33,33	0
54	MG	1A	3045	1/1	0.95	0.57	56,56,56,56	0
54	MG	1A	3418	1/1	0.95	0.19	42,42,42,42	0
54	MG	2A	3443	1/1	0.95	0.24	61,61,61,61	0
54	MG	2A	3259	1/1	0.95	0.29	49,49,49,49	0
54	MG	1A	3473	1/1	0.95	0.12	39,39,39,39	0
54	MG	1a	1714	1/1	0.95	0.19	73,73,73,73	0
54	MG	1A	3066	1/1	0.95	0.43	39,39,39,39	0
54	MG	1a	1716	1/1	0.95	0.12	46,46,46,46	0
54	MG	1A	3272	1/1	0.95	0.54	39,39,39,39	0
54	MG	2A	3450	1/1	0.95	0.17	70,70,70,70	0
54	MG	1A	3031	1/1	0.95	0.14	22,22,22,22	0
54	MG	17	103	1/1	0.95	0.43	41,41,41,41	0
54	MG	2A	3648	1/1	0.95	0.10	65,65,65,65	0
54	MG	1A	3112	1/1	0.95	0.72	42,42,42,42	0
54	MG	1A	3247	1/1	0.95	0.26	42,42,42,42	0
54	MG	2A	3456	1/1	0.95	0.11	75,75,75,75	0
54	MG	2A	3457	1/1	0.95	0.04	84,84,84,84	0
54	MG	17	107	1/1	0.95	0.16	52,52,52,52	0
54	MG	1a	1726	1/1	0.95	0.05	82,82,82,82	0
54	MG	1A	3687	1/1	0.95	0.23	31,31,31,31	0
54	MG	1A	3160	1/1	0.95	0.10	56,56,56,56	0
54	MG	1A	3056	1/1	0.95	0.40	36,36,36,36	0
54	MG	19	101	1/1	0.95	0.23	56,56,56,56	0
54	MG	1A	3608	1/1	0.95	0.13	56,56,56,56	0
54	MG	1A	3692	1/1	0.95	0.08	65,65,65,65	0
54	MG	2A	3278	1/1	0.95	0.22	60,60,60,60	0
54	MG	1A	3791	1/1	0.95	0.23	65,65,65,65	0
54	MG	2A	3117	1/1	0.95	0.19	44,44,44,44	0
54	MG	2A	3281	1/1	0.95	0.19	24,24,24,24	0
54	MG	1A	3538	1/1	0.95	0.20	63,63,63,63	0
54	MG	1A	3989	1/1	0.95	0.14	53,53,53,53	0
54	MG	2A	3120	1/1	0.95	0.27	53,53,53,53	0
54	MG	2A	3287	1/1	0.95	0.23	65,65,65,65	0
54	MG	1B	229	1/1	0.95	0.11	62,62,62,62	0
54	MG	1D	301	1/1	0.95	0.55	44,44,44,44	0
54	MG	2A	3673	1/1	0.95	0.15	41,41,41,41	0
54	MG	1D	303	1/1	0.95	0.34	41,41,41,41	0
54	MG	1a	1609	1/1	0.95	0.18	60,60,60,60	0
54	MG	2A	3295	1/1	0.95	0.17	44,44,44,44	0
54	MG	1a	1610	1/1	0.95	0.29	56,56,56,56	0
54	MG	1a	1746	1/1	0.95	0.06	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	1D	305	1/1	0.95	0.31	46,46,46,46	0
54	MG	1D	307	1/1	0.95	0.18	40,40,40,40	0
54	MG	1A	3115	1/1	0.95	0.26	35,35,35,35	0
54	MG	2A	3135	1/1	0.95	0.26	43,43,43,43	0
54	MG	1A	3047	1/1	0.95	0.74	48,48,48,48	0
54	MG	1g	203	1/1	0.95	0.12	66,66,66,66	0
54	MG	2A	3492	1/1	0.95	0.19	54,54,54,54	0
54	MG	1A	3429	1/1	0.95	0.26	29,29,29,29	0
54	MG	2a	3086	1/1	0.95	0.15	62,62,62,62	0
54	MG	1A	3797	1/1	0.95	0.12	77,77,77,77	0
54	MG	1A	3254	1/1	0.95	0.10	76,76,76,76	0
54	MG	1A	3431	1/1	0.95	0.16	31,31,31,31	0
54	MG	1A	3701	1/1	0.95	0.39	41,41,41,41	0
54	MG	2A	3500	1/1	0.95	0.10	61,61,61,61	0
54	MG	1A	3547	1/1	0.95	0.12	41,41,41,41	0
54	MG	2A	3145	1/1	0.95	0.27	52,52,52,52	0
54	MG	1A	3998	1/1	0.95	0.13	83,83,83,83	0
54	MG	2A	3317	1/1	0.95	0.24	53,53,53,53	0
54	MG	2A	3506	1/1	0.95	0.13	62,62,62,62	0
54	MG	1A	3802	1/1	0.95	0.21	29,29,29,29	0
54	MG	2a	3101	1/1	0.95	0.18	66,66,66,66	0
54	MG	1A	3548	1/1	0.95	0.14	38,38,38,38	0
54	MG	2A	3702	1/1	0.95	0.12	60,60,60,60	0
54	MG	2A	3704	1/1	0.95	0.16	60,60,60,60	0
54	MG	1E	305	1/1	0.95	0.21	27,27,27,27	0
54	MG	1A	3229	1/1	0.95	0.52	40,40,40,40	0
54	MG	1A	3390	1/1	0.95	0.20	28,28,28,28	0
54	MG	1A	3491	1/1	0.95	0.18	28,28,28,28	0
54	MG	1a	1628	1/1	0.95	0.10	77,77,77,77	0
54	MG	2A	3326	1/1	0.95	0.26	63,63,63,63	0
54	MG	2a	3111	1/1	0.95	0.11	66,66,66,66	0
54	MG	2A	3713	1/1	0.95	0.10	69,69,69,69	0
54	MG	2A	3154	1/1	0.95	0.14	59,59,59,59	0
54	MG	2A	3155	1/1	0.95	0.08	67,67,67,67	0
54	MG	1A	3032	1/1	0.95	0.15	51,51,51,51	0
54	MG	2A	3158	1/1	0.95	0.39	44,44,44,44	0
54	MG	1A	3809	1/1	0.95	0.19	61,61,61,61	0
54	MG	1A	3257	1/1	0.95	0.47	39,39,39,39	0
54	MG	2A	3161	1/1	0.95	0.11	84,84,84,84	0
54	MG	1A	3438	1/1	0.95	0.14	61,61,61,61	0
54	MG	1a	1633	1/1	0.95	0.11	47,47,47,47	0
54	MG	1a	1634	1/1	0.95	0.08	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3165	1/1	0.95	0.24	55,55,55,55	0
54	MG	1A	3711	1/1	0.95	0.06	39,39,39,39	0
54	MG	1A	3557	1/1	0.95	0.10	56,56,56,56	0
54	MG	2a	3129	1/1	0.95	0.08	65,65,65,65	0
54	MG	1A	3005	1/1	0.95	0.14	29,29,29,29	0
54	MG	1A	3714	1/1	0.95	0.14	39,39,39,39	0
54	MG	2A	3531	1/1	0.95	0.18	32,32,32,32	0
54	MG	1F	316	1/1	0.95	0.21	57,57,57,57	0
54	MG	1F	317	1/1	0.95	0.20	43,43,43,43	0
54	MG	2a	3135	1/1	0.95	0.06	69,69,69,69	0
54	MG	2A	3733	1/1	0.95	0.24	64,64,64,64	0
54	MG	1A	3287	1/1	0.95	0.13	18,18,18,18	0
54	MG	1A	3633	1/1	0.95	0.14	34,34,34,34	0
54	MG	1A	3717	1/1	0.95	0.20	48,48,48,48	0
54	MG	2A	3350	1/1	0.95	0.32	55,55,55,55	0
54	MG	1G	203	1/1	0.95	0.19	64,64,64,64	0
54	MG	1G	204	1/1	0.95	0.12	60,60,60,60	0
54	MG	2A	3740	1/1	0.95	0.17	69,69,69,69	0
54	MG	1A	3259	1/1	0.95	0.34	45,45,45,45	0
54	MG	1A	3636	1/1	0.95	0.13	68,68,68,68	0
54	MG	2A	3543	1/1	0.95	0.29	56,56,56,56	0
54	MG	1A	3721	1/1	0.95	0.24	40,40,40,40	0
54	MG	1A	3637	1/1	0.95	0.07	46,46,46,46	0
54	MG	1a	1653	1/1	0.95	0.15	59,59,59,59	0
54	MG	1A	3396	1/1	0.95	0.18	24,24,24,24	0
54	MG	1A	3233	1/1	0.95	0.63	38,38,38,38	0
54	MG	1A	3563	1/1	0.95	0.17	51,51,51,51	0
54	MG	1A	3323	1/1	0.95	0.33	37,37,37,37	0
54	MG	1a	1794	1/1	0.95	0.17	92,92,92,92	0
54	MG	2A	3191	1/1	0.95	0.36	57,57,57,57	0
54	MG	1A	3446	1/1	0.95	0.25	58,58,58,58	0
54	MG	1A	3361	1/1	0.95	0.14	50,50,50,50	0
54	MG	2B	214	1/1	0.95	0.10	70,70,70,70	0
54	MG	1a	1797	1/1	0.95	0.11	56,56,56,56	0
54	MG	1a	1798	1/1	0.95	0.13	80,80,80,80	0
54	MG	1A	4028	1/1	0.95	0.18	51,51,51,51	0
54	MG	2A	3559	1/1	0.95	0.11	62,62,62,62	0
54	MG	2A	3197	1/1	0.95	0.30	63,63,63,63	0
54	MG	1A	3932	1/1	0.95	0.43	61,61,61,61	0
54	MG	2a	3166	1/1	0.95	0.12	68,68,68,68	0
54	MG	2a	3167	1/1	0.95	0.11	51,51,51,51	0
54	MG	2A	3200	1/1	0.95	0.20	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	1A	3569	1/1	0.95	0.10	51,51,51,51	0
54	MG	1A	3934	1/1	0.95	0.17	63,63,63,63	0
54	MG	2A	3565	1/1	0.95	0.24	72,72,72,72	0
54	MG	1A	3024	1/1	0.95	0.26	26,26,26,26	0
54	MG	1A	3571	1/1	0.95	0.27	46,46,46,46	0
54	MG	2A	3569	1/1	0.95	0.48	71,71,71,71	0
54	MG	2E	301	1/1	0.95	0.22	73,73,73,73	0
54	MG	1a	1806	1/1	0.95	0.10	74,74,74,74	0
54	MG	2E	303	1/1	0.95	0.11	47,47,47,47	0
54	MG	1A	3363	1/1	0.95	0.11	63,63,63,63	0
54	MG	1A	3452	1/1	0.95	0.12	53,53,53,53	0
54	MG	1A	3651	1/1	0.95	0.15	43,43,43,43	0
54	MG	2E	307	1/1	0.95	0.26	67,67,67,67	0
54	MG	1A	3207	1/1	0.95	0.78	46,46,46,46	0
54	MG	1a	1670	1/1	0.95	0.41	69,69,69,69	0
54	MG	2a	3188	1/1	0.95	0.11	65,65,65,65	0
54	MG	2a	3189	1/1	0.95	0.14	60,60,60,60	0
54	MG	1A	3455	1/1	0.95	0.16	31,31,31,31	0
54	MG	2F	304	1/1	0.95	0.24	46,46,46,46	0
54	MG	1A	3405	1/1	0.95	0.14	24,24,24,24	0
54	MG	1A	3171	1/1	0.95	0.29	36,36,36,36	0
54	MG	1A	3659	1/1	0.95	0.19	68,68,68,68	0
54	MG	1a	1819	1/1	0.95	0.11	61,61,61,61	0
54	MG	1U	204	1/1	0.95	0.58	40,40,40,40	0
54	MG	1A	3844	1/1	0.95	0.22	47,47,47,47	0
54	MG	1A	3328	1/1	0.95	0.15	65,65,65,65	0
54	MG	1a	1823	1/1	0.95	0.09	65,65,65,65	0
54	MG	1A	3513	1/1	0.95	0.22	23,23,23,23	0
54	MG	1A	3847	1/1	0.95	0.15	26,26,26,26	0
54	MG	1A	3460	1/1	0.95	0.11	63,63,63,63	0
54	MG	2A	3225	1/1	0.95	0.69	49,49,49,49	0
54	MG	1A	4048	1/1	0.95	0.13	54,54,54,54	0
54	MG	1W	201	1/1	0.95	0.31	50,50,50,50	0
55	CPF	2A	3741	24/24	0.95	0.24	39,44,56,58	0
54	MG	1A	3515	1/1	0.95	0.15	28,28,28,28	0
54	MG	2A	3597	1/1	0.95	0.15	41,41,41,41	0
54	MG	1W	203	1/1	0.95	0.30	35,35,35,35	0
54	MG	2A	3068	1/1	0.95	0.58	41,41,41,41	0
54	MG	2A	3408	1/1	0.95	0.09	56,56,56,56	0
54	MG	2A	3069	1/1	0.95	0.38	55,55,55,55	0
54	MG	2A	3603	1/1	0.95	0.11	36,36,36,36	0
54	MG	1A	3583	1/1	0.95	0.23	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	27	101	1/1	0.95	0.61	45,45,45,45	0
54	MG	2A	3605	1/1	0.95	0.09	68,68,68,68	0
54	MG	10	101	1/1	0.95	0.33	47,47,47,47	0
54	MG	2A	3234	1/1	0.95	0.24	75,75,75,75	0
54	MG	2A	3073	1/1	0.95	0.56	49,49,49,49	0
54	MG	2A	3237	1/1	0.95	0.37	48,48,48,48	0
54	MG	2A	3411	1/1	0.96	0.39	49,49,49,49	0
54	MG	2A	3268	1/1	0.96	0.56	58,58,58,58	0
54	MG	1a	1702	1/1	0.96	0.25	56,56,56,56	0
54	MG	1A	3457	1/1	0.96	0.13	64,64,64,64	0
54	MG	1a	1704	1/1	0.96	0.13	46,46,46,46	0
54	MG	2a	3065	1/1	0.96	0.15	64,64,64,64	0
54	MG	1A	3653	1/1	0.96	0.13	54,54,54,54	0
54	MG	1a	1707	1/1	0.96	0.08	45,45,45,45	0
54	MG	1A	3062	1/1	0.96	0.17	44,44,44,44	0
54	MG	2A	3566	1/1	0.96	0.14	59,59,59,59	0
54	MG	1A	3053	1/1	0.96	0.18	48,48,48,48	0
54	MG	1A	3953	1/1	0.96	0.14	26,26,26,26	0
54	MG	1A	3544	1/1	0.96	0.12	24,24,24,24	0
54	MG	1A	3793	1/1	0.96	0.24	64,64,64,64	0
54	MG	1A	3657	1/1	0.96	0.41	56,56,56,56	0
54	MG	2A	3726	1/1	0.96	0.08	61,61,61,61	0
54	MG	2A	3427	1/1	0.96	0.12	37,37,37,37	0
54	MG	1A	3545	1/1	0.96	0.14	44,44,44,44	0
54	MG	2A	3575	1/1	0.96	0.14	55,55,55,55	0
54	MG	1A	3720	1/1	0.96	0.50	43,43,43,43	0
54	MG	1A	3873	1/1	0.96	0.09	47,47,47,47	0
54	MG	1a	1717	1/1	0.96	0.10	70,70,70,70	0
54	MG	1a	1718	1/1	0.96	0.14	40,40,40,40	0
54	MG	1A	3596	1/1	0.96	0.16	19,19,19,19	0
54	MG	2A	3288	1/1	0.96	0.21	35,35,35,35	0
54	MG	2A	3289	1/1	0.96	0.25	53,53,53,53	0
54	MG	1N	204	1/1	0.96	0.13	55,55,55,55	0
54	MG	2A	3040	1/1	0.96	0.15	44,44,44,44	0
54	MG	1A	3133	1/1	0.96	0.84	51,51,51,51	0
54	MG	1A	3723	1/1	0.96	0.14	32,32,32,32	0
54	MG	2a	3091	1/1	0.96	0.13	69,69,69,69	0
54	MG	1A	3724	1/1	0.96	0.10	54,54,54,54	0
54	MG	2a	3093	1/1	0.96	0.27	76,76,76,76	0
54	MG	1A	3016	1/1	0.96	0.43	38,38,38,38	0
54	MG	1A	3663	1/1	0.96	0.16	29,29,29,29	0
54	MG	1A	3004	1/1	0.96	0.17	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	2A	3172	1/1	0.96	0.15	65,65,65,65	0
54	MG	1A	3728	1/1	0.96	0.11	39,39,39,39	0
54	MG	1a	1838	1/1	0.96	0.12	74,74,74,74	0
54	MG	1a	1729	1/1	0.96	0.07	69,69,69,69	0
54	MG	1a	1841	1/1	0.96	0.05	63,63,63,63	0
54	MG	1A	3503	1/1	0.96	0.18	43,43,43,43	0
54	MG	1a	1843	1/1	0.96	0.06	58,58,58,58	0
54	MG	1A	3601	1/1	0.96	0.19	66,66,66,66	0
54	MG	1A	3286	1/1	0.96	0.14	22,22,22,22	0
54	MG	1A	3732	1/1	0.96	0.19	57,57,57,57	0
54	MG	1R	203	1/1	0.96	0.14	56,56,56,56	0
54	MG	1A	3234	1/1	0.96	0.30	31,31,31,31	0
54	MG	2A	3315	1/1	0.96	0.24	30,30,30,30	0
54	MG	2A	3184	1/1	0.96	0.10	66,66,66,66	0
54	MG	1A	3552	1/1	0.96	0.15	55,55,55,55	0
54	MG	2D	301	1/1	0.96	0.53	48,48,48,48	0
54	MG	2D	303	1/1	0.96	0.53	45,45,45,45	0
54	MG	2A	3186	1/1	0.96	0.39	54,54,54,54	0
54	MG	1a	1851	1/1	0.96	0.22	72,72,72,72	0
54	MG	1A	3553	1/1	0.96	0.23	59,59,59,59	0
54	MG	1A	3356	1/1	0.96	0.19	27,27,27,27	0
54	MG	1A	3114	1/1	0.96	0.23	33,33,33,33	0
54	MG	1A	3028	1/1	0.96	0.55	33,33,33,33	0
54	MG	1A	3896	1/1	0.96	0.18	49,49,49,49	0
54	MG	1a	1858	1/1	0.96	0.06	61,61,61,61	0
54	MG	1A	3897	1/1	0.96	0.13	32,32,32,32	0
54	MG	1A	3740	1/1	0.96	0.19	31,31,31,31	0
54	MG	2A	3472	1/1	0.96	0.20	62,62,62,62	0
54	MG	2A	3070	1/1	0.96	0.19	28,28,28,28	0
54	MG	1A	3818	1/1	0.96	0.09	48,48,48,48	0
54	MG	1a	1643	1/1	0.96	0.16	56,56,56,56	0
54	MG	2A	3199	1/1	0.96	0.08	53,53,53,53	0
54	MG	2A	3626	1/1	0.96	0.10	60,60,60,60	0
54	MG	1A	3143	1/1	0.96	0.14	40,40,40,40	0
54	MG	1A	3742	1/1	0.96	0.19	23,23,23,23	0
54	MG	1A	3744	1/1	0.96	0.22	53,53,53,53	0
54	MG	1A	3745	1/1	0.96	0.23	42,42,42,42	0
54	MG	1a	1648	1/1	0.96	0.13	51,51,51,51	0
54	MG	1A	3613	1/1	0.96	0.31	40,40,40,40	0
54	MG	1A	3021	1/1	0.96	0.24	41,41,41,41	0
54	MG	1A	3239	1/1	0.96	0.30	37,37,37,37	0
54	MG	1A	3211	1/1	0.96	0.37	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3296	1/1	0.96	0.23	33,33,33,33	0
54	MG	1A	3475	1/1	0.96	0.17	51,51,51,51	0
54	MG	1A	3041	1/1	0.96	0.15	23,23,23,23	0
54	MG	2R	202	1/1	0.96	0.20	46,46,46,46	0
54	MG	1A	3621	1/1	0.96	0.16	34,34,34,34	0
54	MG	1A	3915	1/1	0.96	0.22	25,25,25,25	0
54	MG	2T	202	1/1	0.96	0.13	68,68,68,68	0
54	MG	1A	3400	1/1	0.96	0.16	45,45,45,45	0
54	MG	1A	3623	1/1	0.96	0.06	47,47,47,47	0
54	MG	1A	3042	1/1	0.96	0.45	29,29,29,29	0
54	MG	2A	3646	1/1	0.96	0.25	59,59,59,59	0
54	MG	2A	3353	1/1	0.96	0.14	42,42,42,42	0
54	MG	1A	3919	1/1	0.96	0.15	19,19,19,19	0
54	MG	1A	3479	1/1	0.96	0.23	42,42,42,42	0
54	MG	11	102	1/1	0.96	0.14	59,59,59,59	0
54	MG	1A	3568	1/1	0.96	0.11	52,52,52,52	0
54	MG	1A	3084	1/1	0.96	0.46	39,39,39,39	0
54	MG	2A	3505	1/1	0.96	0.29	64,64,64,64	0
54	MG	2A	3223	1/1	0.96	0.49	40,40,40,40	0
54	MG	1A	3763	1/1	0.96	0.14	65,65,65,65	0
54	MG	1a	1774	1/1	0.96	0.07	78,78,78,78	0
54	MG	13	101	1/1	0.96	0.23	36,36,36,36	0
54	MG	1A	3174	1/1	0.96	0.29	36,36,36,36	0
54	MG	1D	310	1/1	0.96	0.32	29,29,29,29	0
54	MG	2A	3103	1/1	0.96	0.14	30,30,30,30	0
54	MG	1A	3301	1/1	0.96	0.37	44,44,44,44	0
54	MG	1A	3841	1/1	0.96	0.30	49,49,49,49	0
54	MG	15	101	1/1	0.96	0.32	41,41,41,41	0
54	MG	2A	3372	1/1	0.96	0.09	71,71,71,71	0
54	MG	2A	3665	1/1	0.96	0.15	66,66,66,66	0
54	MG	15	102	1/1	0.96	0.41	39,39,39,39	0
54	MG	1k	201	1/1	0.96	0.12	46,46,46,46	0
54	MG	15	103	1/1	0.96	0.61	43,43,43,43	0
54	MG	2A	3236	1/1	0.96	0.29	62,62,62,62	0
54	MG	1A	3086	1/1	0.96	0.09	49,49,49,49	0
54	MG	1a	1784	1/1	0.96	0.14	66,66,66,66	0
54	MG	1A	3043	1/1	0.96	0.20	17,17,17,17	0
54	MG	2A	3114	1/1	0.96	0.11	49,49,49,49	0
54	MG	1A	3768	1/1	0.96	0.43	55,55,55,55	0
54	MG	1A	3338	1/1	0.96	0.22	34,34,34,34	0
54	MG	1A	3526	1/1	0.96	0.18	27,27,27,27	0
54	MG	1A	3072	1/1	0.96	0.38	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	1A	3248	1/1	0.96	0.35	45,45,45,45	0
54	MG	1A	3530	1/1	0.96	0.29	31,31,31,31	0
54	MG	2a	3028	1/1	0.96	0.21	67,67,67,67	0
54	MG	1A	3447	1/1	0.96	0.15	32,32,32,32	0
54	MG	1A	3375	1/1	0.96	0.12	48,48,48,48	0
54	MG	1A	3939	1/1	0.96	0.08	61,61,61,61	0
54	MG	2A	3390	1/1	0.96	0.17	37,37,37,37	0
54	MG	1A	3490	1/1	0.96	0.09	63,63,63,63	0
54	MG	2a	3036	1/1	0.96	0.18	58,58,58,58	0
54	MG	1A	3073	1/1	0.96	0.29	42,42,42,42	0
54	MG	1A	3377	1/1	0.96	0.12	32,32,32,32	0
54	MG	2A	3689	1/1	0.96	0.13	59,59,59,59	0
54	MG	2n	101	1/1	0.96	0.09	81,81,81,81	0
54	MG	2A	3128	1/1	0.96	0.18	62,62,62,62	0
54	MG	2A	3130	1/1	0.96	0.12	64,64,64,64	0
54	MG	2A	3541	1/1	0.96	0.17	64,64,64,64	0
54	MG	1A	3198	1/1	0.96	0.37	45,45,45,45	0
54	MG	1F	308	1/1	0.96	0.39	31,31,31,31	0
54	MG	1F	309	1/1	0.96	0.33	34,34,34,34	0
54	MG	2A	3399	1/1	0.96	0.23	39,39,39,39	0
54	MG	2a	3047	1/1	0.96	0.08	57,57,57,57	0
56	MPD	18	104	8/8	0.96	0.32	32,39,43,43	0
54	MG	1A	3414	1/1	0.96	0.32	59,59,59,59	0
54	MG	1a	1695	1/1	0.96	0.21	65,65,65,65	0
54	MG	1A	3025	1/1	0.96	0.41	41,41,41,41	0
54	MG	2A	3403	1/1	0.96	0.11	39,39,39,39	0
54	MG	1A	3539	1/1	0.96	0.23	64,64,64,64	0
54	MG	2A	3703	1/1	0.96	0.11	55,55,55,55	0
58	ZN	1Y	501	1/1	0.96	0.19	58,58,58,58	0
54	MG	2A	3139	1/1	0.96	0.28	43,43,43,43	0
54	MG	2A	3013	1/1	0.96	0.13	26,26,26,26	0
54	MG	1A	3226	1/1	0.96	0.44	34,34,34,34	0
54	MG	1a	1807	1/1	0.96	0.11	60,60,60,60	0
54	MG	1a	1606	1/1	0.96	0.08	55,55,55,55	0
54	MG	1a	1809	1/1	0.96	0.12	72,72,72,72	0
54	MG	1V	202	1/1	0.97	0.39	35,35,35,35	0
54	MG	1A	3276	1/1	0.97	0.33	37,37,37,37	0
54	MG	1A	3921	1/1	0.97	0.58	44,44,44,44	0
54	MG	1A	3607	1/1	0.97	0.11	49,49,49,49	0
54	MG	1A	3780	1/1	0.97	0.19	48,48,48,48	0
54	MG	1A	3224	1/1	0.97	0.61	42,42,42,42	0
54	MG	1a	1744	1/1	0.97	0.11	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	3609	1/1	0.97	0.26	40,40,40,40	0
54	MG	2D	302	1/1	0.97	0.29	46,46,46,46	0
54	MG	1A	3179	1/1	0.97	0.25	40,40,40,40	0
54	MG	1B	227	1/1	0.97	0.18	61,61,61,61	0
54	MG	2A	3635	1/1	0.97	0.15	59,59,59,59	0
54	MG	1a	1848	1/1	0.97	0.20	66,66,66,66	0
54	MG	1A	3850	1/1	0.97	0.10	44,44,44,44	0
54	MG	1A	3137	1/1	0.97	0.21	35,35,35,35	0
54	MG	2A	3639	1/1	0.97	0.19	42,42,42,42	0
54	MG	1A	4006	1/1	0.97	0.18	18,18,18,18	0
54	MG	1A	3612	1/1	0.97	0.24	62,62,62,62	0
54	MG	1A	3387	1/1	0.97	0.19	41,41,41,41	0
54	MG	1A	3388	1/1	0.97	0.14	31,31,31,31	0
54	MG	1D	308	1/1	0.97	0.23	33,33,33,33	0
54	MG	1A	3350	1/1	0.97	0.13	37,37,37,37	0
54	MG	1A	3252	1/1	0.97	0.41	31,31,31,31	0
54	MG	1A	3003	1/1	0.97	0.12	27,27,27,27	0
54	MG	1A	3017	1/1	0.97	0.25	34,34,34,34	0
54	MG	1A	3141	1/1	0.97	0.55	37,37,37,37	0
54	MG	1A	3436	1/1	0.97	0.16	34,34,34,34	0
54	MG	1A	3674	1/1	0.97	0.21	48,48,48,48	0
54	MG	1A	3231	1/1	0.97	0.36	39,39,39,39	0
54	MG	1A	3019	1/1	0.97	0.51	33,33,33,33	0
54	MG	1A	3162	1/1	0.97	0.37	42,42,42,42	0
54	MG	1A	3397	1/1	0.97	0.22	27,27,27,27	0
54	MG	1A	4021	1/1	0.97	0.13	30,30,30,30	0
54	MG	1A	3626	1/1	0.97	0.24	29,29,29,29	0
54	MG	2a	3114	1/1	0.97	0.27	79,79,79,79	0
54	MG	1A	3013	1/1	0.97	0.19	26,26,26,26	0
54	MG	1A	3007	1/1	0.97	0.16	43,43,43,43	0
54	MG	2a	3117	1/1	0.97	0.10	71,71,71,71	0
54	MG	1A	4025	1/1	0.97	0.20	55,55,55,55	0
54	MG	1A	3322	1/1	0.97	0.17	44,44,44,44	0
54	MG	2A	3291	1/1	0.97	0.15	50,50,50,50	0
54	MG	1A	3083	1/1	0.97	0.50	46,46,46,46	0
54	MG	1a	1773	1/1	0.97	0.07	74,74,74,74	0
54	MG	1A	3262	1/1	0.97	0.52	51,51,51,51	0
54	MG	2A	3413	1/1	0.97	0.32	59,59,59,59	0
54	MG	2V	201	1/1	0.97	0.24	60,60,60,60	0
54	MG	2V	202	1/1	0.97	0.31	44,44,44,44	0
54	MG	2V	203	1/1	0.97	0.15	69,69,69,69	0
54	MG	2W	201	1/1	0.97	0.45	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	1A	3806	1/1	0.97	0.38	42,42,42,42	0
54	MG	2A	3668	1/1	0.97	0.08	44,44,44,44	0
54	MG	1A	3876	1/1	0.97	0.13	29,29,29,29	0
54	MG	2A	3078	1/1	0.97	0.18	53,53,53,53	0
54	MG	1A	3291	1/1	0.97	0.21	36,36,36,36	0
54	MG	2A	3418	1/1	0.97	0.13	31,31,31,31	0
54	MG	1F	311	1/1	0.97	0.20	37,37,37,37	0
54	MG	1A	3326	1/1	0.97	0.24	44,44,44,44	0
54	MG	1A	3879	1/1	0.97	0.23	35,35,35,35	0
54	MG	1A	3263	1/1	0.97	0.43	38,38,38,38	0
54	MG	1A	3881	1/1	0.97	0.13	42,42,42,42	0
54	MG	1A	3746	1/1	0.97	0.21	57,57,57,57	0
54	MG	1A	3635	1/1	0.97	0.19	31,31,31,31	0
54	MG	1A	3210	1/1	0.97	0.12	55,55,55,55	0
54	MG	2a	3001	1/1	0.97	0.24	49,49,49,49	0
54	MG	1A	3690	1/1	0.97	0.12	51,51,51,51	0
54	MG	1A	3146	1/1	0.97	0.71	39,39,39,39	0
54	MG	2a	3147	1/1	0.97	0.14	64,64,64,64	0
54	MG	2A	3312	1/1	0.97	0.21	44,44,44,44	0
54	MG	1A	3751	1/1	0.97	0.11	32,32,32,32	0
54	MG	2A	3685	1/1	0.97	0.16	47,47,47,47	0
54	MG	1a	1692	1/1	0.97	0.14	66,66,66,66	0
54	MG	1a	1693	1/1	0.97	0.23	68,68,68,68	0
54	MG	1A	3816	1/1	0.97	0.14	53,53,53,53	0
54	MG	2A	3435	1/1	0.97	0.13	59,59,59,59	0
54	MG	1A	3368	1/1	0.97	0.13	24,24,24,24	0
54	MG	2A	3095	1/1	0.97	0.16	51,51,51,51	0
54	MG	1A	3639	1/1	0.97	0.17	46,46,46,46	0
54	MG	1a	1697	1/1	0.97	0.26	68,68,68,68	0
54	MG	2a	3017	1/1	0.97	0.21	58,58,58,58	0
54	MG	1a	1698	1/1	0.97	0.09	60,60,60,60	0
54	MG	1A	3640	1/1	0.97	0.20	48,48,48,48	0
54	MG	2A	3323	1/1	0.97	0.22	36,36,36,36	0
54	MG	2A	3697	1/1	0.97	0.08	68,68,68,68	0
54	MG	1A	3695	1/1	0.97	0.19	48,48,48,48	0
54	MG	1A	3971	1/1	0.97	0.15	45,45,45,45	0
54	MG	1A	3127	1/1	0.97	0.53	40,40,40,40	0
54	MG	2A	3213	1/1	0.97	0.16	64,64,64,64	0
54	MG	2a	3026	1/1	0.97	0.09	78,78,78,78	0
54	MG	2A	3572	1/1	0.97	0.11	41,41,41,41	0
54	MG	2a	3170	1/1	0.97	0.11	68,68,68,68	0
54	MG	1A	3894	1/1	0.97	0.18	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	3029	1/1	0.97	0.12	40,40,40,40	0
54	MG	1A	3148	1/1	0.97	0.10	51,51,51,51	0
54	MG	2A	3331	1/1	0.97	0.18	37,37,37,37	0
54	MG	2a	3175	1/1	0.97	0.08	75,75,75,75	0
54	MG	1A	3698	1/1	0.97	0.36	50,50,50,50	0
54	MG	1a	1706	1/1	0.97	0.10	60,60,60,60	0
54	MG	1A	3215	1/1	0.97	0.43	38,38,38,38	0
54	MG	2A	3335	1/1	0.97	0.15	37,37,37,37	0
54	MG	1P	204	1/1	0.97	0.29	52,52,52,52	0
54	MG	2A	3712	1/1	0.97	0.12	61,61,61,61	0
54	MG	2A	3581	1/1	0.97	0.13	34,34,34,34	0
54	MG	2a	3183	1/1	0.97	0.13	70,70,70,70	0
54	MG	1A	3040	1/1	0.97	0.18	35,35,35,35	0
54	MG	1A	3978	1/1	0.97	0.16	33,33,33,33	0
54	MG	1Q	201	1/1	0.97	0.18	36,36,36,36	0
54	MG	1Q	202	1/1	0.97	0.15	36,36,36,36	0
54	MG	1A	3334	1/1	0.97	0.15	28,28,28,28	0
54	MG	2a	3190	1/1	0.97	0.10	62,62,62,62	0
54	MG	1a	1812	1/1	0.97	0.22	63,63,63,63	0
54	MG	1A	3762	1/1	0.97	0.30	38,38,38,38	0
54	MG	1A	3828	1/1	0.97	0.15	18,18,18,18	0
54	MG	1A	3129	1/1	0.97	0.34	35,35,35,35	0
54	MG	1A	3151	1/1	0.97	0.20	41,41,41,41	0
54	MG	1A	3337	1/1	0.97	0.15	18,18,18,18	0
54	MG	1A	3085	1/1	0.97	0.20	44,44,44,44	0
54	MG	2A	3015	1/1	0.97	0.35	39,39,39,39	0
54	MG	1A	3339	1/1	0.97	0.21	37,37,37,37	0
54	MG	1a	1721	1/1	0.97	0.12	63,63,63,63	0
54	MG	2A	3126	1/1	0.97	0.22	67,67,67,67	0
54	MG	1A	3707	1/1	0.97	0.38	50,50,50,50	0
54	MG	2A	3475	1/1	0.97	0.21	37,37,37,37	0
54	MG	1A	3419	1/1	0.97	0.14	29,29,29,29	0
54	MG	1A	3652	1/1	0.97	0.11	39,39,39,39	0
54	MG	2A	3131	1/1	0.97	0.13	64,64,64,64	0
54	MG	2A	3357	1/1	0.97	0.20	34,34,34,34	0
54	MG	2A	3021	1/1	0.97	0.13	43,43,43,43	0
54	MG	1a	1824	1/1	0.97	0.15	55,55,55,55	0
54	MG	1T	205	1/1	0.97	0.11	62,62,62,62	0
54	MG	1A	3153	1/1	0.97	0.29	38,38,38,38	0
54	MG	2A	3484	1/1	0.97	0.17	58,58,58,58	0
54	MG	1A	3119	1/1	0.97	0.34	54,54,54,54	0
54	MG	1A	3773	1/1	0.97	0.16	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	1637	1/1	0.97	0.19	72,72,72,72	0
54	MG	2A	3365	1/1	0.97	0.17	65,65,65,65	0
54	MG	1A	3001	1/1	0.97	0.11	40,40,40,40	0
54	MG	2A	3029	1/1	0.97	0.15	45,45,45,45	0
54	MG	1A	3470	1/1	0.97	0.15	48,48,48,48	0
54	MG	1U	206	1/1	0.97	0.35	43,43,43,43	0
54	MG	1a	1733	1/1	0.97	0.14	62,62,62,62	0
54	MG	1A	3776	1/1	0.97	0.17	45,45,45,45	0
58	ZN	26	501	1/1	0.97	0.14	67,67,67,67	0
54	MG	2A	3495	1/1	0.97	0.17	70,70,70,70	0
54	MG	1A	3306	1/1	0.97	0.19	24,24,24,24	0
54	MG	1A	3955	1/1	0.98	0.16	31,31,31,31	0
54	MG	1A	3318	1/1	0.98	0.19	30,30,30,30	0
54	MG	2A	3007	1/1	0.98	0.13	42,42,42,42	0
54	MG	1A	3132	1/1	0.98	0.20	51,51,51,51	0
54	MG	1A	3590	1/1	0.98	0.12	50,50,50,50	0
54	MG	1B	222	1/1	0.98	0.11	58,58,58,58	0
54	MG	1F	319	1/1	0.98	0.12	53,53,53,53	0
54	MG	1A	3099	1/1	0.98	0.44	36,36,36,36	0
54	MG	2A	3285	1/1	0.98	0.14	54,54,54,54	0
54	MG	1a	1737	1/1	0.98	0.22	79,79,79,79	0
54	MG	1a	1738	1/1	0.98	0.07	56,56,56,56	0
54	MG	1A	3134	1/1	0.98	0.17	38,38,38,38	0
54	MG	1A	3734	1/1	0.98	0.14	39,39,39,39	0
54	MG	1A	3135	1/1	0.98	0.18	26,26,26,26	0
54	MG	1A	3566	1/1	0.98	0.05	61,61,61,61	0
54	MG	1A	4042	1/1	0.98	0.08	67,67,67,67	0
54	MG	1A	3442	1/1	0.98	0.17	18,18,18,18	0
54	MG	2A	3609	1/1	0.98	0.18	62,62,62,62	0
54	MG	1a	1803	1/1	0.98	0.10	50,50,50,50	0
54	MG	1N	201	1/1	0.98	0.23	46,46,46,46	0
54	MG	2A	3370	1/1	0.98	0.20	73,73,73,73	0
54	MG	2A	3527	1/1	0.98	0.22	54,54,54,54	0
54	MG	2A	3156	1/1	0.98	0.27	46,46,46,46	0
54	MG	1A	3341	1/1	0.98	0.19	34,34,34,34	0
54	MG	1D	302	1/1	0.98	0.16	55,55,55,55	0
54	MG	1A	3966	1/1	0.98	0.16	49,49,49,49	0
54	MG	1D	304	1/1	0.98	0.21	46,46,46,46	0
54	MG	1A	3110	1/1	0.98	0.29	35,35,35,35	0
54	MG	2Q	203	1/1	0.98	0.06	61,61,61,61	0
54	MG	2R	201	1/1	0.98	0.39	49,49,49,49	0
54	MG	2A	3302	1/1	0.98	0.23	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	3454	1/1	0.98	0.17	47,47,47,47	0
54	MG	2A	3303	1/1	0.98	0.11	27,27,27,27	0
54	MG	1A	3862	1/1	0.98	0.15	45,45,45,45	0
54	MG	2A	3709	1/1	0.98	0.38	74,74,74,74	0
54	MG	1A	3104	1/1	0.98	0.40	37,37,37,37	0
54	MG	1A	3931	1/1	0.98	0.14	47,47,47,47	0
54	MG	1A	3138	1/1	0.98	0.24	39,39,39,39	0
54	MG	1A	3865	1/1	0.98	0.09	55,55,55,55	0
54	MG	2A	3309	1/1	0.98	0.20	55,55,55,55	0
54	MG	1A	3090	1/1	0.98	0.27	26,26,26,26	0
54	MG	2A	3463	1/1	0.98	0.14	56,56,56,56	0
54	MG	2A	3168	1/1	0.98	0.28	51,51,51,51	0
54	MG	1A	3743	1/1	0.98	0.18	53,53,53,53	0
54	MG	2A	3035	1/1	0.98	0.15	68,68,68,68	0
54	MG	2A	3101	1/1	0.98	0.14	78,78,78,78	0
54	MG	2A	3549	1/1	0.98	0.14	25,25,25,25	0
54	MG	1A	3227	1/1	0.98	0.21	29,29,29,29	0
54	MG	1A	4055	1/1	0.98	0.34	57,57,57,57	0
54	MG	2a	3088	1/1	0.98	0.16	49,49,49,49	0
54	MG	2A	3104	1/1	0.98	0.21	72,72,72,72	0
54	MG	1A	3901	1/1	0.98	0.12	43,43,43,43	0
54	MG	1R	201	1/1	0.98	0.21	42,42,42,42	0
54	MG	2A	3473	1/1	0.98	0.12	66,66,66,66	0
54	MG	1A	3902	1/1	0.98	0.17	28,28,28,28	0
54	MG	2A	3041	1/1	0.98	0.16	34,34,34,34	0
54	MG	17	105	1/1	0.98	0.56	49,49,49,49	0
54	MG	1A	3106	1/1	0.98	0.50	34,34,34,34	0
54	MG	2A	3044	1/1	0.98	0.19	65,65,65,65	0
54	MG	1E	301	1/1	0.98	0.62	45,45,45,45	0
54	MG	1R	205	1/1	0.98	0.17	45,45,45,45	0
54	MG	2A	3327	1/1	0.98	0.16	42,42,42,42	0
54	MG	1E	302	1/1	0.98	0.40	41,41,41,41	0
54	MG	1A	3293	1/1	0.98	0.63	49,49,49,49	0
54	MG	2a	3011	1/1	0.98	0.16	49,49,49,49	0
54	MG	1A	3349	1/1	0.98	0.22	28,28,28,28	0
54	MG	2a	3013	1/1	0.98	0.17	54,54,54,54	0
54	MG	1A	3006	1/1	0.98	0.14	25,25,25,25	0
54	MG	1A	3943	1/1	0.98	0.06	65,65,65,65	0
54	MG	1a	1831	1/1	0.98	0.20	66,66,66,66	0
54	MG	1A	3454	1/1	0.98	0.20	28,28,28,28	0
54	MG	1E	308	1/1	0.98	0.12	62,62,62,62	0
54	MG	1A	3168	1/1	0.98	0.28	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	1F	301	1/1	0.98	0.32	39,39,39,39	0
54	MG	1A	3529	1/1	0.98	0.14	25,25,25,25	0
54	MG	1F	304	1/1	0.98	0.19	34,34,34,34	0
54	MG	1F	305	1/1	0.98	0.28	38,38,38,38	0
54	MG	1a	1839	1/1	0.98	0.10	55,55,55,55	0
54	MG	1A	3432	1/1	0.98	0.14	18,18,18,18	0
54	MG	1A	3130	1/1	0.98	0.60	35,35,35,35	0
54	MG	2A	3498	1/1	0.98	0.14	73,73,73,73	0
54	MG	1A	3912	1/1	0.98	0.15	49,49,49,49	0
54	MG	2a	3121	1/1	0.98	0.12	67,67,67,67	0
54	MG	1V	203	1/1	0.98	0.17	44,44,44,44	0
54	MG	1A	3063	1/1	0.98	0.30	42,42,42,42	0
54	MG	1A	3200	1/1	0.98	0.45	39,39,39,39	0
54	MG	2a	3032	1/1	0.98	0.07	92,92,92,92	0
54	MG	2A	3585	1/1	0.98	0.08	61,61,61,61	0
54	MG	1A	3156	1/1	0.98	0.33	39,39,39,39	0
54	MG	2A	3587	1/1	0.98	0.05	46,46,46,46	0
58	ZN	25	102	1/1	0.98	0.16	71,71,71,71	0
54	MG	2A	3424	1/1	0.98	0.10	39,39,39,39	0
54	MG	1A	3614	1/1	0.98	0.34	39,39,39,39	0
54	MG	1A	3461	1/1	0.98	0.09	52,52,52,52	0
59	SF4	2d	302	8/8	0.98	0.13	71,83,87,87	0
54	MG	1A	3507	1/1	0.99	0.14	46,46,46,46	0
54	MG	1A	3451	1/1	0.99	0.18	57,57,57,57	0
54	MG	1A	3166	1/1	0.99	0.29	41,41,41,41	0
54	MG	1D	306	1/1	0.99	0.18	17,17,17,17	0
54	MG	2A	3282	1/1	0.99	0.20	53,53,53,53	0
54	MG	2A	3129	1/1	0.99	0.21	33,33,33,33	0
54	MG	1A	3116	1/1	0.99	0.20	39,39,39,39	0
54	MG	1A	3222	1/1	0.99	0.62	42,42,42,42	0
54	MG	1A	3307	1/1	0.99	0.37	40,40,40,40	0
54	MG	1A	3212	1/1	0.99	0.41	33,33,33,33	0
54	MG	1A	3789	1/1	0.99	0.10	29,29,29,29	0
54	MG	1A	3018	1/1	0.99	0.30	28,28,28,28	0
54	MG	1A	3169	1/1	0.99	0.24	31,31,31,31	0
58	ZN	16	501	1/1	0.99	0.23	48,48,48,48	0
58	ZN	19	103	1/1	0.99	0.19	50,50,50,50	0
58	ZN	1n	104	1/1	0.99	0.11	77,77,77,77	0
54	MG	1N	202	1/1	0.99	0.19	42,42,42,42	0
54	MG	1A	3858	1/1	0.99	0.27	39,39,39,39	0
54	MG	1a	1852	1/1	0.99	0.12	40,40,40,40	0
54	MG	2a	3184	1/1	0.99	0.12	58,58,58,58	0

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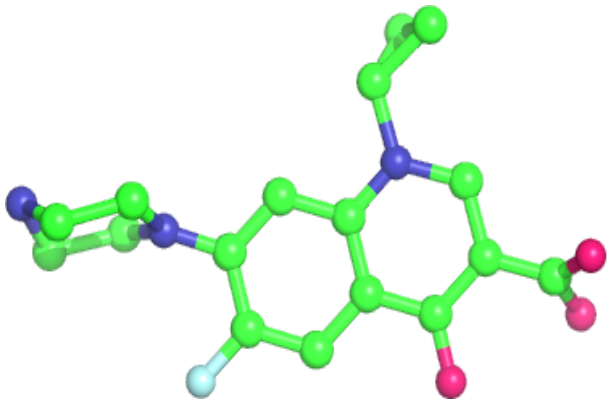
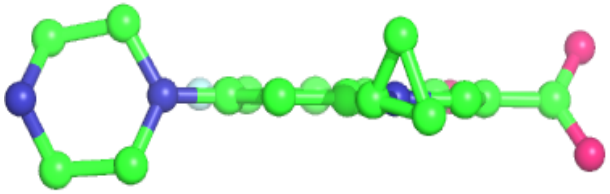
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3661	1/1	0.99	0.08	31,31,31,31	0
54	MG	2A	3601	1/1	0.99	0.21	46,46,46,46	0
59	SF4	1d	306	8/8	0.99	0.16	60,71,79,80	0
54	MG	1F	302	1/1	0.99	0.18	34,34,34,34	0
54	MG	1A	3582	1/1	1.00	0.22	28,28,28,28	0

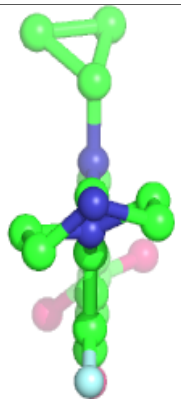
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CPF 1A 4056:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

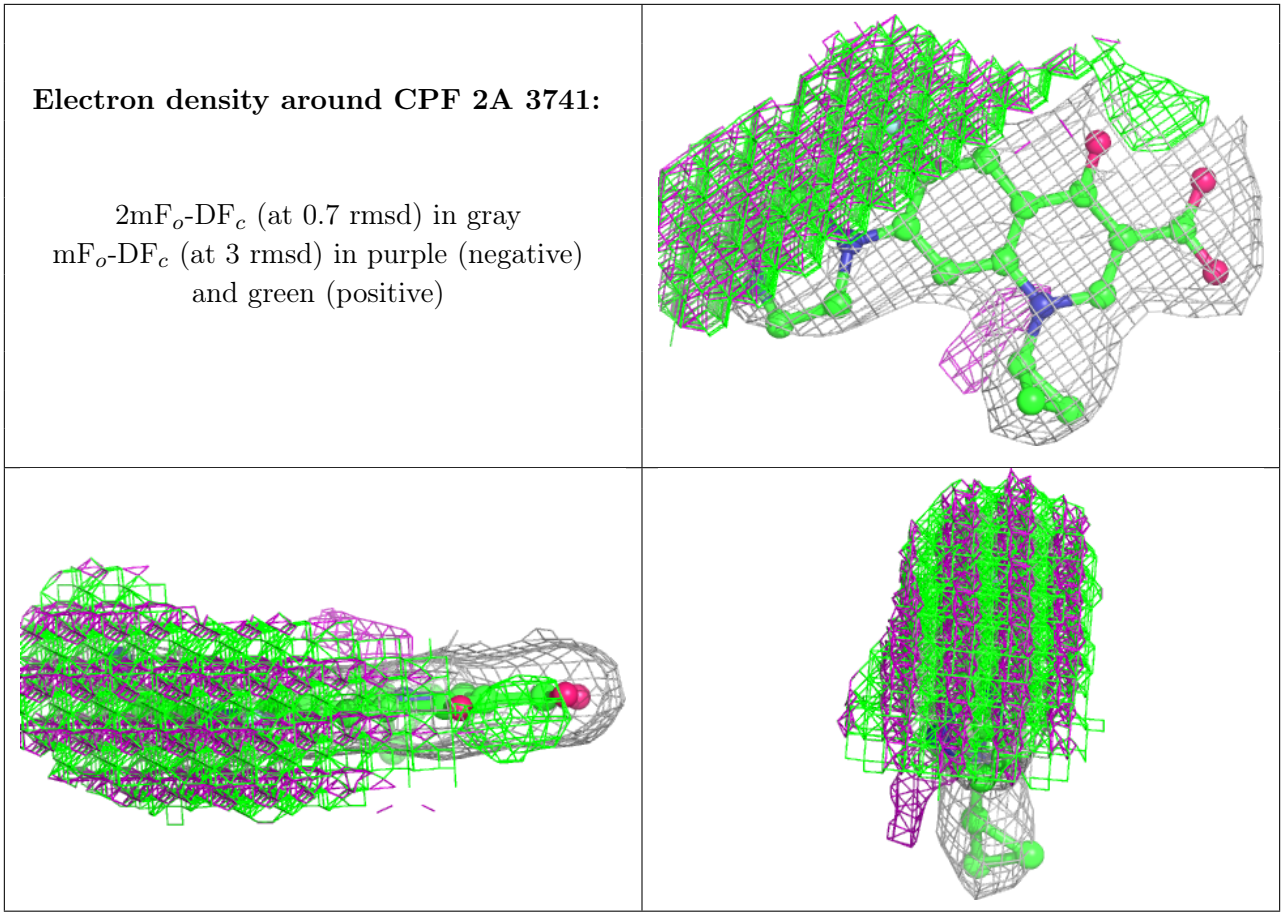






Electron density around CPF 2A 3741:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.