Full wwPDB X-ray Structure Validation Report (i)

Dec 20, 2023 – 08:55 PM EST

PDB ID	:	8G29
Title	:	Crystal structure of the A2503-C2,C8-dimethylated Thermus thermophilus 70S ribosome in complex with mRNA, aminoacylated A-site Phe-tRNAphe, aminoacylated P-site fMet-tRNAmet, and deacylated E-site tRNAphe at 2.55A resolution
Authors	:	Aleksandrova, E.V.; Wu, K.J.Y.; Tresco, B.I.C.; Syroegin, E.A.; Killeavy, E.E.; Balasanyants, S.M.; Svetlov, M.S.; Gregory, S.T.; Atkinson, G.C.; Myers, A.G.; Polikanov, Y.S.
Deposited on	:	2023-02-03
Resolution	:	2.55 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 (i) symbol.

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

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

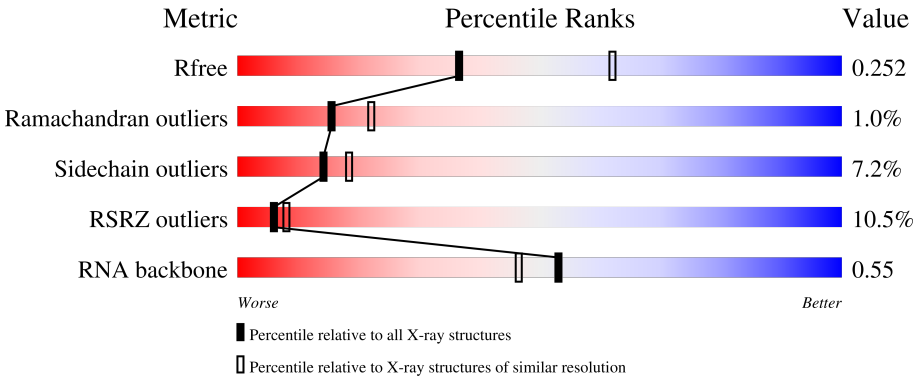
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 2.55 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	1284 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)
RNA backbone	3102	1026 (2.88-2.20)

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	6% 83% 15%
1	2A	2915	5% 79% 16%
2	1B	121	93% 7%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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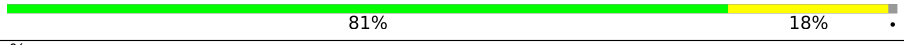
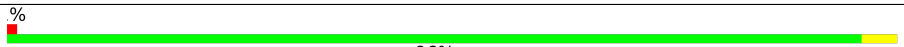
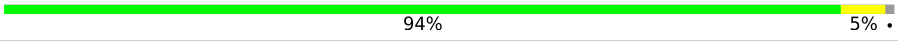
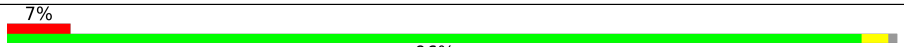
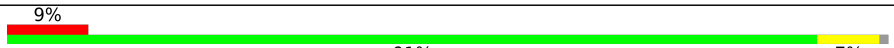
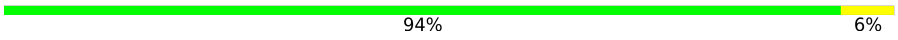
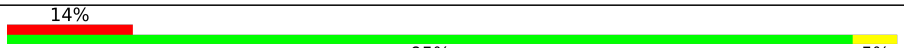
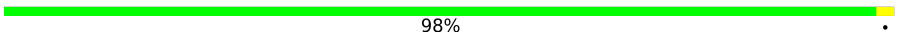
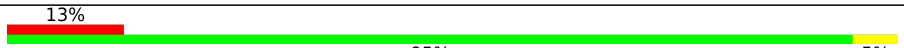
Mol	Chain	Length	Quality of chain
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
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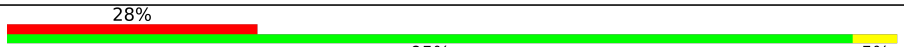
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	

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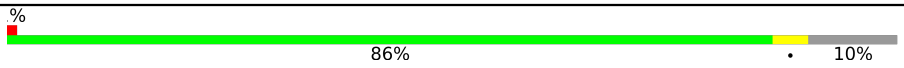
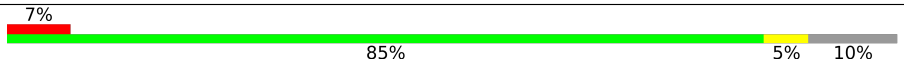
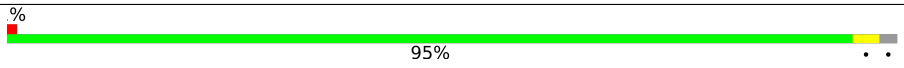
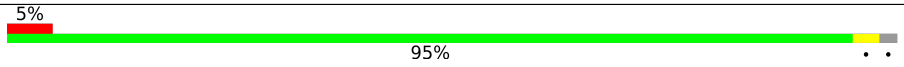
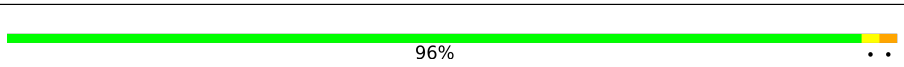
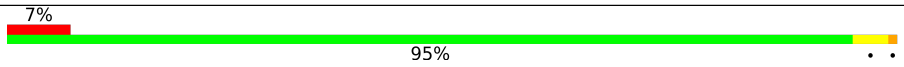
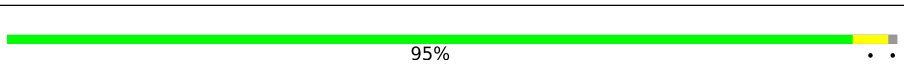
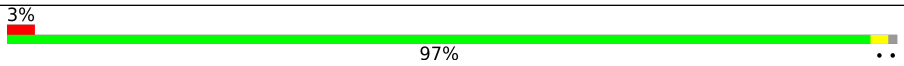
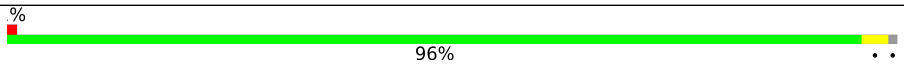
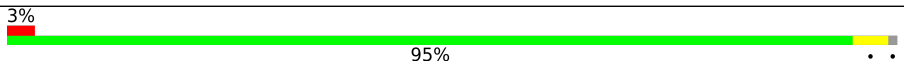
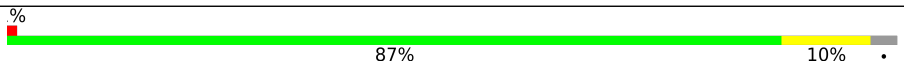
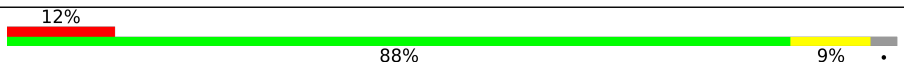
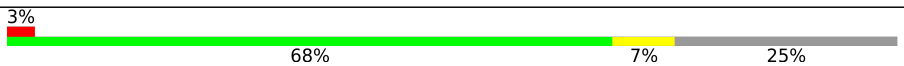
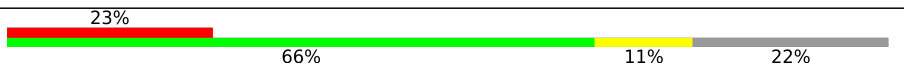
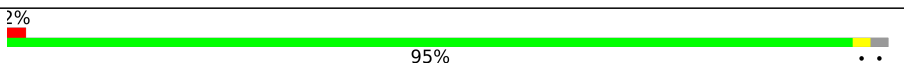
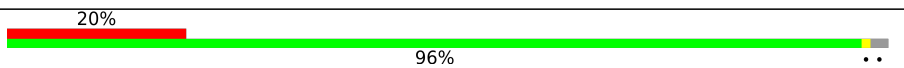
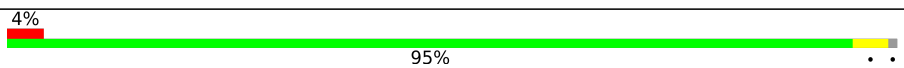
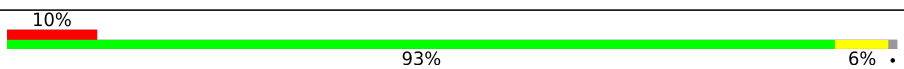
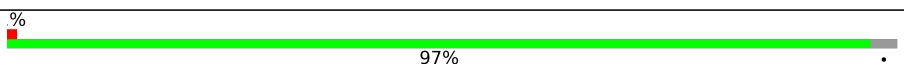
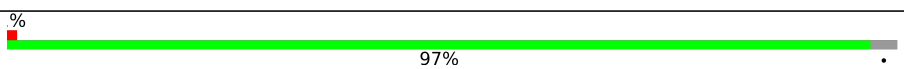
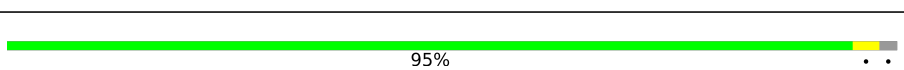
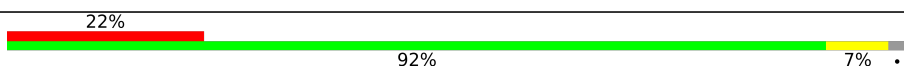
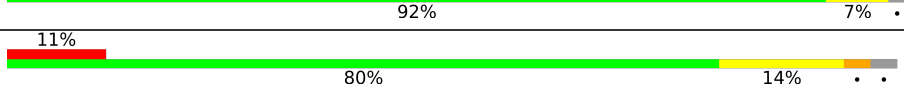
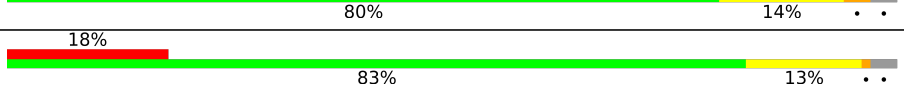
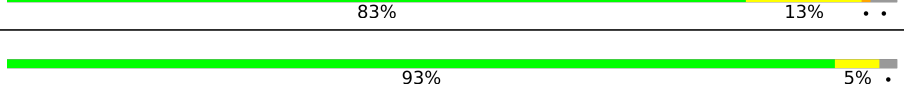
Mol	Chain	Length	Quality of chain
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	

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Mol	Chain	Length	Quality of chain
27	25	60	2% 93% 5%
28	16	54	87% 11%
28	26	54	15% 93% 6%
29	17	49	6% 90% 8%
29	27	49	10% 90% 8%
30	18	65	94% 5%
30	28	65	25% 94% 5%
31	19	37	3% 100%
31	29	37	81% 100%
32	1a	1521	5% 83% 15%
32	2a	1521	6% 81% 18%
33	1b	256	30% 79% 11% 10%
33	2b	256	27% 75% 14% 10%
34	1c	239	19% 80% 6% 14%
34	2c	239	28% 82% 14%
35	1d	209	8% 93% 6%
35	2d	209	7% 89% 11%
36	1e	162	9% 86% 6% 9%
36	2e	162	7% 86% 5% 9%
37	1f	101	90% 9%
37	2f	101	2% 96%
38	1g	156	16% 90% 10%
38	2g	156	16% 91% 8%
39	1h	138	5% 94% 5%
39	2h	138	11% 93% 6%

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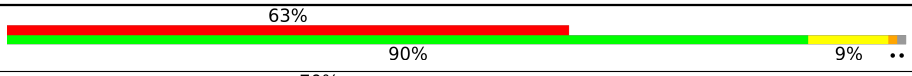
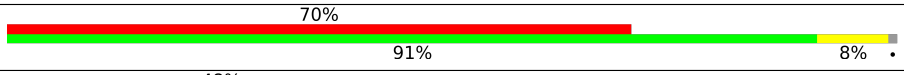
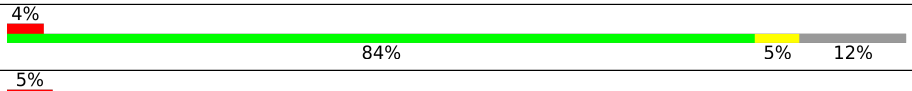
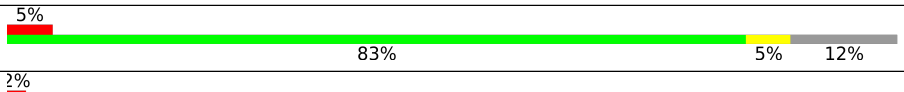
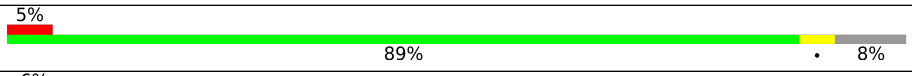
Mol	Chain	Length	Quality of chain
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
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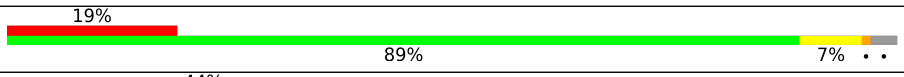
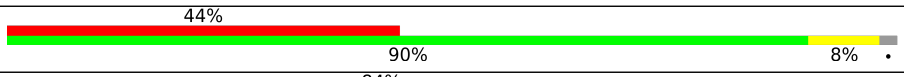
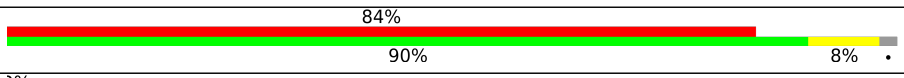
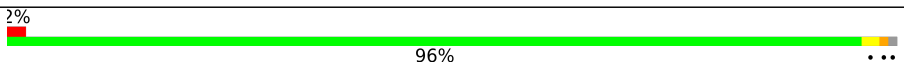
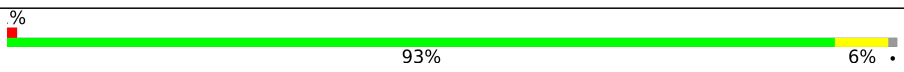
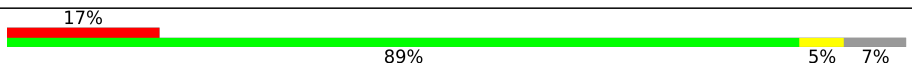
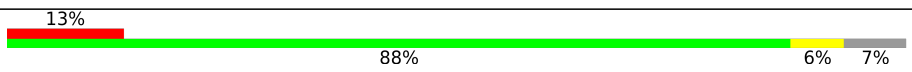
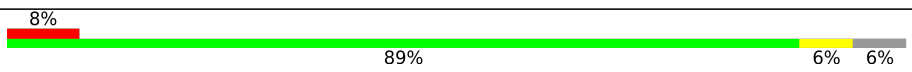
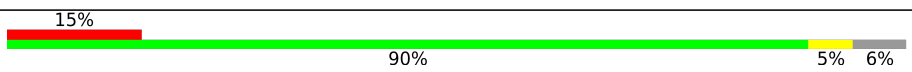
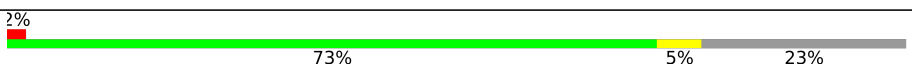
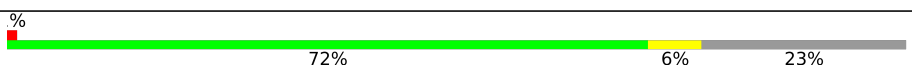
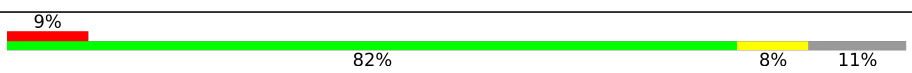
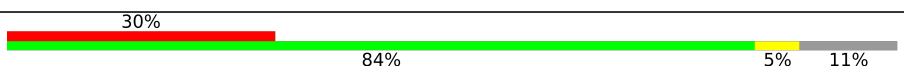
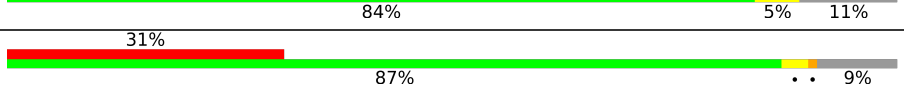
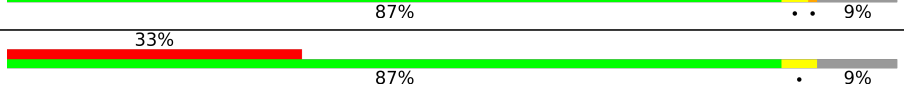
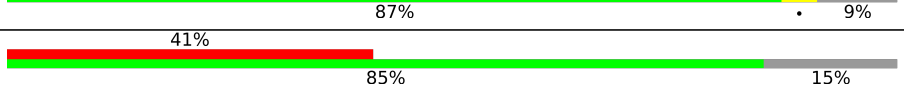
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	

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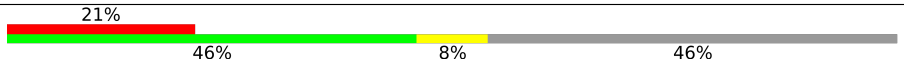
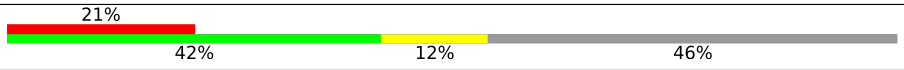
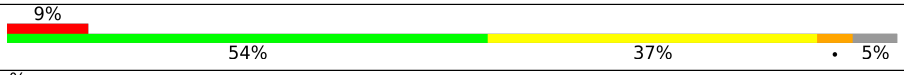
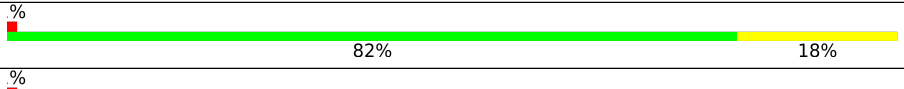
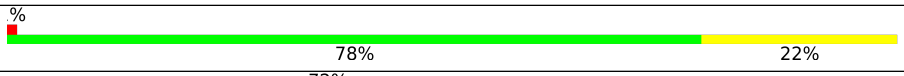
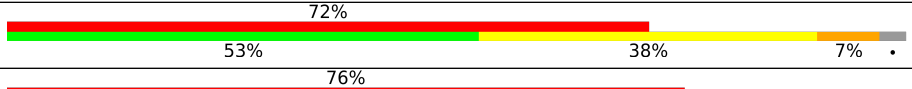
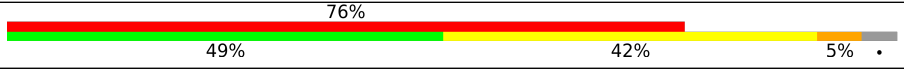
Mol	Chain	Length	Quality of chain
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	2y	76	

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
56	MIA	1y	37	-	-	-	X
56	5MU	1y	54	-	-	-	X
56	PSU	1y	55	-	-	-	X
56	PSU	2y	32	-	-	-	X
56	MIA	2y	37	-	-	-	X
56	5MU	2y	54	-	-	-	X
56	PSU	2y	55	-	-	-	X
57	MG	15	108	-	-	-	X
57	MG	18	105	-	-	-	X
57	MG	1A	3051	-	-	-	X
57	MG	1A	3072	-	-	-	X
57	MG	1A	3101	-	-	-	X
57	MG	1A	3186	-	-	-	X
57	MG	1A	3292	-	-	-	X
57	MG	1A	3329	-	-	-	X
57	MG	1A	3399	-	-	-	X
57	MG	1A	3428	-	-	-	X
57	MG	1A	3436	-	-	-	X
57	MG	1A	3437	-	-	-	X
57	MG	1A	3447	-	-	-	X
57	MG	1A	3452	-	-	-	X
57	MG	1A	3502	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1A	3563	-	-	-	X
57	MG	1A	3953	-	-	-	X
57	MG	1A	4024	-	-	-	X
57	MG	1A	4042	-	-	-	X
57	MG	1N	202	-	-	-	X
57	MG	1N	205	-	-	-	X
57	MG	1T	203	-	-	-	X
57	MG	1a	1651	-	-	-	X
57	MG	1a	1655	-	-	-	X
57	MG	2A	3082	-	-	-	X
57	MG	2A	3084	-	-	-	X
57	MG	2A	3139	-	-	-	X
57	MG	2A	3175	-	-	-	X
57	MG	2A	3189	-	-	-	X
57	MG	2A	3206	-	-	-	X
57	MG	2A	3226	-	-	-	X
57	MG	2A	3279	-	-	-	X
57	MG	2A	3285	-	-	-	X
57	MG	2A	3301	-	-	-	X
57	MG	2A	3308	-	-	-	X
57	MG	2A	3317	-	-	-	X
57	MG	2A	3318	-	-	-	X
57	MG	2A	3346	-	-	-	X
57	MG	2A	3362	-	-	-	X
57	MG	2A	3384	-	-	-	X
57	MG	2A	3387	-	-	-	X
57	MG	2A	3398	-	-	-	X
57	MG	2A	3592	-	-	-	X
57	MG	2A	3686	-	-	-	X
57	MG	2D	303	-	-	-	X
57	MG	2U	202	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 299618 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	2871	Total	C	N	O	P	0	0	0
			61853	27532	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60323	26849	11284	19390	2800			

- 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
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

- 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
			2136	1349	423	361	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	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
5	2F	202	Total	C	N	O	S	0	0	0
			1579	1007	296	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
			1423	913	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	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	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1097	701	191	204	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	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
			1117	719	207	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 873	C 550	N 174	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
			771	495	140	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
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
21	2Z	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	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
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	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
			588	365	118	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
			552	349	99	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			532	339	97	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
			455	285	89	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	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

- 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
			1846	1179	331	331	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
			1548	973	301	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
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	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
			1129	714	213	198	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
			810	514	144	149	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
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	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
			1088	689	206	191	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
			983	623	193	167			
40	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

- 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
			709	440	138	131			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	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
			829	516	155	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	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	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
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	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
			728	446	156	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			727	446	155	124	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 RNA chain called MF-mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
53	2v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 54 is a RNA chain called A-site Aminoacylated Phe-tRNAphe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1603	722	287	518	74	2			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1555	699	280	502	72	2			

- Molecule 55 is a RNA chain called P-site Aminoacylated fMet-tRNAmet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1656	740	299	538	77	2			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1656	740	299	538	77	2			

- Molecule 56 is a RNA chain called E-site Deacylated tRNAphe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
56	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
56	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1113	Total	Mg	0	0
			1113	1113		
57	1B	38	Total	Mg	0	0
			38	38		
57	1D	12	Total	Mg	0	0
			12	12		
57	1E	14	Total	Mg	0	0
			14	14		
57	1F	13	Total	Mg	0	0
			13	13		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1G	5	Total Mg 5 5	0	0
57	1H	1	Total Mg 1 1	0	0
57	1N	6	Total Mg 6 6	0	0
57	1O	4	Total Mg 4 4	0	0
57	1P	5	Total Mg 5 5	0	0
57	1Q	7	Total Mg 7 7	0	0
57	1R	6	Total Mg 6 6	0	0
57	1S	3	Total Mg 3 3	0	0
57	1T	3	Total Mg 3 3	0	0
57	1U	6	Total Mg 6 6	0	0
57	1V	7	Total Mg 7 7	0	0
57	1W	6	Total Mg 6 6	0	0
57	1X	7	Total Mg 7 7	0	0
57	1Y	2	Total Mg 2 2	0	0
57	1Z	3	Total Mg 3 3	0	0
57	10	7	Total Mg 7 7	0	0
57	11	6	Total Mg 6 6	0	0
57	12	2	Total Mg 2 2	0	0
57	13	3	Total Mg 3 3	0	0
57	14	1	Total Mg 1 1	0	0
57	15	8	Total Mg 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	16	2	Total Mg 2 2	0	0
57	17	6	Total Mg 6 6	0	0
57	18	5	Total Mg 5 5	0	0
57	19	1	Total Mg 1 1	0	0
57	1a	220	Total Mg 220 220	0	0
57	1b	1	Total Mg 1 1	0	0
57	1d	1	Total Mg 1 1	0	0
57	1e	2	Total Mg 2 2	0	0
57	1f	2	Total Mg 2 2	0	0
57	1l	2	Total Mg 2 2	0	0
57	1m	1	Total Mg 1 1	0	0
57	1n	1	Total Mg 1 1	0	0
57	1p	1	Total Mg 1 1	0	0
57	1q	1	Total Mg 1 1	0	0
57	1t	1	Total Mg 1 1	0	0
57	1v	1	Total Mg 1 1	0	0
57	1w	9	Total Mg 9 9	0	0
57	1x	14	Total Mg 14 14	0	0
57	2A	804	Total Mg 804 804	0	0
57	2B	16	Total Mg 16 16	0	0
57	2D	6	Total Mg 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2E	7	Total Mg 7 7	0	0
57	2F	6	Total Mg 6 6	0	0
57	2G	1	Total Mg 1 1	0	0
57	2O	1	Total Mg 1 1	0	0
57	2P	1	Total Mg 1 1	0	0
57	2Q	4	Total Mg 4 4	0	0
57	2R	2	Total Mg 2 2	0	0
57	2T	3	Total Mg 3 3	0	0
57	2U	3	Total Mg 3 3	0	0
57	2V	1	Total Mg 1 1	0	0
57	2W	3	Total Mg 3 3	0	0
57	2X	2	Total Mg 2 2	0	0
57	2Z	1	Total Mg 1 1	0	0
57	20	2	Total Mg 2 2	0	0
57	21	3	Total Mg 3 3	0	0
57	23	2	Total Mg 2 2	0	0
57	25	3	Total Mg 3 3	0	0
57	27	2	Total Mg 2 2	0	0
57	28	2	Total Mg 2 2	0	0
57	2a	2	Total Mg 2 2	0	0
57	2w	6	Total Mg 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2x	7	Total Mg 7 7	0	0
57	2y	7	Total Mg 7 7	0	0

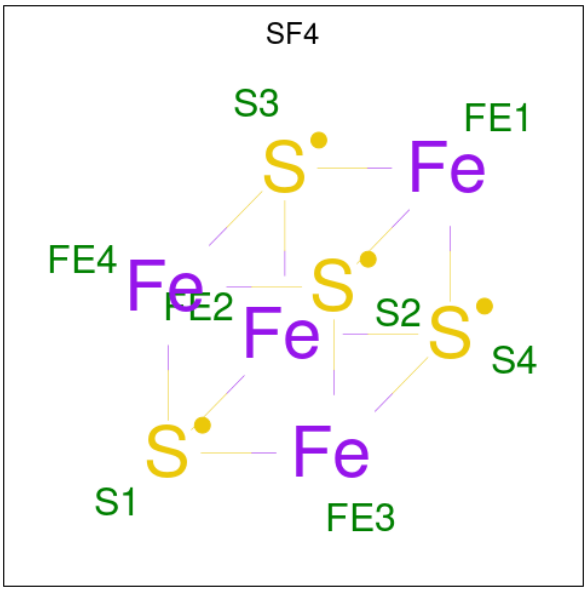
- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total K 1 1	0	0
58	2A	1	Total K 1 1	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1Y	1	Total Zn 1 1	0	0
59	14	1	Total Zn 1 1	0	0
59	15	1	Total Zn 1 1	0	0
59	16	1	Total Zn 1 1	0	0
59	19	1	Total Zn 1 1	0	0
59	1n	1	Total Zn 1 1	0	0
59	2Y	1	Total Zn 1 1	0	0
59	24	1	Total Zn 1 1	0	0
59	25	1	Total Zn 1 1	0	0
59	26	1	Total Zn 1 1	0	0
59	29	1	Total Zn 1 1	0	0
59	2n	1	Total Zn 1 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1d	1	Total Fe S 8 4 4	0	0
60	2d	1	Total Fe S 8 4 4	0	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	2067	Total O 2067 2067	0	0
61	1B	61	Total O 61 61	0	0
61	1D	32	Total O 32 32	0	0
61	1E	26	Total O 26 26	0	0
61	1F	20	Total O 20 20	0	0
61	1G	1	Total O 1 1	0	0
61	1H	2	Total O 2 2	0	0
61	1N	6	Total O 6 6	0	0
61	1O	6	Total O 6 6	0	0
61	1P	21	Total O 21 21	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1Q	7	Total O 7 7	0	0
61	1R	7	Total O 7 7	0	0
61	1S	5	Total O 5 5	0	0
61	1T	9	Total O 9 9	0	0
61	1U	14	Total O 14 14	0	0
61	1V	7	Total O 7 7	0	0
61	1W	6	Total O 6 6	0	0
61	1X	5	Total O 5 5	0	0
61	1Y	3	Total O 3 3	0	0
61	1Z	1	Total O 1 1	0	0
61	10	12	Total O 12 12	0	0
61	11	7	Total O 7 7	0	0
61	12	4	Total O 4 4	0	0
61	13	4	Total O 4 4	0	0
61	14	1	Total O 1 1	0	0
61	15	10	Total O 10 10	0	0
61	16	5	Total O 5 5	0	0
61	17	10	Total O 10 10	0	0
61	18	10	Total O 10 10	0	0
61	1a	425	Total O 425 425	0	0
61	1b	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1f	1	Total O 1 1	0	0
61	1i	1	Total O 1 1	0	0
61	1l	8	Total O 8 8	0	0
61	1m	2	Total O 2 2	0	0
61	1n	1	Total O 1 1	0	0
61	1o	3	Total O 3 3	0	0
61	1p	1	Total O 1 1	0	0
61	1q	2	Total O 2 2	0	0
61	1r	2	Total O 2 2	0	0
61	1u	2	Total O 2 2	0	0
61	1v	4	Total O 4 4	0	0
61	1w	12	Total O 12 12	0	0
61	1x	17	Total O 17 17	0	0
61	1y	1	Total O 1 1	0	0
61	2A	1094	Total O 1094 1094	0	0
61	2B	18	Total O 18 18	0	0
61	2D	22	Total O 22 22	0	0
61	2E	9	Total O 9 9	0	0
61	2F	11	Total O 11 11	0	0
61	2I	3	Total O 3 3	0	0
61	2N	1	Total O 1 1	0	0

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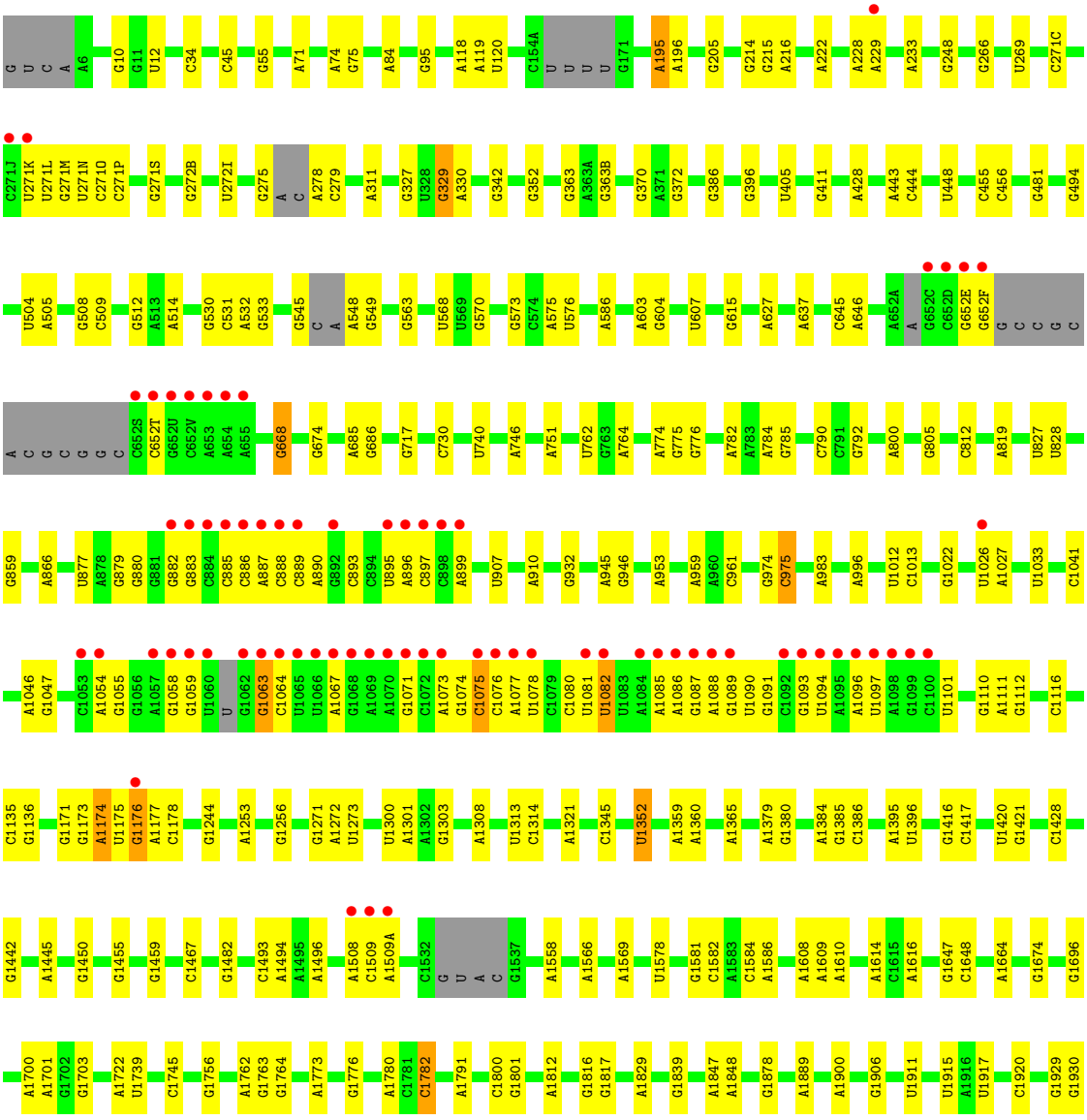
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2O	1	Total O 1 1	0	0
61	2P	9	Total O 9 9	0	0
61	2Q	1	Total O 1 1	0	0
61	2R	1	Total O 1 1	0	0
61	2T	5	Total O 5 5	0	0
61	2U	3	Total O 3 3	0	0
61	2W	3	Total O 3 3	0	0
61	2X	2	Total O 2 2	0	0
61	20	1	Total O 1 1	0	0
61	21	6	Total O 6 6	0	0
61	23	2	Total O 2 2	0	0
61	27	5	Total O 5 5	0	0
61	28	4	Total O 4 4	0	0
61	29	1	Total O 1 1	0	0
61	2w	1	Total O 1 1	0	0
61	2x	6	Total O 6 6	0	0
61	2y	2	Total O 2 2	0	0

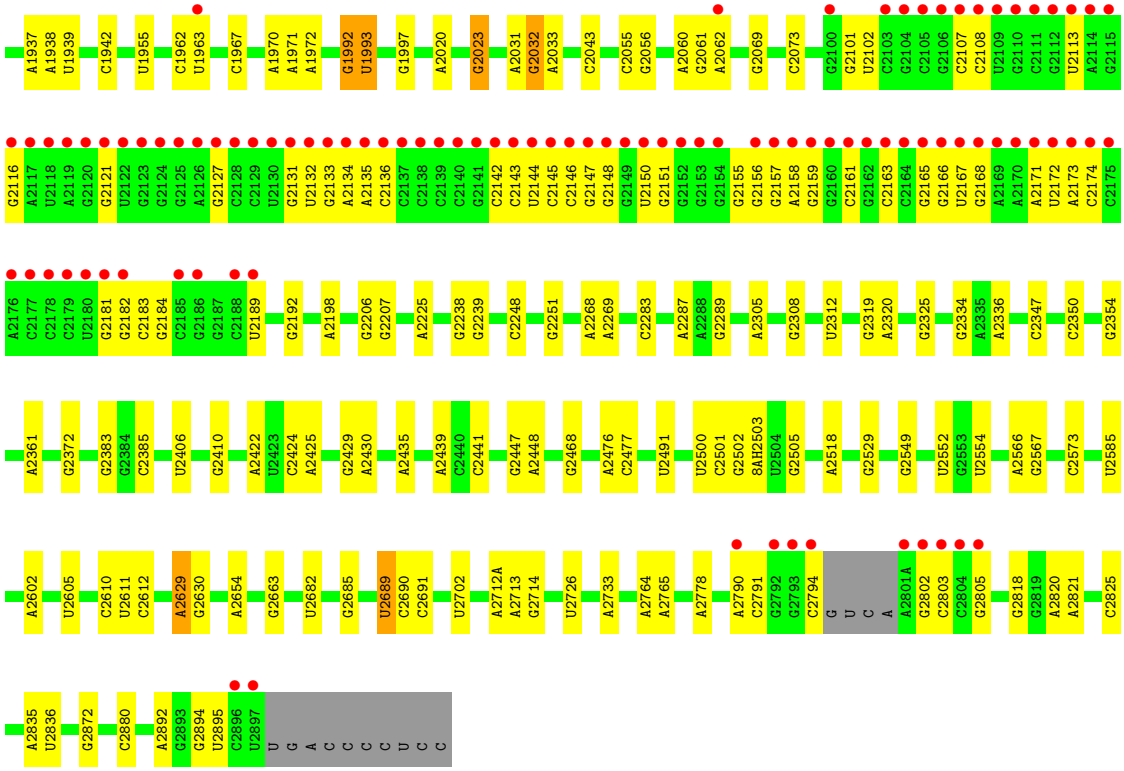
3 Residue-property plots (i)

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

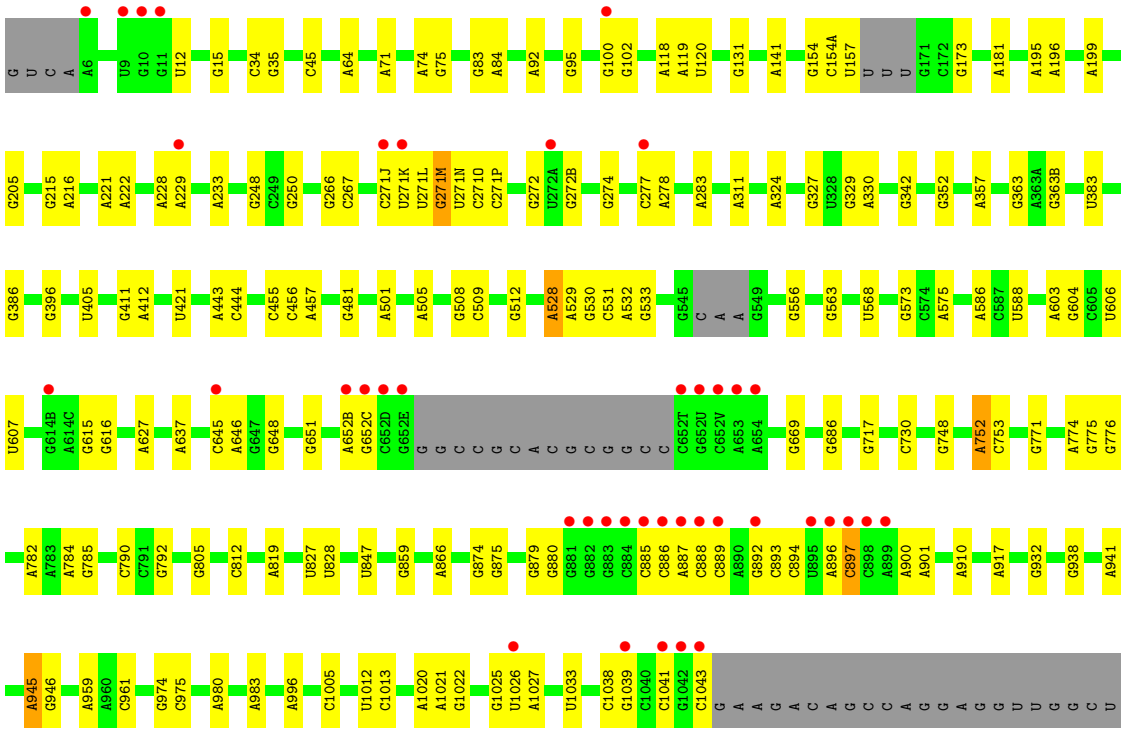
Chain 1A:

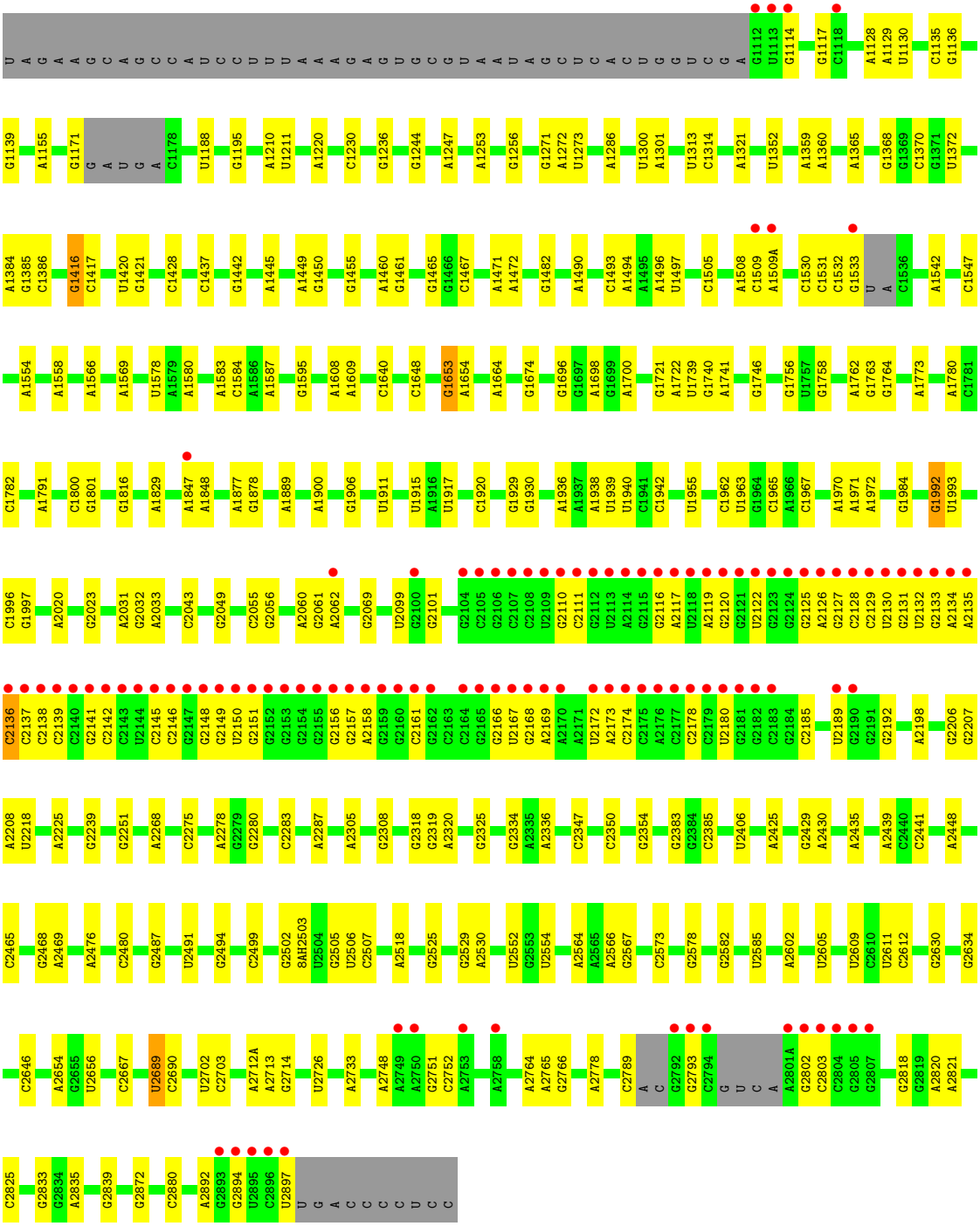




• Molecule 1: 23S Ribosomal RNA

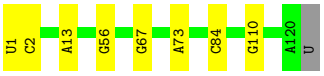
Chain 2A:





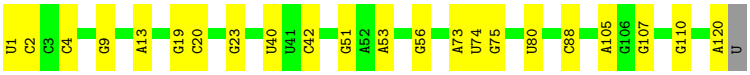
• Molecule 2: 5S Ribosomal RNA

Chain 1B:

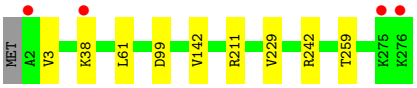


• Molecule 2: 5S Ribosomal RNA

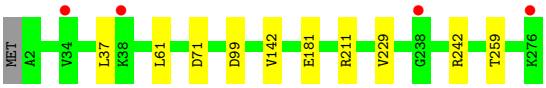
Chain 2B:



• Molecule 3: 50S ribosomal protein L2

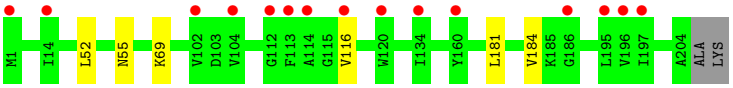


• Molecule 3: 50S ribosomal protein L2

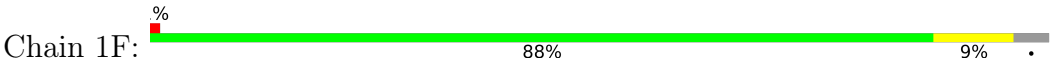


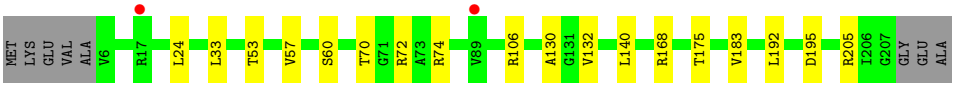
• Molecule 4: 50S ribosomal protein L3

• Molecule 4: 50S ribosomal protein L3

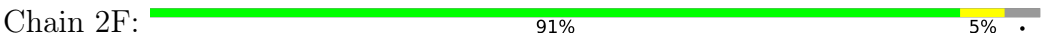


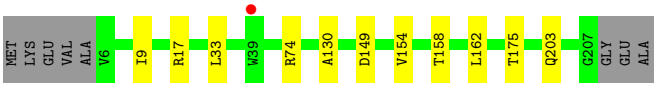
• Molecule 5: 50S ribosomal protein L4





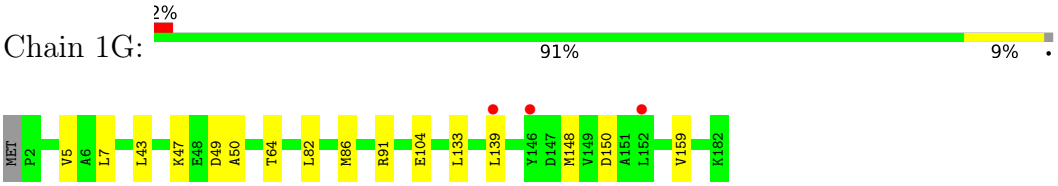
• Molecule 5: 50S ribosomal protein L4





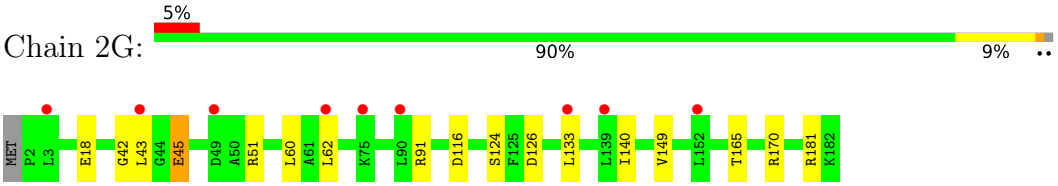
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



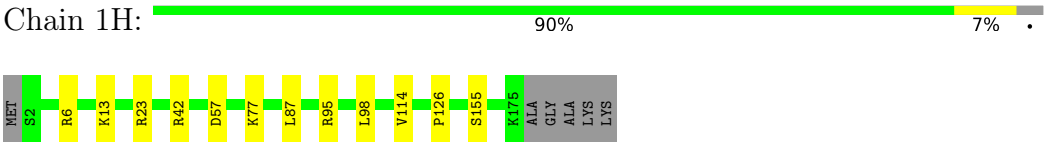
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



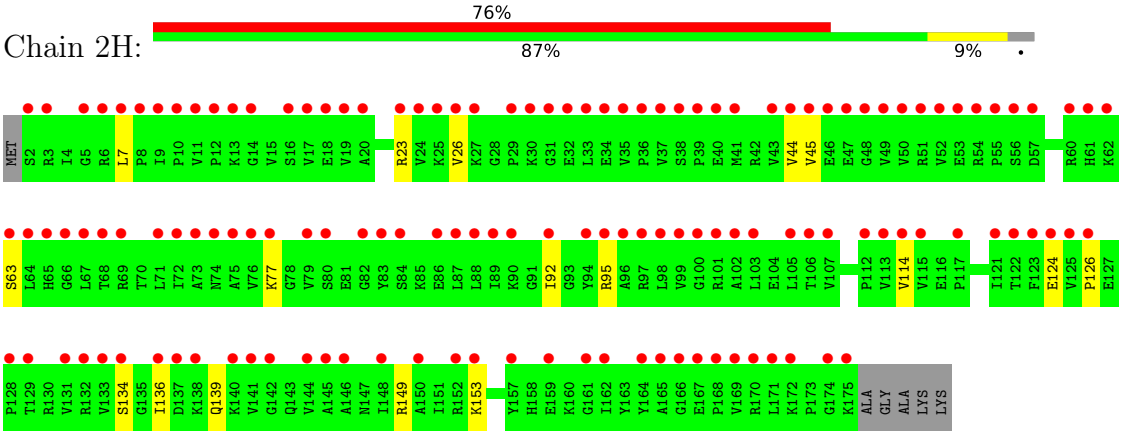
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



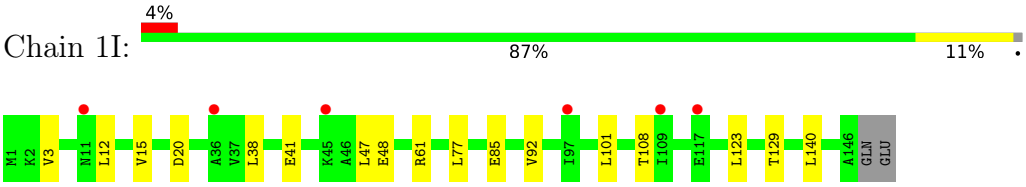
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



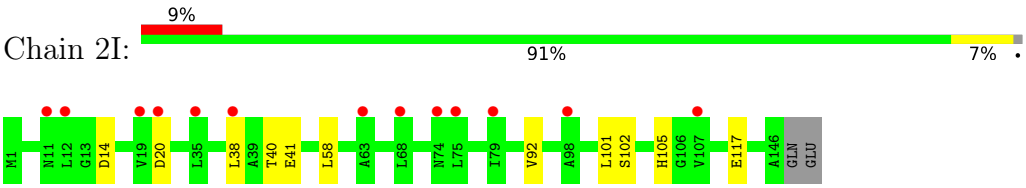
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



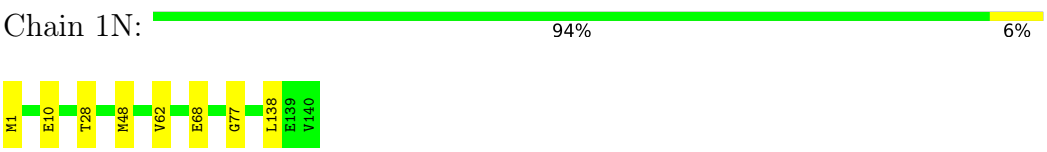
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



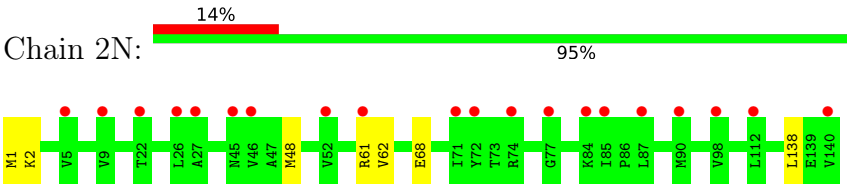
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



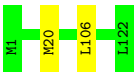
• Molecule 9: 50S ribosomal protein L13

Chain 2N:



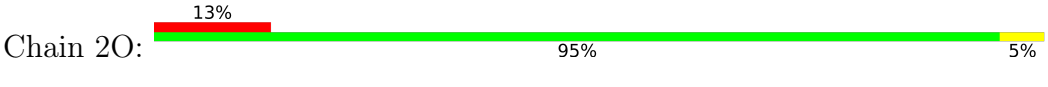
• Molecule 10: 50S ribosomal protein L14

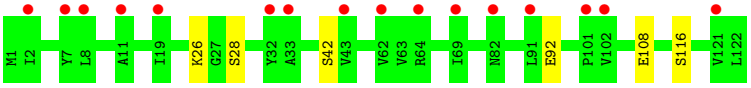
Chain 1O:



• Molecule 10: 50S ribosomal protein L14

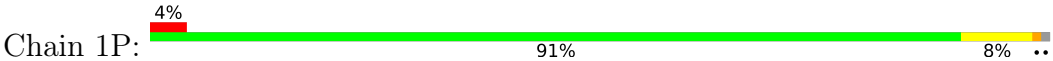
Chain 2O:

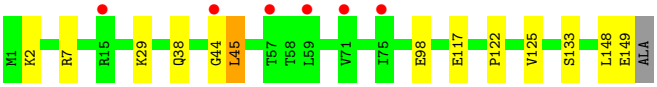




• Molecule 11: 50S ribosomal protein L15

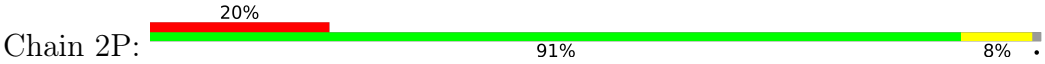
Chain 1P:

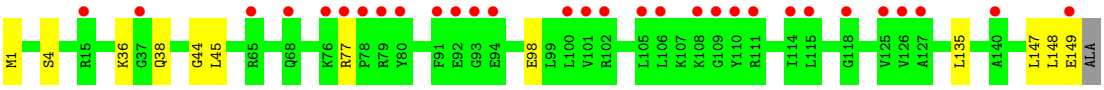




• Molecule 11: 50S ribosomal protein L15

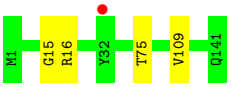
Chain 2P:





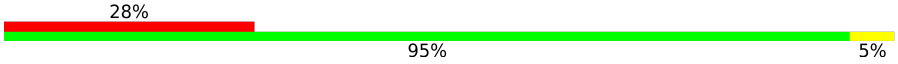
• Molecule 12: 50S ribosomal protein L16

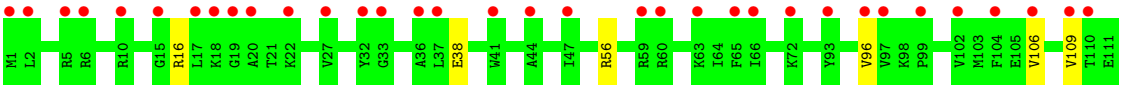
Chain 1Q:

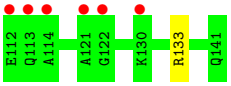


• Molecule 12: 50S ribosomal protein L16

Chain 2Q:

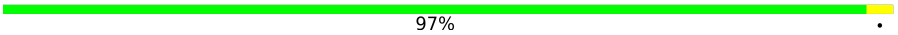






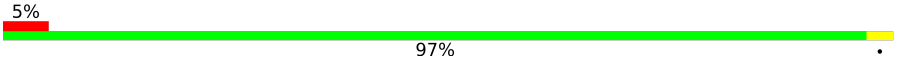
• Molecule 13: 50S ribosomal protein L17

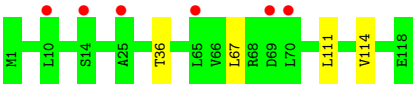
Chain 1R:



• Molecule 13: 50S ribosomal protein L17

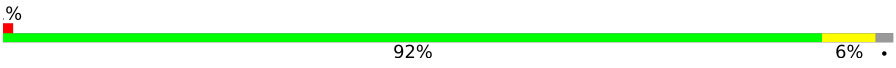
Chain 2R:





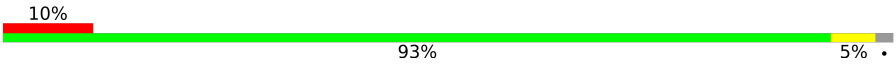
• Molecule 14: 50S ribosomal protein L18

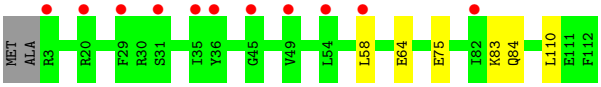
Chain 1S:



• Molecule 14: 50S ribosomal protein L18

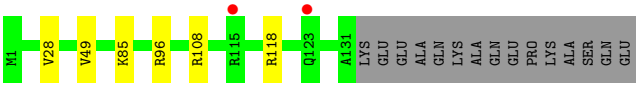
Chain 2S:





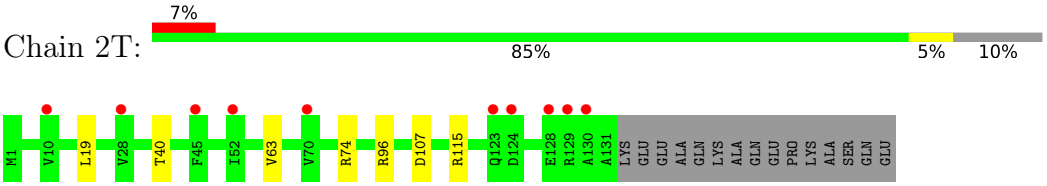
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



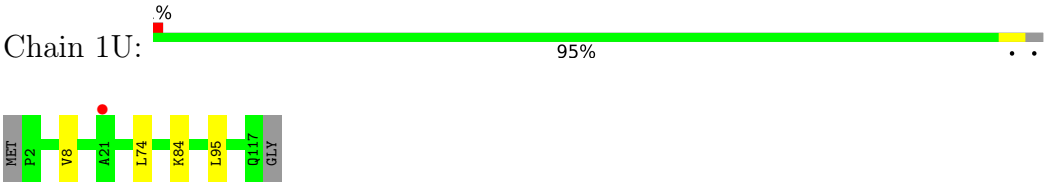
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



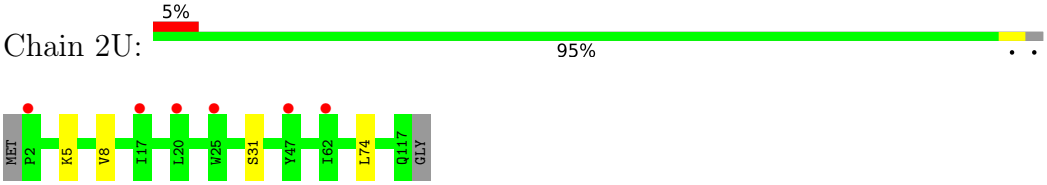
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



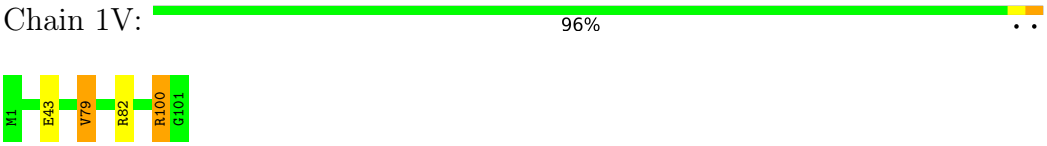
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



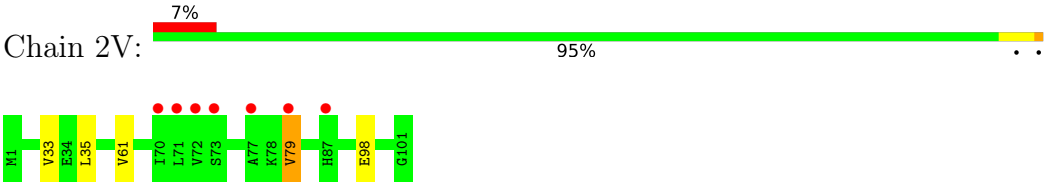
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



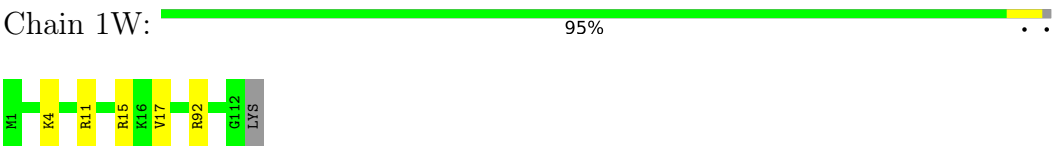
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



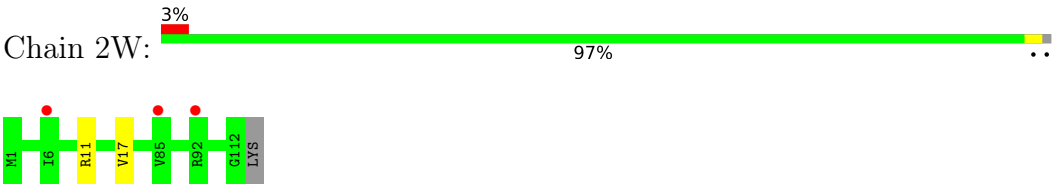
• Molecule 18: 50S ribosomal protein L22

Chain 1W:



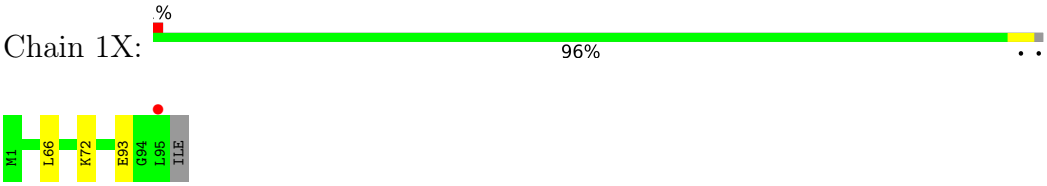
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



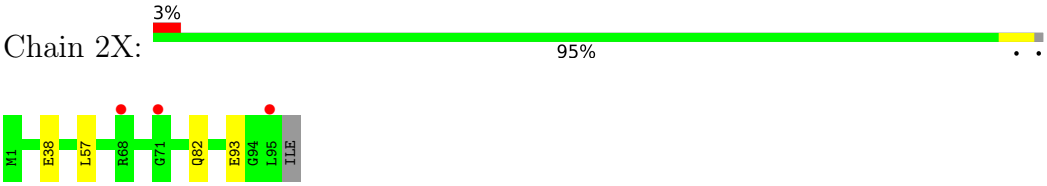
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



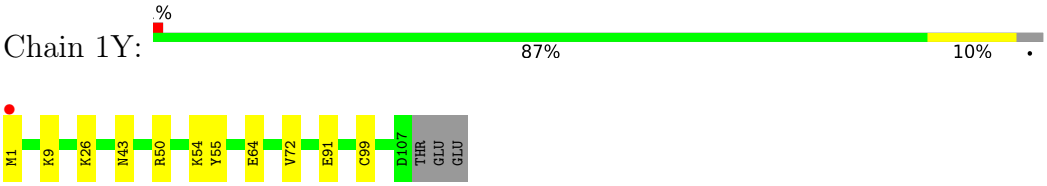
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



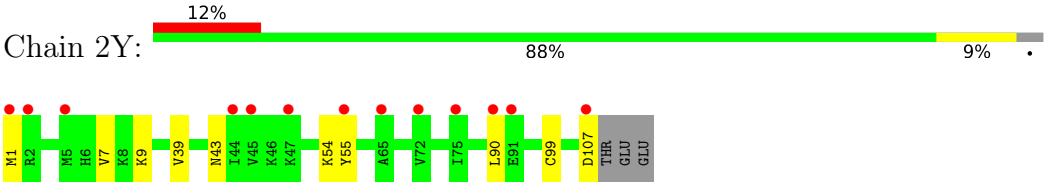
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



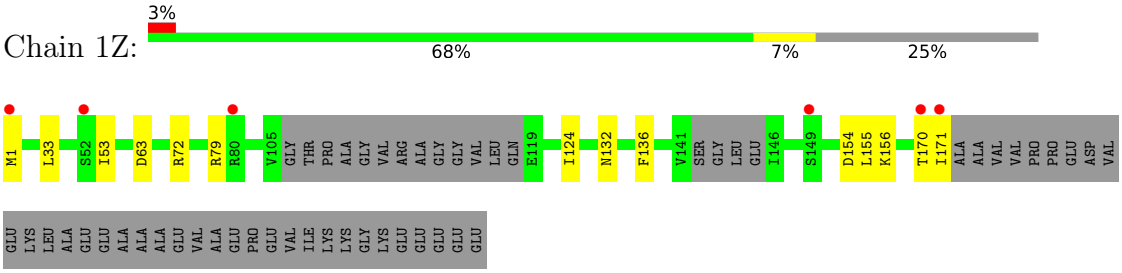
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



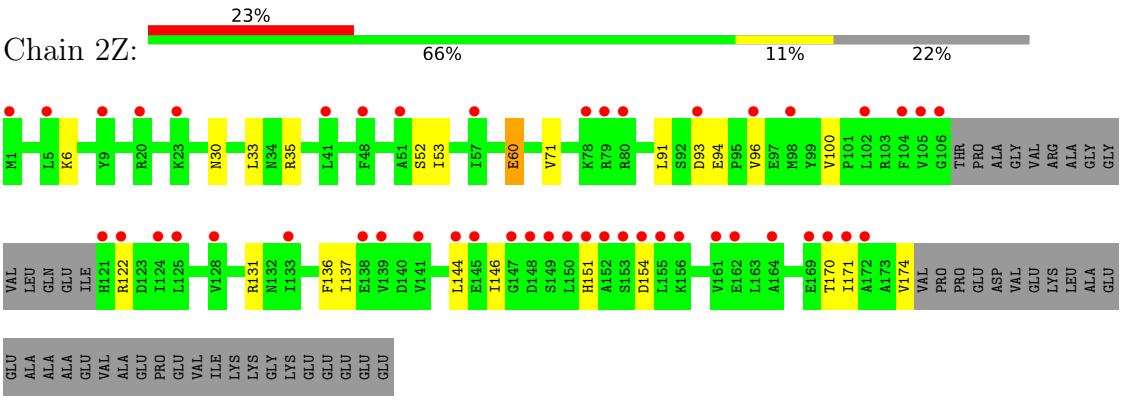
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



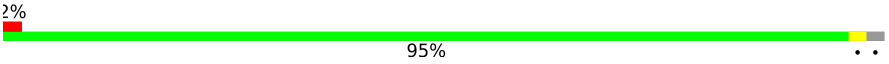
• Molecule 21: 50S ribosomal protein L25

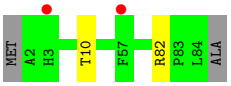
Chain 2Z:



• Molecule 22: 50S ribosomal protein L27

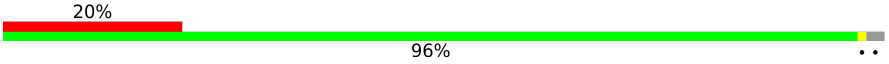
Chain 10:

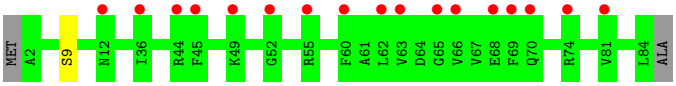




• Molecule 22: 50S ribosomal protein L27

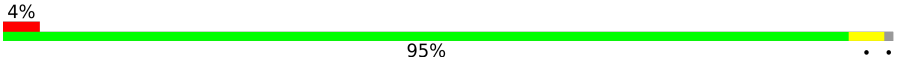
Chain 20:





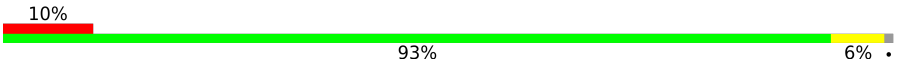
• Molecule 23: 50S ribosomal protein L28

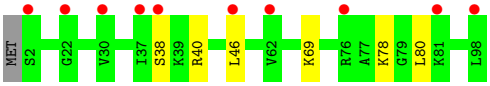
Chain 11:



• Molecule 23: 50S ribosomal protein L28

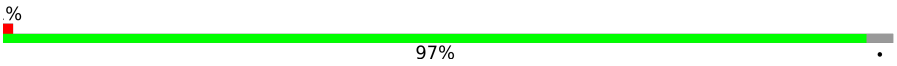
Chain 21:

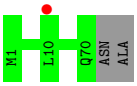




• Molecule 24: 50S ribosomal protein L29

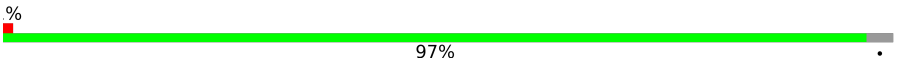
Chain 12:





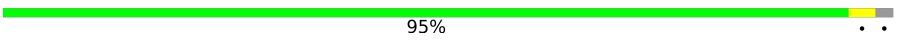
• Molecule 24: 50S ribosomal protein L29

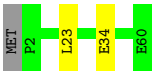
Chain 22:



• Molecule 25: 50S ribosomal protein L30

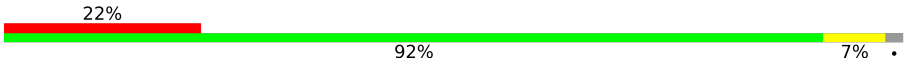
Chain 13:

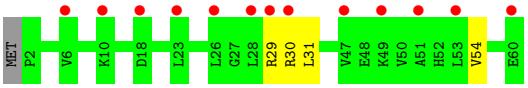




• Molecule 25: 50S ribosomal protein L30

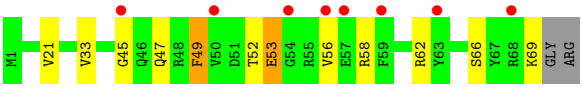
Chain 23:





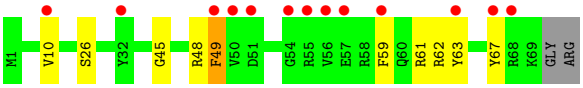
• Molecule 26: 50S ribosomal protein L31

Chain 14:



• Molecule 26: 50S ribosomal protein L31

Chain 24:

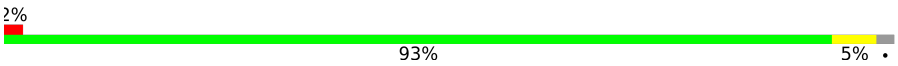


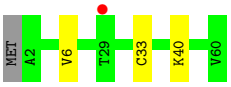
• Molecule 27: 50S ribosomal protein L32

Chain 15:

• Molecule 27: 50S ribosomal protein L32

Chain 25:



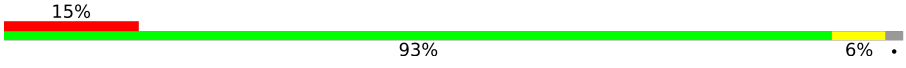


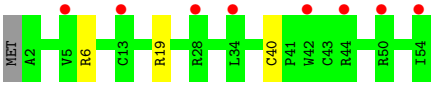
• Molecule 28: 50S ribosomal protein L33

Chain 16:

• Molecule 28: 50S ribosomal protein L33

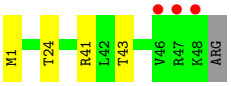
Chain 26:





• Molecule 29: 50S ribosomal protein L34

Chain 17:

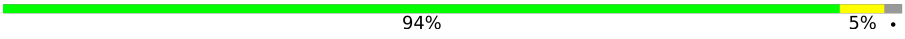


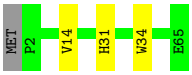
• Molecule 29: 50S ribosomal protein L34

Chain 27:

• Molecule 30: 50S ribosomal protein L35

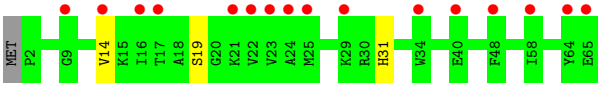
Chain 18:





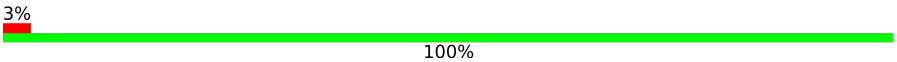
• Molecule 30: 50S ribosomal protein L35

Chain 28:



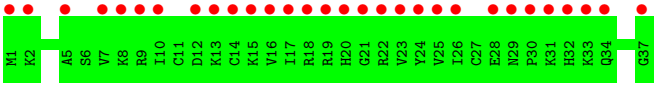
• Molecule 31: 50S ribosomal protein L36

Chain 19:



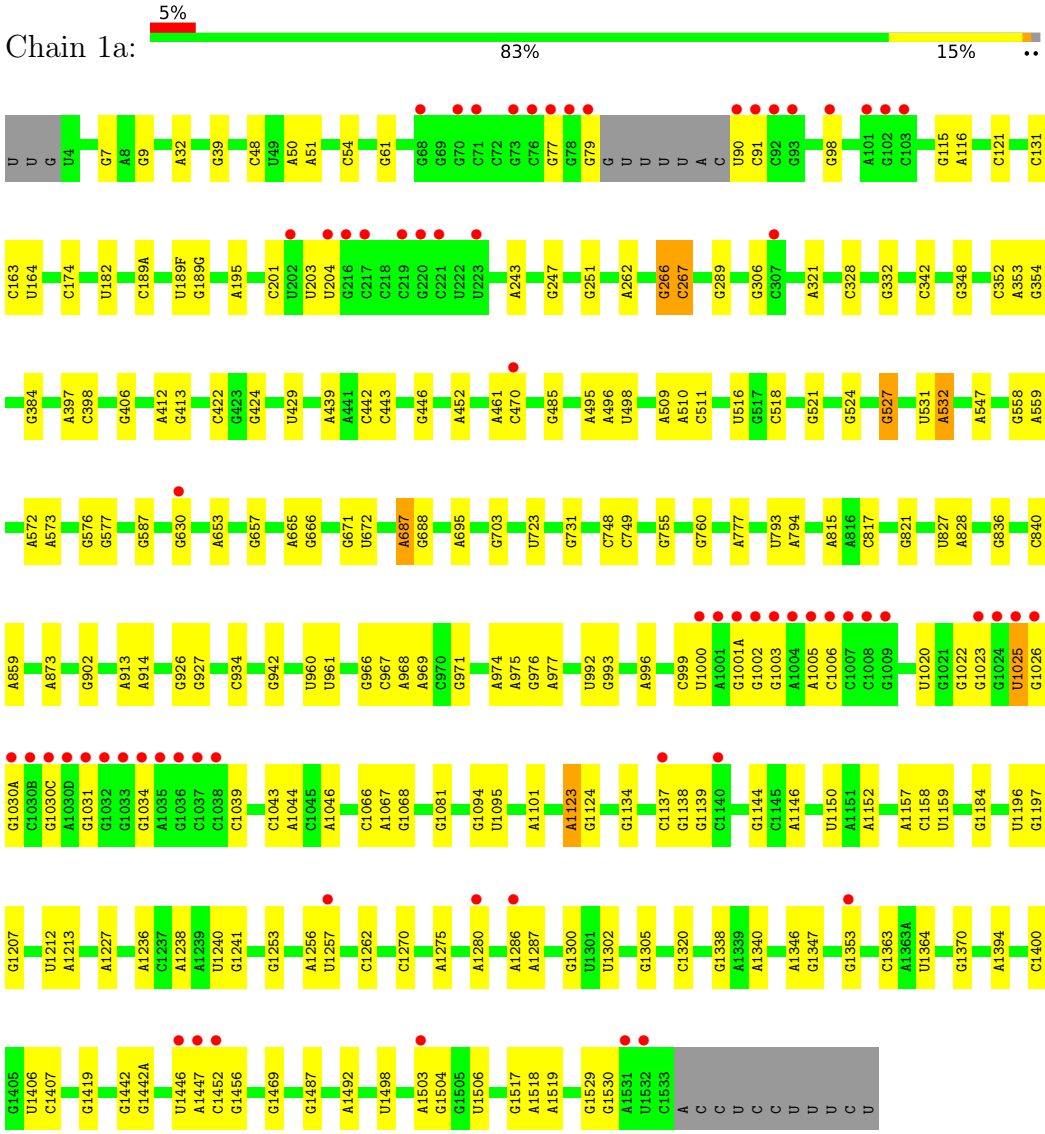
• Molecule 31: 50S ribosomal protein L36

Chain 29:



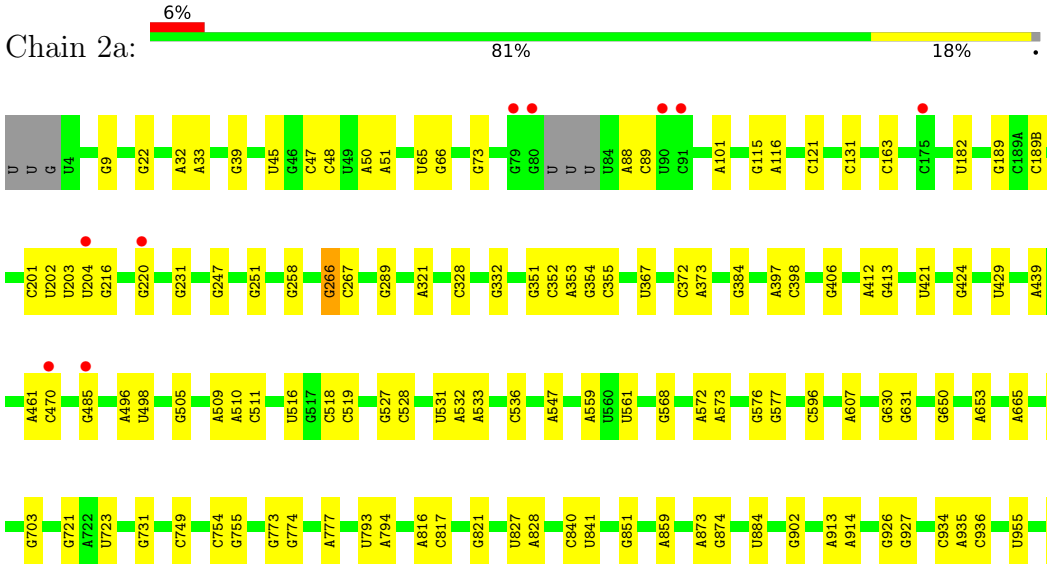
• Molecule 32: 16S Ribosomal RNA

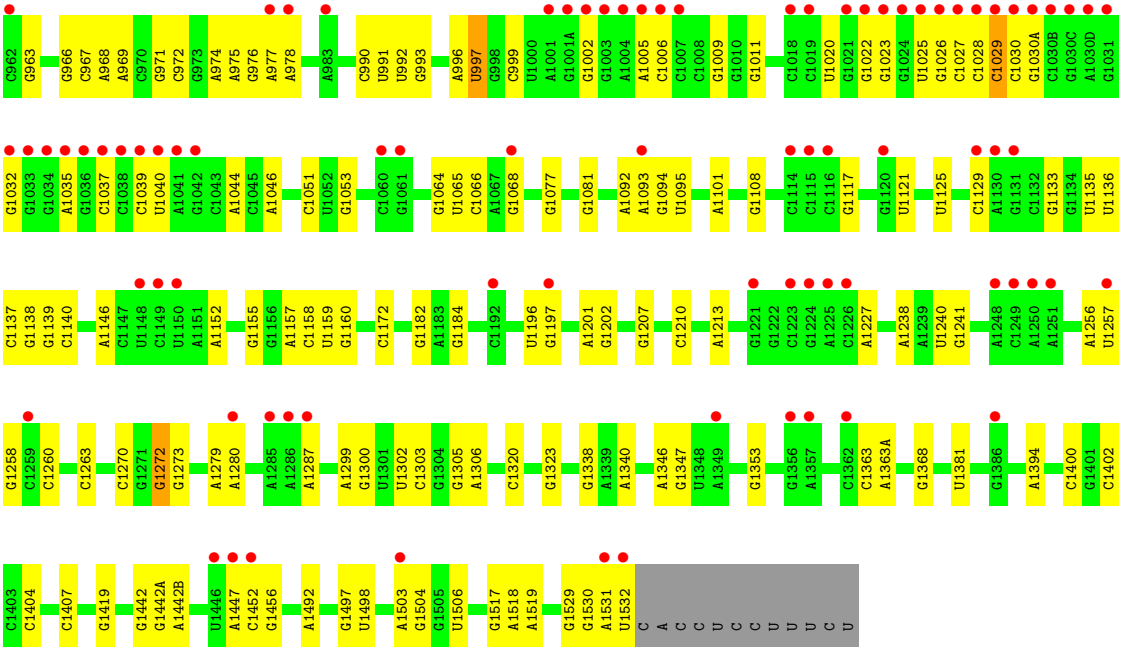
Chain 1a:



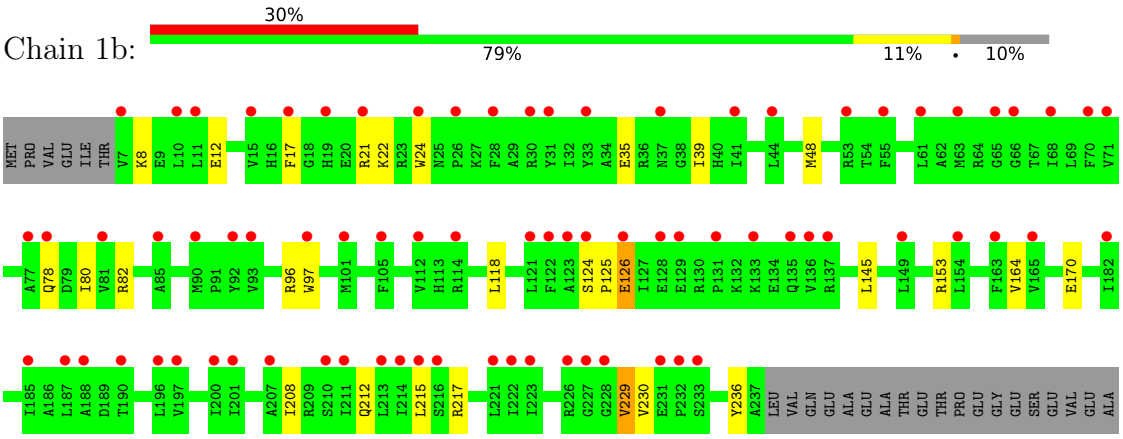
• Molecule 32: 16S Ribosomal RNA

Chain 2a:

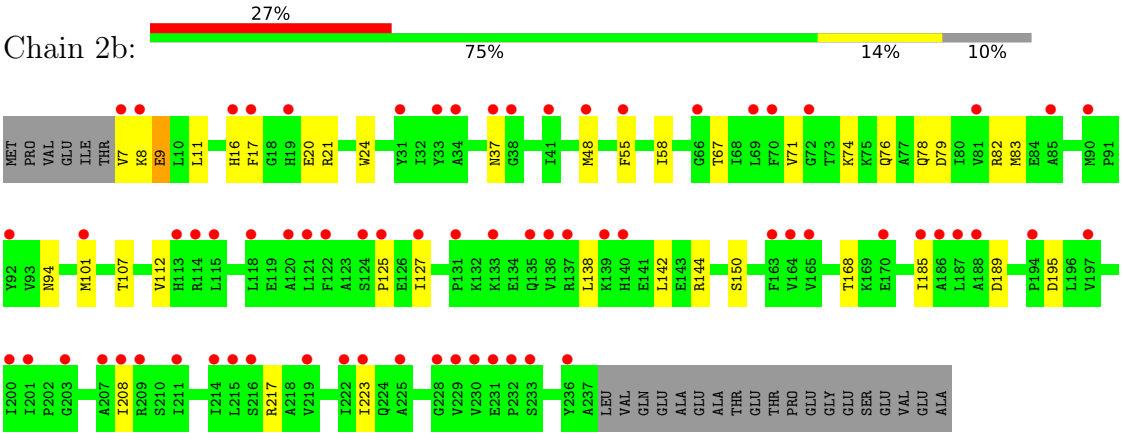




• Molecule 33: 30S ribosomal protein S2

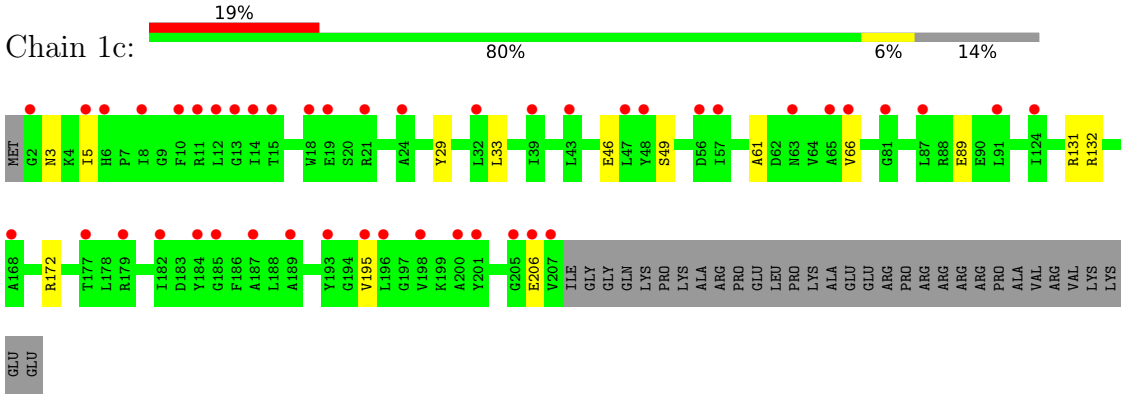


• Molecule 33: 30S ribosomal protein S2



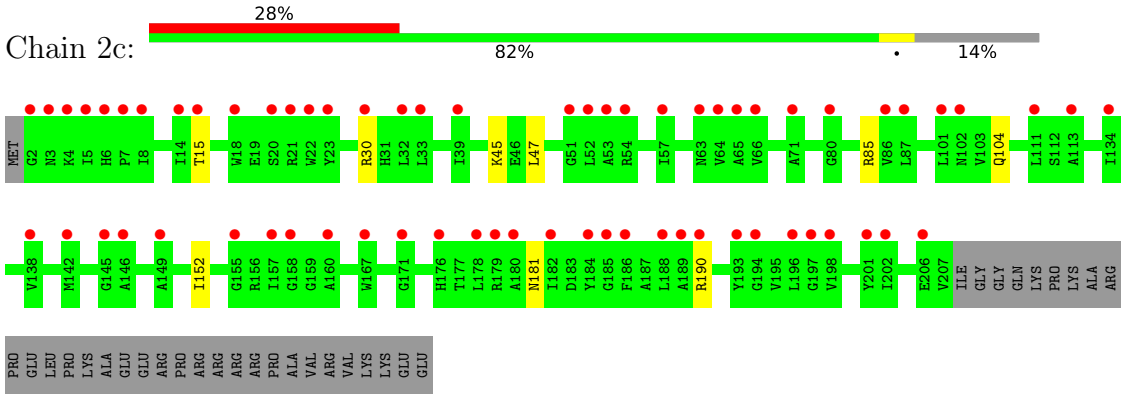
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



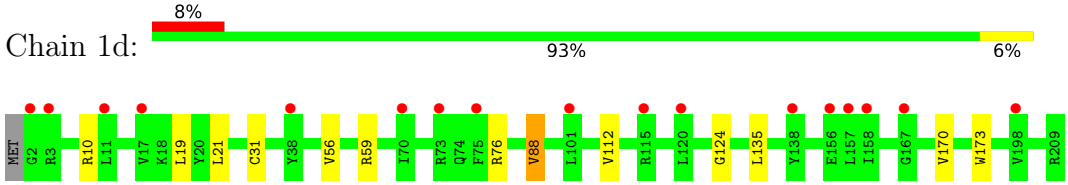
• Molecule 34: 30S ribosomal protein S3

Chain 2c:



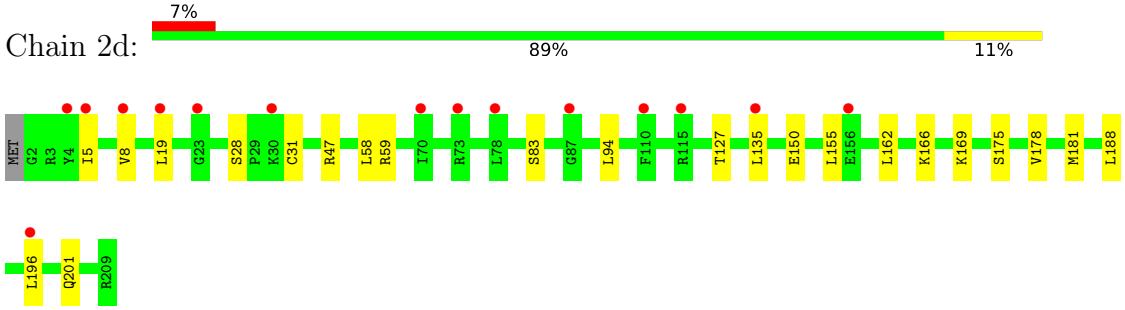
• Molecule 35: 30S ribosomal protein S4

Chain 1d:



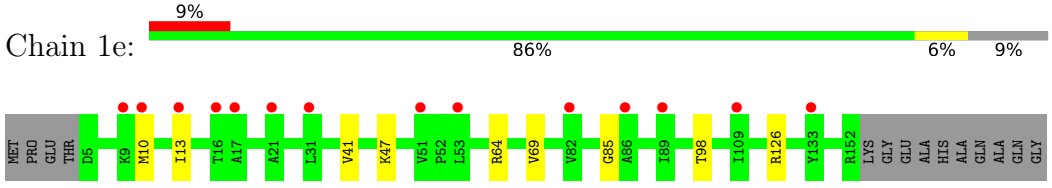
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



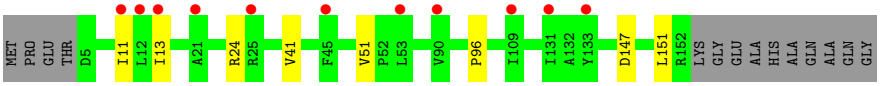
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



• Molecule 36: 30S ribosomal protein S5

Chain 2e:

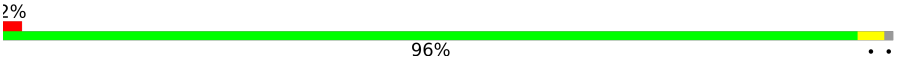


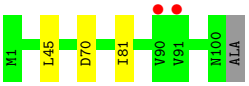
• Molecule 37: 30S ribosomal protein S6

Chain 1f:

• Molecule 37: 30S ribosomal protein S6

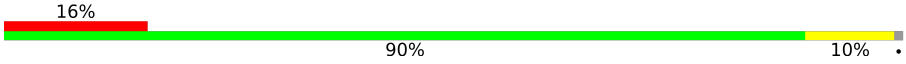
Chain 2f:

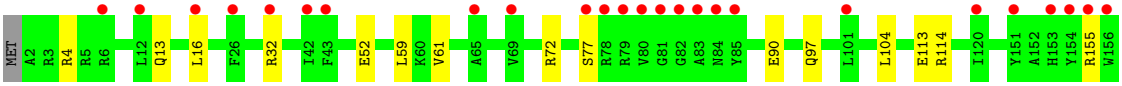




• Molecule 38: 30S ribosomal protein S7

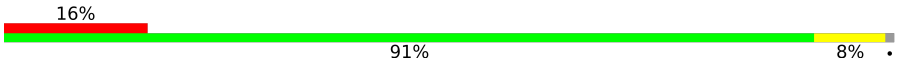
Chain 1g:

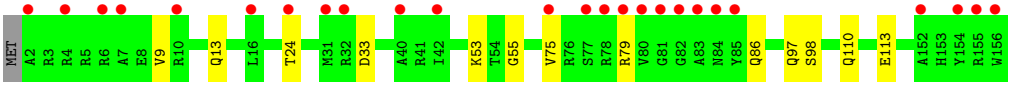




• Molecule 38: 30S ribosomal protein S7

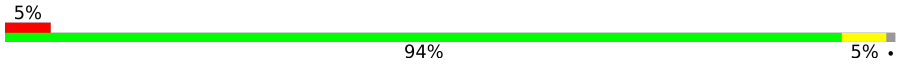
Chain 2g:

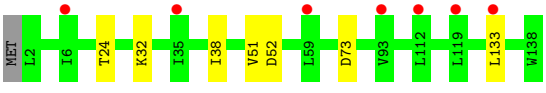




• Molecule 39: 30S ribosomal protein S8

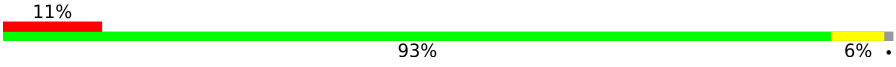
Chain 1h:





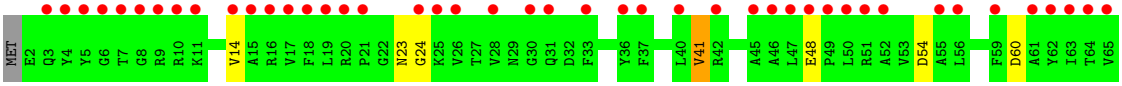
• Molecule 39: 30S ribosomal protein S8

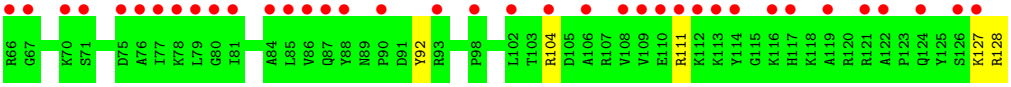
Chain 2h:



• Molecule 40: 30S ribosomal protein S9

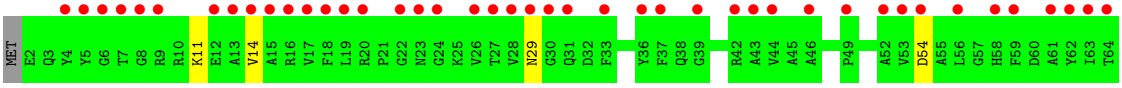
Chain 1i:

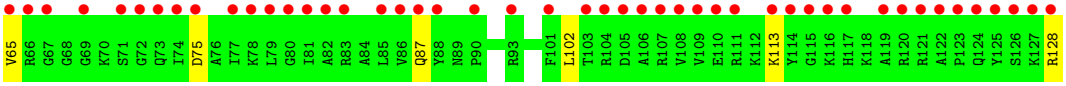




• Molecule 40: 30S ribosomal protein S9

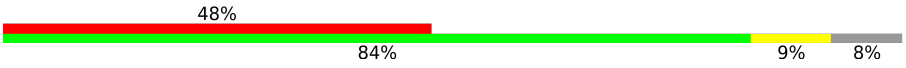
Chain 2i:

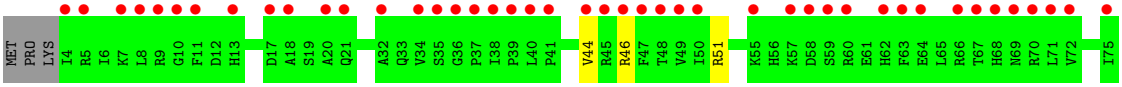


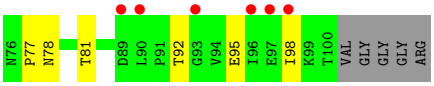


• Molecule 41: 30S ribosomal protein S10

Chain 1j:

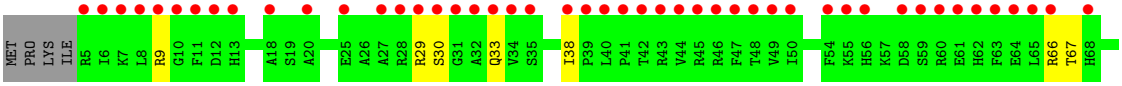


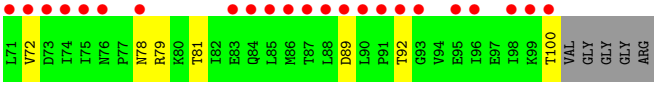




• Molecule 41: 30S ribosomal protein S10

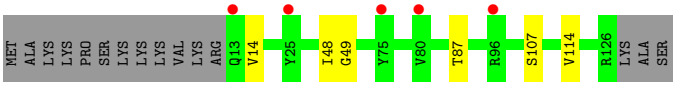
Chain 2j:





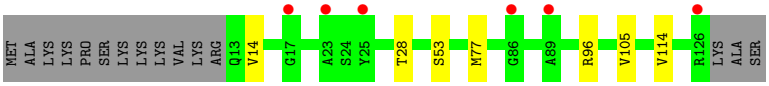
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



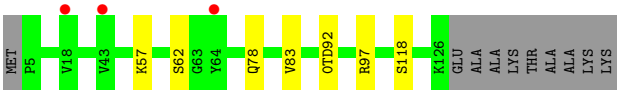
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



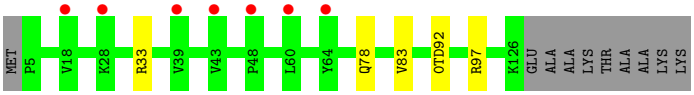
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



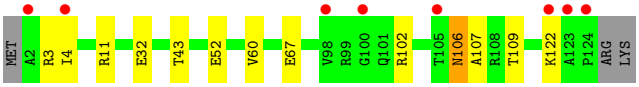
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



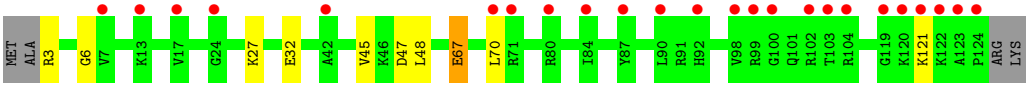
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



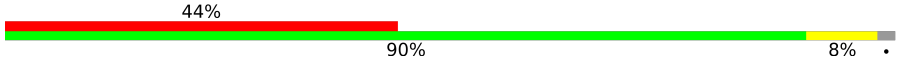
• Molecule 44: 30S ribosomal protein S13

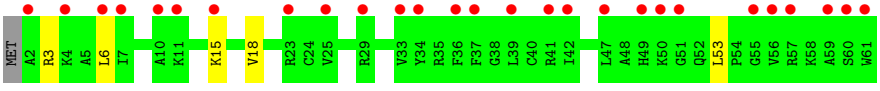
Chain 2m:



• Molecule 45: 30S ribosomal protein S14 type Z

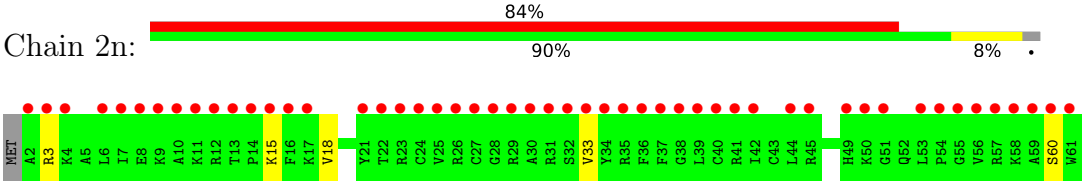
Chain 1n:





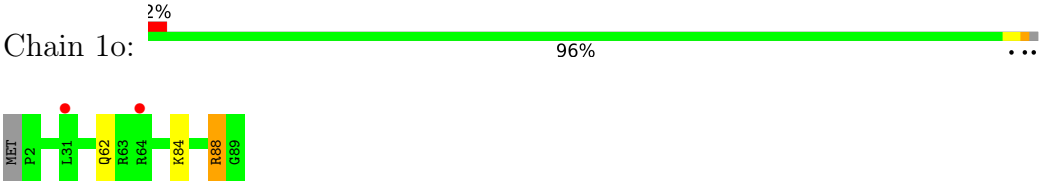
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



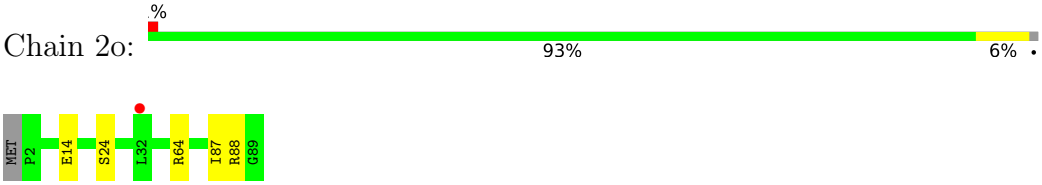
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



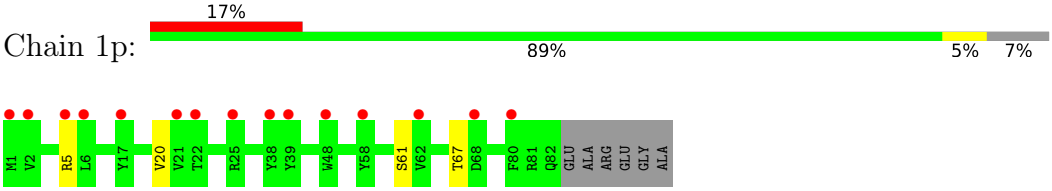
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



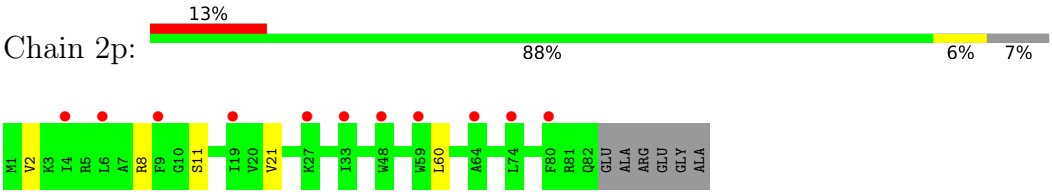
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



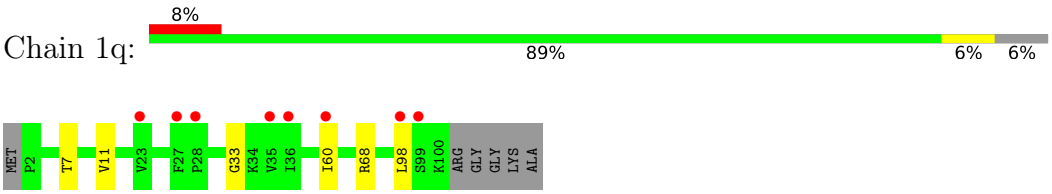
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



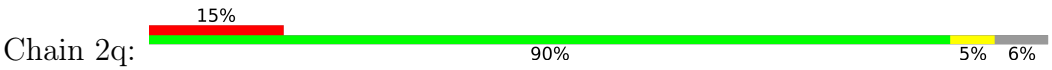
• Molecule 48: 30S ribosomal protein S17

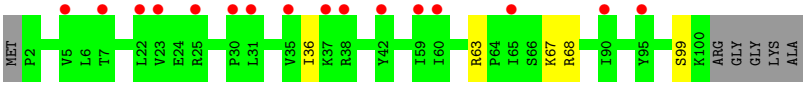
Chain 1q:



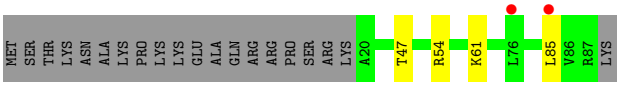
• Molecule 48: 30S ribosomal protein S17

Chain 2q:

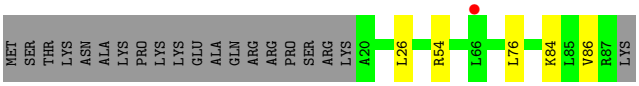




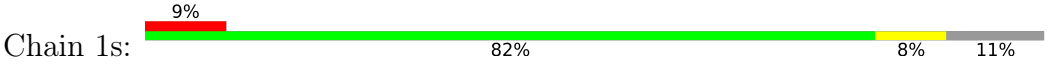
• Molecule 49: 30S ribosomal protein S18

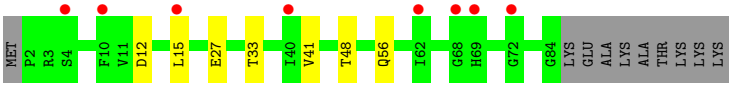


• Molecule 49: 30S ribosomal protein S18

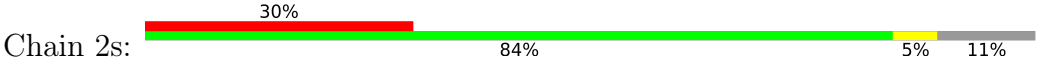


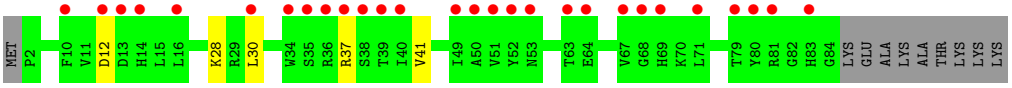
• Molecule 50: 30S ribosomal protein S19



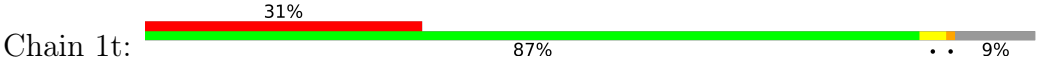


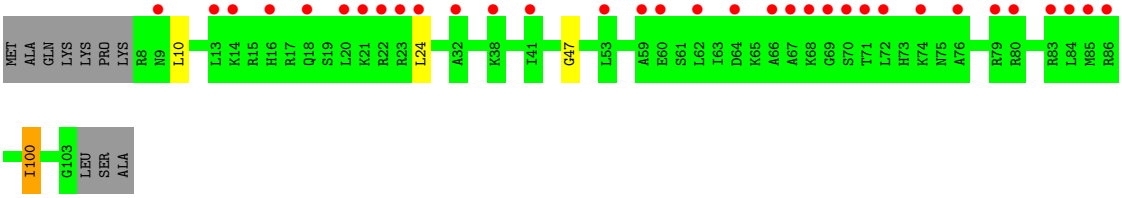
• Molecule 50: 30S ribosomal protein S19



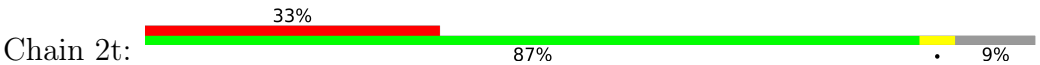


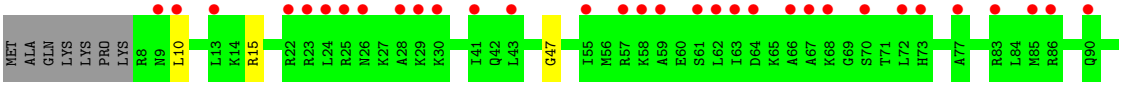
• Molecule 51: 30S ribosomal protein S20

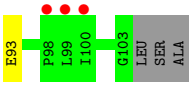




• Molecule 51: 30S ribosomal protein S20

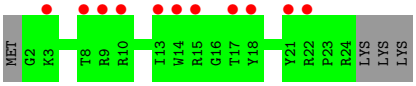






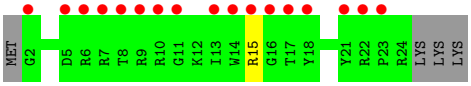
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



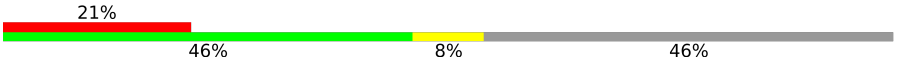
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



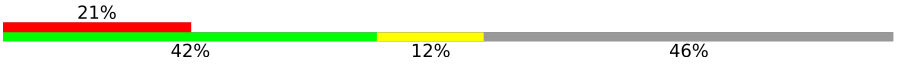
• Molecule 53: MF-mRNA

Chain 1v:



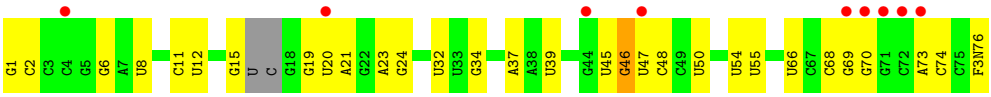
• Molecule 53: MF-mRNA

Chain 2v:



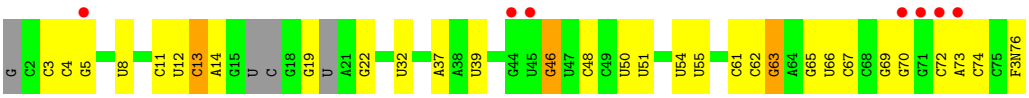
• Molecule 54: A-site Aminoacylated Phe-tRNAphe

Chain 1w:



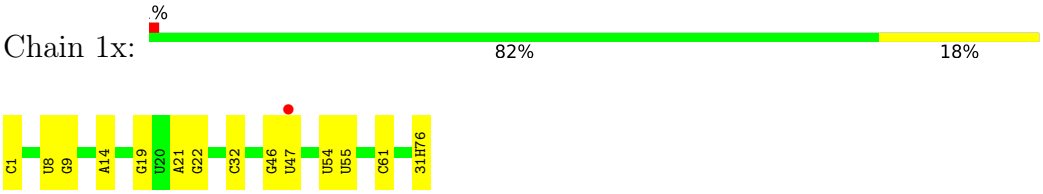
• Molecule 54: A-site Aminoacylated Phe-tRNAphe

Chain 2w:



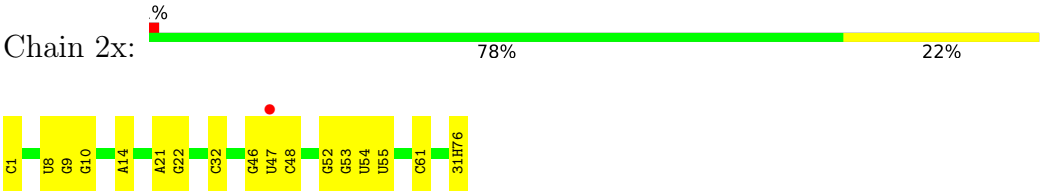
• Molecule 55: P-site Aminoacylated fMet-tRNAmet

Chain 1x:



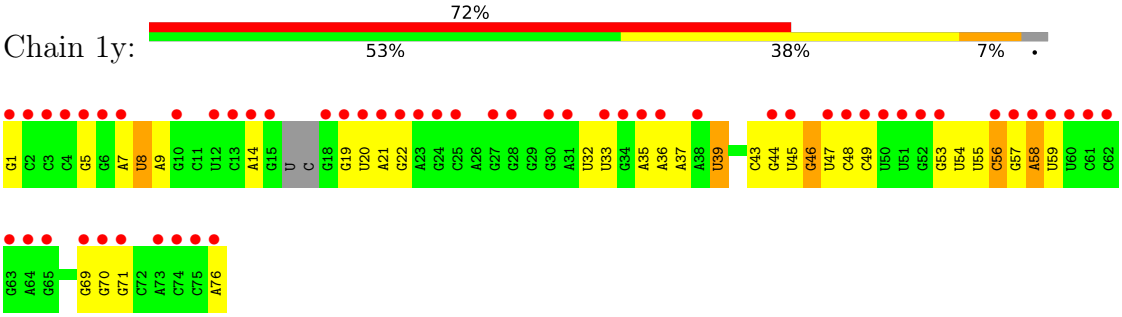
• Molecule 55: P-site Aminoacylated fMet-tRNAmet

Chain 2x:



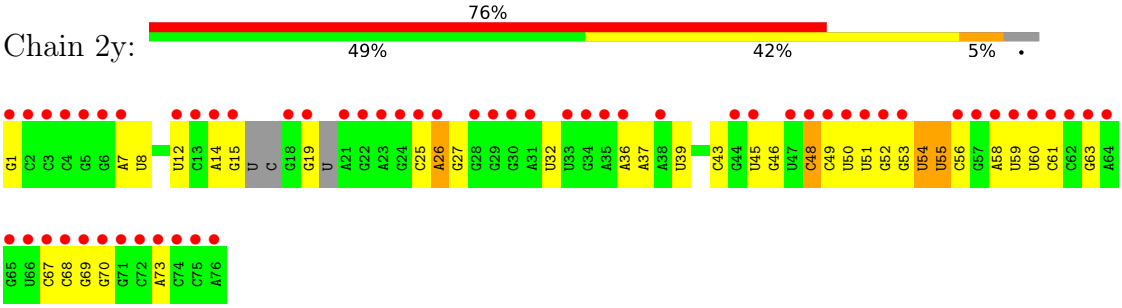
• Molecule 56: E-site Deacylated tRNAphe

Chain 1y:



• Molecule 56: E-site Deacylated tRNAphe

Chain 2y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.09Å 449.74Å 625.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.52 – 2.55 182.09 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.0 (153.52-2.55) 99.1 (182.09-2.55)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.213 , 0.252 0.213 , 0.252	Depositor DCC
R_{free} test set	94286 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	299618	wwPDB-VP
Average B, all atoms (Å^2)	61.0	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, 4SU, 5MC, 2MU, F3N, G7M, OMG, K, PSU, ZN, MIA, MA6, 5MU, 0TD, SF4, 31H, UR3, MG, 8AH, 2MG, OMC, 4OC

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	0.48	0/69010	0.94	64/107716 (0.1%)
1	2A	0.37	0/67294	0.84	28/105038 (0.0%)
2	1B	0.43	1/2882 (0.0%)	0.85	0/4494
2	2B	0.38	1/2879 (0.0%)	0.82	1/4487 (0.0%)
3	1D	0.35	0/2186	0.56	0/2944
3	2D	0.30	0/2186	0.51	0/2944
4	1E	0.33	0/1592	0.52	0/2149
4	2E	0.28	0/1592	0.49	0/2149
5	1F	0.32	0/1618	0.54	0/2191
5	2F	0.29	0/1614	0.50	0/2186
6	1G	0.30	0/1448	0.50	0/1957
6	2G	0.28	0/1453	0.46	0/1963
7	1H	0.32	0/1356	0.50	0/1834
7	2H	0.28	0/1356	0.48	0/1834
8	1I	0.28	0/1112	0.50	0/1514
8	2I	0.28	0/1079	0.48	0/1475
9	1N	0.33	0/1144	0.53	1/1543 (0.1%)
9	2N	0.28	0/1144	0.44	0/1543
10	1O	0.34	0/943	0.54	0/1269
10	2O	0.30	0/943	0.50	0/1269
11	1P	0.30	0/1152	0.58	0/1533
11	2P	0.30	0/1152	0.54	0/1533
12	1Q	0.35	0/1143	0.52	0/1527
12	2Q	0.29	0/1143	0.48	0/1527
13	1R	0.32	0/982	0.54	0/1312
13	2R	0.27	0/982	0.49	0/1312
14	1S	0.31	0/883	0.51	0/1176
14	2S	0.28	0/880	0.48	0/1172
15	1T	0.32	0/1105	0.50	0/1477
15	2T	0.28	0/1097	0.46	0/1468
16	1U	0.36	0/977	0.54	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.29	0/977	0.42	0/1301
17	1V	0.34	0/782	0.54	0/1049
17	2V	0.28	0/782	0.49	0/1049
18	1W	0.35	0/897	0.51	0/1205
18	2W	0.30	0/897	0.47	0/1205
19	1X	0.33	0/764	0.53	0/1025
19	2X	0.32	0/764	0.52	0/1025
20	1Y	0.34	0/819	0.54	0/1095
20	2Y	0.30	0/819	0.51	0/1095
21	1Z	0.30	0/1267	0.51	0/1717
21	2Z	0.31	0/1299	0.49	0/1763
22	10	0.32	0/662	0.55	0/881
22	20	0.28	0/662	0.47	0/881
23	11	0.32	0/762	0.51	0/1014
23	21	0.31	0/762	0.51	0/1014
24	12	0.37	0/590	0.47	0/781
24	22	0.28	0/590	0.39	0/781
25	13	0.33	0/474	0.52	0/635
25	23	0.26	0/469	0.45	0/630
26	14	0.32	0/565	0.54	0/761
26	24	0.32	0/545	0.52	0/737
27	15	0.33	0/469	0.54	0/635
27	25	0.29	0/469	0.48	0/635
28	16	0.34	0/460	0.53	0/613
28	26	0.29	0/456	0.48	0/608
29	17	0.35	0/426	0.56	0/561
29	27	0.30	0/426	0.52	0/561
30	18	0.30	0/525	0.51	0/691
30	28	0.29	0/525	0.48	0/691
31	19	0.35	0/310	0.54	0/407
31	29	0.27	0/310	0.49	0/407
32	1a	0.35	0/35795	0.85	19/55864 (0.0%)
32	2a	0.35	3/35886 (0.0%)	0.88	30/56005 (0.1%)
33	1b	0.30	0/1881	0.48	0/2542
33	2b	0.30	0/1860	0.46	0/2518
34	1c	0.29	0/1572	0.45	0/2126
34	2c	0.29	0/1566	0.47	0/2119
35	1d	0.28	0/1685	0.46	0/2262
35	2d	0.29	0/1704	0.46	0/2284
36	1e	0.29	0/1145	0.53	0/1543
36	2e	0.31	0/1149	0.50	0/1548
37	1f	0.28	0/823	0.48	0/1115
37	2f	0.28	0/829	0.48	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.28	0/1250	0.42	0/1679
38	2g	0.28	0/1254	0.43	0/1683
39	1h	0.29	0/1108	0.49	0/1494
39	2h	0.27	0/1108	0.46	0/1494
40	1i	0.29	0/1002	0.49	0/1346
40	2i	0.29	0/997	0.52	0/1343
41	1j	0.28	0/722	0.47	0/982
41	2j	0.28	0/727	0.49	0/988
42	1k	0.27	0/844	0.49	0/1145
42	2k	0.28	0/848	0.48	0/1149
43	1l	0.31	0/937	0.51	0/1260
43	2l	0.27	0/937	0.47	0/1260
44	1m	0.27	0/969	0.49	0/1302
44	2m	0.28	0/961	0.47	0/1291
45	1n	0.28	0/501	0.47	0/664
45	2n	0.30	0/501	0.48	0/664
46	1o	0.28	0/739	0.44	0/985
46	2o	0.26	0/739	0.41	0/985
47	1p	0.28	0/697	0.52	0/939
47	2p	0.28	0/693	0.47	0/935
48	1q	0.29	0/836	0.50	0/1117
48	2q	0.28	0/836	0.47	0/1117
49	1r	0.29	0/560	0.46	0/746
49	2r	0.28	0/560	0.47	0/746
50	1s	0.27	0/667	0.53	0/900
50	2s	0.28	0/661	0.54	1/893 (0.1%)
51	1t	0.27	0/730	0.42	0/965
51	2t	0.28	0/729	0.43	0/965
52	1u	0.27	0/203	0.47	0/266
52	2u	0.27	0/203	0.49	0/266
53	1v	0.46	0/310	0.95	0/480
53	2v	0.42	0/310	1.00	0/480
54	1w	0.51	1/1581 (0.1%)	1.00	0/2458
54	2w	0.44	0/1531	1.01	2/2379 (0.1%)
55	1x	0.58	4/1723 (0.2%)	1.12	19/2684 (0.7%)
55	2x	0.53	2/1723 (0.1%)	1.07	19/2684 (0.7%)
56	1y	0.56	1/1606 (0.1%)	1.05	4/2497 (0.2%)
56	2y	0.53	1/1583 (0.1%)	1.01	4/2459 (0.2%)
All	All	0.38	14/316632 (0.0%)	0.81	192/474029 (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
21	1Z	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1272	G	N1-C2	-10.71	1.29	1.37
32	2a	1272	G	C6-N1	-10.61	1.32	1.39
55	1x	1	C	OP3-P	-10.49	1.48	1.61
2	1B	1	U	OP3-P	-10.28	1.48	1.61
54	1w	1	G	OP3-P	-10.14	1.49	1.61
55	2x	1	C	OP3-P	-10.11	1.49	1.61
2	2B	1	U	OP3-P	-10.09	1.49	1.61
56	1y	1	G	OP3-P	-10.01	1.49	1.61
56	2y	1	G	OP3-P	-9.96	1.49	1.61
32	2a	1263	C	N3-C4	-6.84	1.29	1.33
55	1x	14	A	N7-C5	-6.16	1.35	1.39
55	2x	22	G	N7-C5	5.54	1.42	1.39
55	1x	14	A	C8-N7	-5.40	1.27	1.31
55	1x	22	G	N7-C5	5.04	1.42	1.39

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1263	C	N1-C2-O2	29.02	136.31	118.90
32	2a	1272	G	N3-C2-N2	24.63	137.14	119.90
32	2a	1272	G	C5-C6-O6	23.65	142.79	128.60
32	2a	1272	G	N1-C2-N2	-21.37	96.97	116.20
32	2a	1263	C	N3-C2-O2	-17.16	109.89	121.90
32	2a	1263	C	C2-N3-C4	16.71	128.26	119.90
32	2a	1272	G	N1-C6-O6	-15.29	110.73	119.90
32	2a	1272	G	C6-N1-C2	13.12	132.97	125.10
55	2x	46	G	C6-N1-C2	-11.43	118.24	125.10
1	1A	1086	A	N1-C6-N6	-11.30	111.82	118.60
55	1x	14	A	C4-C5-C6	11.10	122.55	117.00
55	1x	14	A	C5-N7-C8	10.95	109.37	103.90
32	2a	1263	C	C5-C4-N4	10.91	127.83	120.20
55	1x	46	G	C6-N1-C2	-10.74	118.66	125.10
1	1A	1063	G	C5-C6-O6	10.46	134.87	128.60
32	2a	1263	C	C5-C6-N1	10.36	126.18	121.00
32	2a	1263	C	N3-C4-N4	-10.36	110.75	118.00
32	2a	1272	G	C5-C6-N1	-10.15	106.42	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	14	A	C5-N7-C8	9.88	108.84	103.90
1	1A	512	G	O4'-C1'-N9	9.55	115.84	108.20
32	2a	1272	G	C2-N3-C4	-9.55	107.13	111.90
1	1A	1075	C	N1-C2-O2	9.54	124.63	118.90
2	2B	80	U	O4'-C1'-N1	9.23	115.59	108.20
32	2a	1263	C	C2-N1-C1'	8.96	128.65	118.80
55	2x	14	A	C4-C5-C6	8.90	121.45	117.00
1	1A	576	U	O5'-P-OP1	-8.65	97.92	105.70
32	2a	1263	C	C4-C5-C6	-8.63	113.09	117.40
1	1A	1075	C	C2-N3-C4	8.60	124.20	119.90
1	1A	975	C	N1-C2-O2	-8.54	113.78	118.90
55	1x	14	A	C5-C6-N1	-8.38	113.51	117.70
55	1x	46	G	N3-C2-N2	-7.93	114.35	119.90
32	2a	1263	C	C6-N1-C2	-7.86	117.16	120.30
1	1A	1782	C	O5'-P-OP1	-7.83	98.65	105.70
55	1x	22	G	C5-N7-C8	-7.77	100.41	104.30
55	2x	22	G	C5-N7-C8	-7.74	100.43	104.30
32	2a	1263	C	N1-C2-N3	-7.73	113.79	119.20
1	1A	570	G	C5-C6-N1	7.70	115.35	111.50
32	1a	1025	U	N1-C2-O2	7.66	128.16	122.80
1	1A	2682	U	O5'-P-OP2	-7.56	98.89	105.70
1	1A	1063	G	C6-N1-C2	7.55	129.63	125.10
1	1A	1082	U	N3-C4-O4	-7.43	114.20	119.40
32	2a	1272	G	C4-N9-C1'	7.38	136.10	126.50
32	2a	1272	G	C8-N9-C1'	-7.31	117.50	127.00
55	2x	22	G	N1-C6-O6	-7.31	115.52	119.90
1	1A	2023	G	O5'-P-OP1	-7.29	99.14	105.70
1	1A	975	C	C2-N1-C1'	-7.29	110.79	118.80
1	1A	1063	G	N1-C6-O6	-7.11	115.63	119.90
1	1A	570	G	C5-C6-O6	-7.05	124.37	128.60
1	1A	1075	C	C5-C4-N4	7.04	125.13	120.20
1	1A	1352	U	O5'-P-OP1	-7.02	99.39	105.70
32	1a	90	U	C2-N1-C1'	6.88	125.96	117.70
55	2x	46	G	C5-C6-N1	6.85	114.92	111.50
1	2A	897	C	C2-N1-C1'	6.75	126.23	118.80
1	2A	512	G	O4'-C1'-N9	6.71	113.57	108.20
1	1A	2689	U	P-O3'-C3'	6.66	127.69	119.70
55	1x	46	G	C5-C6-N1	6.62	114.81	111.50
1	2A	141	A	N7-C8-N9	6.54	117.07	113.80
55	2x	22	G	C4-C5-C6	-6.50	114.90	118.80
1	1A	1992	G	P-O3'-C3'	6.46	127.45	119.70
32	2a	1029	C	N1-C2-O2	6.46	122.77	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1993	U	O5'-P-OP1	-6.43	99.91	105.70
1	1A	1063	G	N3-C2-N2	6.42	124.39	119.90
55	2x	14	A	C5-C6-N1	-6.41	114.50	117.70
55	2x	14	A	C4-C5-N7	-6.39	107.50	110.70
55	2x	22	G	C5-C6-N1	6.37	114.68	111.50
32	2a	754	C	C2-N1-C1'	6.34	125.78	118.80
55	1x	22	G	C5-C6-N1	6.31	114.66	111.50
55	1x	22	G	C4-C5-C6	-6.26	115.05	118.80
32	1a	266	G	P-O3'-C3'	6.17	127.10	119.70
56	2y	26	A	N1-C6-N6	6.16	122.29	118.60
1	2A	2318	G	O4'-C1'-N9	6.12	113.10	108.20
1	2A	1416	G	O4'-C1'-N9	6.11	113.08	108.20
1	1A	2825	C	N3-C4-N4	-6.05	113.77	118.00
55	1x	22	G	N1-C6-O6	-6.02	116.29	119.90
1	2A	2499	C	O5'-P-OP2	-6.02	100.28	105.70
55	2x	46	G	N3-C2-N2	-6.01	115.69	119.90
32	1a	1158	C	C2-N1-C1'	5.99	125.38	118.80
32	1a	913	A	P-O3'-C3'	5.96	126.86	119.70
32	2a	1158	C	C2-N1-C1'	5.96	125.36	118.80
1	1A	1080	C	N1-C2-O2	5.96	122.48	118.90
1	1A	2248	C	O5'-P-OP2	-5.96	100.34	105.70
56	2y	48	C	N1-C2-O2	-5.93	115.34	118.90
55	2x	46	G	N1-C2-N3	5.91	127.45	123.90
32	1a	1067	A	P-O3'-C3'	5.90	126.78	119.70
32	1a	532	A	O4'-C1'-N9	5.90	112.92	108.20
32	1a	1123	A	C5-C6-N6	5.88	128.40	123.70
1	1A	1074	G	N3-C4-N9	5.83	129.50	126.00
1	1A	800	A	O5'-P-OP1	-5.80	100.48	105.70
1	1A	1082	U	N3-C4-C5	5.80	118.08	114.60
1	2A	885	C	C5-C6-N1	5.79	123.89	121.00
55	1x	14	A	C8-N9-C1'	-5.77	117.31	127.70
55	1x	46	G	N9-C4-C5	5.75	107.70	105.40
55	1x	14	A	C4-C5-N7	-5.75	107.83	110.70
55	2x	22	G	N7-C8-N9	5.72	115.96	113.10
1	2A	2689	U	N3-C2-O2	-5.71	118.20	122.20
1	1A	668	G	OP2-P-O3'	5.71	117.75	105.20
1	1A	1174	A	OP1-P-O3'	5.70	117.75	105.20
1	2A	945	A	N1-C6-N6	5.68	122.01	118.60
50	2s	30	LEU	CA-CB-CG	5.67	128.34	115.30
1	2A	141	A	C8-N9-C4	-5.65	103.54	105.80
32	1a	267	C	O5'-P-OP1	-5.64	100.62	105.70
1	1A	1074	G	C5-C6-O6	-5.64	125.22	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	22	G	N7-C8-N9	5.63	115.92	113.10
1	1A	1086	A	C5-C6-N6	5.63	128.21	123.70
1	1A	1074	G	N9-C4-C5	-5.63	103.15	105.40
56	2y	48	C	C2-N1-C1'	-5.62	112.61	118.80
32	1a	90	U	N1-C2-O2	5.61	126.73	122.80
55	1x	14	A	C4-N9-C1'	5.61	136.39	126.30
1	2A	383	U	O4'-C1'-N1	5.60	112.68	108.20
55	1x	22	G	C8-N9-C1'	5.60	134.28	127.00
1	1A	975	C	C6-N1-C1'	5.59	127.51	120.80
1	2A	1698	A	O4'-C1'-N9	5.59	112.67	108.20
32	2a	1263	C	C6-N1-C1'	-5.58	114.11	120.80
9	1N	77	GLY	C-N-CA	5.58	135.64	121.70
1	2A	897	C	C6-N1-C1'	-5.57	114.12	120.80
1	1A	2629	A	P-O3'-C3'	5.55	126.36	119.70
55	2x	46	G	N3-C4-C5	-5.54	125.83	128.60
1	1A	570	G	C4-C5-N7	5.51	113.00	110.80
1	1A	2319	G	N3-C4-N9	-5.50	122.70	126.00
54	2w	63	G	C5-C6-O6	5.49	131.89	128.60
1	1A	1176	G	OP1-P-O3'	5.48	117.26	105.20
1	1A	1082	U	C2-N3-C4	-5.44	123.73	127.00
55	2x	46	G	C5-C6-O6	-5.43	125.34	128.60
1	1A	975	C	C2-N3-C4	-5.43	117.19	119.90
1	1A	2610	C	N3-C2-O2	-5.42	118.10	121.90
1	1A	1174	A	P-O3'-C3'	5.41	126.20	119.70
1	2A	528	A	P-O3'-C3'	5.40	126.18	119.70
54	2w	13	C	P-O3'-C3'	5.40	126.18	119.70
1	1A	1075	C	N3-C2-O2	-5.39	118.12	121.90
1	1A	1074	G	C4-C5-N7	5.38	112.95	110.80
1	1A	1614	A	O5'-P-OP1	-5.38	100.85	105.70
1	1A	2685	G	C5-C6-N1	5.38	114.19	111.50
1	1A	2689	U	N3-C2-O2	-5.37	118.44	122.20
32	2a	955	U	C5-C4-O4	5.37	129.12	125.90
32	2a	913	A	P-O3'-C3'	5.37	126.14	119.70
1	2A	2136	C	N1-C2-O2	5.36	122.12	118.90
1	1A	1776	G	O5'-P-OP2	-5.36	100.88	105.70
1	1A	2500	U	O4'-C1'-N1	5.34	112.47	108.20
1	1A	195	A	P-O3'-C3'	5.33	126.09	119.70
55	2x	46	G	N9-C4-C5	5.32	107.53	105.40
1	2A	271(M)	G	P-O3'-C3'	5.32	126.08	119.70
1	1A	329	G	O5'-P-OP2	-5.29	100.94	105.70
32	2a	115	G	P-O3'-C3'	5.29	126.05	119.70
1	2A	885	C	C6-N1-C2	-5.28	118.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	14	A	C4-N9-C1'	5.28	135.81	126.30
1	1A	2319	G	N3-C4-C5	5.26	131.23	128.60
32	2a	1158	C	C6-N1-C2	-5.26	118.20	120.30
32	2a	266	G	P-O3'-C3'	5.26	126.01	119.70
55	1x	46	G	C5-C6-O6	-5.24	125.45	128.60
55	2x	14	A	C8-N9-C1'	-5.24	118.27	127.70
1	1A	570	G	N3-C4-N9	5.24	129.14	126.00
1	1A	1080	C	C2-N3-C4	5.23	122.51	119.90
1	1A	1314	C	C2-N1-C1'	5.22	124.54	118.80
1	1A	975	C	C5-C6-N1	-5.21	118.39	121.00
1	2A	847	U	C2-N1-C1'	5.21	123.95	117.70
1	2A	271(M)	G	OP1-P-O3'	5.19	116.62	105.20
1	2A	2318	G	N7-C8-N9	5.18	115.69	113.10
1	2A	1992	G	P-O3'-C3'	5.17	125.90	119.70
56	2y	26	A	C5-C6-N6	-5.16	119.57	123.70
1	1A	1308	A	O5'-P-OP2	-5.15	101.07	105.70
56	1y	58	A	OP1-P-O3'	5.14	116.51	105.20
1	2A	1653	G	P-O3'-C3'	5.14	125.87	119.70
32	1a	115	G	P-O3'-C3'	5.13	125.86	119.70
56	1y	33	U	N3-C2-O2	-5.13	118.61	122.20
55	1x	14	A	N1-C2-N3	5.13	131.86	129.30
32	1a	90	U	N3-C2-O2	-5.12	118.62	122.20
1	1A	1064	C	C5-C4-N4	-5.11	116.62	120.20
1	1A	2073	C	OP2-P-O3'	5.11	116.43	105.20
32	1a	1150	U	C5-C4-O4	5.11	128.96	125.90
32	2a	997	U	C5-C4-O4	5.10	128.96	125.90
1	2A	1313	U	C2-N1-C1'	5.10	123.82	117.70
32	2a	65	U	P-O3'-C3'	5.09	125.81	119.70
1	1A	674	G	C5-C6-O6	-5.09	125.55	128.60
55	2x	46	G	C4-C5-N7	-5.09	108.76	110.80
32	1a	558	G	O5'-P-OP1	-5.09	101.12	105.70
1	2A	748	G	O4'-C1'-N9	5.09	112.27	108.20
32	1a	1150	U	C2-N3-C4	5.09	130.05	127.00
32	1a	1201	A	P-O3'-C3'	5.08	125.80	119.70
1	2A	2318	G	C4-N9-C1'	5.08	133.11	126.50
32	1a	748	C	P-O3'-C3'	5.08	125.80	119.70
1	2A	2689	U	P-O3'-C3'	5.08	125.80	119.70
32	1a	1034	G	C5-C6-O6	5.08	131.65	128.60
56	1y	56	C	C2-N3-C4	5.08	122.44	119.90
1	1A	568	U	N3-C4-C5	5.04	117.63	114.60
56	1y	33	U	C2-N1-C1'	5.04	123.75	117.70
32	1a	687	A	P-O3'-C3'	5.04	125.75	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1372	U	C5-C4-O4	-5.03	122.88	125.90
1	1A	2032	G	C5-N7-C8	5.02	106.81	104.30
1	1A	751	A	O5'-P-OP1	-5.02	101.18	105.70
1	2A	752	A	C8-N9-C4	-5.01	103.79	105.80
1	1A	2501	C	C2-N1-C1'	-5.01	113.29	118.80
55	1x	46	G	C4-C5-N7	-5.00	108.80	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	1Z	136	PHE	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	1D	273/276 (99%)	256 (94%)	17 (6%)	0	100 100
3	2D	273/276 (99%)	259 (95%)	14 (5%)	0	100 100
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	29 40
4	2E	202/206 (98%)	187 (93%)	14 (7%)	1 (0%)	29 40
5	1F	200/210 (95%)	195 (98%)	4 (2%)	1 (0%)	29 40
5	2F	200/210 (95%)	188 (94%)	11 (6%)	1 (0%)	29 40
6	1G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	25 34
6	2G	179/182 (98%)	157 (88%)	19 (11%)	3 (2%)	9 11
7	1H	172/180 (96%)	159 (92%)	12 (7%)	1 (1%)	25 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	2H	172/180 (96%)	158 (92%)	13 (8%)	1 (1%)	25 34
8	1I	144/148 (97%)	128 (89%)	16 (11%)	0	100 100
8	2I	144/148 (97%)	128 (89%)	14 (10%)	2 (1%)	11 15
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100 100
9	2N	138/140 (99%)	125 (91%)	12 (9%)	1 (1%)	22 30
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100 100
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	19 27
11	1P	147/150 (98%)	132 (90%)	10 (7%)	5 (3%)	3 2
11	2P	147/150 (98%)	132 (90%)	11 (8%)	4 (3%)	5 4
12	1Q	139/141 (99%)	134 (96%)	3 (2%)	2 (1%)	11 15
12	2Q	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	22 30
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100 100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100 100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100 100
14	2S	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	17 24
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100 100
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100 100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100 100
17	1V	99/101 (98%)	92 (93%)	4 (4%)	3 (3%)	4 3
17	2V	99/101 (98%)	88 (89%)	10 (10%)	1 (1%)	15 22
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
19	1X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	14 19
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14 19
20	1Y	105/110 (96%)	99 (94%)	5 (5%)	1 (1%)	15 22
20	2Y	105/110 (96%)	96 (91%)	7 (7%)	2 (2%)	8 9
21	1Z	148/206 (72%)	132 (89%)	14 (10%)	2 (1%)	11 15
21	2Z	156/206 (76%)	124 (80%)	25 (16%)	7 (4%)	2 1
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100 100
22	20	81/85 (95%)	78 (96%)	3 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14 19
23	21	95/98 (97%)	92 (97%)	3 (3%)	0	100 100
24	12	68/72 (94%)	65 (96%)	3 (4%)	0	100 100
24	22	68/72 (94%)	68 (100%)	0	0	100 100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
25	23	57/60 (95%)	52 (91%)	5 (9%)	0	100 100
26	14	67/71 (94%)	54 (81%)	6 (9%)	7 (10%)	0 0
26	24	67/71 (94%)	50 (75%)	14 (21%)	3 (4%)	2 1
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%)	48 (94%)	3 (6%)	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%)	60 (97%)	2 (3%)	0	100 100
31	19	35/37 (95%)	35 (100%)	0	0	100 100
31	29	35/37 (95%)	35 (100%)	0	0	100 100
33	1b	229/256 (90%)	197 (86%)	26 (11%)	6 (3%)	5 5
33	2b	229/256 (90%)	185 (81%)	37 (16%)	7 (3%)	4 3
34	1c	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	29 40
34	2c	204/239 (85%)	185 (91%)	18 (9%)	1 (0%)	29 40
35	1d	206/209 (99%)	193 (94%)	9 (4%)	4 (2%)	8 9
35	2d	206/209 (99%)	197 (96%)	9 (4%)	0	100 100
36	1e	146/162 (90%)	131 (90%)	13 (9%)	2 (1%)	11 15
36	2e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	11 15
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100 100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100 100
38	1g	153/156 (98%)	147 (96%)	5 (3%)	1 (1%)	22 30
38	2g	153/156 (98%)	140 (92%)	12 (8%)	1 (1%)	22 30
39	1h	135/138 (98%)	127 (94%)	7 (5%)	1 (1%)	22 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
39	2h	135/138 (98%)	128 (95%)	7 (5%)	0	100 100
40	1i	125/128 (98%)	110 (88%)	12 (10%)	3 (2%)	6 5
40	2i	125/128 (98%)	110 (88%)	14 (11%)	1 (1%)	19 27
41	1j	95/105 (90%)	84 (88%)	9 (10%)	2 (2%)	7 7
41	2j	94/105 (90%)	79 (84%)	12 (13%)	3 (3%)	4 3
42	1k	112/129 (87%)	98 (88%)	13 (12%)	1 (1%)	17 24
42	2k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	17 24
43	1l	119/132 (90%)	114 (96%)	5 (4%)	0	100 100
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100 100
44	1m	121/126 (96%)	108 (89%)	10 (8%)	3 (2%)	5 5
44	2m	120/126 (95%)	109 (91%)	9 (8%)	2 (2%)	9 11
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100 100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100 100
46	1o	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	13 17
46	2o	86/89 (97%)	83 (96%)	3 (4%)	0	100 100
47	1p	80/88 (91%)	71 (89%)	9 (11%)	0	100 100
47	2p	80/88 (91%)	76 (95%)	4 (5%)	0	100 100
48	1q	97/105 (92%)	89 (92%)	6 (6%)	2 (2%)	7 7
48	2q	97/105 (92%)	90 (93%)	5 (5%)	2 (2%)	7 7
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100 100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100 100
50	1s	81/93 (87%)	71 (88%)	9 (11%)	1 (1%)	13 17
50	2s	81/93 (87%)	71 (88%)	10 (12%)	0	100 100
51	1t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	7 7
51	2t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	7 7
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
All	All	11368/12128 (94%)	10523 (93%)	737 (6%)	108 (1%)	15 22

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA

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Mol	Chain	Res	Type
11	1P	29	LYS
11	1P	38	GLN
11	1P	44	GLY
17	1V	79	VAL
21	1Z	53	ILE
26	14	49	PHE
26	14	62	ARG
33	1b	17	PHE
33	1b	22	LYS
40	1i	54	ASP
44	1m	67	GLU
44	1m	107	ALA
5	2F	130	ALA
8	2I	40	THR
11	2P	36	LYS
21	2Z	154	ASP
26	24	45	GLY
33	2b	9	GLU
33	2b	17	PHE
44	2m	67	GLU
12	1Q	16	ARG
23	11	3	LYS
26	14	45	GLY
26	14	47	GLN
35	1d	88	VAL
38	1g	52	GLU
42	1k	49	GLY
48	1q	68	ARG
6	2G	51	ARG
8	2I	41	GLU
17	2V	79	VAL
19	2X	93	GLU
21	2Z	53	ILE
21	2Z	93	ASP
26	24	48	ARG
33	2b	21	ARG
38	2g	55	GLY
48	2q	68	ARG
51	2t	10	LEU
11	1P	45	LEU
17	1V	100	ARG
20	1Y	54	LYS

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Mol	Chain	Res	Type
26	14	52	THR
33	1b	124	SER
35	1d	173	TRP
36	1e	85	GLY
11	2P	38	GLN
12	2Q	16	ARG
14	2S	84	GLN
20	2Y	54	LYS
21	2Z	52	SER
26	24	49	PHE
33	2b	20	GLU
41	2j	79	ARG
4	1E	52	LEU
7	1H	126	PRO
17	1V	43	GLU
19	1X	93	GLU
21	1Z	156	LYS
26	14	53	GLU
33	1b	126	GLU
34	1c	61	ALA
41	1j	78	ASN
44	1m	106	ASN
46	1o	88	ARG
51	1t	100	ILE
4	2E	52	LEU
6	2G	45	GLU
7	2H	126	PRO
9	2N	2	LYS
10	2O	26	LYS
11	2P	44	GLY
21	2Z	60	GLU
21	2Z	144	LEU
34	2c	181	ASN
48	2q	67	LYS
50	1s	27	GLU
11	2P	45	LEU
40	2i	11	LYS
41	2j	29	ARG
44	2m	6	GLY
6	1G	50	ALA
12	1Q	15	GLY
33	2b	74	LYS

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Mol	Chain	Res	Type
33	2b	78	GLN
41	2j	78	ASN
35	1d	170	VAL
36	1e	69	VAL
40	1i	41	VAL
41	1j	77	PRO
48	1q	33	GLY
51	1t	47	GLY
21	2Z	146	ILE
33	2b	125	PRO
51	2t	47	GLY
6	2G	42	GLY
36	2e	11	ILE
11	1P	122	PRO
26	14	56	VAL
35	1d	124	GLY
42	2k	105	VAL
33	1b	229	VAL
39	1h	73	ASP
40	1i	24	GLY
20	2Y	55	TYR
36	2e	96	PRO
33	1b	125	PRO

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	215/218 (99%)	206 (96%)	9 (4%)	30 40
3	2D	215/218 (99%)	205 (95%)	10 (5%)	26 35
4	1E	164/166 (99%)	154 (94%)	10 (6%)	18 24
4	2E	164/166 (99%)	159 (97%)	5 (3%)	41 55
5	1F	160/166 (96%)	143 (89%)	17 (11%)	6 7
5	2F	159/166 (96%)	149 (94%)	10 (6%)	18 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	1G	143/156 (92%)	128 (90%)	15 (10%)	7 7
6	2G	143/156 (92%)	128 (90%)	15 (10%)	7 7
7	1H	144/148 (97%)	133 (92%)	11 (8%)	13 17
7	2H	144/148 (97%)	128 (89%)	16 (11%)	6 6
8	1I	113/124 (91%)	96 (85%)	17 (15%)	3 2
8	2I	105/124 (85%)	96 (91%)	9 (9%)	10 13
9	1N	118/119 (99%)	111 (94%)	7 (6%)	19 25
9	2N	118/119 (99%)	112 (95%)	6 (5%)	24 32
10	1O	100/100 (100%)	98 (98%)	2 (2%)	55 70
10	2O	100/100 (100%)	95 (95%)	5 (5%)	24 33
11	1P	115/116 (99%)	106 (92%)	9 (8%)	12 16
11	2P	115/116 (99%)	107 (93%)	8 (7%)	15 19
12	1Q	111/111 (100%)	109 (98%)	2 (2%)	59 74
12	2Q	111/111 (100%)	105 (95%)	6 (5%)	22 29
13	1R	101/101 (100%)	97 (96%)	4 (4%)	31 43
13	2R	101/101 (100%)	97 (96%)	4 (4%)	31 43
14	1S	86/88 (98%)	79 (92%)	7 (8%)	11 14
14	2S	85/88 (97%)	80 (94%)	5 (6%)	19 25
15	1T	115/127 (91%)	109 (95%)	6 (5%)	23 30
15	2T	113/127 (89%)	106 (94%)	7 (6%)	18 24
16	1U	93/94 (99%)	89 (96%)	4 (4%)	29 39
16	2U	93/94 (99%)	89 (96%)	4 (4%)	29 39
17	1V	80/82 (98%)	77 (96%)	3 (4%)	33 45
17	2V	80/82 (98%)	75 (94%)	5 (6%)	18 23
18	1W	90/92 (98%)	85 (94%)	5 (6%)	21 28
18	2W	90/92 (98%)	88 (98%)	2 (2%)	52 66
19	1X	77/78 (99%)	75 (97%)	2 (3%)	46 61
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32 44
20	1Y	85/91 (93%)	75 (88%)	10 (12%)	5 5
20	2Y	85/91 (93%)	77 (91%)	8 (9%)	8 10
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	2Z	137/179 (76%)	119 (87%)	18 (13%)	4 3
22	10	65/67 (97%)	63 (97%)	2 (3%)	40 54
22	20	65/67 (97%)	64 (98%)	1 (2%)	65 77
23	11	80/83 (96%)	77 (96%)	3 (4%)	33 45
23	21	80/83 (96%)	74 (92%)	6 (8%)	13 17
24	12	65/67 (97%)	65 (100%)	0	100 100
24	22	65/67 (97%)	65 (100%)	0	100 100
25	13	51/52 (98%)	49 (96%)	2 (4%)	32 44
25	23	50/52 (96%)	46 (92%)	4 (8%)	12 15
26	14	59/63 (94%)	52 (88%)	7 (12%)	5 5
26	24	53/63 (84%)	45 (85%)	8 (15%)	3 2
27	15	50/52 (96%)	47 (94%)	3 (6%)	19 25
27	25	50/52 (96%)	47 (94%)	3 (6%)	19 25
28	16	51/52 (98%)	45 (88%)	6 (12%)	5 5
28	26	50/52 (96%)	47 (94%)	3 (6%)	19 25
29	17	41/42 (98%)	37 (90%)	4 (10%)	8 9
29	27	41/42 (98%)	37 (90%)	4 (10%)	8 9
30	18	54/55 (98%)	51 (94%)	3 (6%)	21 28
30	28	54/55 (98%)	51 (94%)	3 (6%)	21 28
31	19	34/34 (100%)	34 (100%)	0	100 100
31	29	34/34 (100%)	34 (100%)	0	100 100
33	1b	192/220 (87%)	167 (87%)	25 (13%)	4 3
33	2b	187/220 (85%)	155 (83%)	32 (17%)	2 2
34	1c	142/188 (76%)	129 (91%)	13 (9%)	9 11
34	2c	140/188 (74%)	132 (94%)	8 (6%)	20 27
35	1d	169/181 (93%)	159 (94%)	10 (6%)	19 25
35	2d	173/181 (96%)	150 (87%)	23 (13%)	4 3
36	1e	113/123 (92%)	106 (94%)	7 (6%)	18 24
36	2e	114/123 (93%)	108 (95%)	6 (5%)	22 30
37	1f	84/90 (93%)	75 (89%)	9 (11%)	6 7
37	2f	85/90 (94%)	82 (96%)	3 (4%)	36 49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	1g	119/127 (94%)	105 (88%)	14 (12%)	5 5
38	2g	120/127 (94%)	108 (90%)	12 (10%)	7 8
39	1h	114/119 (96%)	108 (95%)	6 (5%)	22 30
39	2h	114/119 (96%)	106 (93%)	8 (7%)	15 19
40	1i	90/99 (91%)	80 (89%)	10 (11%)	6 6
40	2i	89/99 (90%)	80 (90%)	9 (10%)	7 8
41	1j	66/92 (72%)	59 (89%)	7 (11%)	6 7
41	2j	69/92 (75%)	58 (84%)	11 (16%)	2 2
42	1k	82/99 (83%)	77 (94%)	5 (6%)	18 24
42	2k	83/99 (84%)	77 (93%)	6 (7%)	14 18
43	1l	96/108 (89%)	90 (94%)	6 (6%)	18 23
43	2l	96/108 (89%)	92 (96%)	4 (4%)	30 40
44	1m	93/101 (92%)	82 (88%)	11 (12%)	5 5
44	2m	92/101 (91%)	83 (90%)	9 (10%)	8 9
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7 8
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7 8
46	1o	78/80 (98%)	75 (96%)	3 (4%)	33 45
46	2o	78/80 (98%)	73 (94%)	5 (6%)	17 23
47	1p	69/74 (93%)	65 (94%)	4 (6%)	20 26
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13 18
48	1q	94/97 (97%)	90 (96%)	4 (4%)	29 39
48	2q	94/97 (97%)	91 (97%)	3 (3%)	39 53
49	1r	59/77 (77%)	55 (93%)	4 (7%)	16 20
49	2r	59/77 (77%)	54 (92%)	5 (8%)	10 13
50	1s	69/80 (86%)	63 (91%)	6 (9%)	10 12
50	2s	67/80 (84%)	63 (94%)	4 (6%)	19 25
51	1t	70/82 (85%)	67 (96%)	3 (4%)	29 39
51	2t	70/82 (85%)	68 (97%)	2 (3%)	42 57
52	1u	18/22 (82%)	18 (100%)	0	100 100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	21 28
All	All	9303/10064 (92%)	8631 (93%)	672 (7%)	14 18

All (672) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	38	LYS
3	1D	61	LEU
3	1D	99	ASP
3	1D	142	VAL
3	1D	211	ARG
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
4	1E	2	LYS
4	1E	45	THR
4	1E	47	VAL
4	1E	49	LEU
4	1E	78	LEU
4	1E	113	PHE
4	1E	116	VAL
4	1E	181	LEU
4	1E	184	VAL
4	1E	195	LEU
5	1F	24	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	60	SER
5	1F	70	THR
5	1F	72	ARG
5	1F	74	ARG
5	1F	106	ARG
5	1F	132	VAL
5	1F	140	LEU
5	1F	168	ARG
5	1F	175	THR
5	1F	183	VAL
5	1F	192	LEU
5	1F	195	ASP
5	1F	205	ARG
6	1G	5	VAL
6	1G	7	LEU
6	1G	43	LEU
6	1G	47	LYS
6	1G	49	ASP
6	1G	64	THR

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Mol	Chain	Res	Type
6	1G	82	LEU
6	1G	86	MET
6	1G	91	ARG
6	1G	104	GLU
6	1G	133	LEU
6	1G	139	LEU
6	1G	148	MET
6	1G	150	ASP
6	1G	159	VAL
7	1H	6	ARG
7	1H	13	LYS
7	1H	23	ARG
7	1H	42	ARG
7	1H	57	ASP
7	1H	77	LYS
7	1H	87	LEU
7	1H	95	ARG
7	1H	98	LEU
7	1H	114	VAL
7	1H	155	SER
8	1I	3	VAL
8	1I	12	LEU
8	1I	15	VAL
8	1I	20	ASP
8	1I	38	LEU
8	1I	41	GLU
8	1I	47	LEU
8	1I	48	GLU
8	1I	61	ARG
8	1I	77	LEU
8	1I	85	GLU
8	1I	92	VAL
8	1I	101	LEU
8	1I	108	THR
8	1I	123	LEU
8	1I	129	THR
8	1I	140	LEU
9	1N	1	MET
9	1N	10	GLU
9	1N	28	THR
9	1N	48	MET
9	1N	62	VAL

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Mol	Chain	Res	Type
9	1N	68	GLU
9	1N	138	LEU
10	1O	20	MET
10	1O	106	LEU
11	1P	2	LYS
11	1P	7	ARG
11	1P	45	LEU
11	1P	98	GLU
11	1P	117	GLU
11	1P	125	VAL
11	1P	133	SER
11	1P	148	LEU
11	1P	149	GLU
12	1Q	75	THR
12	1Q	109	VAL
13	1R	36	THR
13	1R	67	LEU
13	1R	114	VAL
13	1R	117	VAL
14	1S	3	ARG
14	1S	14	VAL
14	1S	25	ARG
14	1S	46	VAL
14	1S	69	VAL
14	1S	73	LEU
14	1S	75	GLU
15	1T	28	VAL
15	1T	49	VAL
15	1T	85	LYS
15	1T	96	ARG
15	1T	108	ARG
15	1T	118	ARG
16	1U	8	VAL
16	1U	74	LEU
16	1U	84	LYS
16	1U	95	LEU
17	1V	79	VAL
17	1V	82	ARG
17	1V	100	ARG
18	1W	4	LYS
18	1W	11	ARG
18	1W	15	ARG

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Mol	Chain	Res	Type
18	1W	17	VAL
18	1W	92	ARG
19	1X	66	LEU
19	1X	72	LYS
20	1Y	1	MET
20	1Y	9	LYS
20	1Y	26	LYS
20	1Y	43	ASN
20	1Y	50	ARG
20	1Y	55	TYR
20	1Y	64	GLU
20	1Y	72	VAL
20	1Y	91	GLU
20	1Y	99	CYS
21	1Z	1	MET
21	1Z	33	LEU
21	1Z	63	ASP
21	1Z	72	ARG
21	1Z	79	ARG
21	1Z	124	ILE
21	1Z	132	ASN
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	170	THR
21	1Z	171	ILE
22	10	10	THR
22	10	82	ARG
23	11	40	ARG
23	11	46	LEU
23	11	56	GLN
25	13	23	LEU
25	13	34	GLU
26	14	21	VAL
26	14	33	VAL
26	14	49	PHE
26	14	53	GLU
26	14	58	ARG
26	14	66	SER
26	14	69	LYS
27	15	6	VAL
27	15	15	ARG
27	15	40	LYS

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Mol	Chain	Res	Type
28	16	5	VAL
28	16	6	ARG
28	16	14	THR
28	16	19	ARG
28	16	35	GLU
28	16	41	PRO
29	17	1	MET
29	17	24	THR
29	17	41	ARG
29	17	43	THR
30	18	14	VAL
30	18	31	HIS
30	18	34	TRP
33	1b	8	LYS
33	1b	12	GLU
33	1b	21	ARG
33	1b	24	TRP
33	1b	35	GLU
33	1b	39	ILE
33	1b	48	MET
33	1b	78	GLN
33	1b	80	ILE
33	1b	82	ARG
33	1b	96	ARG
33	1b	97	TRP
33	1b	118	LEU
33	1b	126	GLU
33	1b	145	LEU
33	1b	153	ARG
33	1b	164	VAL
33	1b	170	GLU
33	1b	208	ILE
33	1b	212	GLN
33	1b	215	LEU
33	1b	217	ARG
33	1b	229	VAL
33	1b	230	VAL
33	1b	236	TYR
34	1c	3	ASN
34	1c	5	ILE
34	1c	29	TYR
34	1c	33	LEU

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Mol	Chain	Res	Type
34	1c	46	GLU
34	1c	49	SER
34	1c	66	VAL
34	1c	89	GLU
34	1c	131	ARG
34	1c	132	ARG
34	1c	172	ARG
34	1c	195	VAL
34	1c	206	GLU
35	1d	10	ARG
35	1d	19	LEU
35	1d	21	LEU
35	1d	31	CYS
35	1d	56	VAL
35	1d	59	ARG
35	1d	76	ARG
35	1d	88	VAL
35	1d	112	VAL
35	1d	135	LEU
36	1e	10	MET
36	1e	13	ILE
36	1e	41	VAL
36	1e	47	LYS
36	1e	64	ARG
36	1e	98	THR
36	1e	126	ARG
37	1f	10	LEU
37	1f	19	LEU
37	1f	36	ARG
37	1f	37	VAL
37	1f	45	LEU
37	1f	57	GLN
37	1f	72	VAL
37	1f	75	LEU
37	1f	92	LYS
38	1g	4	ARG
38	1g	13	GLN
38	1g	16	LEU
38	1g	32	ARG
38	1g	59	LEU
38	1g	61	VAL
38	1g	72	ARG

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Mol	Chain	Res	Type
38	1g	77	SER
38	1g	90	GLU
38	1g	97	GLN
38	1g	104	LEU
38	1g	113	GLU
38	1g	114	ARG
38	1g	155	ARG
39	1h	24	THR
39	1h	32	LYS
39	1h	38	ILE
39	1h	51	VAL
39	1h	52	ASP
39	1h	133	LEU
40	1i	14	VAL
40	1i	23	ASN
40	1i	41	VAL
40	1i	48	GLU
40	1i	60	ASP
40	1i	92	TYR
40	1i	104	ARG
40	1i	111	ARG
40	1i	127	LYS
40	1i	128	ARG
41	1j	44	VAL
41	1j	46	ARG
41	1j	51	ARG
41	1j	81	THR
41	1j	92	THR
41	1j	95	GLU
41	1j	98	ILE
42	1k	14	VAL
42	1k	48	ILE
42	1k	87	THR
42	1k	107	SER
42	1k	114	VAL
43	1l	57	LYS
43	1l	62	SER
43	1l	78	GLN
43	1l	83	VAL
43	1l	97	ARG
43	1l	118	SER
44	1m	3	ARG

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Mol	Chain	Res	Type
44	1m	4	ILE
44	1m	11	ARG
44	1m	32	GLU
44	1m	43	THR
44	1m	52	GLU
44	1m	60	VAL
44	1m	102	ARG
44	1m	106	ASN
44	1m	109	THR
44	1m	122	LYS
45	1n	3	ARG
45	1n	6	LEU
45	1n	15	LYS
45	1n	18	VAL
45	1n	53	LEU
46	1o	62	GLN
46	1o	84	LYS
46	1o	88	ARG
47	1p	5	ARG
47	1p	20	VAL
47	1p	61	SER
47	1p	67	THR
48	1q	7	THR
48	1q	11	VAL
48	1q	60	ILE
48	1q	98	LEU
49	1r	47	THR
49	1r	54	ARG
49	1r	61	LYS
49	1r	85	LEU
50	1s	12	ASP
50	1s	15	LEU
50	1s	33	THR
50	1s	41	VAL
50	1s	48	THR
50	1s	56	GLN
51	1t	10	LEU
51	1t	24	LEU
51	1t	100	ILE
3	2D	37	LEU
3	2D	61	LEU
3	2D	71	ASP

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Mol	Chain	Res	Type
3	2D	99	ASP
3	2D	142	VAL
3	2D	181	GLU
3	2D	211	ARG
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
4	2E	55	ASN
4	2E	69	LYS
4	2E	116	VAL
4	2E	181	LEU
4	2E	184	VAL
5	2F	9	ILE
5	2F	17	ARG
5	2F	33	LEU
5	2F	74	ARG
5	2F	149	ASP
5	2F	154	VAL
5	2F	158	THR
5	2F	162	LEU
5	2F	175	THR
5	2F	203	GLN
6	2G	18	GLU
6	2G	43	LEU
6	2G	45	GLU
6	2G	60	LEU
6	2G	62	LEU
6	2G	91	ARG
6	2G	116	ASP
6	2G	124	SER
6	2G	126	ASP
6	2G	133	LEU
6	2G	140	ILE
6	2G	149	VAL
6	2G	165	THR
6	2G	170	ARG
6	2G	181	ARG
7	2H	7	LEU
7	2H	23	ARG
7	2H	26	VAL
7	2H	44	VAL
7	2H	45	VAL

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Mol	Chain	Res	Type
7	2H	63	SER
7	2H	77	LYS
7	2H	92	ILE
7	2H	95	ARG
7	2H	114	VAL
7	2H	124	GLU
7	2H	134	SER
7	2H	136	ILE
7	2H	139	GLN
7	2H	149	ARG
7	2H	153	LYS
8	2I	14	ASP
8	2I	20	ASP
8	2I	38	LEU
8	2I	58	LEU
8	2I	92	VAL
8	2I	101	LEU
8	2I	102	SER
8	2I	105	HIS
8	2I	117	GLU
9	2N	1	MET
9	2N	48	MET
9	2N	61	ARG
9	2N	62	VAL
9	2N	68	GLU
9	2N	138	LEU
10	2O	28	SER
10	2O	42	SER
10	2O	92	GLU
10	2O	108	GLU
10	2O	116	SER
11	2P	1	MET
11	2P	4	SER
11	2P	77	ARG
11	2P	98	GLU
11	2P	135	LEU
11	2P	147	LEU
11	2P	148	LEU
11	2P	149	GLU
12	2Q	38	GLU
12	2Q	56	ARG
12	2Q	96	VAL

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Mol	Chain	Res	Type
12	2Q	106	VAL
12	2Q	109	VAL
12	2Q	133	ARG
13	2R	36	THR
13	2R	67	LEU
13	2R	111	LEU
13	2R	114	VAL
14	2S	58	LEU
14	2S	64	GLU
14	2S	75	GLU
14	2S	83	LYS
14	2S	110	LEU
15	2T	19	LEU
15	2T	40	THR
15	2T	63	VAL
15	2T	74	ARG
15	2T	96	ARG
15	2T	107	ASP
15	2T	115	ARG
16	2U	5	LYS
16	2U	8	VAL
16	2U	31	SER
16	2U	74	LEU
17	2V	33	VAL
17	2V	35	LEU
17	2V	61	VAL
17	2V	79	VAL
17	2V	98	GLU
18	2W	11	ARG
18	2W	17	VAL
19	2X	38	GLU
19	2X	57	LEU
19	2X	82	GLN
20	2Y	1	MET
20	2Y	7	VAL
20	2Y	9	LYS
20	2Y	39	VAL
20	2Y	43	ASN
20	2Y	90	LEU
20	2Y	99	CYS
20	2Y	107	ASP
21	2Z	6	LYS

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Mol	Chain	Res	Type
21	2Z	30	ASN
21	2Z	33	LEU
21	2Z	35	ARG
21	2Z	60	GLU
21	2Z	71	VAL
21	2Z	91	LEU
21	2Z	94	GLU
21	2Z	96	VAL
21	2Z	100	VAL
21	2Z	122	ARG
21	2Z	131	ARG
21	2Z	136	PHE
21	2Z	137	ILE
21	2Z	151	HIS
21	2Z	170	THR
21	2Z	171	ILE
21	2Z	174	VAL
22	20	9	SER
23	21	38	SER
23	21	40	ARG
23	21	46	LEU
23	21	69	LYS
23	21	78	LYS
23	21	80	LEU
25	23	29	ARG
25	23	30	ARG
25	23	31	LEU
25	23	54	VAL
26	24	10	VAL
26	24	26	SER
26	24	49	PHE
26	24	59	PHE
26	24	61	ARG
26	24	62	ARG
26	24	63	TYR
26	24	67	TYR
27	25	6	VAL
27	25	33	CYS
27	25	40	LYS
28	26	6	ARG
28	26	19	ARG
28	26	40	CYS

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Mol	Chain	Res	Type
29	27	1	MET
29	27	23	ARG
29	27	43	THR
29	27	46	VAL
30	28	14	VAL
30	28	19	SER
30	28	31	HIS
33	2b	7	VAL
33	2b	8	LYS
33	2b	9	GLU
33	2b	11	LEU
33	2b	16	HIS
33	2b	24	TRP
33	2b	37	ASN
33	2b	48	MET
33	2b	55	PHE
33	2b	58	ILE
33	2b	67	THR
33	2b	71	VAL
33	2b	76	GLN
33	2b	79	ASP
33	2b	82	ARG
33	2b	83	MET
33	2b	94	ASN
33	2b	101	MET
33	2b	107	THR
33	2b	112	VAL
33	2b	127	ILE
33	2b	138	LEU
33	2b	142	LEU
33	2b	144	ARG
33	2b	150	SER
33	2b	168	THR
33	2b	185	ILE
33	2b	189	ASP
33	2b	195	ASP
33	2b	208	ILE
33	2b	217	ARG
33	2b	223	ILE
34	2c	15	THR
34	2c	30	ARG
34	2c	45	LYS

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Mol	Chain	Res	Type
34	2c	47	LEU
34	2c	85	ARG
34	2c	104	GLN
34	2c	152	ILE
34	2c	190	ARG
35	2d	5	ILE
35	2d	8	VAL
35	2d	19	LEU
35	2d	28	SER
35	2d	31	CYS
35	2d	47	ARG
35	2d	58	LEU
35	2d	59	ARG
35	2d	83	SER
35	2d	94	LEU
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	155	LEU
35	2d	162	LEU
35	2d	166	LYS
35	2d	169	LYS
35	2d	175	SER
35	2d	178	VAL
35	2d	181	MET
35	2d	188	LEU
35	2d	196	LEU
35	2d	201	GLN
36	2e	13	ILE
36	2e	24	ARG
36	2e	41	VAL
36	2e	51	VAL
36	2e	147	ASP
36	2e	151	LEU
37	2f	45	LEU
37	2f	70	ASP
37	2f	81	ILE
38	2g	9	VAL
38	2g	13	GLN
38	2g	24	THR
38	2g	33	ASP
38	2g	53	LYS

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Mol	Chain	Res	Type
38	2g	75	VAL
38	2g	79	ARG
38	2g	86	GLN
38	2g	97	GLN
38	2g	98	SER
38	2g	110	GLN
38	2g	113	GLU
39	2h	29	SER
39	2h	51	VAL
39	2h	52	ASP
39	2h	56	LYS
39	2h	68	ARG
39	2h	86	ILE
39	2h	95	VAL
39	2h	97	VAL
40	2i	14	VAL
40	2i	29	ASN
40	2i	54	ASP
40	2i	65	VAL
40	2i	75	ASP
40	2i	87	GLN
40	2i	102	LEU
40	2i	113	LYS
40	2i	128	ARG
41	2j	9	ARG
41	2j	30	SER
41	2j	33	GLN
41	2j	38	ILE
41	2j	66	ARG
41	2j	67	THR
41	2j	72	VAL
41	2j	81	THR
41	2j	89	ASP
41	2j	92	THR
41	2j	100	THR
42	2k	14	VAL
42	2k	28	THR
42	2k	53	SER
42	2k	77	MET
42	2k	96	ARG
42	2k	114	VAL
43	2l	33	ARG

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Mol	Chain	Res	Type
43	2l	78	GLN
43	2l	83	VAL
43	2l	97	ARG
44	2m	3	ARG
44	2m	27	LYS
44	2m	32	GLU
44	2m	45	VAL
44	2m	47	ASP
44	2m	48	LEU
44	2m	67	GLU
44	2m	70	LEU
44	2m	121	LYS
45	2n	3	ARG
45	2n	15	LYS
45	2n	18	VAL
45	2n	33	VAL
45	2n	60	SER
46	2o	14	GLU
46	2o	24	SER
46	2o	64	ARG
46	2o	87	ILE
46	2o	88	ARG
47	2p	2	VAL
47	2p	8	ARG
47	2p	11	SER
47	2p	21	VAL
47	2p	60	LEU
48	2q	36	ILE
48	2q	63	ARG
48	2q	99	SER
49	2r	26	LEU
49	2r	54	ARG
49	2r	76	LEU
49	2r	84	LYS
49	2r	86	VAL
50	2s	12	ASP
50	2s	28	LYS
50	2s	37	ARG
50	2s	41	VAL
51	2t	15	ARG
51	2t	93	GLU
52	2u	15	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	48	GLN
4	1E	143	ASN
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
7	1H	74	ASN
8	1I	74	ASN
9	1N	131	GLN
12	1Q	12	GLN
12	1Q	57	HIS
13	1R	31	HIS
14	1S	68	GLN
14	1S	95	HIS
15	1T	58	ASN
16	1U	81	HIS
19	1X	31	HIS
19	1X	82	GLN
21	1Z	73	GLN
22	10	50	ASN
23	11	56	GLN
25	13	32	GLN
34	1c	6	HIS
34	1c	104	GLN
34	1c	162	GLN
34	1c	181	ASN
35	1d	116	GLN
35	1d	125	HIS
36	1e	78	HIS
37	1f	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
40	1i	31	GLN
40	1i	34	ASN
41	1j	56	HIS
41	1j	62	HIS
42	1k	99	GLN
43	1l	99	HIS
44	1m	12	ASN
44	1m	77	ASN
44	1m	92	HIS

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Mol	Chain	Res	Type
46	1o	9	GLN
46	1o	62	GLN
47	1p	13	HIS
47	1p	14	ASN
48	1q	26	GLN
50	1s	23	ASN
50	1s	47	HIS
50	1s	83	HIS
51	1t	90	GLN
3	2D	87	ASN
4	2E	48	GLN
4	2E	143	ASN
5	2F	69	HIS
5	2F	75	HIS
7	2H	139	GLN
8	2I	104	GLN
9	2N	131	GLN
10	2O	3	GLN
10	2O	5	GLN
11	2P	27	HIS
12	2Q	123	HIS
13	2R	71	GLN
14	2S	38	GLN
15	2T	43	GLN
15	2T	58	ASN
16	2U	81	HIS
19	2X	31	HIS
19	2X	82	GLN
20	2Y	6	HIS
20	2Y	43	ASN
21	2Z	32	HIS
21	2Z	55	HIS
21	2Z	65	GLN
21	2Z	73	GLN
23	21	56	GLN
25	23	32	GLN
26	24	46	GLN
33	2b	40	HIS
33	2b	94	ASN
33	2b	113	HIS
33	2b	135	GLN
34	2c	6	HIS

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Mol	Chain	Res	Type
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
36	2e	78	HIS
37	2f	57	GLN
37	2f	100	ASN
38	2g	13	GLN
38	2g	28	ASN
38	2g	56	GLN
40	2i	3	GLN
40	2i	29	ASN
40	2i	31	GLN
40	2i	58	HIS
40	2i	117	HIS
41	2j	33	GLN
42	2k	78	GLN
42	2k	104	GLN
42	2k	117	ASN
43	2l	99	HIS
44	2m	92	HIS
50	2s	47	HIS
50	2s	56	GLN
50	2s	69	HIS
50	2s	83	HIS
51	2t	9	ASN
51	2t	75	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2862/2915 (98%)	412 (14%)	31 (1%)
1	2A	2789/2915 (95%)	456 (16%)	25 (0%)
2	1B	119/121 (98%)	7 (5%)	0
2	2B	118/121 (97%)	20 (16%)	0
32	1a	1494/1521 (98%)	222 (14%)	0
32	2a	1498/1521 (98%)	255 (17%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	70/76 (92%)	22 (31%)	0
54	2w	67/76 (88%)	24 (35%)	0
55	1x	75/77 (97%)	5 (6%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	2x	75/77 (97%)	8 (10%)	0
56	1y	71/76 (93%)	28 (39%)	0
56	2y	69/76 (90%)	30 (43%)	0
All	All	9331/9620 (96%)	1494 (16%)	56 (0%)

All (1494) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	55	G
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	196	A
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(C)	C
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	271(P)	C
1	1A	271(S)	G
1	1A	272(B)	G
1	1A	272(I)	U

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Mol	Chain	Res	Type
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	327	G
1	1A	329	G
1	1A	330	A
1	1A	342	G
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	370	G
1	1A	372	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	428	A
1	1A	443	A
1	1A	444	C
1	1A	448	U
1	1A	455	C
1	1A	456	C
1	1A	481	G
1	1A	494	G
1	1A	504	U
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	514	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
1	1A	604	G
1	1A	607	U

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Mol	Chain	Res	Type
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	668	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	740	U
1	1A	762	U
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	819	A
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	877	U
1	1A	879	G
1	1A	880	G
1	1A	882	G
1	1A	883	G
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	893	C
1	1A	896	A
1	1A	897	C

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Mol	Chain	Res	Type
1	1A	899	A
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
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	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1041	C
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G
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	1081	U
1	1A	1082	U
1	1A	1085	A
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G

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Mol	Chain	Res	Type
1	1A	1094	U
1	1A	1096	A
1	1A	1097	U
1	1A	1101	U
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1116	C
1	1A	1135	C
1	1A	1136	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	1244	G
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	1313	U
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	1386	C
1	1A	1395	A
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U

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Mol	Chain	Res	Type
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1459	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1496	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1581	G
1	1A	1582	C
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1616	A
1	1A	1647	G
1	1A	1648	C
1	1A	1664	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	1745	C
1	1A	1756	G
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C

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Mol	Chain	Res	Type
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1812	A
1	1A	1816	G
1	1A	1817	G
1	1A	1829	A
1	1A	1839	G
1	1A	1847	A
1	1A	1848	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
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
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2101	G
1	1A	2102	U
1	1A	2107	C

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Mol	Chain	Res	Type
1	1A	2108	C
1	1A	2113	U
1	1A	2116	G
1	1A	2121	G
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2145	C
1	1A	2146	C
1	1A	2147	G
1	1A	2148	G
1	1A	2150	U
1	1A	2151	G
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2161	C
1	1A	2163	C
1	1A	2165	G
1	1A	2166	G
1	1A	2167	U
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2189	U
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G

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Mol	Chain	Res	Type
1	1A	2207	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G
1	1A	2312	U
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	2354	G
1	1A	2361	A
1	1A	2372	G
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2410	G
1	1A	2422	A
1	1A	2424	C
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	2447	G
1	1A	2448	A
1	1A	2468	G
1	1A	2476	A
1	1A	2477	C
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A

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Mol	Chain	Res	Type
1	1A	2529	G
1	1A	2549	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2585	U
1	1A	2602	A
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2663	G
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2702	U
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2764	A
1	1A	2765	A
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2794	C
1	1A	2802	G
1	1A	2803	C
1	1A	2805	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2836	U
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U

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Mol	Chain	Res	Type
2	1B	2	C
2	1B	13	A
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	84	C
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	54	C
32	1a	61	G
32	1a	77	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	163	C
32	1a	164	U
32	1a	174	C
32	1a	182	U
32	1a	189(A)	C
32	1a	189(F)	U
32	1a	189(G)	G
32	1a	195	A
32	1a	201	C
32	1a	203	U
32	1a	204	U
32	1a	243	A
32	1a	247	G
32	1a	251	G
32	1a	262	A
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	306	G

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Mol	Chain	Res	Type
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	342	C
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	443	C
32	1a	446	G
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	485	G
32	1a	495	A
32	1a	496	A
32	1a	498	U
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	524	G
32	1a	527	G7M
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U

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Mol	Chain	Res	Type
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	587	G
32	1a	630	G
32	1a	653	A
32	1a	657	G
32	1a	665	A
32	1a	666	G
32	1a	671	G
32	1a	672	U
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	703	G
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	755	G
32	1a	760	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	827	U
32	1a	828	A
32	1a	836	G
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	859	A
32	1a	873	A
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	942	G

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Mol	Chain	Res	Type
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	996	A
32	1a	999	C
32	1a	1000	U
32	1a	1001(A)	G
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1020	U
32	1a	1022	G
32	1a	1023	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(C)	G
32	1a	1031	G
32	1a	1039	C
32	1a	1043	C
32	1a	1044	A
32	1a	1046	A
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1123	A

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Mol	Chain	Res	Type
32	1a	1124	G
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1144	G
32	1a	1146	A
32	1a	1152	A
32	1a	1157	A
32	1a	1159	U
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1240	U
32	1a	1241	G
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
32	1a	1262	C
32	1a	1270	C
32	1a	1275	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1320	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U

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Mol	Chain	Res	Type
32	1a	1370	G
32	1a	1394	A
32	1a	1406	U
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1469	G
32	1a	1487	G
32	1a	1492	A
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	24	A
54	1w	2	C
54	1w	6	G
54	1w	11	C
54	1w	12	U
54	1w	15	G
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	34	G
54	1w	45	U
54	1w	46	G7M
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	66	U
54	1w	68	C
54	1w	69	G
54	1w	70	G
54	1w	73	A

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Mol	Chain	Res	Type
54	1w	74	C
55	1x	9	G
55	1x	19	G
55	1x	21	A
55	1x	47	U
55	1x	61	C
56	1y	5	G
56	1y	7	A
56	1y	8	4SU
56	1y	9	A
56	1y	14	A
56	1y	19	G
56	1y	20	U
56	1y	21	A
56	1y	22	G
56	1y	35	A
56	1y	36	A
56	1y	39	PSU
56	1y	43	C
56	1y	44	G
56	1y	45	U
56	1y	46	G7M
56	1y	47	U
56	1y	48	C
56	1y	49	C
56	1y	53	G
56	1y	56	C
56	1y	57	G
56	1y	58	A
56	1y	59	U
56	1y	69	G
56	1y	70	G
56	1y	71	G
56	1y	76	A
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	64	A
1	2A	71	A
1	2A	74	A

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Mol	Chain	Res	Type
1	2A	75	G
1	2A	83	G
1	2A	84	A
1	2A	92	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	131	G
1	2A	154	G
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	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	228	A
1	2A	229	A
1	2A	233	A
1	2A	248	G
1	2A	250	G
1	2A	266	G
1	2A	267	C
1	2A	271(J)	C
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	271(P)	C
1	2A	272	G
1	2A	272(B)	G
1	2A	274	G
1	2A	277	C
1	2A	278	A

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Mol	Chain	Res	Type
1	2A	283	A
1	2A	311	A
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	352	G
1	2A	357	A
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	396	G
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	443	A
1	2A	444	C
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	501	A
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	528	A
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	556	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	603	A
1	2A	604	G

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Mol	Chain	Res	Type
1	2A	606	U
1	2A	607	U
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	648	G
1	2A	651	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	859	G
1	2A	866	A
1	2A	874	G
1	2A	875	G
1	2A	879	G
1	2A	880	G
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	892	G

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Mol	Chain	Res	Type
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	980	A
1	2A	983	A
1	2A	996	A
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1020	A
1	2A	1021	A
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1114	G
1	2A	1117	G
1	2A	1128	A
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G

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Mol	Chain	Res	Type
1	2A	1155	A
1	2A	1171	G
1	2A	1188	U
1	2A	1195	G
1	2A	1211	U
1	2A	1220	A
1	2A	1230	C
1	2A	1236	G
1	2A	1244	G
1	2A	1247	A
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1286	A
1	2A	1300	U
1	2A	1301	A
1	2A	1314	C
1	2A	1321	A
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1421	G
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1461	G
1	2A	1465	G
1	2A	1467	C

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Mol	Chain	Res	Type
1	2A	1471	A
1	2A	1472	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1496	A
1	2A	1497	U
1	2A	1505	C
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1542	A
1	2A	1547	C
1	2A	1554	A
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	1587	A
1	2A	1595	G
1	2A	1608	A
1	2A	1609	A
1	2A	1640	C
1	2A	1648	C
1	2A	1653	G
1	2A	1654	A
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1741	A

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Mol	Chain	Res	Type
1	2A	1746	G
1	2A	1756	G
1	2A	1758	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	1829	A
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	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A
1	2A	1940	U
1	2A	1955	U
1	2A	1963	U
1	2A	1965	C
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1993	U
1	2A	1996	C
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A

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Mol	Chain	Res	Type
1	2A	2043	C
1	2A	2049	G
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	2099	U
1	2A	2101	G
1	2A	2110	G
1	2A	2111	C
1	2A	2116	G
1	2A	2117	A
1	2A	2120	G
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	2130	U
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C
1	2A	2141	G
1	2A	2142	C
1	2A	2145	C
1	2A	2146	C
1	2A	2148	G
1	2A	2149	G
1	2A	2150	U
1	2A	2151	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A

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Mol	Chain	Res	Type
1	2A	2161	C
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2178	C
1	2A	2180	U
1	2A	2185	C
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	2239	G
1	2A	2268	A
1	2A	2275	C
1	2A	2278	A
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2305	A
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2383	G
1	2A	2385	C
1	2A	2406	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A

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Mol	Chain	Res	Type
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2465	C
1	2A	2468	G
1	2A	2469	A
1	2A	2476	A
1	2A	2480	C
1	2A	2487	G
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2525	G
1	2A	2529	G
1	2A	2530	A
1	2A	2554	U
1	2A	2564	A
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2582	G
1	2A	2585	U
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2634	G
1	2A	2646	C
1	2A	2654	A
1	2A	2656	U
1	2A	2667	C
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C

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Mol	Chain	Res	Type
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2748	A
1	2A	2751	G
1	2A	2752	C
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
1	2A	2802	G
1	2A	2803	C
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2825	C
1	2A	2833	G
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	4	C
2	2B	9	G
2	2B	13	A
2	2B	19	G
2	2B	20	C
2	2B	23	G
2	2B	40	U
2	2B	42	C
2	2B	51	G
2	2B	53	A
2	2B	56	G
2	2B	73	A
2	2B	74	U

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Mol	Chain	Res	Type
2	2B	75	G
2	2B	88	C
2	2B	105	A
2	2B	107	G
2	2B	110	G
2	2B	120	A
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	33	A
32	2a	39	G
32	2a	45	U
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	66	G
32	2a	73	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	163	C
32	2a	182	U
32	2a	189	G
32	2a	189(B)	C
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	220	G
32	2a	231	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C

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Mol	Chain	Res	Type
32	2a	289	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	355	C
32	2a	367	U
32	2a	372	C
32	2a	373	A
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	421	U
32	2a	424	G
32	2a	429	U
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	519	C
32	2a	528	C
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	536	C
32	2a	547	A
32	2a	559	A

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Mol	Chain	Res	Type
32	2a	561	U
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	607	A
32	2a	630	G
32	2a	631	G
32	2a	650	G
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	703	G
32	2a	721	G
32	2a	723	U
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	773	G
32	2a	774	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	827	U
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	859	A
32	2a	873	A
32	2a	874	G
32	2a	884	U
32	2a	902	G
32	2a	914	A
32	2a	926	G

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Mol	Chain	Res	Type
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	936	C
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	963	G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	978	A
32	2a	990	C
32	2a	991	U
32	2a	992	U
32	2a	993	G
32	2a	996	A
32	2a	997	U
32	2a	999	C
32	2a	1002	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	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	C
32	2a	1030(A)	G
32	2a	1032	G
32	2a	1035	A
32	2a	1037	C

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Mol	Chain	Res	Type
32	2a	1039	C
32	2a	1040	U
32	2a	1044	A
32	2a	1046	A
32	2a	1051	C
32	2a	1053	G
32	2a	1064	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1092	A
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1108	G
32	2a	1117	G
32	2a	1121	U
32	2a	1125	U
32	2a	1129	C
32	2a	1133	G
32	2a	1135	U
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	1152	A
32	2a	1155	G
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1172	C
32	2a	1182	G
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1201	A
32	2a	1202	G

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Mol	Chain	Res	Type
32	2a	1210	C
32	2a	1213	A
32	2a	1227	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1299	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1320	C
32	2a	1323	G
32	2a	1338	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1368	G
32	2a	1381	U
32	2a	1394	A
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A

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Mol	Chain	Res	Type
32	2a	1497	G
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	14	A
53	2v	24	A
54	2w	3	C
54	2w	4	C
54	2w	5	G
54	2w	11	C
54	2w	12	U
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	46	G7M
54	2w	48	C
54	2w	50	U
54	2w	51	U
54	2w	61	C
54	2w	62	C
54	2w	63	G
54	2w	65	G
54	2w	66	U
54	2w	67	C
54	2w	69	G
54	2w	70	G
54	2w	72	C
54	2w	73	A
54	2w	74	C
55	2x	9	G
55	2x	10	G
55	2x	21	A
55	2x	47	U
55	2x	48	C
55	2x	52	G

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Mol	Chain	Res	Type
55	2x	53	G
55	2x	61	C
56	2y	7	A
56	2y	12	U
56	2y	14	A
56	2y	15	G
56	2y	19	G
56	2y	25	C
56	2y	26	A
56	2y	27	G
56	2y	36	A
56	2y	43	C
56	2y	45	U
56	2y	48	C
56	2y	49	C
56	2y	50	U
56	2y	51	U
56	2y	52	G
56	2y	53	G
56	2y	54	5MU
56	2y	55	PSU
56	2y	56	C
56	2y	58	A
56	2y	59	U
56	2y	60	U
56	2y	61	C
56	2y	63	G
56	2y	67	C
56	2y	68	C
56	2y	69	G
56	2y	70	G
56	2y	73	A

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	195	A
1	1A	196	A
1	1A	266	G
1	1A	278	A
1	1A	548	A
1	1A	685	A

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Mol	Chain	Res	Type
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	827	U
1	1A	895	U
1	1A	974	G
1	1A	1067	A
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1379	A
1	1A	1420	U
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1762	A
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2439	A
1	1A	2611	U
1	1A	2629	A
1	1A	2689	U
1	2A	195	A
1	2A	196	A
1	2A	228	A
1	2A	229	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	774	A
1	2A	827	U
1	2A	893	C
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1420	U

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Mol	Chain	Res	Type
1	2A	1442	G
1	2A	1530	C
1	2A	1608	A
1	2A	1653	G
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2689	U

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

88 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	$\#\|Z\| > 2$
54	MIA	1w	37	54	24,31,32	2.17	3 (12%)	26,44,47	2.88	10 (38%)
1	5MC	1A	1942	57,1	18,22,23	0.96	2 (11%)	26,32,35	1.22	3 (11%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	22,30,33	2.05	3 (13%)
55	5MC	2x	32	55	18,22,23	0.97	2 (11%)	26,32,35	1.23	2 (7%)
32	5MC	2a	1400	32	18,22,23	0.93	2 (11%)	26,32,35	1.17	2 (7%)
32	PSU	1a	516	32	18,21,22	1.34	2 (11%)	22,30,33	1.81	4 (18%)
55	PSU	2x	55	55	18,21,22	1.31	2 (11%)	22,30,33	1.78	4 (18%)
1	5MU	2A	1915	1	19,22,23	1.44	6 (31%)	28,32,35	2.31	7 (25%)
43	0TD	2l	92	43	7,9,10	4.69	1 (14%)	6,11,13	4.98	3 (50%)
55	PSU	1x	55	57,55	18,21,22	1.28	2 (11%)	22,30,33	1.84	4 (18%)
1	5MU	1A	1915	1	19,22,23	1.38	4 (21%)	28,32,35	2.15	7 (25%)
1	8AH	1A	2503	57,1	20,26,27	0.70	0	23,39,42	1.99	4 (17%)
32	M2G	2a	966	32	20,27,28	1.42	2 (10%)	22,40,43	1.08	2 (9%)
32	UR3	2a	1498	32	19,22,23	1.07	2 (10%)	26,32,35	1.43	2 (7%)
54	G7M	1w	46	54	20,26,27	1.22	2 (10%)	17,39,42	0.73	0
32	5MC	1a	967	32	18,22,23	0.94	2 (11%)	26,32,35	1.16	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5MU	1A	1939	57,1	19,22,23	1.47	5 (26%)	28,32,35	2.16	6 (21%)
56	PSU	2y	39	56	18,21,22	1.38	2 (11%)	22,30,33	1.62	2 (9%)
56	5MU	2y	54	56	19,22,23	1.41	4 (21%)	28,32,35	2.18	6 (21%)
32	UR3	1a	1498	32	19,22,23	0.93	1 (5%)	26,32,35	1.48	2 (7%)
1	2MU	1A	2552	1	19,22,24	1.18	2 (10%)	26,31,36	1.89	6 (23%)
32	MA6	1a	1518	32	19,26,27	0.86	0	18,38,41	1.31	2 (11%)
1	OMC	1A	1920	1	19,22,23	0.79	0	26,31,34	0.95	1 (3%)
32	MA6	2a	1518	32	19,26,27	0.82	0	18,38,41	1.38	2 (11%)
56	MIA	2y	37	56	18,24,32	1.10	2 (11%)	18,35,47	1.19	2 (11%)
55	31H	2x	76	57,55	28,34,35	1.09	3 (10%)	23,47,50	1.59	3 (13%)
55	5MU	1x	54	57,55	19,22,23	1.46	5 (26%)	28,32,35	1.90	6 (21%)
54	PSU	1w	39	54	18,21,22	1.41	3 (16%)	22,30,33	1.45	2 (9%)
54	5MU	1w	54	54	19,22,23	1.50	5 (26%)	28,32,35	1.70	5 (17%)
56	PSU	2y	32	56	18,21,22	1.32	2 (11%)	22,30,33	1.89	3 (13%)
32	5MC	1a	1407	32	18,22,23	0.99	1 (5%)	26,32,35	1.11	2 (7%)
54	MIA	2w	37	54	20,27,32	1.81	3 (15%)	22,39,47	1.80	6 (27%)
32	G7M	1a	527	32	20,26,27	1.14	2 (10%)	17,39,42	0.63	0
54	PSU	1w	32	57,54	18,21,22	1.30	2 (11%)	22,30,33	1.84	3 (13%)
32	MA6	1a	1519	32	19,26,27	0.83	0	18,38,41	1.52	2 (11%)
56	PSU	1y	32	56	18,21,22	1.34	2 (11%)	22,30,33	1.84	3 (13%)
1	OMG	1A	2251	57,55,1	18,26,27	0.97	1 (5%)	19,38,41	1.11	2 (10%)
43	0TD	1l	92	43	7,9,10	4.74	1 (14%)	6,11,13	5.99	2 (33%)
32	2MG	1a	1207	57,32	18,26,27	0.95	1 (5%)	16,38,41	1.06	2 (12%)
54	PSU	2w	32	54	18,21,22	1.32	2 (11%)	22,30,33	1.75	3 (13%)
56	G7M	1y	46	56	20,26,27	1.31	2 (10%)	17,39,42	0.61	0
32	5MC	1a	1400	32	18,22,23	0.94	2 (11%)	26,32,35	1.08	2 (7%)
32	PSU	2a	516	32	18,21,22	1.28	2 (11%)	22,30,33	1.90	3 (13%)
56	PSU	2y	55	56	18,21,22	1.35	3 (16%)	22,30,33	1.86	4 (18%)
55	4SU	1x	8	55	18,21,22	2.27	6 (33%)	26,30,33	1.89	7 (26%)
1	5MC	2A	1942	1	18,22,23	0.96	2 (11%)	26,32,35	1.13	3 (11%)
1	OMC	2A	1920	1	19,22,23	0.82	1 (5%)	26,31,34	0.98	1 (3%)
32	5MC	2a	1404	32	18,22,23	1.00	2 (11%)	26,32,35	1.11	2 (7%)
55	5MU	2x	54	55	19,22,23	1.45	5 (26%)	28,32,35	1.90	7 (25%)
32	MA6	2a	1519	32	19,26,27	0.87	0	18,38,41	1.46	2 (11%)
56	MIA	1y	37	56	18,24,32	1.19	2 (11%)	18,35,47	1.21	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
56	4SU	2y	8	56	18,21,22	1.72	5 (27%)	26,30,33	1.76	4 (15%)
55	5MC	1x	32	55	18,22,23	1.01	2 (11%)	26,32,35	1.20	3 (11%)
54	4SU	1w	8	54	18,21,22	1.78	4 (22%)	26,30,33	2.07	5 (19%)
56	PSU	1y	39	56	18,21,22	1.40	2 (11%)	22,30,33	1.65	3 (13%)
56	5MU	1y	54	56	19,22,23	1.42	4 (21%)	28,32,35	2.06	6 (21%)
55	31H	1x	76	57,55	28,34,35	1.02	3 (10%)	23,47,50	1.68	5 (21%)
54	4SU	2w	8	54	18,21,22	1.74	5 (27%)	26,30,33	2.36	5 (19%)
1	OMG	2A	2251	55,1	18,26,27	0.99	1 (5%)	19,38,41	1.07	3 (15%)
1	PSU	1A	1911	1	18,21,22	1.39	2 (11%)	22,30,33	1.83	3 (13%)
56	G7M	2y	46	56	20,26,27	1.34	2 (10%)	17,39,42	0.71	0
1	PSU	1A	2605	57,1	18,21,22	1.40	2 (11%)	22,30,33	2.08	3 (13%)
32	G7M	2a	527	32	20,26,27	1.19	2 (10%)	17,39,42	0.61	0
32	2MG	2a	1207	32	18,26,27	0.97	1 (5%)	16,38,41	1.05	2 (12%)
1	5MC	1A	1962	57,1	18,22,23	0.91	2 (11%)	26,32,35	1.25	4 (15%)
54	G7M	2w	46	54	20,26,27	1.21	1 (5%)	17,39,42	0.64	0
32	5MC	2a	967	32	18,22,23	0.98	2 (11%)	26,32,35	1.13	2 (7%)
1	5MU	2A	1939	57,1	19,22,23	1.44	6 (31%)	28,32,35	2.17	6 (21%)
54	PSU	1w	55	54	18,21,22	1.33	2 (11%)	22,30,33	1.91	3 (13%)
56	PSU	1y	55	56	18,21,22	1.34	2 (11%)	22,30,33	1.90	3 (13%)
1	PSU	2A	1917	1	18,21,22	1.33	2 (11%)	22,30,33	1.80	3 (13%)
55	4SU	2x	8	55	18,21,22	1.98	6 (33%)	26,30,33	1.23	5 (19%)
56	4SU	1y	8	56	18,21,22	1.69	6 (33%)	26,30,33	1.67	4 (15%)
1	PSU	1A	1917	1	18,21,22	1.32	2 (11%)	22,30,33	1.98	3 (13%)
32	M2G	1a	966	32	20,27,28	1.45	3 (15%)	22,40,43	1.06	3 (13%)
32	5MC	2a	1407	57,32	18,22,23	0.98	2 (11%)	26,32,35	1.22	3 (11%)
32	4OC	1a	1402	32	20,23,24	0.81	0	26,32,35	0.84	1 (3%)
32	4OC	2a	1402	32	20,23,24	0.79	0	26,32,35	1.00	1 (3%)
1	PSU	2A	2605	1	18,21,22	1.23	2 (11%)	22,30,33	1.91	3 (13%)
1	8AH	2A	2503	57,1	20,26,27	0.79	1 (5%)	23,39,42	2.00	4 (17%)
54	PSU	2w	55	54	18,21,22	1.38	2 (11%)	22,30,33	1.79	3 (13%)
1	2MU	2A	2552	57,1	19,22,24	1.19	2 (10%)	26,31,36	1.74	6 (23%)
32	5MC	1a	1404	32	18,22,23	1.01	2 (11%)	26,32,35	1.16	2 (7%)
54	PSU	2w	39	54	18,21,22	1.35	2 (11%)	22,30,33	1.77	3 (13%)
54	F3N	1w	76	54,1	30,36,37	1.51	4 (13%)	29,51,54	1.26	1 (3%)
54	5MU	2w	54	54	19,22,23	1.35	3 (15%)	28,32,35	1.78	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	F3N	2w	76	54,1	30,36,37	1.47	5 (16%)	29,51,54	1.19	1 (3%)
1	5MC	2A	1962	57,1	18,22,23	0.93	2 (11%)	26,32,35	1.19	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
54	MIA	1w	37	54	-	3/11/33/34	0/3/3/3
1	5MC	1A	1942	57,1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	5/7/12/14	-
55	PSU	1x	55	57,55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	8AH	1A	2503	57,1	-	2/3/25/26	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/3/25/26	0/3/3/3
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
1	5MU	1A	1939	57,1	-	0/7/25/26	0/2/2/2
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
56	5MU	2y	54	56	-	2/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	1	-	0/9/27/28	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
56	MIA	2y	37	56	-	2/3/25/34	0/3/3/3
55	31H	2x	76	57,55	-	4/18/40/41	0/3/3/3
55	5MU	1x	54	57,55	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/7/29/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	G7M	1a	527	32	-	3/3/25/26	0/3/3/3
54	PSU	1w	32	57,54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	57,55,1	-	0/5/27/28	0/3/3/3
43	0TD	1l	92	43	-	4/7/12/14	-
32	2MG	1a	1207	57,32	-	1/5/27/28	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
56	G7M	1y	46	56	-	3/3/25/26	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	5/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
56	MIA	1y	37	56	-	0/3/25/34	0/3/3/3
56	4SU	2y	8	56	-	1/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	1/7/25/26	0/2/2/2
55	31H	1x	76	57,55	-	4/18/40/41	0/3/3/3
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/5/27/28	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
56	G7M	2y	46	56	-	0/3/25/26	0/3/3/3
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32	-	3/3/25/26	0/3/3/3
32	2MG	2a	1207	32	-	1/5/27/28	0/3/3/3
1	5MC	1A	1962	57,1	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	1/3/25/26	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	57,1	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	2/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	4SU	1y	8	56	-	3/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	5MC	2a	1407	57,32	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	8AH	2A	2503	57,1	-	1/3/25/26	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	57,1	-	0/9/27/28	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
54	F3N	1w	76	54,1	-	0/15/37/38	0/4/4/4
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	F3N	2w	76	54,1	-	0/15/37/38	0/4/4/4
1	5MC	2A	1962	57,1	-	0/7/25/26	0/2/2/2

All (208) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.11	1.69	1.82
43	1l	92	0TD	CB-SB	-12.07	1.69	1.82
54	1w	37	MIA	C13-C14	7.00	1.52	1.32
54	1w	37	MIA	C2-S10	-6.95	1.69	1.75
54	2w	37	MIA	C2-S10	-6.71	1.70	1.75
55	1x	8	4SU	C4-N3	-6.01	1.31	1.37
54	1w	76	F3N	CB-CG	-4.92	1.39	1.51
55	2x	8	4SU	C4-N3	-4.90	1.32	1.37
54	2w	76	F3N	CB-CG	-4.77	1.39	1.51
32	1a	966	M2G	C2-N3	4.67	1.36	1.30
54	1w	8	4SU	C4-S4	-4.66	1.59	1.68
54	2w	8	4SU	C4-S4	-4.61	1.59	1.68
32	2a	966	M2G	C2-N3	4.49	1.36	1.30
56	2y	8	4SU	C4-S4	-4.29	1.60	1.68
55	1x	8	4SU	C2-N3	-4.24	1.30	1.38
56	1y	46	G7M	C5-C4	4.05	1.47	1.39
56	2y	46	G7M	C5-C4	4.03	1.47	1.39
55	1x	8	4SU	C4-S4	-3.99	1.60	1.68
56	1y	39	PSU	C6-C5	3.95	1.39	1.35
56	1y	8	4SU	C4-S4	-3.94	1.60	1.68
1	1A	1911	PSU	C6-C5	3.88	1.39	1.35
55	2x	8	4SU	C4-S4	-3.78	1.61	1.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	39	PSU	C6-C5	3.78	1.39	1.35
54	1w	46	G7M	C5-C4	3.76	1.46	1.39
54	2w	46	G7M	C5-C4	3.75	1.46	1.39
54	2w	55	PSU	C6-C5	3.75	1.39	1.35
54	1w	76	F3N	O4'-C1'	3.74	1.46	1.41
56	1y	55	PSU	C6-C5	3.74	1.39	1.35
56	1y	32	PSU	C6-C5	3.70	1.39	1.35
54	2w	39	PSU	C6-C5	3.65	1.39	1.35
56	2y	32	PSU	C6-C5	3.65	1.39	1.35
54	1w	55	PSU	C6-C5	3.62	1.39	1.35
32	2a	527	G7M	C5-C4	3.53	1.46	1.39
1	1A	2605	PSU	C6-C5	3.48	1.39	1.35
54	1w	32	PSU	C6-C5	3.44	1.39	1.35
32	1a	527	G7M	C5-C4	3.31	1.45	1.39
1	2A	1917	PSU	C6-C5	3.31	1.39	1.35
54	2w	32	PSU	C6-C5	3.30	1.39	1.35
1	2A	1911	PSU	C6-C5	3.30	1.39	1.35
32	1a	516	PSU	C6-C5	3.29	1.39	1.35
54	2w	8	4SU	C4-N3	-3.27	1.34	1.37
55	2x	55	PSU	C6-C5	3.25	1.39	1.35
32	2a	516	PSU	C6-C5	3.23	1.39	1.35
56	1y	8	4SU	C4-N3	-3.23	1.34	1.37
55	2x	8	4SU	C2-N3	-3.20	1.32	1.38
54	1w	39	PSU	C6-C5	3.16	1.39	1.35
56	2y	8	4SU	C4-N3	-3.16	1.34	1.37
55	1x	8	4SU	C5-C4	-3.14	1.38	1.42
32	2a	966	M2G	C2-N2	3.13	1.41	1.35
32	2a	1404	5MC	C6-C5	3.12	1.39	1.34
56	2y	55	PSU	C6-C5	3.11	1.38	1.35
54	1w	54	5MU	C6-C5	3.10	1.39	1.34
1	1A	1939	5MU	C6-C5	3.06	1.39	1.34
1	1A	1939	5MU	C4-N3	-3.03	1.33	1.38
54	2w	76	F3N	O4'-C1'	3.02	1.45	1.41
55	1x	55	PSU	C6-C5	3.01	1.38	1.35
32	1a	1407	5MC	C6-C5	2.97	1.39	1.34
54	1w	8	4SU	C4-N3	-2.97	1.34	1.37
55	1x	54	5MU	C6-C5	2.96	1.39	1.34
1	1A	1942	5MC	C6-C5	2.94	1.39	1.34
32	1a	966	M2G	C2-N2	2.94	1.40	1.35
55	1x	32	5MC	C6-C5	2.93	1.39	1.34
55	2x	54	5MU	C6-C5	2.93	1.39	1.34
54	1w	54	5MU	C4-N3	-2.92	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	8	4SU	C5-C4	-2.92	1.38	1.42
56	1y	54	5MU	C6-C5	2.91	1.39	1.34
56	2y	54	5MU	C6-C5	2.91	1.39	1.34
54	2w	76	F3N	C5-C4	-2.90	1.33	1.40
54	2w	37	MIA	C5-C4	2.88	1.48	1.40
32	2a	1407	5MC	C6-C5	2.88	1.39	1.34
32	1a	967	5MC	C6-C5	2.85	1.39	1.34
32	1a	1400	5MC	C6-C5	2.85	1.39	1.34
32	1a	1404	5MC	C6-C5	2.83	1.39	1.34
1	1A	1917	PSU	C4-N3	-2.82	1.33	1.38
54	1w	76	F3N	C5-C4	-2.81	1.33	1.40
56	1y	37	MIA	C2-N3	2.80	1.36	1.32
1	1A	2251	OMG	C6-N1	-2.79	1.33	1.37
55	1x	76	31H	C5-C4	-2.79	1.33	1.40
56	1y	37	MIA	C5-C4	2.79	1.48	1.40
54	1w	8	4SU	C5-C4	-2.78	1.39	1.42
1	2A	1939	5MU	C4-N3	-2.78	1.33	1.38
54	1w	39	PSU	C4-N3	-2.78	1.33	1.38
1	1A	1915	5MU	C6-C5	2.74	1.39	1.34
1	2A	1939	5MU	C6-C5	2.74	1.39	1.34
1	1A	1917	PSU	C6-C5	2.73	1.38	1.35
56	2y	55	PSU	C4-N3	-2.72	1.33	1.38
55	2x	76	31H	C5-C4	-2.70	1.33	1.40
56	2y	54	5MU	C2-N1	2.69	1.42	1.38
56	2y	37	MIA	C5-C4	2.68	1.48	1.40
1	2A	2251	OMG	C6-N1	-2.68	1.33	1.37
55	1x	54	5MU	C4-C5	2.67	1.49	1.44
55	2x	54	5MU	C4-N3	-2.67	1.33	1.38
32	2a	967	5MC	C6-C5	2.67	1.39	1.34
1	2A	1915	5MU	C6-C5	2.65	1.38	1.34
1	2A	1915	5MU	C4-N3	-2.65	1.33	1.38
55	2x	32	5MC	C6-C5	2.64	1.38	1.34
56	1y	54	5MU	C4-C5	2.63	1.49	1.44
54	2w	54	5MU	C4-N3	-2.62	1.34	1.38
55	1x	54	5MU	C4-N3	-2.62	1.34	1.38
1	1A	1962	5MC	C6-C5	2.61	1.38	1.34
56	2y	39	PSU	C4-N3	-2.61	1.34	1.38
32	1a	516	PSU	C4-N3	-2.60	1.34	1.38
1	2A	2605	PSU	C6-C5	2.60	1.38	1.35
1	1A	1915	5MU	C2-N1	2.60	1.42	1.38
54	2w	54	5MU	C6-C5	2.59	1.38	1.34
1	1A	2605	PSU	C4-N3	-2.59	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	76	31H	C6-C5	-2.58	1.33	1.43
55	2x	76	31H	C6-C5	-2.57	1.33	1.43
54	1w	76	F3N	C6-C5	-2.56	1.33	1.43
55	2x	54	5MU	C4-C5	2.56	1.49	1.44
56	2y	37	MIA	C2-N3	2.56	1.36	1.32
1	1A	1915	5MU	C4-N3	-2.56	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.54	1.34	1.37
1	2A	1942	5MC	C6-C5	2.54	1.38	1.34
32	2a	1400	5MC	C6-C5	2.53	1.38	1.34
56	1y	39	PSU	C4-N3	-2.53	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.52	1.34	1.38
56	2y	8	4SU	C5-C4	-2.52	1.39	1.42
56	1y	54	5MU	C2-N1	2.52	1.42	1.38
54	2w	55	PSU	C4-N3	-2.51	1.34	1.38
1	2A	2552	2MU	C4-N3	-2.50	1.34	1.38
54	2w	8	4SU	C5-C4	-2.50	1.39	1.42
1	1A	1911	PSU	C4-N3	-2.50	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.48	1.34	1.37
1	2A	1962	5MC	C6-N1	-2.48	1.33	1.38
54	2w	76	F3N	C6-C5	-2.47	1.34	1.43
1	2A	1915	5MU	C4-C5	2.47	1.48	1.44
1	2A	1911	PSU	C4-N3	-2.47	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.47	1.33	1.38
54	1w	32	PSU	C4-N3	-2.46	1.34	1.38
55	1x	55	PSU	C4-N3	-2.46	1.34	1.38
54	2w	39	PSU	C4-N3	-2.46	1.34	1.38
1	2A	1915	5MU	C2-N1	2.45	1.42	1.38
1	2A	1942	5MC	C6-N1	-2.43	1.33	1.38
32	2a	967	5MC	C6-N1	-2.42	1.33	1.38
56	1y	55	PSU	C4-N3	-2.42	1.34	1.38
55	2x	55	PSU	C4-N3	-2.42	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.41	1.33	1.38
32	2a	1498	UR3	C2-N1	2.40	1.42	1.38
32	2a	527	G7M	C6-N1	-2.40	1.34	1.37
54	1w	55	PSU	C4-N3	-2.39	1.34	1.38
54	1w	37	MIA	C5-C4	2.38	1.47	1.40
56	1y	32	PSU	C4-N3	-2.38	1.34	1.38
56	1y	54	5MU	C4-N3	-2.37	1.34	1.38
55	2x	32	5MC	C6-N1	-2.35	1.34	1.38
54	1w	54	5MU	C2-N1	2.35	1.42	1.38
54	1w	54	5MU	C4-C5	2.35	1.48	1.44
54	2w	32	PSU	C4-N3	-2.34	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1939	5MU	C6-N1	-2.34	1.34	1.38
1	2A	1962	5MC	C6-C5	2.33	1.38	1.34
54	1w	8	4SU	C2-N1	2.33	1.42	1.38
32	2a	516	PSU	C4-N3	-2.33	1.34	1.38
56	2y	54	5MU	C4-C5	2.31	1.48	1.44
1	2A	2605	PSU	C4-N3	-2.31	1.34	1.38
1	1A	1939	5MU	C4-C5	2.30	1.48	1.44
56	1y	8	4SU	C5-C4	-2.29	1.39	1.42
55	1x	32	5MC	C6-N1	-2.29	1.34	1.38
56	2y	54	5MU	C4-N3	-2.29	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.28	1.34	1.38
56	1y	8	4SU	C2-N1	2.28	1.42	1.38
32	2a	1400	5MC	C6-N1	-2.27	1.34	1.38
1	2A	2503	8AH	C5-C4	2.26	1.46	1.40
56	2y	46	G7M	C6-N1	-2.26	1.34	1.37
1	2A	1939	5MU	C2-N1	2.25	1.42	1.38
56	2y	8	4SU	C2-N3	-2.24	1.34	1.38
1	1A	2552	2MU	C4-N3	-2.24	1.34	1.38
55	1x	8	4SU	O2-C2	2.24	1.27	1.23
54	2w	54	5MU	C4-C5	2.23	1.48	1.44
32	2a	1407	5MC	C6-N1	-2.21	1.34	1.38
54	1w	46	G7M	C6-N1	-2.21	1.34	1.37
32	2a	1404	5MC	C6-N1	-2.21	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.21	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.20	1.34	1.38
54	1w	54	5MU	C2-N3	-2.20	1.34	1.38
54	1w	39	PSU	C2-N3	-2.19	1.33	1.37
32	1a	527	G7M	C6-N1	-2.19	1.34	1.37
1	1A	1939	5MU	C2-N3	-2.19	1.34	1.38
55	2x	8	4SU	O2-C2	2.17	1.27	1.23
55	2x	76	31H	C5-N7	-2.16	1.31	1.39
55	2x	54	5MU	C2-N3	-2.16	1.34	1.38
1	1A	1915	5MU	C4-C5	2.15	1.48	1.44
54	2w	37	MIA	C2-N3	2.15	1.37	1.34
1	1A	1942	5MC	C6-N1	-2.15	1.34	1.38
54	2w	76	F3N	C5-N7	-2.15	1.31	1.39
32	1a	1400	5MC	C6-N1	-2.14	1.34	1.38
56	2y	32	PSU	C4-N3	-2.13	1.34	1.38
55	2x	8	4SU	C6-C5	2.12	1.40	1.35
32	1a	966	M2G	C6-N1	-2.12	1.34	1.37
32	2a	1498	UR3	C6-C5	2.12	1.39	1.35
1	1A	2552	2MU	C2-N1	2.10	1.41	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	8	4SU	C2-N3	-2.10	1.34	1.38
56	2y	8	4SU	C2-N1	2.10	1.41	1.38
1	2A	1915	5MU	C2-N3	-2.09	1.34	1.38
55	1x	54	5MU	C2-N1	2.08	1.41	1.38
32	1a	1498	UR3	C6-C5	2.07	1.39	1.35
56	1y	8	4SU	C2-N3	-2.06	1.34	1.38
55	1x	54	5MU	C6-N1	-2.06	1.34	1.38
1	2A	1939	5MU	C4-C5	2.05	1.48	1.44
55	2x	54	5MU	C6-N1	-2.05	1.34	1.38
32	1a	967	5MC	C6-N1	-2.04	1.34	1.38
56	1y	46	G7M	C6-N1	-2.04	1.34	1.37
55	1x	8	4SU	C6-C5	2.04	1.39	1.35
1	2A	2552	2MU	C5-C4	2.04	1.48	1.43
1	2A	1920	OMC	C6-C5	2.04	1.39	1.35
56	2y	55	PSU	C2-N3	-2.03	1.34	1.37
55	1x	76	31H	C5-N7	-2.03	1.32	1.39
56	1y	8	4SU	C6-C5	2.02	1.39	1.35
54	2w	8	4SU	C2-N1	2.00	1.41	1.38

All (280) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	-14.20	76.74	102.44
43	2l	92	0TD	CSB-SB-CB	-11.41	81.80	102.44
54	1w	37	MIA	C12-C13-C14	-9.36	108.93	127.14
54	2w	8	4SU	C4-N3-C2	-7.37	120.18	127.34
1	2A	2503	8AH	C2-N3-C4	7.23	121.40	115.52
1	1A	2503	8AH	C2-N3-C4	6.65	120.93	115.52
54	2w	8	4SU	C5-C4-N3	6.49	120.71	114.69
1	2A	1911	PSU	N1-C2-N3	6.39	122.38	115.13
1	1A	1917	PSU	N1-C2-N3	6.30	122.27	115.13
54	1w	8	4SU	C5-C4-N3	6.24	120.48	114.69
1	1A	2605	PSU	N1-C2-N3	6.23	122.19	115.13
32	1a	1498	UR3	C4-N3-C2	-6.04	118.88	124.56
56	2y	55	PSU	N1-C2-N3	5.98	121.91	115.13
56	2y	32	PSU	N1-C2-N3	5.92	121.84	115.13
1	1A	1911	PSU	N1-C2-N3	5.91	121.82	115.13
32	2a	1498	UR3	C4-N3-C2	-5.83	119.07	124.56
1	2A	2605	PSU	N1-C2-N3	5.82	121.72	115.13
56	1y	55	PSU	N1-C2-N3	5.82	121.72	115.13
1	2A	1915	5MU	C4-N3-C2	-5.81	119.83	127.35
56	1y	32	PSU	N1-C2-N3	5.77	121.67	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	76	F3N	N3-C2-N1	-5.73	119.72	128.68
1	2A	1915	5MU	C5-C4-N3	5.71	120.19	115.31
55	2x	76	31H	N3-C2-N1	-5.70	119.77	128.68
54	1w	32	PSU	N1-C2-N3	5.68	121.56	115.13
55	1x	76	31H	N3-C2-N1	-5.67	119.81	128.68
54	1w	55	PSU	N1-C2-N3	5.66	121.54	115.13
54	2w	76	F3N	N3-C2-N1	-5.66	119.83	128.68
54	2w	55	PSU	N1-C2-N3	5.61	121.49	115.13
1	2A	1917	PSU	N1-C2-N3	5.60	121.47	115.13
32	2a	516	PSU	N1-C2-N3	5.57	121.44	115.13
55	1x	55	PSU	N1-C2-N3	5.54	121.40	115.13
54	2w	39	PSU	N1-C2-N3	5.51	121.38	115.13
54	2w	32	PSU	N1-C2-N3	5.51	121.37	115.13
54	1w	8	4SU	C4-N3-C2	-5.49	122.01	127.34
32	1a	516	PSU	N1-C2-N3	5.47	121.33	115.13
1	2A	1939	5MU	C4-N3-C2	-5.46	120.28	127.35
55	2x	55	PSU	N1-C2-N3	5.44	121.29	115.13
1	1A	1939	5MU	C4-N3-C2	-5.42	120.34	127.35
56	2y	54	5MU	C4-N3-C2	-5.36	120.42	127.35
1	1A	1915	5MU	C4-N3-C2	-5.23	120.59	127.35
56	1y	54	5MU	N3-C2-N1	5.21	121.81	114.89
56	2y	8	4SU	C5-C4-N3	5.14	119.46	114.69
1	1A	1915	5MU	N3-C2-N1	5.11	121.68	114.89
56	1y	54	5MU	C4-N3-C2	-5.05	120.81	127.35
56	2y	54	5MU	O4-C4-C5	-5.04	119.05	124.90
1	2A	1939	5MU	N3-C2-N1	5.03	121.56	114.89
56	2y	39	PSU	N1-C2-N3	5.02	120.82	115.13
56	1y	39	PSU	N1-C2-N3	5.01	120.81	115.13
54	1w	37	MIA	C12-N6-C6	-5.00	115.15	122.55
1	1A	1939	5MU	N3-C2-N1	4.97	121.49	114.89
1	2A	1915	5MU	N3-C2-N1	4.95	121.46	114.89
56	2y	54	5MU	N3-C2-N1	4.95	121.46	114.89
1	2A	1939	5MU	C5-C4-N3	4.92	119.51	115.31
32	1a	1519	MA6	N3-C2-N1	-4.90	121.02	128.68
1	1A	1939	5MU	C5-C4-N3	4.90	119.49	115.31
56	2y	54	5MU	C5-C4-N3	4.89	119.48	115.31
1	1A	2552	2MU	N3-C2-N1	4.80	121.26	114.89
55	1x	8	4SU	S4-C4-N3	-4.77	115.51	120.21
1	2A	1911	PSU	O2-C2-N1	-4.75	117.56	122.79
1	1A	1939	5MU	C5-C6-N1	-4.74	118.46	123.34
55	1x	54	5MU	N3-C2-N1	4.74	121.18	114.89
56	1y	8	4SU	C4-N3-C2	-4.73	122.75	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	54	5MU	N3-C2-N1	4.69	121.11	114.89
1	2A	2552	2MU	N3-C2-N1	4.67	121.09	114.89
32	2a	1519	MA6	N3-C2-N1	-4.67	121.38	128.68
55	1x	54	5MU	C4-N3-C2	-4.66	121.31	127.35
32	2a	1518	MA6	N3-C2-N1	-4.64	121.43	128.68
56	1y	8	4SU	C5-C4-N3	4.58	118.94	114.69
54	1w	39	PSU	N1-C2-N3	4.57	120.31	115.13
1	1A	1915	5MU	C5-C4-N3	4.57	119.21	115.31
55	2x	54	5MU	C4-N3-C2	-4.57	121.44	127.35
1	1A	2552	2MU	C4-N3-C2	-4.55	120.58	126.58
1	2A	1939	5MU	O4-C4-C5	-4.51	119.67	124.90
56	2y	8	4SU	C4-N3-C2	-4.43	123.04	127.34
55	1x	8	4SU	C6-C5-C4	-4.42	116.12	119.95
1	2A	1915	5MU	O4-C4-C5	-4.36	119.84	124.90
54	1w	54	5MU	N3-C2-N1	4.36	120.68	114.89
54	2w	37	MIA	C5-C6-N1	-4.35	117.19	120.81
54	2w	8	4SU	N3-C2-N1	4.33	120.64	114.89
1	1A	2605	PSU	C4-N3-C2	-4.32	120.11	126.34
54	1w	37	MIA	C15-C14-C13	-4.32	110.17	122.65
1	1A	2605	PSU	O2-C2-N1	-4.31	118.04	122.79
1	1A	1915	5MU	O4-C4-C5	-4.26	119.96	124.90
54	1w	8	4SU	C5-C4-S4	-4.23	119.02	124.47
32	2a	516	PSU	C4-N3-C2	-4.19	120.30	126.34
54	2w	54	5MU	N3-C2-N1	4.17	120.42	114.89
1	2A	2552	2MU	C4-N3-C2	-4.16	121.09	126.58
56	1y	54	5MU	C5-C4-N3	4.13	118.83	115.31
1	1A	1917	PSU	C4-N3-C2	-4.12	120.41	126.34
1	2A	2605	PSU	C4-N3-C2	-4.11	120.41	126.34
32	1a	1518	MA6	N3-C2-N1	-4.10	122.27	128.68
1	1A	1942	5MC	C5-C6-N1	-4.10	119.12	123.34
54	1w	32	PSU	C4-N3-C2	-4.09	120.44	126.34
54	2w	54	5MU	C4-N3-C2	-4.09	122.06	127.35
54	1w	55	PSU	C4-N3-C2	-4.07	120.48	126.34
55	1x	55	PSU	C4-N3-C2	-4.05	120.51	126.34
54	1w	37	MIA	C16-C14-C13	-4.04	110.98	122.65
32	1a	967	5MC	C5-C6-N1	-3.99	119.23	123.34
32	1a	516	PSU	C4-N3-C2	-3.98	120.60	126.34
54	1w	37	MIA	C11-S10-C2	-3.97	99.30	102.27
56	2y	32	PSU	O2-C2-N1	-3.96	118.43	122.79
55	2x	54	5MU	C5-C4-N3	3.94	118.67	115.31
54	1w	37	MIA	C2-N3-C4	3.94	120.75	115.32
55	1x	8	4SU	O2-C2-N1	3.93	128.01	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	55	PSU	C4-N3-C2	-3.92	120.69	126.34
1	2A	1939	5MU	C5-C6-N1	-3.92	119.31	123.34
56	1y	55	PSU	C4-N3-C2	-3.90	120.72	126.34
54	1w	54	5MU	C4-N3-C2	-3.89	122.32	127.35
56	1y	54	5MU	O4-C4-C5	-3.88	120.41	124.90
32	1a	1404	5MC	C5-C6-N1	-3.88	119.35	123.34
56	2y	55	PSU	C4-N3-C2	-3.87	120.76	126.34
1	2A	1917	PSU	C4-N3-C2	-3.87	120.76	126.34
1	2A	1911	PSU	C4-N3-C2	-3.87	120.76	126.34
54	2w	54	5MU	C5-C4-N3	3.87	118.61	115.31
1	2A	2503	8AH	C5-C6-N1	-3.84	118.49	121.01
1	1A	1939	5MU	O4-C4-C5	-3.84	120.46	124.90
32	2a	967	5MC	C5-C6-N1	-3.83	119.40	123.34
1	2A	1915	5MU	C5-C6-N1	-3.83	119.40	123.34
1	1A	2503	8AH	C5-C6-N1	-3.82	118.50	121.01
55	1x	32	5MC	C5-C6-N1	-3.82	119.41	123.34
55	1x	54	5MU	C5-C4-N3	3.81	118.56	115.31
1	1A	1917	PSU	O2-C2-N1	-3.81	118.60	122.79
1	2A	1962	5MC	C5-C6-N1	-3.80	119.43	123.34
54	2w	8	4SU	C5-C4-S4	-3.76	119.62	124.47
56	1y	32	PSU	C4-N3-C2	-3.75	120.93	126.34
55	1x	54	5MU	C5-C6-N1	-3.74	119.49	123.34
1	1A	1911	PSU	C4-N3-C2	-3.74	120.95	126.34
32	2a	1400	5MC	C5-C6-N1	-3.72	119.51	123.34
32	2a	1407	5MC	C5-C6-N1	-3.72	119.51	123.34
54	2w	39	PSU	C4-N3-C2	-3.71	120.99	126.34
54	1w	54	5MU	C5-C4-N3	3.69	118.46	115.31
54	2w	32	PSU	C4-N3-C2	-3.66	121.07	126.34
56	2y	32	PSU	C4-N3-C2	-3.65	121.08	126.34
55	2x	54	5MU	C5-C6-N1	-3.63	119.60	123.34
54	2w	37	MIA	C2-N3-C4	3.61	120.30	115.32
32	1a	1407	5MC	C5-C6-N1	-3.59	119.64	123.34
54	2w	55	PSU	C4-N3-C2	-3.57	121.19	126.34
1	2A	1942	5MC	C5-C6-N1	-3.57	119.66	123.34
1	1A	2552	2MU	C2'-C1'-N1	-3.54	107.36	114.22
32	2a	516	PSU	O2-C2-N1	-3.52	118.92	122.79
56	2y	54	5MU	C5-C6-N1	-3.50	119.74	123.34
1	2A	2605	PSU	O2-C2-N1	-3.49	118.95	122.79
54	2w	54	5MU	O4-C4-C5	-3.48	120.87	124.90
56	1y	55	PSU	O2-C2-N1	-3.47	118.97	122.79
55	2x	32	5MC	C5-C6-N1	-3.44	119.80	123.34
56	1y	32	PSU	O2-C2-N1	-3.39	119.06	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1400	5MC	C5-C6-N1	-3.35	119.89	123.34
54	1w	54	5MU	C5-C6-N1	-3.35	119.89	123.34
55	1x	55	PSU	O2-C2-N1	-3.34	119.11	122.79
32	2a	1404	5MC	C5-C6-N1	-3.32	119.93	123.34
32	1a	1519	MA6	C4-C5-N7	-3.30	105.96	109.40
54	1w	55	PSU	O2-C2-N1	-3.29	119.16	122.79
1	1A	2552	2MU	O4-C4-C5	-3.29	119.38	125.16
56	1y	37	MIA	N3-C2-N1	-3.29	123.54	128.68
32	2a	1519	MA6	C4-C5-N7	-3.29	105.97	109.40
56	1y	39	PSU	C4-N3-C2	-3.25	121.66	126.34
56	1y	8	4SU	N3-C2-N1	3.23	119.18	114.89
55	2x	54	5MU	O4-C4-C5	-3.22	121.17	124.90
1	1A	1962	5MC	C5-C6-N1	-3.21	120.03	123.34
43	2l	92	0TD	OD2-CG-CB	3.19	120.04	113.15
1	2A	2503	8AH	C4-C5-N7	-3.18	106.24	109.47
1	2A	1917	PSU	O2-C2-N1	-3.17	119.30	122.79
54	1w	54	5MU	O4-C4-C5	-3.17	121.23	124.90
56	2y	37	MIA	N3-C2-N1	-3.14	123.78	128.68
56	2y	39	PSU	C4-N3-C2	-3.11	121.85	126.34
1	1A	1915	5MU	C5-C6-N1	-3.09	120.16	123.34
55	2x	8	4SU	C6-C5-C4	-3.07	117.29	119.95
55	2x	76	31H	O4'-C1'-C2'	-3.05	102.48	106.93
1	1A	2552	2MU	O2-C2-N1	-3.03	118.76	122.79
55	1x	54	5MU	O4-C4-C5	-3.02	121.40	124.90
54	1w	37	MIA	C5-C6-N1	-3.01	118.31	120.81
1	2A	2552	2MU	C5-C4-N3	3.01	119.34	114.84
54	2w	37	MIA	C12-N6-C6	-3.00	120.29	122.87
54	2w	55	PSU	O2-C2-N1	-2.96	119.53	122.79
54	2w	32	PSU	O2-C2-N1	-2.95	119.54	122.79
1	1A	2503	8AH	C2-N1-C6	2.93	122.66	118.08
56	1y	54	5MU	C5-C6-N1	-2.92	120.33	123.34
32	1a	1404	5MC	C5-C4-N3	-2.91	118.53	121.67
55	1x	32	5MC	C5-C4-N3	-2.90	118.54	121.67
55	1x	8	4SU	C4-N3-C2	2.90	130.16	127.34
1	1A	2552	2MU	C5-C4-N3	2.89	119.16	114.84
54	1w	37	MIA	C2-N1-C6	2.89	122.36	117.19
56	2y	8	4SU	N3-C2-N1	2.87	118.70	114.89
54	2w	54	5MU	C5-C6-N1	-2.86	120.40	123.34
56	2y	8	4SU	C5-C4-S4	-2.85	120.79	124.47
1	1A	1911	PSU	O2-C2-N1	-2.81	119.70	122.79
55	1x	76	31H	O4'-C1'-C2'	-2.81	102.82	106.93
32	2a	1404	5MC	C5-C4-N3	-2.79	118.66	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	8	4SU	C5-C4-N3	2.79	117.28	114.69
1	2A	2552	2MU	O4-C4-C5	-2.77	120.28	125.16
43	1l	92	0TD	OD2-CG-CB	2.77	119.14	113.15
32	2a	1518	MA6	C4-C5-N7	-2.75	106.53	109.40
54	1w	8	4SU	N3-C2-N1	2.74	118.53	114.89
56	2y	55	PSU	O2-C2-N1	-2.74	119.77	122.79
54	2w	37	MIA	C2-N1-C6	2.74	122.09	117.19
56	1y	37	MIA	C4-C5-N7	-2.71	106.58	109.40
1	1A	1962	5MC	CM5-C5-C6	-2.69	119.25	122.85
32	2a	1407	5MC	C5-C4-N3	-2.69	118.77	121.67
54	1w	37	MIA	C4-C5-N7	-2.67	106.61	109.40
54	2w	39	PSU	O2-C2-N1	-2.67	119.85	122.79
32	1a	1518	MA6	C4-C5-N7	-2.67	106.62	109.40
1	1A	1942	5MC	C5-C4-N3	-2.66	118.80	121.67
1	2A	1920	OMC	O2-C2-N3	-2.66	118.00	122.33
55	1x	76	31H	CA-N-CN	-2.65	118.75	122.82
54	1w	32	PSU	O2-C2-N1	-2.63	119.89	122.79
32	1a	1207	2MG	C8-N7-C5	2.63	108.00	102.99
56	2y	37	MIA	C4-C5-N7	-2.60	106.69	109.40
32	1a	967	5MC	C5-C4-N3	-2.60	118.87	121.67
1	2A	1915	5MU	C5M-C5-C4	2.57	121.59	118.77
55	2x	55	PSU	O2-C2-N1	-2.56	119.97	122.79
32	1a	516	PSU	O2-C2-N1	-2.56	119.97	122.79
55	1x	76	31H	O2'-C2'-C3'	2.56	117.44	111.16
56	1y	8	4SU	C5-C4-S4	-2.55	121.17	124.47
55	2x	32	5MC	C5-C4-N3	-2.55	118.92	121.67
32	1a	1498	UR3	C3U-N3-C4	2.55	121.53	117.89
32	2a	1407	5MC	O2-C2-N3	-2.53	118.22	122.33
1	1A	2251	OMG	C8-N7-C5	2.52	107.79	102.99
1	2A	2552	2MU	C2'-C1'-N1	-2.52	109.33	114.22
1	1A	1915	5MU	O2-C2-N1	-2.52	119.44	122.79
56	1y	54	5MU	O2-C2-N1	-2.51	119.45	122.79
54	1w	8	4SU	C1'-N1-C2	2.51	122.11	117.57
54	1w	39	PSU	C4-N3-C2	-2.51	122.73	126.34
43	2l	92	0TD	OD1-CG-CB	-2.50	117.21	122.44
1	1A	2503	8AH	C4-C5-N7	-2.47	106.96	109.47
1	1A	1920	OMC	O2-C2-N3	-2.46	118.32	122.33
1	2A	2251	OMG	C8-N7-C5	2.45	107.66	102.99
56	1y	39	PSU	C6-C5-C4	-2.45	116.48	118.20
55	1x	54	5MU	O2-C2-N1	-2.45	119.54	122.79
32	2a	1207	2MG	C8-N7-C5	2.43	107.63	102.99
32	2a	1402	4OC	C6-C5-C4	2.43	119.94	116.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	966	M2G	C8-N7-C5	2.42	107.61	102.99
54	2w	54	5MU	O2-C2-N1	-2.42	119.57	122.79
55	2x	8	4SU	C5-C4-N3	2.42	116.93	114.69
1	2A	1962	5MC	C5-C4-N3	-2.38	119.10	121.67
1	2A	2503	8AH	C2-N1-C6	2.38	121.79	118.08
32	1a	966	M2G	C5-C6-N1	2.35	118.11	113.95
1	2A	1939	5MU	O2-C2-N1	-2.35	119.66	122.79
1	1A	1939	5MU	O2-C2-N1	-2.35	119.66	122.79
54	2w	37	MIA	C4-C5-N7	-2.33	106.97	109.40
32	1a	1400	5MC	C5-C4-N3	-2.33	119.16	121.67
32	2a	967	5MC	C5-C4-N3	-2.33	119.16	121.67
1	1A	1962	5MC	C5-C4-N3	-2.32	119.17	121.67
32	1a	1407	5MC	C5-C4-N3	-2.31	119.18	121.67
54	1w	37	MIA	N3-C2-N1	-2.29	122.76	126.98
55	1x	32	5MC	O2-C2-N3	-2.29	118.60	122.33
55	1x	76	31H	OCN-CN-N	-2.29	119.23	125.27
1	2A	1942	5MC	C5-C4-N3	-2.29	119.20	121.67
55	2x	54	5MU	O2-C2-N1	-2.28	119.75	122.79
1	2A	2251	OMG	C5-C6-N1	2.27	117.97	113.95
1	2A	1915	5MU	O2-C2-N1	-2.27	119.77	122.79
1	1A	2251	OMG	C5-C6-N1	2.27	117.96	113.95
32	2a	966	M2G	C5-C6-N1	2.26	117.95	113.95
54	2w	54	5MU	C5M-C5-C4	2.23	121.22	118.77
32	1a	966	M2G	O6-C6-C5	-2.21	120.05	124.37
32	1a	966	M2G	C8-N7-C5	2.19	107.17	102.99
54	2w	37	MIA	C11-S10-C2	-2.19	100.64	102.27
1	2A	2552	2MU	O2-C2-N1	-2.18	119.89	122.79
32	2a	1400	5MC	C5-C4-N3	-2.15	119.35	121.67
55	2x	8	4SU	C1'-N1-C2	2.15	121.46	117.57
55	1x	8	4SU	O2-C2-N3	-2.14	117.51	121.50
1	1A	1942	5MC	O2-C2-N3	-2.14	118.85	122.33
55	1x	8	4SU	C5-C4-S4	2.13	127.20	124.47
32	1a	516	PSU	C5-C6-N1	-2.12	118.92	122.11
32	2a	1498	UR3	C3U-N3-C4	2.12	120.92	117.89
55	1x	55	PSU	C5-C6-N1	-2.11	118.94	122.11
55	2x	8	4SU	O2-C2-N1	2.10	125.58	122.79
32	2a	1207	2MG	C5-C6-N1	2.10	117.66	113.95
32	1a	1402	4OC	C6-C5-C4	2.10	119.53	116.96
32	1a	1207	2MG	C5-C6-N1	2.08	117.62	113.95
56	2y	55	PSU	O4'-C1'-C2'	2.07	108.06	105.14
55	2x	76	31H	O2'-C2'-C3'	2.07	116.23	111.16
55	2x	8	4SU	S4-C4-N3	-2.06	118.18	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1962	5MC	C1'-N1-C6	-2.06	117.70	121.12
55	2x	54	5MU	C5M-C5-C4	2.05	121.02	118.77
1	1A	1915	5MU	C5M-C5-C4	2.05	121.02	118.77
55	2x	55	PSU	C5-C6-N1	-2.04	119.04	122.11
56	2y	54	5MU	C1'-N1-C2	2.04	121.27	117.57
54	2w	8	4SU	O2-C2-N1	-2.04	120.07	122.79
1	2A	1942	5MC	CM5-C5-C6	-2.04	120.13	122.85
1	2A	2251	OMG	O6-C6-C5	-2.01	120.45	124.37

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N3-C2-N2-CM2
43	1l	92	0TD	O-C-CA-CB
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	N6-C12-C13-C14
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16
55	1x	76	31H	C3'-C4'-C5'-O5'
55	1x	76	31H	O4'-C4'-C5'-O5'
56	1y	46	G7M	C4'-C5'-O5'-P
32	2a	1207	2MG	N3-C2-N2-CM2
43	2l	92	0TD	O-C-CA-CB
43	2l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	SB-CB-CG-OD2
54	2w	37	MIA	C5-C6-N6-C12
54	2w	37	MIA	N1-C6-N6-C12
55	2x	76	31H	C3'-C4'-C5'-O5'
55	2x	76	31H	O4'-C4'-C5'-O5'
56	2y	54	5MU	C3'-C4'-C5'-O5'
56	2y	54	5MU	O4'-C4'-C5'-O5'
56	2y	55	PSU	C2'-C1'-C5-C4
56	2y	55	PSU	C2'-C1'-C5-C6
56	2y	55	PSU	C3'-C4'-C5'-O5'
55	2x	76	31H	CB-CG-SD-CE
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
56	2y	55	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	1a	527	G7M	C3'-C4'-C5'-O5'
56	1y	46	G7M	C3'-C4'-C5'-O5'
55	1x	76	31H	CB-CG-SD-CE
56	1y	8	4SU	C3'-C4'-C5'-O5'
56	1y	8	4SU	O4'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
54	2w	46	G7M	C4'-C5'-O5'-P
56	2y	37	MIA	C3'-C4'-C5'-O5'
54	1w	46	G7M	C4'-C5'-O5'-P
43	2l	92	0TD	SB-CB-CG-OD1
32	1a	527	G7M	O4'-C4'-C5'-O5'
55	1x	76	31H	C4'-C5'-O5'-P
55	2x	76	31H	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
32	2a	527	G7M	C4'-C5'-O5'-P
32	1a	1402	4OC	O4'-C4'-C5'-O5'
1	1A	2503	8AH	C4'-C5'-O5'-P
32	1a	1519	MA6	C4'-C5'-O5'-P
32	1a	527	G7M	C4'-C5'-O5'-P
56	1y	46	G7M	O4'-C4'-C5'-O5'
56	1y	55	PSU	O4'-C1'-C5-C4
56	2y	55	PSU	O4'-C1'-C5-C4
56	1y	8	4SU	C4'-C5'-O5'-P
43	2l	92	0TD	CA-CB-SB-CSB
56	1y	54	5MU	O4'-C4'-C5'-O5'
1	1A	1920	OMC	C2'-C1'-N1-C2
32	2a	527	G7M	O4'-C4'-C5'-O5'
56	1y	55	PSU	O4'-C1'-C5-C6
32	1a	967	5MC	O4'-C4'-C5'-O5'
56	2y	37	MIA	O4'-C4'-C5'-O5'
1	1A	2503	8AH	O4'-C4'-C5'-O5'
1	2A	2503	8AH	O4'-C4'-C5'-O5'
43	1l	92	0TD	SB-CB-CG-OD1
32	2a	1402	4OC	O4'-C4'-C5'-O5'
56	2y	8	4SU	C2'-C1'-N1-C2

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 2472 ligands modelled in this entry, 2470 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
60	SF4	2d	501	35	0,12,12	-	-	-		
60	SF4	1d	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
60	SF4	2d	501	35	-	-	0/6/5/5
60	SF4	1d	302	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	2860/2915 (98%)	0.60	169 (5%) 22 26	22, 39, 97, 108	0
1	2A	2789/2915 (95%)	0.52	149 (5%) 26 31	38, 59, 96, 109	0
2	1B	120/121 (99%)	0.01	0 100 100	34, 53, 65, 87	0
2	2B	120/121 (99%)	-0.16	0 100 100	62, 73, 84, 97	0
3	1D	275/276 (99%)	0.80	4 (1%) 73 79	24, 39, 53, 84	0
3	2D	275/276 (99%)	0.89	4 (1%) 73 79	34, 50, 62, 78	0
4	1E	204/206 (99%)	0.56	1 (0%) 91 94	21, 41, 60, 73	0
4	2E	204/206 (99%)	0.75	15 (7%) 14 18	41, 64, 76, 83	0
5	1F	202/210 (96%)	0.53	2 (0%) 82 86	21, 44, 68, 82	0
5	2F	202/210 (96%)	0.53	1 (0%) 91 94	38, 64, 78, 85	0
6	1G	181/182 (99%)	0.37	3 (1%) 70 76	46, 58, 72, 86	0
6	2G	181/182 (99%)	0.53	9 (4%) 28 34	63, 74, 82, 88	0
7	1H	174/180 (96%)	0.39	0 100 100	39, 54, 67, 72	0
7	2H	174/180 (96%)	3.23	136 (78%) 0 0	73, 86, 92, 97	0
8	1I	146/148 (98%)	0.38	6 (4%) 37 44	51, 73, 80, 84	0
8	2I	146/148 (98%)	0.74	13 (8%) 9 11	52, 73, 84, 91	0
9	1N	140/140 (100%)	0.55	0 100 100	26, 38, 59, 75	0
9	2N	140/140 (100%)	0.99	20 (14%) 2 3	51, 69, 80, 84	0
10	1O	122/122 (100%)	0.59	0 100 100	30, 42, 59, 62	0
10	2O	122/122 (100%)	1.03	16 (13%) 3 4	50, 63, 73, 78	0
11	1P	149/150 (99%)	0.56	6 (4%) 38 45	24, 52, 69, 77	0
11	2P	149/150 (99%)	1.32	30 (20%) 1 1	42, 64, 79, 88	0
12	1Q	141/141 (100%)	0.56	1 (0%) 87 90	26, 42, 57, 71	0
12	2Q	141/141 (100%)	1.52	40 (28%) 0 0	46, 68, 78, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	0.49	0 100 100	28, 37, 51, 57	0
13	2R	118/118 (100%)	0.66	6 (5%) 28 33	48, 58, 66, 76	0
14	1S	110/112 (98%)	0.38	1 (0%) 84 88	40, 53, 64, 69	0
14	2S	110/112 (98%)	0.85	11 (10%) 7 9	59, 70, 78, 84	0
15	1T	131/146 (89%)	0.52	2 (1%) 73 79	37, 46, 72, 84	0
15	2T	131/146 (89%)	0.75	10 (7%) 13 17	56, 66, 81, 84	0
16	1U	116/118 (98%)	0.64	1 (0%) 84 88	22, 31, 44, 62	0
16	2U	116/118 (98%)	0.76	6 (5%) 27 32	45, 66, 76, 81	0
17	1V	101/101 (100%)	0.37	0 100 100	24, 38, 55, 65	0
17	2V	101/101 (100%)	0.48	7 (6%) 16 20	47, 72, 79, 84	0
18	1W	112/113 (99%)	0.52	0 100 100	25, 33, 56, 80	0
18	2W	112/113 (99%)	0.75	3 (2%) 54 61	43, 52, 67, 90	0
19	1X	95/96 (98%)	0.65	1 (1%) 80 85	30, 42, 65, 75	0
19	2X	95/96 (98%)	0.72	3 (3%) 47 55	49, 58, 76, 82	0
20	1Y	107/110 (97%)	0.54	1 (0%) 84 88	39, 52, 69, 82	0
20	2Y	107/110 (97%)	0.95	13 (12%) 4 5	58, 70, 84, 89	0
21	1Z	154/206 (74%)	0.50	6 (3%) 39 45	41, 66, 84, 89	0
21	2Z	160/206 (77%)	1.43	47 (29%) 0 0	72, 82, 90, 92	0
22	10	83/85 (97%)	0.75	2 (2%) 59 65	27, 40, 52, 63	0
22	20	83/85 (97%)	1.19	17 (20%) 1 1	45, 62, 70, 77	0
23	11	97/98 (98%)	0.74	4 (4%) 37 44	31, 50, 71, 76	0
23	21	97/98 (98%)	0.95	10 (10%) 6 8	42, 56, 75, 84	0
24	12	70/72 (97%)	0.73	1 (1%) 75 81	38, 50, 61, 76	0
24	22	70/72 (97%)	0.36	1 (1%) 75 81	56, 68, 76, 86	0
25	13	59/60 (98%)	0.50	0 100 100	27, 37, 63, 82	0
25	23	59/60 (98%)	1.33	13 (22%) 0 0	53, 67, 78, 85	0
26	14	69/71 (97%)	0.55	8 (11%) 4 6	59, 75, 87, 90	0
26	24	69/71 (97%)	1.01	13 (18%) 1 1	71, 84, 91, 93	0
27	15	59/60 (98%)	0.65	0 100 100	22, 34, 49, 57	0
27	25	59/60 (98%)	0.63	1 (1%) 70 76	41, 57, 69, 78	0
28	16	53/54 (98%)	0.44	0 100 100	36, 45, 57, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	1.16	8 (15%) 2 2	47, 59, 67, 77	0
29	17	48/49 (97%)	0.94	3 (6%) 20 23	26, 31, 56, 66	0
29	27	48/49 (97%)	1.17	5 (10%) 6 8	38, 42, 67, 71	0
30	18	64/65 (98%)	0.63	0 100 100	29, 37, 44, 56	0
30	28	64/65 (98%)	1.53	16 (25%) 0 0	46, 56, 61, 68	0
31	19	37/37 (100%)	0.74	1 (2%) 54 61	32, 40, 61, 62	0
31	29	37/37 (100%)	3.32	30 (81%) 0 0	64, 73, 84, 88	0
32	1a	1488/1521 (97%)	0.38	73 (4%) 29 35	35, 67, 94, 109	0
32	2a	1491/1521 (98%)	0.44	92 (6%) 20 24	45, 72, 94, 108	0
33	1b	231/256 (90%)	1.55	78 (33%) 0 0	62, 78, 87, 93	0
33	2b	231/256 (90%)	1.63	70 (30%) 0 0	69, 83, 89, 93	0
34	1c	206/239 (86%)	1.20	45 (21%) 0 0	63, 73, 83, 90	0
34	2c	206/239 (86%)	1.50	66 (32%) 0 0	70, 79, 86, 90	0
35	1d	208/209 (99%)	0.82	17 (8%) 11 14	57, 69, 78, 89	0
35	2d	208/209 (99%)	0.68	15 (7%) 15 18	56, 66, 75, 85	0
36	1e	148/162 (91%)	0.84	14 (9%) 8 10	48, 64, 75, 81	0
36	2e	148/162 (91%)	0.79	11 (7%) 14 18	54, 71, 80, 87	0
37	1f	100/101 (99%)	0.32	0 100 100	55, 68, 76, 80	0
37	2f	100/101 (99%)	0.37	2 (2%) 65 72	55, 66, 74, 81	0
38	1g	155/156 (99%)	1.20	25 (16%) 1 2	61, 71, 85, 91	0
38	2g	155/156 (99%)	1.08	25 (16%) 1 2	68, 75, 85, 96	0
39	1h	137/138 (99%)	0.55	7 (5%) 28 33	55, 65, 72, 76	0
39	2h	137/138 (99%)	0.85	15 (10%) 5 7	64, 72, 78, 81	0
40	1i	127/128 (99%)	2.61	81 (63%) 0 0	51, 78, 85, 88	0
40	2i	127/128 (99%)	2.99	90 (70%) 0 0	68, 83, 88, 91	0
41	1j	97/105 (92%)	1.90	50 (51%) 0 0	57, 78, 87, 93	0
41	2j	96/105 (91%)	2.97	70 (72%) 0 0	72, 83, 89, 96	0
42	1k	114/129 (88%)	0.70	5 (4%) 34 41	44, 64, 76, 80	0
42	2k	114/129 (88%)	0.69	6 (5%) 26 31	54, 71, 80, 84	0
43	1l	121/132 (91%)	0.51	3 (2%) 57 63	48, 54, 65, 71	0
43	2l	121/132 (91%)	0.70	7 (5%) 23 27	58, 65, 73, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.75	8 (6%) 18 22	54, 70, 77, 86	0
44	2m	122/126 (96%)	1.12	24 (19%) 1 1	67, 78, 84, 90	0
45	1n	60/61 (98%)	2.07	27 (45%) 0 0	61, 69, 77, 78	0
45	2n	60/61 (98%)	3.82	51 (85%) 0 0	72, 79, 87, 89	0
46	1o	88/89 (98%)	0.46	2 (2%) 60 67	45, 65, 73, 77	0
46	2o	88/89 (98%)	0.48	1 (1%) 80 85	54, 66, 78, 86	0
47	1p	82/88 (93%)	1.18	15 (18%) 1 1	59, 71, 79, 84	0
47	2p	82/88 (93%)	0.96	11 (13%) 3 4	58, 68, 77, 79	0
48	1q	99/105 (94%)	0.78	8 (8%) 12 15	53, 66, 74, 76	0
48	2q	99/105 (94%)	0.99	16 (16%) 1 2	58, 70, 79, 80	0
49	1r	68/88 (77%)	0.52	2 (2%) 51 59	56, 64, 77, 79	0
49	2r	68/88 (77%)	0.49	1 (1%) 73 79	58, 67, 76, 79	0
50	1s	83/93 (89%)	0.74	8 (9%) 8 10	62, 73, 81, 86	0
50	2s	83/93 (89%)	1.64	28 (33%) 0 0	72, 82, 88, 90	0
51	1t	96/106 (90%)	1.60	33 (34%) 0 0	61, 71, 80, 85	0
51	2t	96/106 (90%)	1.65	35 (36%) 0 0	60, 72, 82, 85	0
52	1u	23/27 (85%)	2.00	11 (47%) 0 0	62, 66, 72, 78	0
52	2u	23/27 (85%)	3.33	17 (73%) 0 0	67, 75, 81, 84	0
53	1v	13/24 (54%)	1.97	5 (38%) 0 0	48, 55, 91, 97	0
53	2v	13/24 (54%)	1.60	5 (38%) 0 0	60, 70, 96, 103	0
54	1w	66/76 (86%)	0.89	9 (13%) 3 3	31, 86, 98, 102	0
54	2w	64/76 (84%)	0.80	7 (10%) 5 7	50, 95, 100, 104	0
55	1x	72/77 (93%)	0.12	1 (1%) 75 81	28, 60, 79, 90	0
55	2x	72/77 (93%)	-0.10	1 (1%) 75 81	45, 72, 84, 100	0
56	1y	67/76 (88%)	3.85	55 (82%) 0 0	58, 99, 103, 105	0
56	2y	66/76 (86%)	4.47	58 (87%) 0 0	69, 101, 104, 107	0
All	All	20871/21748 (95%)	0.78	2182 (10%) 6 8	21, 64, 89, 109	0

All (2182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2A	652(V)	C	20.3
1	2A	652(U)	G	19.9

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Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	19.1
1	2A	653	A	16.3
1	1A	652(C)	G	15.8
1	1A	653	A	14.5
44	1m	123	ALA	14.0
1	2A	652(C)	G	13.6
44	2m	123	ALA	13.6
1	1A	652(S)	C	12.7
1	2A	2802	G	12.5
1	1A	652(V)	C	12.3
1	2A	654	A	12.1
44	1m	124	PRO	12.1
1	2A	652(T)	C	11.7
1	1A	652(U)	G	11.6
1	1A	652(T)	C	11.3
1	2A	652(D)	C	11.0
45	2n	39	LEU	10.6
35	1d	167	GLY	10.6
56	1y	34	G	10.2
1	2A	2145	C	10.1
45	2n	2	ALA	10.0
40	1i	15	ALA	9.9
1	1A	654	A	9.4
54	2w	71	G	9.3
56	1y	35	A	9.3
32	2a	1030(B)	C	9.0
1	2A	883	G	9.0
1	1A	2145	C	8.9
32	1a	1030(B)	C	8.8
38	2g	80	VAL	8.7
40	2i	14	VAL	8.7
56	1y	36	A	8.6
41	2j	10	GLY	8.5
38	2g	81	GLY	8.5
32	2a	1001(A)	G	8.5
3	1D	276	LYS	8.5
41	2j	47	PHE	8.4
45	2n	34	TYR	8.4
38	1g	80	VAL	8.2
56	2y	1	G	8.2
41	2j	32	ALA	8.1
56	2y	34	G	8.1

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Mol	Chain	Res	Type	RSRZ
1	2A	884	C	8.1
56	2y	36	A	8.0
1	2A	2112	G	8.0
21	2Z	144	LEU	8.0
1	2A	2111	C	8.0
32	2a	1033	G	8.0
7	2H	35	VAL	7.9
38	2g	82	GLY	7.9
45	2n	13	THR	7.9
1	1A	2115	G	7.9
1	1A	1096	A	7.8
1	1A	2159	G	7.8
54	1w	71	G	7.7
1	1A	2129	C	7.6
1	2A	2146	C	7.6
54	1w	70	G	7.6
1	1A	1095	A	7.5
32	2a	1030(A)	G	7.5
1	1A	2114	A	7.5
45	2n	6	LEU	7.4
38	2g	156	TRP	7.4
1	1A	2110	G	7.4
56	2y	15	G	7.4
44	1m	2	ALA	7.4
7	2H	123	PHE	7.3
1	1A	2160	G	7.3
1	1A	2111	C	7.2
40	2i	36	TYR	7.2
1	1A	2131	G	7.2
23	21	2	SER	7.2
1	2A	652(E)	G	7.2
31	29	17	ILE	7.2
40	1i	14	VAL	7.2
56	2y	18	G	7.2
7	2H	24	VAL	7.2
7	2H	141	VAL	7.2
38	1g	83	ALA	7.2
56	2y	21	A	7.1
40	2i	8	GLY	7.1
32	1a	1036	G	7.1
1	1A	652(E)	G	7.1
38	1g	156	TRP	7.1

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Mol	Chain	Res	Type	RSRZ
1	2A	2110	G	7.1
1	1A	884	C	7.1
40	2i	15	ALA	7.1
1	2A	888	C	7.0
1	2A	2147	G	7.0
56	2y	35	A	7.0
1	1A	1094	U	7.0
1	1A	2128	C	7.0
52	2u	14	TRP	7.0
38	1g	79	ARG	7.0
1	1A	2130	U	7.0
1	2A	2128	C	7.0
1	2A	896	A	6.9
32	2a	1257	U	6.9
56	1y	47	U	6.9
45	2n	35	ARG	6.9
1	1A	652(F)	G	6.8
40	2i	9	ARG	6.8
7	2H	113	VAL	6.8
56	1y	19	G	6.8
1	1A	1068	G	6.7
1	2A	2160	G	6.7
32	1a	1030(C)	G	6.7
32	1a	1030(A)	G	6.7
45	2n	61	TRP	6.7
7	2H	52	VAL	6.7
40	2i	114	TYR	6.6
40	1i	19	LEU	6.6
56	1y	15	G	6.6
7	2H	29	PRO	6.6
1	1A	2117	A	6.6
40	1i	79	LEU	6.6
41	2j	65	LEU	6.6
51	2t	28	ALA	6.6
38	1g	81	GLY	6.6
1	1A	2158	A	6.6
56	2y	73	A	6.6
1	1A	2166	G	6.5
1	2A	2179	C	6.5
32	2a	1032	G	6.5
56	2y	19	G	6.5
53	1v	13	A	6.5

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Mol	Chain	Res	Type	RSRZ
38	1g	154	TYR	6.5
52	2u	16	GLY	6.5
1	2A	2174	C	6.5
1	2A	2803	C	6.5
45	2n	11	LYS	6.4
31	29	16	VAL	6.4
1	1A	652(D)	C	6.4
1	2A	2127	G	6.4
1	2A	2125	G	6.4
51	1t	76	ALA	6.4
1	1A	1509	C	6.4
41	2j	63	PHE	6.3
56	2y	53	G	6.3
44	2m	122	LYS	6.3
53	2v	12	A	6.3
1	1A	2116	G	6.3
31	29	13	LYS	6.3
1	2A	2135	A	6.3
56	2y	66	U	6.3
1	2A	229	A	6.2
7	2H	43	VAL	6.2
1	1A	888	C	6.2
1	2A	2148	G	6.2
32	2a	1035	A	6.2
40	1i	106	ALA	6.2
32	2a	1030(C)	G	6.2
1	1A	1064	C	6.2
38	2g	79	ARG	6.2
40	2i	108	VAL	6.2
44	2m	121	LYS	6.2
56	2y	58	A	6.2
56	1y	1	G	6.2
40	2i	106	ALA	6.1
1	1A	2108	C	6.1
1	1A	2170	A	6.1
1	2A	2113	U	6.1
1	1A	2112	G	6.1
32	1a	1257	U	6.0
40	2i	66	ARG	6.0
1	1A	2181	G	6.0
21	2Z	106	GLY	6.0
56	1y	53	G	6.0

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Mol	Chain	Res	Type	RSRZ
38	2g	154	TYR	6.0
32	2a	1030	C	6.0
56	1y	20	U	5.9
56	2y	57	G	5.9
1	1A	1057	A	5.9
45	2n	25	VAL	5.9
1	2A	2149	G	5.9
45	1n	2	ALA	5.9
1	1A	2141	G	5.9
32	1a	1035	A	5.8
40	1i	8	GLY	5.8
40	1i	59	PHE	5.8
1	2A	2896	C	5.8
56	2y	4	C	5.8
1	2A	2801(A)	A	5.8
7	2H	128	PRO	5.8
1	2A	2123	G	5.8
32	2a	1034	G	5.8
33	1b	61	LEU	5.8
33	2b	118	LEU	5.8
1	2A	1509	C	5.8
32	2a	1003	G	5.8
33	2b	188	ALA	5.8
40	2i	109	VAL	5.7
33	2b	187	LEU	5.7
38	1g	85	TYR	5.7
20	2Y	1	MET	5.7
31	29	19	ARG	5.7
32	1a	1003	G	5.7
1	1A	2135	A	5.7
50	2s	80	TYR	5.7
1	1A	2174	C	5.7
56	2y	3	C	5.7
7	2H	99	VAL	5.7
56	2y	62	C	5.7
1	1A	1058	G	5.7
1	1A	2147	G	5.7
44	2m	102	ARG	5.6
56	1y	22	G	5.6
1	1A	2109	U	5.6
41	2j	31	GLY	5.6
1	2A	885	C	5.6

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Mol	Chain	Res	Type	RSRZ
56	1y	61	C	5.6
41	2j	59	SER	5.6
50	2s	36	ARG	5.6
52	2u	17	THR	5.6
1	1A	2146	C	5.5
41	2j	44	VAL	5.5
1	1A	885	C	5.5
56	1y	74	C	5.5
1	2A	2134	A	5.5
1	2A	2165	G	5.5
56	2y	52	G	5.5
7	2H	174	GLY	5.5
1	1A	1098	A	5.5
1	2A	2170	A	5.5
31	29	20	HIS	5.5
33	1b	232	PRO	5.5
1	2A	1043	C	5.5
33	1b	165	VAL	5.5
1	1A	2120	G	5.5
21	2Z	139	VAL	5.4
1	2A	2138	C	5.4
23	11	2	SER	5.4
56	2y	74	C	5.4
40	2i	115	GLY	5.4
40	1i	47	LEU	5.4
45	2n	55	GLY	5.4
40	2i	30	GLY	5.4
56	2y	65	G	5.4
1	1A	2180	U	5.4
40	1i	65	VAL	5.4
45	2n	38	GLY	5.4
33	2b	232	PRO	5.4
56	2y	64	A	5.4
7	2H	64	LEU	5.4
7	2H	92	ILE	5.4
40	2i	62	TYR	5.3
1	1A	2132	U	5.3
7	2H	10	PRO	5.3
1	2A	2159	G	5.3
33	1b	222	ILE	5.3
1	2A	2109	U	5.3
11	2P	79	ARG	5.3

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Mol	Chain	Res	Type	RSRZ
7	2H	48	GLY	5.3
1	1A	1059	G	5.3
52	2u	6	ARG	5.3
48	2q	23	VAL	5.3
56	2y	14	A	5.3
33	1b	133	LYS	5.3
1	1A	2113	U	5.3
32	2a	1031	G	5.3
33	2b	121	LEU	5.3
41	2j	72	VAL	5.3
40	2i	27	THR	5.3
41	2j	66	ARG	5.3
42	2k	25	TYR	5.3
1	2A	2181	G	5.3
52	2u	13	ILE	5.3
7	2H	94	TYR	5.2
1	2A	2175	C	5.2
34	1c	184	TYR	5.2
40	2i	16	ARG	5.2
40	1i	113	LYS	5.2
32	2a	1286	A	5.2
1	1A	2151	G	5.2
7	2H	171	LEU	5.2
56	2y	72	C	5.2
33	2b	225	ALA	5.2
1	2A	2117	A	5.2
1	1A	2107	C	5.2
1	2A	2129	C	5.2
56	2y	48	C	5.2
56	2y	61	C	5.2
7	2H	79	VAL	5.2
56	1y	5	G	5.2
34	2c	4	LYS	5.1
7	2H	47	GLU	5.1
32	1a	204	U	5.1
56	1y	21	A	5.1
56	2y	47	U	5.1
7	2H	103	LEU	5.1
31	29	22	ARG	5.1
1	2A	2168	G	5.1
32	1a	1026	G	5.1
1	2A	2144	U	5.1

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Mol	Chain	Res	Type	RSRZ
40	1i	17	VAL	5.1
1	1A	2123	G	5.1
1	1A	2168	G	5.1
32	1a	1447	A	5.1
41	2j	55	LYS	5.1
40	1i	33	PHE	5.1
1	2A	2115	G	5.1
32	2a	1002	G	5.1
53	1v	12	A	5.0
1	2A	2180	U	5.0
33	1b	70	PHE	5.0
40	2i	126	SER	5.0
40	2i	125	TYR	5.0
7	2H	159	GLU	5.0
21	2Z	149	SER	5.0
32	1a	1030	C	5.0
56	2y	75	C	5.0
31	29	37	GLY	5.0
40	2i	17	VAL	5.0
40	1i	117	HIS	5.0
11	2P	76	LYS	5.0
56	1y	75	C	5.0
33	1b	136	VAL	5.0
1	1A	1082	U	5.0
1	2A	882	G	5.0
7	2H	2	SER	5.0
7	2H	37	VAL	5.0
38	2g	85	TYR	5.0
32	1a	1002	G	4.9
7	2H	67	LEU	4.9
7	2H	98	LEU	4.9
45	2n	12	ARG	4.9
1	1A	2175	C	4.9
7	2H	162	ILE	4.9
1	2A	2126	A	4.9
32	2a	1532	U	4.9
40	2i	19	LEU	4.9
50	2s	71	LEU	4.9
7	2H	26	VAL	4.9
1	1A	889	C	4.9
1	1A	2161	C	4.9
1	1A	2144	U	4.9

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Mol	Chain	Res	Type	RSRZ
31	29	25	VAL	4.9
34	1c	14	ILE	4.9
45	2n	7	ILE	4.9
56	1y	71	G	4.9
56	1y	56	C	4.9
34	2c	101	LEU	4.9
1	1A	896	A	4.9
33	1b	231	GLU	4.9
51	2t	24	LEU	4.9
1	1A	2173	A	4.9
43	2l	18	VAL	4.9
41	2j	74	ILE	4.9
56	2y	2	C	4.8
1	2A	2114	A	4.8
56	2y	51	U	4.8
44	2m	100	GLY	4.8
34	1c	39	ILE	4.8
1	1A	897	C	4.8
41	2j	48	THR	4.8
56	2y	6	G	4.8
7	2H	145	ALA	4.8
45	2n	4	LYS	4.8
48	1q	98	LEU	4.8
54	1w	20	U	4.8
56	1y	33	U	4.8
1	1A	2143	C	4.8
32	2a	1039	C	4.8
47	1p	22	THR	4.8
54	1w	72	C	4.8
1	2A	2133	G	4.8
7	2H	157	TYR	4.8
32	2a	1001	A	4.8
56	1y	24	G	4.8
56	1y	57	G	4.8
56	2y	30	G	4.8
41	2j	40	LEU	4.8
32	1a	1532	U	4.8
1	1A	2164	C	4.8
40	2i	63	ILE	4.8
41	2j	6	ILE	4.8
1	2A	2182	G	4.8
21	2Z	170	THR	4.8

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Mol	Chain	Res	Type	RSRZ
34	2c	180	ALA	4.8
1	1A	2167	U	4.7
1	1A	2121	G	4.7
56	1y	6	G	4.7
7	2H	13	LYS	4.7
40	1i	63	ILE	4.7
32	1a	1024	G	4.7
32	2a	1036	G	4.7
11	2P	110	TYR	4.7
33	2b	165	VAL	4.7
45	2n	56	VAL	4.7
32	1a	1030(D)	A	4.7
7	2H	102	ALA	4.7
1	1A	2162	G	4.7
1	2A	2164	C	4.7
32	2a	1030(D)	A	4.7
45	2n	16	PHE	4.7
56	2y	5	G	4.7
26	24	63	TYR	4.7
1	2A	2139	C	4.7
41	1j	46	ARG	4.7
32	1a	1531	A	4.7
1	2A	2121	G	4.7
56	2y	56	C	4.7
1	1A	1069	A	4.6
1	1A	2169	A	4.6
1	1A	2801(A)	A	4.6
56	2y	26	A	4.6
32	1a	1023	G	4.6
45	2n	17	LYS	4.6
7	2H	105	LEU	4.6
1	1A	1081	U	4.6
7	2H	6	ARG	4.6
41	2j	73	ASP	4.6
45	2n	31	ARG	4.6
29	27	48	LYS	4.6
41	1j	62	HIS	4.6
31	29	18	ARG	4.6
40	1i	4	TYR	4.6
56	2y	63	G	4.6
52	1u	9	ARG	4.6
7	2H	129	THR	4.6

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Mol	Chain	Res	Type	RSRZ
51	1t	68	LYS	4.6
7	2H	88	LEU	4.6
1	2A	2154	G	4.6
32	1a	1033	G	4.6
1	1A	887	A	4.6
12	2Q	59	ARG	4.6
56	2y	59	U	4.6
1	2A	1112	G	4.6
33	2b	34	ALA	4.6
54	2w	72	C	4.5
40	2i	79	LEU	4.5
56	1y	2	C	4.5
56	2y	67	C	4.5
40	1i	45	ALA	4.5
1	1A	2127	G	4.5
32	2a	1005	A	4.5
44	2m	120	LYS	4.5
56	1y	51	U	4.5
56	2y	60	U	4.5
34	2c	198	VAL	4.5
33	2b	92	TYR	4.5
32	1a	1031	G	4.5
54	2w	70	G	4.5
56	2y	70	G	4.5
1	1A	1066	U	4.5
56	1y	50	U	4.5
1	2A	2804	C	4.5
40	1i	64	THR	4.5
26	24	68	ARG	4.5
1	1A	2140	C	4.5
1	2A	2161	C	4.5
1	2A	2177	C	4.5
40	2i	37	PHE	4.5
51	2t	25	ARG	4.5
1	1A	2165	G	4.5
40	1i	56	LEU	4.5
1	2A	2173	A	4.4
1	2A	2157	G	4.4
1	2A	2794	C	4.4
7	2H	121	ILE	4.4
12	2Q	47	ILE	4.4
38	2g	155	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	1A	2119	A	4.4
33	2b	201	ILE	4.4
32	1a	1001(A)	G	4.4
40	2i	28	VAL	4.4
40	2i	74	ILE	4.4
1	2A	2143	C	4.4
29	27	47	ARG	4.4
56	2y	71	G	4.4
11	2P	109	GLY	4.4
7	2H	17	VAL	4.4
40	1i	26	VAL	4.4
12	2Q	63	LYS	4.4
31	29	24	TYR	4.4
1	1A	2136	C	4.4
1	1A	2802	G	4.4
45	2n	37	PHE	4.3
1	2A	2805	G	4.3
32	2a	1024	G	4.3
12	2Q	6	ARG	4.3
45	2n	50	LYS	4.3
41	2j	85	LEU	4.3
33	2b	17	PHE	4.3
33	2b	70	PHE	4.3
40	2i	18	PHE	4.3
52	2u	2	GLY	4.3
1	1A	882	G	4.3
1	1A	2154	G	4.3
1	2A	2120	G	4.3
32	1a	79	G	4.3
56	2y	44	G	4.3
34	1c	12	LEU	4.3
41	1j	72	VAL	4.3
21	2Z	152	ALA	4.3
31	29	26	ILE	4.3
52	1u	14	TRP	4.3
1	1A	1065	U	4.3
21	2Z	150	LEU	4.3
34	2c	179	ARG	4.3
40	2i	64	THR	4.3
40	1i	80	GLY	4.3
48	2q	22	LEU	4.3
40	2i	5	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
7	2H	131	VAL	4.3
33	1b	81	VAL	4.3
1	2A	2108	C	4.3
1	2A	2178	C	4.3
40	2i	77	ILE	4.3
33	2b	215	LEU	4.3
1	2A	2116	G	4.3
56	2y	29	G	4.3
41	2j	88	LEU	4.2
7	2H	97	ARG	4.2
1	1A	2803	C	4.2
1	2A	887	A	4.2
32	2a	1004	A	4.2
45	1n	57	ARG	4.2
22	20	63	VAL	4.2
45	2n	33	VAL	4.2
25	23	29	ARG	4.2
51	2t	72	LEU	4.2
33	1b	19	HIS	4.2
7	2H	45	VAL	4.2
7	2H	55	PRO	4.2
40	1i	30	GLY	4.2
38	1g	84	ASN	4.2
45	1n	25	VAL	4.2
28	26	28	ARG	4.2
1	1A	2134	A	4.2
52	2u	15	ARG	4.2
53	2v	13	A	4.2
56	1y	38	A	4.2
56	1y	58	A	4.2
7	2H	142	GLY	4.2
45	2n	30	ALA	4.2
1	2A	2156	G	4.1
34	2c	8	ILE	4.1
41	2j	96	ILE	4.1
45	1n	7	ILE	4.1
1	2A	2118	U	4.1
1	2A	2167	U	4.1
41	2j	71	LEU	4.1
7	2H	100	GLY	4.1
41	2j	86	MET	4.1
12	2Q	102	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
50	2s	38	SER	4.1
42	1k	25	TYR	4.1
33	2b	203	GLY	4.1
33	1b	188	ALA	4.1
1	1A	2178	C	4.1
40	1i	18	PHE	4.1
1	1A	1086	A	4.1
32	2a	1447	A	4.1
35	2d	5	ILE	4.1
51	1t	24	LEU	4.1
7	2H	20	ALA	4.1
51	2t	59	ALA	4.1
31	29	21	GLY	4.1
33	2b	127	ILE	4.1
34	2c	184	TYR	4.1
34	2c	178	LEU	4.1
56	1y	14	A	4.1
29	17	47	ARG	4.1
40	1i	7	THR	4.1
34	2c	186	PHE	4.1
41	1j	7	LYS	4.1
54	2w	45	U	4.1
4	2E	1	MET	4.1
7	2H	138	LYS	4.1
1	2A	2793	G	4.0
32	1a	216	G	4.0
40	2i	105	ASP	4.0
55	2x	47	U	4.0
56	2y	33	U	4.0
1	2A	2107	C	4.0
51	1t	9	ASN	4.0
41	1j	47	PHE	4.0
41	2j	56	HIS	4.0
1	1A	1063	G	4.0
1	1A	2157	G	4.0
1	1A	2794	C	4.0
12	2Q	121	ALA	4.0
7	2H	76	VAL	4.0
33	1b	68	ILE	4.0
21	2Z	164	ALA	4.0
56	1y	52	G	4.0
33	2b	164	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	1A	1077	A	4.0
56	2y	31	A	4.0
33	2b	200	ILE	4.0
3	1D	275	LYS	4.0
40	1i	116	LYS	4.0
7	2H	133	VAL	4.0
56	1y	13	C	4.0
1	2A	2124	G	4.0
1	1A	1070	A	4.0
40	1i	37	PHE	4.0
38	1g	16	LEU	4.0
50	2s	16	LEU	4.0
9	2N	90	MET	4.0
52	2u	21	TYR	4.0
21	2Z	153	SER	4.0
50	2s	30	LEU	4.0
51	1t	69	GLY	4.0
7	2H	148	ILE	4.0
32	1a	1025	U	4.0
38	2g	32	ARG	4.0
41	2j	46	ARG	4.0
43	2l	39	VAL	4.0
7	2H	82	GLY	4.0
7	2H	71	LEU	3.9
56	1y	4	C	3.9
38	2g	78	ARG	3.9
7	2H	41	MET	3.9
32	2a	1021	G	3.9
33	2b	207	ALA	3.9
48	2q	42	TYR	3.9
7	2H	169	VAL	3.9
26	24	50	VAL	3.9
51	1t	14	LYS	3.9
33	1b	215	LEU	3.9
33	2b	122	PHE	3.9
1	2A	2119	A	3.9
45	1n	61	TRP	3.9
54	2w	73	A	3.9
1	2A	2155	G	3.9
31	29	8	LYS	3.9
38	1g	78	ARG	3.9
41	2j	64	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
41	2j	98	ILE	3.9
7	2H	23	ARG	3.9
40	2i	67	GLY	3.9
33	2b	233	SER	3.9
40	2i	110	GLU	3.9
40	2i	59	PHE	3.9
45	2n	22	THR	3.9
1	1A	2163	C	3.9
40	2i	90	PRO	3.9
1	1A	1087	G	3.9
12	2Q	2	LEU	3.9
33	1b	17	PHE	3.9
11	2P	15	ARG	3.9
21	2Z	133	ILE	3.9
45	2n	26	ARG	3.9
26	24	54	GLY	3.9
1	1A	2142	C	3.9
1	1A	2185	C	3.9
33	2b	133	LYS	3.9
40	2i	86	VAL	3.9
45	1n	39	LEU	3.9
33	2b	163	PHE	3.9
33	1b	211	ILE	3.9
1	1A	2133	G	3.9
1	2A	2190	G	3.9
1	2A	2132	U	3.9
51	1t	59	ALA	3.9
31	29	23	VAL	3.9
40	1i	66	ARG	3.9
47	2p	9	PHE	3.8
34	2c	5	ILE	3.8
51	2t	63	ILE	3.8
11	2P	127	ALA	3.8
40	2i	13	ALA	3.8
1	2A	2897	U	3.8
32	1a	1037	C	3.8
56	1y	62	C	3.8
7	2H	57	ASP	3.8
41	1j	10	GLY	3.8
33	1b	200	ILE	3.8
38	2g	42	ILE	3.8
51	1t	71	THR	3.8

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Mol	Chain	Res	Type	RSRZ
50	2s	50	ALA	3.8
7	2H	54	ARG	3.8
7	2H	95	ARG	3.8
26	24	51	ASP	3.8
7	2H	7	LEU	3.8
32	1a	1028	C	3.8
56	1y	48	C	3.8
34	2c	202	ILE	3.8
45	2n	23	ARG	3.8
52	2u	8	THR	3.8
7	2H	63	SER	3.8
56	1y	7	A	3.8
29	17	48	LYS	3.8
51	2t	9	ASN	3.8
1	1A	2148	G	3.8
51	2t	99	LEU	3.8
33	2b	55	PHE	3.8
1	1A	271(K)	U	3.8
31	29	34	GLN	3.8
1	1A	229	A	3.8
32	1a	152	A	3.8
41	2j	93	GLY	3.8
33	1b	15	VAL	3.8
1	2A	897	C	3.8
41	2j	89	ASP	3.8
21	2Z	147	GLY	3.8
7	2H	33	LEU	3.8
10	2O	102	VAL	3.8
21	2Z	172	ALA	3.8
40	1i	61	ALA	3.8
1	1A	2105	C	3.8
34	2c	138	VAL	3.8
50	2s	51	VAL	3.8
21	2Z	51	ALA	3.7
52	1u	18	TYR	3.7
32	2a	1027	C	3.7
56	2y	22	G	3.7
4	2E	196	VAL	3.7
7	2H	49	VAL	3.7
7	2H	107	VAL	3.7
12	2Q	130	LYS	3.7
32	2a	1287	A	3.7

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Mol	Chain	Res	Type	RSRZ
50	2s	52	TYR	3.7
1	1A	1100	C	3.7
25	23	49	LYS	3.7
45	2n	57	ARG	3.7
50	2s	37	ARG	3.7
1	1A	2152	G	3.7
33	2b	136	VAL	3.7
56	2y	24	G	3.7
34	1c	2	GLY	3.7
7	2H	72	ILE	3.7
1	2A	2130	U	3.7
7	2H	164	TYR	3.7
7	2H	132	ARG	3.7
40	2i	93	ARG	3.7
41	1j	41	PRO	3.7
36	1e	10	MET	3.7
33	2b	211	ILE	3.7
40	1i	77	ILE	3.7
7	2H	12	PRO	3.7
7	2H	44	VAL	3.7
51	2t	86	ARG	3.7
33	2b	214	ILE	3.7
1	1A	2790	A	3.7
34	2c	193	TYR	3.7
40	1i	11	LYS	3.7
1	1A	2177	C	3.7
33	1b	71	VAL	3.7
40	2i	53	VAL	3.7
8	2I	98	ALA	3.7
41	1j	66	ARG	3.7
45	2n	49	HIS	3.7
50	2s	14	HIS	3.7
33	2b	222	ILE	3.7
1	2A	881	G	3.7
45	1n	51	GLY	3.7
12	2Q	5	ARG	3.7
20	2Y	91	GLU	3.7
40	2i	123	PRO	3.7
29	17	46	VAL	3.7
1	1A	2896	C	3.7
40	2i	46	ALA	3.7
41	1j	57	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
56	1y	12	U	3.6
1	2A	2176	A	3.6
32	1a	1286	A	3.6
56	1y	65	G	3.6
31	29	15	LYS	3.6
36	2e	133	TYR	3.6
12	2Q	109	VAL	3.6
1	1A	2804	C	3.6
12	2Q	104	PHE	3.6
21	1Z	149	SER	3.6
21	2Z	148	ASP	3.6
25	23	53	LEU	3.6
34	2c	201	TYR	3.6
41	1j	97	GLU	3.6
7	2H	106	THR	3.6
9	2N	140	VAL	3.6
32	2a	1250	A	3.6
30	28	29	LYS	3.6
40	1i	6	GLY	3.6
41	1j	98	ILE	3.6
1	1A	1060	U	3.6
1	2A	2136	C	3.6
32	1a	1137	C	3.6
33	2b	231	GLU	3.6
45	2n	32	SER	3.6
33	1b	121	LEU	3.6
41	1j	67	THR	3.6
39	2h	93	VAL	3.6
26	14	54	GLY	3.6
34	1c	185	GLY	3.6
1	2A	2183	C	3.6
32	1a	1034	G	3.6
32	2a	1023	G	3.6
7	2H	51	ARG	3.6
40	2i	78	LYS	3.6
53	1v	15	A	3.6
56	1y	64	A	3.6
41	2j	60	ARG	3.6
49	2r	66	LEU	3.6
40	2i	29	ASN	3.6
42	2k	86	GLY	3.6
11	2P	101	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
21	1Z	1	MET	3.6
1	1A	2172	U	3.5
45	2n	44	LEU	3.5
33	1b	207	ALA	3.5
40	2i	82	ALA	3.5
51	2t	30	LYS	3.5
1	2A	2166	G	3.5
32	2a	1026	G	3.5
40	2i	65	VAL	3.5
40	1i	110	GLU	3.5
1	2A	652(B)	A	3.5
44	1m	122	LYS	3.5
40	2i	128	ARG	3.5
41	2j	83	GLU	3.5
52	2u	18	TYR	3.5
33	2b	131	PRO	3.5
54	1w	44	G	3.5
45	2n	36	PHE	3.5
25	23	18	ASP	3.5
23	21	98	LEU	3.5
33	2b	69	LEU	3.5
35	2d	78	LEU	3.5
34	2c	15	THR	3.5
1	1A	1053	C	3.5
32	2a	470	C	3.5
45	1n	56	VAL	3.5
34	2c	7	PRO	3.5
33	2b	135	GLN	3.5
38	2g	4	ARG	3.5
45	1n	55	GLY	3.5
45	2n	29	ARG	3.5
56	1y	18	G	3.5
40	1i	76	ALA	3.5
7	2H	125	VAL	3.5
1	1A	886	C	3.5
1	1A	2179	C	3.5
50	2s	12	ASP	3.5
34	2c	14	ILE	3.5
33	2b	124	SER	3.5
1	2A	2169	A	3.5
38	1g	155	ARG	3.5
39	2h	129	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
32	2a	1452	C	3.5
1	2A	1026	U	3.5
28	26	34	LEU	3.5
34	1c	179	ARG	3.5
20	1Y	1	MET	3.5
21	2Z	1	MET	3.5
31	29	1	MET	3.5
40	1i	109	VAL	3.5
32	1a	1027	C	3.4
33	2b	41	ILE	3.4
56	2y	45	U	3.4
25	23	23	LEU	3.4
40	2i	127	LYS	3.4
47	2p	59	TRP	3.4
1	2A	2131	G	3.4
7	2H	18	GLU	3.4
41	1j	64	GLU	3.4
7	2H	87	LEU	3.4
33	1b	124	SER	3.4
33	2b	101	MET	3.4
40	2i	80	GLY	3.4
23	11	93	GLU	3.4
1	2A	2792	G	3.4
7	2H	175	LYS	3.4
32	2a	79	G	3.4
39	2h	13	ILE	3.4
50	1s	10	PHE	3.4
1	1A	895	U	3.4
1	2A	272(A)	U	3.4
1	2A	2158	A	3.4
8	2I	68	LEU	3.4
11	2P	106	LEU	3.4
12	2Q	37	LEU	3.4
32	1a	1001	A	3.4
35	1d	120	LEU	3.4
40	1i	85	LEU	3.4
45	1n	49	HIS	3.4
32	2a	1116	C	3.4
56	1y	3	C	3.4
38	2g	6	ARG	3.4
7	2H	19	VAL	3.4
1	1A	2118	U	3.4

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Mol	Chain	Res	Type	RSRZ
12	2Q	17	LEU	3.4
34	1c	201	TYR	3.4
1	1A	1084	A	3.4
1	1A	1093	G	3.4
10	2O	11	ALA	3.4
11	2P	93	GLY	3.4
41	2j	87	THR	3.4
56	1y	63	G	3.4
56	2y	28	G	3.4
14	2S	20	ARG	3.4
40	1i	51	ARG	3.4
51	2t	83	ARG	3.4
20	2Y	45	VAL	3.4
40	2i	44	VAL	3.4
50	2s	49	ILE	3.4
8	2I	75	LEU	3.4
33	1b	228	GLY	3.4
40	2i	72	GLY	3.4
51	1t	84	LEU	3.4
1	1A	1088	A	3.4
1	1A	2793	G	3.4
33	2b	209	ARG	3.4
38	1g	82	GLY	3.4
34	2c	111	LEU	3.4
34	2c	182	ILE	3.4
51	1t	23	ARG	3.4
56	1y	59	U	3.4
12	2Q	99	PRO	3.4
7	2H	144	VAL	3.4
32	2a	1037	C	3.4
12	2Q	10	ARG	3.4
38	1g	32	ARG	3.4
44	2m	80	ARG	3.4
41	1j	48	THR	3.3
32	2a	1149	C	3.3
7	2H	34	GLU	3.3
34	2c	57	ILE	3.3
34	2c	142	MET	3.3
7	2H	65	HIS	3.3
1	1A	1076	C	3.3
7	2H	137	ASP	3.3
38	1g	42	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
39	2h	111	ILE	3.3
51	2t	13	LEU	3.3
7	2H	3	ARG	3.3
32	1a	70	G	3.3
32	1a	78	G	3.3
40	2i	7	THR	3.3
41	2j	61	GLU	3.3
41	1j	59	SER	3.3
50	2s	13	ASP	3.3
50	2s	35	SER	3.3
1	2A	899	A	3.3
11	2P	91	PHE	3.3
26	24	49	PHE	3.3
41	1j	9	ARG	3.3
1	2A	271(K)	U	3.3
32	2a	1150	U	3.3
1	2A	2106	G	3.3
40	1i	5	TYR	3.3
34	1c	18	TRP	3.3
7	2H	56	SER	3.3
40	1i	20	ARG	3.3
40	2i	33	PHE	3.3
41	1j	50	ILE	3.3
7	2H	30	LYS	3.3
32	2a	1248	A	3.3
45	1n	59	ALA	3.3
56	2y	68	C	3.3
40	1i	114	TYR	3.3
41	2j	45	ARG	3.3
7	2H	115	VAL	3.3
40	1i	28	VAL	3.3
3	2D	276	LYS	3.3
40	1i	3	GLN	3.3
11	2P	100	LEU	3.3
39	2h	2	LEU	3.3
33	2b	186	ALA	3.3
33	2b	223	ILE	3.3
7	2H	124	GLU	3.3
7	2H	69	ARG	3.3
40	2i	121	ARG	3.3
7	2H	83	TYR	3.3
1	2A	2100	G	3.2

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Mol	Chain	Res	Type	RSRZ
1	2A	2104	G	3.2
40	1i	21	PRO	3.2
19	1X	95	LEU	3.2
21	2Z	104	PHE	3.2
1	1A	1097	U	3.2
52	2u	10	ARG	3.2
1	1A	2126	A	3.2
8	2I	19	VAL	3.2
13	2R	10	LEU	3.2
34	2c	6	HIS	3.2
34	2c	176	HIS	3.2
51	1t	22	ARG	3.2
31	29	12	ASP	3.2
48	1q	27	PHE	3.2
1	1A	1078	U	3.2
7	2H	77	LYS	3.2
1	2A	645	C	3.2
1	2A	2137	C	3.2
7	2H	38	SER	3.2
7	2H	134	SER	3.2
32	2a	1251	A	3.2
56	2y	76	A	3.2
33	1b	93	VAL	3.2
34	2c	189	ALA	3.2
36	2e	13	ILE	3.2
56	1y	44	G	3.2
41	2j	28	ARG	3.2
44	2m	104	ARG	3.2
6	2G	49	ASP	3.2
53	1v	14	A	3.2
7	2H	150	ALA	3.2
32	1a	841	U	3.2
33	1b	90	MET	3.2
1	1A	2106	G	3.2
41	1j	68	HIS	3.2
1	1A	2137	C	3.2
34	1c	207	VAL	3.2
47	1p	62	VAL	3.2
1	1A	2171	A	3.2
7	2H	73	ALA	3.2
7	2H	172	LYS	3.2
32	2a	204	U	3.2

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Mol	Chain	Res	Type	RSRZ
33	1b	201	ILE	3.2
52	1u	13	ILE	3.2
40	2i	42	ARG	3.2
41	1j	45	ARG	3.2
52	2u	9	ARG	3.2
50	2s	34	TRP	3.2
1	1A	2153	G	3.2
7	2H	50	VAL	3.2
12	2Q	72	LYS	3.2
33	2b	31	TYR	3.2
33	2b	236	TYR	3.2
34	2c	188	LEU	3.2
35	1d	38	TYR	3.2
40	2i	113	LYS	3.2
43	1l	64	TYR	3.2
1	1A	1067	A	3.2
31	29	9	ARG	3.2
35	1d	115	ARG	3.2
51	1t	86	ARG	3.2
1	1A	2897	U	3.2
32	1a	202	U	3.2
33	1b	233	SER	3.2
34	2c	51	GLY	3.2
7	2H	75	ALA	3.1
12	2Q	44	ALA	3.1
38	2g	83	ALA	3.1
44	2m	87	TYR	3.1
51	2t	77	ALA	3.1
32	2a	1223	C	3.1
48	1q	36	ILE	3.1
7	2H	25	LYS	3.1
11	2P	108	LYS	3.1
34	1c	198	VAL	3.1
41	1j	44	VAL	3.1
40	1i	88	TYR	3.1
40	2i	54	ASP	3.1
52	1u	21	TYR	3.1
1	2A	2142	C	3.1
32	2a	961	U	3.1
41	1j	4	ILE	3.1
45	2n	58	LYS	3.1
50	1s	40	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
56	1y	49	C	3.1
56	1y	60	U	3.1
45	2n	54	PRO	3.1
56	2y	23	A	3.1
34	1c	87	LEU	3.1
41	2j	34	VAL	3.1
1	1A	2138	C	3.1
34	1c	206	GLU	3.1
45	2n	14	PRO	3.1
1	1A	2156	G	3.1
1	2A	2153	G	3.1
1	2A	2162	G	3.1
56	1y	73	A	3.1
4	2E	120	TRP	3.1
38	2g	2	ALA	3.1
40	2i	56	LEU	3.1
40	1i	10	ARG	3.1
51	1t	70	SER	3.1
33	2b	113	HIS	3.1
41	2j	50	ILE	3.1
7	2H	112	PRO	3.1
32	2a	1028	C	3.1
40	1i	112	LYS	3.1
1	1A	1508	A	3.1
1	1A	1099	G	3.1
1	2A	614(B)	G	3.1
8	1I	117	GLU	3.1
45	2n	10	ALA	3.1
52	1u	10	ARG	3.1
1	2A	2122	U	3.1
18	2W	6	ILE	3.1
41	1j	55	LYS	3.1
41	2j	38	ILE	3.1
45	1n	42	ILE	3.1
7	2H	46	GLU	3.1
15	2T	128	GLU	3.1
33	2b	37	ASN	3.1
35	1d	101	LEU	3.1
29	27	46	VAL	3.1
32	1a	1032	G	3.1
41	2j	68	HIS	3.1
10	2O	19	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
26	24	32	TYR	3.1
32	2a	90	U	3.1
47	1p	80	PHE	3.1
47	2p	33	ILE	3.1
21	2Z	145	GLU	3.1
1	1A	1075	C	3.1
7	2H	5	GLY	3.1
11	2P	118	GLY	3.1
34	2c	53	ALA	3.1
39	1h	119	LEU	3.1
9	2N	98	VAL	3.1
44	1m	98	VAL	3.1
51	2t	70	SER	3.1
25	23	30	ARG	3.0
33	2b	90	MET	3.0
33	2b	185	ILE	3.0
51	1t	79	ARG	3.0
51	2t	23	ARG	3.0
7	2H	68	THR	3.0
32	1a	1452	C	3.0
32	2a	1007	C	3.0
38	2g	152	ALA	3.0
15	2T	123	GLN	3.0
20	2Y	107	ASP	3.0
44	2m	99	ARG	3.0
56	1y	23	A	3.0
6	1G	146	TYR	3.0
45	1n	34	TYR	3.0
1	2A	2151	G	3.0
56	1y	10	G	3.0
7	2H	40	GLU	3.0
7	2H	96	ALA	3.0
40	1i	71	SER	3.0
40	1i	102	LEU	3.0
40	1i	122	ALA	3.0
17	2V	72	VAL	3.0
32	2a	1115	C	3.0
39	1h	93	VAL	3.0
40	1i	108	VAL	3.0
43	1l	18	VAL	3.0
40	2i	81	ILE	3.0
41	1j	11	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
41	1j	63	PHE	3.0
48	2q	59	ILE	3.0
7	2H	53	GLU	3.0
26	24	55	ARG	3.0
8	2I	12	LEU	3.0
33	1b	11	LEU	3.0
33	1b	77	ALA	3.0
34	1c	189	ALA	3.0
36	1e	21	ALA	3.0
1	2A	898	C	3.0
16	2U	62	ILE	3.0
34	2c	2	GLY	3.0
34	2c	157	ILE	3.0
41	1j	38	ILE	3.0
33	2b	8	LYS	3.0
51	1t	83	ARG	3.0
52	2u	22	ARG	3.0
41	2j	58	ASP	3.0
40	2i	52	ALA	3.0
40	2i	61	ALA	3.0
40	2i	103	THR	3.0
28	26	13	CYS	3.0
33	1b	26	PRO	3.0
41	2j	41	PRO	3.0
56	1y	30	G	3.0
7	2H	31	GLY	3.0
1	2A	886	C	3.0
32	1a	76	C	3.0
30	28	48	PHE	3.0
47	2p	19	ILE	3.0
56	2y	50	U	3.0
45	2n	21	TYR	3.0
48	2q	95	TYR	3.0
33	2b	139	LYS	3.0
41	2j	39	PRO	3.0
33	1b	37	ASN	3.0
34	1c	66	VAL	3.0
40	1i	67	GLY	3.0
32	2a	1006	C	3.0
40	2i	101	PHE	3.0
40	1i	78	LYS	3.0
51	2t	43	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
51	2t	66	ALA	3.0
35	1d	3	ARG	3.0
45	2n	51	GLY	3.0
21	2Z	105	VAL	2.9
35	1d	17	VAL	2.9
1	1A	2189	U	2.9
1	2A	1113	U	2.9
41	2j	62	HIS	2.9
12	2Q	65	PHE	2.9
1	1A	2100	G	2.9
32	1a	73	G	2.9
32	2a	1362	C	2.9
11	2P	77	ARG	2.9
33	2b	33	TYR	2.9
44	2m	119	GLY	2.9
48	2q	30	PRO	2.9
31	29	28	GLU	2.9
56	2y	7	A	2.9
34	2c	86	VAL	2.9
50	2s	67	VAL	2.9
38	2g	31	MET	2.9
33	1b	214	ILE	2.9
51	2t	41	ILE	2.9
51	2t	55	ILE	2.9
56	1y	45	U	2.9
34	1c	21	ARG	2.9
1	1A	2149	G	2.9
1	2A	2141	G	2.9
11	2P	140	ALA	2.9
33	1b	227	GLY	2.9
40	2i	43	ALA	2.9
41	1j	37	PRO	2.9
41	2j	27	ALA	2.9
47	1p	6	LEU	2.9
56	2y	69	G	2.9
21	2Z	96	VAL	2.9
7	2H	136	ILE	2.9
32	2a	1148	U	2.9
34	1c	81	GLY	2.9
34	2c	158	GLY	2.9
1	1A	2188	C	2.9
21	2Z	5	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
32	2a	91	C	2.9
56	1y	69	G	2.9
40	1i	104	ARG	2.9
45	1n	41	ARG	2.9
1	1A	2062	A	2.9
1	1A	2176	A	2.9
7	2H	86	GLU	2.9
21	1Z	170	THR	2.9
50	2s	39	THR	2.9
1	1A	1092	C	2.9
40	2i	4	TYR	2.9
1	1A	1062	G	2.9
7	2H	27	LYS	2.9
51	2t	68	LYS	2.9
11	2P	114	ILE	2.9
33	2b	228	GLY	2.9
39	2h	90	GLY	2.9
52	2u	5	ASP	2.9
48	1q	28	PRO	2.9
15	2T	129	ARG	2.9
21	2Z	155	LEU	2.9
22	10	3	HIS	2.9
21	2Z	156	LYS	2.9
1	2A	2105	C	2.9
9	2N	71	ILE	2.9
10	2O	69	ILE	2.9
40	2i	12	GLU	2.9
45	1n	36	PHE	2.9
32	2a	1357	A	2.9
40	1i	9	ARG	2.9
25	23	26	LEU	2.9
40	2i	119	ALA	2.9
50	2s	79	THR	2.9
21	1Z	52	SER	2.8
21	2Z	141	VAL	2.8
32	1a	92	C	2.8
41	2j	43	ARG	2.8
7	2H	168	PRO	2.8
9	2N	84	LYS	2.8
12	2Q	66	ILE	2.8
14	2S	29	PHE	2.8
32	2a	1040	U	2.8

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Mol	Chain	Res	Type	RSRZ
40	2i	73	GLN	2.8
51	1t	41	ILE	2.8
33	1b	149	LEU	2.8
45	2n	8	GLU	2.8
40	2i	6	GLY	2.8
33	1b	197	VAL	2.8
42	1k	96	ARG	2.8
56	2y	49	C	2.8
34	1c	187	ALA	2.8
45	2n	40	CYS	2.8
34	2c	52	LEU	2.8
41	1j	90	LEU	2.8
12	2Q	19	GLY	2.8
38	1g	77	SER	2.8
43	2l	43	VAL	2.8
15	2T	45	PHE	2.8
21	2Z	162	GLU	2.8
32	2a	1029	C	2.8
51	1t	60	GLU	2.8
34	2c	3	ASN	2.8
32	2a	978	A	2.8
30	28	25	MET	2.8
47	1p	48	TRP	2.8
12	2Q	97	VAL	2.8
30	28	22	VAL	2.8
41	2j	91	PRO	2.8
50	2s	69	HIS	2.8
22	10	57	PHE	2.8
22	20	45	PHE	2.8
1	2A	2140	C	2.8
40	1i	121	ARG	2.8
41	1j	32	ALA	2.8
9	2N	87	LEU	2.8
40	1i	50	LEU	2.8
50	1s	15	LEU	2.8
26	14	57	GLU	2.8
7	2H	36	PRO	2.8
33	2b	194	PRO	2.8
47	1p	21	VAL	2.8
9	2N	61	ARG	2.8
34	1c	48	TYR	2.8
21	2Z	93	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
35	2d	73	ARG	2.8
41	2j	29	ARG	2.8
26	24	59	PHE	2.8
12	2Q	113	GLN	2.8
30	28	17	THR	2.8
33	1b	123	ALA	2.8
44	1m	105	THR	2.8
45	1n	10	ALA	2.8
32	1a	1008	C	2.8
34	2c	87	LEU	2.8
40	2i	116	LYS	2.8
43	2l	28	LYS	2.8
51	1t	74	LYS	2.8
21	2Z	122	ARG	2.8
22	20	66	VAL	2.8
40	1i	75	ASP	2.8
20	2Y	65	ALA	2.8
21	2Z	171	ILE	2.8
34	2c	102	ASN	2.8
35	2d	23	GLY	2.8
1	1A	1176	G	2.8
1	1A	2792	G	2.8
8	2I	38	LEU	2.8
33	1b	10	LEU	2.8
12	2Q	22	LYS	2.8
1	2A	271(J)	C	2.8
56	2y	13	C	2.8
45	2n	41	ARG	2.8
32	1a	1005	A	2.7
47	1p	39	TYR	2.7
33	1b	190	THR	2.7
51	1t	66	ALA	2.7
4	2E	195	LEU	2.7
7	2H	84	SER	2.7
34	2c	190	ARG	2.7
1	1A	2139	C	2.7
19	2X	68	ARG	2.7
25	23	51	ALA	2.7
33	1b	33	TYR	2.7
34	1c	65	ALA	2.7
34	2c	71	ALA	2.7
1	1A	1054	A	2.7

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Mol	Chain	Res	Type	RSRZ
33	1b	24	TRP	2.7
41	1j	96	ILE	2.7
33	1b	44	LEU	2.7
45	2n	24	CYS	2.7
51	2t	62	LEU	2.7
7	2H	14	GLY	2.7
26	24	56	VAL	2.7
36	1e	82	VAL	2.7
41	1j	60	ARG	2.7
42	2k	126	ARG	2.7
34	2c	146	ALA	2.7
45	2n	59	ALA	2.7
6	2G	3	LEU	2.7
41	2j	54	PHE	2.7
41	1j	21	GLN	2.7
53	2v	24	A	2.7
16	2U	2	PRO	2.7
4	2E	112	GLY	2.7
42	2k	17	GLY	2.7
21	2Z	20	ARG	2.7
40	2i	83	ARG	2.7
1	1A	2125	G	2.7
54	2w	5	G	2.7
1	2A	2150	U	2.7
13	2R	69	ASP	2.7
33	1b	213	LEU	2.7
51	1t	72	LEU	2.7
1	2A	1509(A)	A	2.7
5	1F	17	ARG	2.7
32	2a	1225	A	2.7
34	1c	13	GLY	2.7
51	1t	80	ARG	2.7
35	2d	8	VAL	2.7
40	2i	122	ALA	2.7
33	1b	223	ILE	2.7
34	1c	10	PHE	2.7
34	1c	43	LEU	2.7
21	2Z	151	HIS	2.7
35	1d	138	TYR	2.7
10	2O	82	ASN	2.7
52	2u	11	GLY	2.7
45	1n	11	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
40	1i	87	GLN	2.7
9	2N	5	VAL	2.7
41	1j	34	VAL	2.7
1	2A	889	C	2.7
7	2H	32	GLU	2.7
21	2Z	41	LEU	2.7
33	1b	55	PHE	2.7
34	1c	182	ILE	2.7
41	1j	8	LEU	2.7
50	2s	83	HIS	2.7
1	1A	2186	G	2.7
14	2S	45	GLY	2.7
45	2n	28	GLY	2.7
31	29	30	PRO	2.7
56	1y	28	G	2.7
21	2Z	169	GLU	2.6
50	2s	64	GLU	2.6
54	1w	73	A	2.6
40	2i	107	ARG	2.6
51	1t	38	LYS	2.6
34	2c	171	GLY	2.6
32	2a	1022	G	2.6
28	26	42	TRP	2.6
33	2b	120	ALA	2.6
1	2A	2189	U	2.6
6	2G	62	LEU	2.6
33	1b	196	LEU	2.6
39	2h	133	LEU	2.6
32	1a	71	C	2.6
39	2h	4	ASP	2.6
12	2Q	32	TYR	2.6
34	2c	23	TYR	2.6
33	1b	226	ARG	2.6
45	2n	15	LYS	2.6
7	2H	11	VAL	2.6
12	2Q	20	ALA	2.6
23	21	62	VAL	2.6
30	28	24	ALA	2.6
38	2g	84	ASN	2.6
1	1A	2122	U	2.6
1	2A	2895	U	2.6
6	1G	139	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
32	2a	1041	A	2.6
56	1y	31	A	2.6
14	2S	35	ILE	2.6
33	2b	137	ARG	2.6
30	28	64	TYR	2.6
33	2b	48	MET	2.6
33	2b	216	SER	2.6
36	1e	17	ALA	2.6
40	1i	52	ALA	2.6
40	1i	119	ALA	2.6
1	1A	2182	G	2.6
32	1a	90	U	2.6
34	2c	32	LEU	2.6
34	2c	196	LEU	2.6
38	2g	16	LEU	2.6
39	1h	112	LEU	2.6
39	2h	112	LEU	2.6
40	1i	40	LEU	2.6
46	1o	31	LEU	2.6
11	2P	78	PRO	2.6
21	2Z	48	PHE	2.6
33	2b	208	ILE	2.6
30	28	40	GLU	2.6
32	2a	1038	C	2.6
45	2n	27	CYS	2.6
40	1i	36	TYR	2.6
3	2D	38	LYS	2.6
12	2Q	33	GLY	2.6
15	2T	70	VAL	2.6
36	2e	90	VAL	2.6
39	2h	118	VAL	2.6
40	2i	111	ARG	2.6
6	2G	139	LEU	2.6
35	2d	19	LEU	2.6
52	2u	23	PRO	2.6
34	2c	134	ILE	2.6
36	2e	131	ILE	2.6
39	1h	6	ILE	2.6
1	1A	2124	G	2.6
12	2Q	112	GLU	2.6
34	2c	206	GLU	2.6
32	2a	1280	A	2.6

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Mol	Chain	Res	Type	RSRZ
41	2j	7	LYS	2.6
7	2H	74	ASN	2.6
40	1i	24	GLY	2.6
43	2l	64	TYR	2.6
50	1s	72	GLY	2.6
5	1F	89	VAL	2.6
48	2q	7	THR	2.6
7	2H	126	PRO	2.6
41	1j	40	LEU	2.6
51	1t	13	LEU	2.6
7	2H	9	ILE	2.6
30	28	16	ILE	2.6
30	28	34	TRP	2.6
33	2b	19	HIS	2.6
42	2k	89	ALA	2.5
9	2N	52	VAL	2.5
30	28	23	VAL	2.5
47	1p	2	VAL	2.5
50	2s	63	THR	2.5
8	2I	35	LEU	2.5
34	1c	91	LEU	2.5
40	1i	127	LYS	2.5
45	1n	15	LYS	2.5
1	2A	895	U	2.5
31	29	10	ILE	2.5
36	1e	89	ILE	2.5
7	2H	60	ARG	2.5
26	14	68	ARG	2.5
40	2i	117	HIS	2.5
44	2m	92	HIS	2.5
32	2a	1285	A	2.5
22	20	49	LYS	2.5
34	2c	149	ALA	2.5
51	2t	67	ALA	2.5
17	2V	79	VAL	2.5
23	21	30	VAL	2.5
31	19	16	VAL	2.5
56	2y	25	C	2.5
41	2j	8	LEU	2.5
48	2q	31	LEU	2.5
48	2q	25	ARG	2.5
1	1A	1509(A)	A	2.5

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Mol	Chain	Res	Type	RSRZ
11	2P	80	TYR	2.5
32	2a	1531	A	2.5
40	2i	88	TYR	2.5
41	2j	84	GLN	2.5
51	1t	18	GLN	2.5
51	2t	90	GLN	2.5
25	23	6	VAL	2.5
1	1A	271(J)	C	2.5
1	2A	1042	G	2.5
32	2a	1224	G	2.5
34	2c	66	VAL	2.5
41	1j	49	VAL	2.5
34	1c	19	GLU	2.5
35	1d	157	LEU	2.5
44	2m	17	VAL	2.5
56	1y	70	G	2.5
1	2A	9	U	2.5
8	1I	109	ILE	2.5
9	2N	85	ILE	2.5
34	1c	57	ILE	2.5
33	1b	78	GLN	2.5
34	2c	65	ALA	2.5
43	2l	48	PRO	2.5
44	2m	42	ALA	2.5
45	2n	3	ARG	2.5
7	2H	117	PRO	2.5
26	14	63	TYR	2.5
9	2N	26	LEU	2.5
10	2O	8	LEU	2.5
13	2R	70	LEU	2.5
22	20	62	LEU	2.5
8	2I	11	ASN	2.5
32	1a	1503	A	2.5
41	1j	58	ASP	2.5
42	1k	80	VAL	2.5
44	2m	13	LYS	2.5
51	1t	20	LEU	2.5
33	2b	140	HIS	2.5
34	2c	185	GLY	2.5
56	1y	25	C	2.5
13	2R	14	SER	2.5
33	1b	30	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
33	1b	137	ARG	2.5
46	1o	64	ARG	2.5
14	2S	36	TYR	2.5
35	1d	2	GLY	2.5
40	2i	26	VAL	2.5
40	2i	58	HIS	2.5
14	2S	3	ARG	2.5
32	1a	217	C	2.5
32	1a	1038	C	2.5
32	2a	1249	C	2.5
38	2g	77	SER	2.5
45	2n	42	ILE	2.5
38	1g	6	ARG	2.5
1	2A	11	G	2.5
1	2A	1533	G	2.5
32	2a	80	G	2.5
47	1p	68	ASP	2.5
25	23	60	GLU	2.5
28	26	5	VAL	2.5
33	2b	197	VAL	2.5
47	2p	48	TRP	2.5
45	1n	60	SER	2.5
7	2H	89	ILE	2.5
36	2e	11	ILE	2.5
40	1i	70	LYS	2.5
41	2j	75	ILE	2.5
1	1A	1072	C	2.5
32	1a	91	C	2.5
32	2a	1197	G	2.5
34	1c	200	ALA	2.5
41	2j	20	ALA	2.5
51	2t	26	ASN	2.5
26	24	57	GLU	2.5
11	1P	15	ARG	2.4
19	2X	95	LEU	2.4
34	1c	196	LEU	2.4
45	1n	29	ARG	2.4
9	2N	72	TYR	2.4
15	2T	28	VAL	2.4
26	14	50	VAL	2.4
33	1b	112	VAL	2.4
32	1a	1000	U	2.4

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Mol	Chain	Res	Type	RSRZ
32	1a	1446	U	2.4
38	1g	43	PHE	2.4
1	2A	2758	A	2.4
21	2Z	23	LYS	2.4
31	29	33	LYS	2.4
35	2d	115	ARG	2.4
38	2g	10	ARG	2.4
1	1A	892	G	2.4
1	2A	1114	G	2.4
11	2P	105	LEU	2.4
32	1a	93	G	2.4
32	1a	102	G	2.4
32	2a	1221	G	2.4
35	1d	11	LEU	2.4
41	2j	90	LEU	2.4
44	2m	70	LEU	2.4
46	2o	32	LEU	2.4
30	28	14	VAL	2.4
16	2U	25	TRP	2.4
30	28	65	GLU	2.4
33	2b	170	GLU	2.4
33	1b	63	MET	2.4
12	2Q	122	GLY	2.4
1	2A	6	A	2.4
40	1i	49	PRO	2.4
32	1a	221	C	2.4
38	1g	65	ALA	2.4
41	2j	13	HIS	2.4
10	2O	91	LEU	2.4
33	1b	187	LEU	2.4
22	20	68	GLU	2.4
1	1A	883	G	2.4
1	2A	2894	G	2.4
31	29	2	LYS	2.4
32	2a	1068	G	2.4
33	1b	122	PHE	2.4
34	1c	5	ILE	2.4
23	21	22	GLY	2.4
40	1i	31	GLN	2.4
36	2e	21	ALA	2.4
1	1A	898	C	2.4
1	2A	1118	C	2.4

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Mol	Chain	Res	Type	RSRZ
51	1t	62	LEU	2.4
7	2H	153	LYS	2.4
8	2I	20	ASP	2.4
33	2b	81	VAL	2.4
40	1i	86	VAL	2.4
47	2p	27	LYS	2.4
1	2A	2172	U	2.4
22	20	44	ARG	2.4
28	26	50	ARG	2.4
47	1p	25	ARG	2.4
51	2t	22	ARG	2.4
4	2E	134	ILE	2.4
7	2H	166	GLY	2.4
22	20	12	ASN	2.4
33	1b	31	TYR	2.4
33	1b	92	TYR	2.4
34	1c	193	TYR	2.4
44	2m	84	ILE	2.4
51	2t	85	MET	2.4
7	2H	8	PRO	2.4
56	1y	27	G	2.4
11	2P	149	GLU	2.4
33	1b	126	GLU	2.4
15	2T	130	ALA	2.4
42	2k	23	ALA	2.4
52	1u	8	THR	2.4
34	2c	20	SER	2.4
34	2c	33	LEU	2.4
38	1g	101	LEU	2.4
50	1s	4	SER	2.4
45	1n	23	ARG	2.4
34	2c	155	GLY	2.4
35	2d	70	ILE	2.4
40	1i	81	ILE	2.4
41	2j	11	PHE	2.4
10	2O	33	ALA	2.4
12	2Q	114	ALA	2.4
1	2A	2893	G	2.4
12	2Q	110	THR	2.4
34	1c	177	THR	2.4
7	2H	80	SER	2.4
33	1b	21	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
45	2n	45	ARG	2.4
34	1c	32	LEU	2.4
36	2e	12	LEU	2.4
39	2h	119	LEU	2.4
11	2P	92	GLU	2.4
22	20	52	GLY	2.4
26	14	56	VAL	2.4
1	1A	1026	U	2.4
33	1b	182	ILE	2.4
36	2e	109	ILE	2.4
47	1p	38	TYR	2.4
51	2t	73	HIS	2.4
17	2V	77	ALA	2.4
21	2Z	80	ARG	2.4
34	1c	24	ALA	2.4
17	2V	73	SER	2.4
34	2c	167	TRP	2.4
40	2i	71	SER	2.4
23	11	98	LEU	2.4
45	2n	53	LEU	2.4
8	2I	74	ASN	2.3
40	2i	22	GLY	2.3
44	2m	24	GLY	2.3
50	1s	68	GLY	2.3
1	2A	1041	C	2.3
10	2O	2	ILE	2.3
17	2V	70	ILE	2.3
21	2Z	57	ILE	2.3
28	26	54	ILE	2.3
29	27	1	MET	2.3
39	1h	35	ILE	2.3
41	2j	9	ARG	2.3
48	2q	90	ILE	2.3
33	1b	163	PHE	2.3
40	1i	84	ALA	2.3
7	2H	90	LYS	2.3
6	2G	152	LEU	2.3
33	1b	97	TRP	2.3
33	2b	72	GLY	2.3
11	2P	125	VAL	2.3
1	1A	1963	U	2.3
1	2A	100	G	2.3

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Mol	Chain	Res	Type	RSRZ
32	1a	68	G	2.3
32	1a	630	G	2.3
34	2c	30	ARG	2.3
36	2e	25	ARG	2.3
54	2w	44	G	2.3
7	2H	39	PRO	2.3
32	2a	1114	C	2.3
40	2i	124	GLN	2.3
41	2j	25	GLU	2.3
38	1g	26	PHE	2.3
10	2O	7	TYR	2.3
26	24	67	TYR	2.3
31	29	31	LYS	2.3
40	1i	126	SER	2.3
41	2j	92	THR	2.3
33	1b	66	GLY	2.3
34	2c	194	GLY	2.3
49	1r	76	LEU	2.3
7	2H	61	HIS	2.3
35	2d	156	GLU	2.3
9	2N	46	VAL	2.3
32	1a	1007	C	2.3
32	2a	1018	C	2.3
40	1i	55	ALA	2.3
56	2y	38	A	2.3
41	2j	76	ASN	2.3
7	2H	161	GLY	2.3
33	2b	38	GLY	2.3
39	2h	71	GLY	2.3
6	1G	152	LEU	2.3
17	2V	71	LEU	2.3
20	2Y	90	LEU	2.3
24	12	10	LEU	2.3
33	1b	53	ARG	2.3
33	1b	114	ARG	2.3
36	1e	31	LEU	2.3
35	2d	30	LYS	2.3
10	2O	43	VAL	2.3
21	2Z	128	VAL	2.3
33	1b	131	PRO	2.3
45	1n	33	VAL	2.3
32	2a	1025	U	2.3

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Mol	Chain	Res	Type	RSRZ
55	1x	47	U	2.3
23	21	37	ILE	2.3
41	1j	75	ILE	2.3
7	2H	167	GLU	2.3
9	2N	22	THR	2.3
28	26	44	ARG	2.3
32	1a	1140	C	2.3
32	2a	1060	C	2.3
40	2i	39	GLY	2.3
40	2i	69	GLY	2.3
1	1A	655	A	2.3
1	2A	2152	G	2.3
1	2A	2750	A	2.3
32	2a	1131	G	2.3
39	2h	94	TYR	2.3
51	2t	57	ARG	2.3
52	1u	22	ARG	2.3
3	1D	38	LYS	2.3
6	2G	43	LEU	2.3
22	20	70	GLN	2.3
23	21	81	LYS	2.3
41	1j	17	ASP	2.3
45	1n	4	LYS	2.3
45	1n	50	LYS	2.3
17	2V	87	HIS	2.3
10	2O	101	PRO	2.3
12	2Q	106	VAL	2.3
31	29	7	VAL	2.3
39	2h	26	VAL	2.3
48	1q	35	VAL	2.3
8	1I	97	ILE	2.3
22	20	69	PHE	2.3
50	2s	68	GLY	2.3
33	2b	85	ALA	2.3
7	2H	122	THR	2.3
41	2j	42	THR	2.3
36	1e	133	TYR	2.3
42	1k	75	TYR	2.3
1	2A	892	G	2.3
53	2v	14	A	2.3
51	2t	98	PRO	2.3
11	2P	65	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
15	2T	10	VAL	2.3
34	1c	195	VAL	2.3
32	2a	1446	U	2.3
52	2u	7	ARG	2.3
45	2n	9	LYS	2.3
48	2q	37	LYS	2.3
33	1b	216	SER	2.3
34	2c	197	GLY	2.3
12	2Q	36	ALA	2.3
41	2j	33	GLN	2.3
50	2s	10	PHE	2.3
21	2Z	125	LEU	2.3
35	2d	196	LEU	2.3
11	2P	111	ARG	2.2
25	23	10	LYS	2.2
30	28	21	LYS	2.2
34	2c	21	ARG	2.2
9	2N	45	ASN	2.2
11	1P	71	VAL	2.2
11	2P	37	GLY	2.2
20	2Y	72	VAL	2.2
25	23	47	VAL	2.2
34	1c	63	ASN	2.2
3	1D	2	ALA	2.2
51	2t	100	ILE	2.2
36	1e	9	LYS	2.2
39	1h	59	LEU	2.2
32	1a	219	C	2.2
32	2a	1019	C	2.2
54	1w	4	C	2.2
1	2A	2749	A	2.2
8	2I	107	VAL	2.2
11	2P	94	GLU	2.2
22	20	60	PHE	2.2
38	2g	7	ALA	2.2
40	1i	46	ALA	2.2
33	2b	16	HIS	2.2
34	1c	15	THR	2.2
38	1g	153	HIS	2.2
44	2m	103	THR	2.2
7	2H	101	ARG	2.2
34	1c	47	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
39	2h	10	LEU	2.2
16	2U	47	TYR	2.2
33	2b	125	PRO	2.2
40	2i	49	PRO	2.2
47	1p	58	TYR	2.2
4	2E	186	GLY	2.2
34	1c	56	ASP	2.2
41	1j	89	ASP	2.2
41	2j	95	GLU	2.2
4	2E	102	VAL	2.2
9	2N	9	VAL	2.2
26	24	10	VAL	2.2
32	1a	1280	A	2.2
7	2H	170	ARG	2.2
30	28	58	ILE	2.2
35	1d	158	ILE	2.2
36	1e	109	ILE	2.2
11	1P	57	THR	2.2
36	2e	45	PHE	2.2
32	2a	1120	G	2.2
33	1b	135	GLN	2.2
33	2b	114	ARG	2.2
41	2j	5	ARG	2.2
45	2n	60	SER	2.2
4	2E	104	VAL	2.2
50	2s	81	ARG	2.2
41	1j	13	HIS	2.2
1	1A	1073	A	2.2
16	1U	21	ALA	2.2
20	2Y	44	ILE	2.2
22	20	36	ILE	2.2
33	1b	28	PHE	2.2
8	1I	11	ASN	2.2
11	2P	115	LEU	2.2
36	2e	53	LEU	2.2
40	2i	85	LEU	2.2
41	1j	36	GLY	2.2
52	1u	3	LYS	2.2
1	2A	10	G	2.2
1	2A	1039	G	2.2
32	2a	1356	G	2.2
4	2E	160	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
51	2t	61	SER	2.2
14	2S	49	VAL	2.2
33	2b	7	VAL	2.2
41	2j	49	VAL	2.2
8	1I	36	ALA	2.2
32	1a	103	C	2.2
32	2a	962	C	2.2
32	2a	1259	C	2.2
47	2p	64	ALA	2.2
51	1t	67	ALA	2.2
44	1m	4	ILE	2.2
1	2A	2753	A	2.2
15	2T	124	ASP	2.2
32	1a	1004	A	2.2
32	2a	1130	A	2.2
41	1j	69	ASN	2.2
41	2j	78	ASN	2.2
22	20	65	GLY	2.2
33	1b	65	GLY	2.2
38	1g	12	LEU	2.2
40	1i	90	PRO	2.2
44	1m	100	GLY	2.2
45	1n	6	LEU	2.2
11	2P	102	ARG	2.2
32	1a	98	G	2.2
33	1b	128	GLU	2.2
34	2c	18	TRP	2.2
47	1p	17	TYR	2.2
12	2Q	18	LYS	2.2
21	2Z	161	VAL	2.2
37	2f	91	VAL	2.2
47	1p	1	MET	2.2
51	1t	85	MET	2.2
4	2E	114	ALA	2.2
34	1c	168	ALA	2.2
38	2g	40	ALA	2.2
1	2A	277	C	2.2
14	1S	82	ILE	2.2
14	2S	82	ILE	2.2
16	2U	17	ILE	2.2
32	1a	470	C	2.2
33	1b	185	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
34	2c	39	ILE	2.2
41	2j	12	ASP	2.2
15	1T	115	ARG	2.2
18	2W	92	ARG	2.2
19	2X	71	GLY	2.2
33	1b	105	PHE	2.2
34	2c	54	ARG	2.2
40	2i	24	GLY	2.2
41	1j	39	PRO	2.2
21	2Z	102	LEU	2.2
33	1b	154	LEU	2.2
35	2d	135	LEU	2.2
47	2p	6	LEU	2.2
41	2j	30	SER	2.2
12	1Q	32	TYR	2.1
12	2Q	1	MET	2.1
1	1A	1071	G	2.1
1	1A	1089	G	2.1
21	2Z	154	ASP	2.1
22	20	81	VAL	2.1
48	2q	5	VAL	2.1
41	1j	18	ALA	2.1
11	1P	44	GLY	2.1
12	2Q	15	GLY	2.1
21	2Z	79	ARG	2.1
26	14	45	GLY	2.1
27	25	29	THR	2.1
34	1c	205	GLY	2.1
35	2d	87	GLY	2.1
38	2g	24	THR	2.1
48	2q	60	ILE	2.1
6	2G	90	LEU	2.1
16	2U	20	LEU	2.1
48	1q	99	SER	2.1
1	1A	2150	U	2.1
7	2H	165	ALA	2.1
11	2P	126	VAL	2.1
37	2f	90	VAL	2.1
38	2g	75	VAL	2.1
40	2i	120	ARG	2.1
41	1j	5	ARG	2.1
21	2Z	138	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
30	28	9	GLY	2.1
32	1a	223	U	2.1
20	2Y	75	ILE	2.1
21	2Z	124	ILE	2.1
32	1a	1009	G	2.1
34	1c	8	ILE	2.1
50	2s	40	ILE	2.1
47	2p	80	PHE	2.1
25	23	28	LEU	2.1
40	1i	124	GLN	2.1
41	2j	35	SER	2.1
1	2A	1847	A	2.1
9	2N	74	ARG	2.1
12	2Q	60	ARG	2.1
22	20	55	ARG	2.1
32	2a	1093	A	2.1
40	1i	16	ARG	2.1
40	1i	93	ARG	2.1
40	2i	20	ARG	2.1
53	2v	15	A	2.1
56	1y	76	A	2.1
8	1I	45	LYS	2.1
10	2O	121	VAL	2.1
18	2W	85	VAL	2.1
33	1b	7	VAL	2.1
33	1b	85	ALA	2.1
35	2d	4	TYR	2.1
36	1e	51	VAL	2.1
51	2t	29	LYS	2.1
56	2y	12	U	2.1
11	2P	68	GLN	2.1
12	2Q	41	TRP	2.1
47	2p	4	ILE	2.1
4	2E	113	PHE	2.1
9	2N	112	LEU	2.1
13	2R	65	LEU	2.1
1	1A	2104	G	2.1
1	1A	2805	G	2.1
23	21	38	SER	2.1
32	2a	1061	G	2.1
41	1j	35	SER	2.1
40	1i	25	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
7	2H	66	GLY	2.1
41	1j	93	GLY	2.1
32	2a	1349	A	2.1
53	1v	24	A	2.1
3	2D	34	VAL	2.1
13	2R	25	ALA	2.1
33	2b	230	VAL	2.1
34	2c	160	ALA	2.1
41	2j	18	ALA	2.1
29	27	4	THR	2.1
54	1w	47	U	2.1
36	1e	13	ILE	2.1
38	1g	120	ILE	2.1
11	1P	59	LEU	2.1
23	21	46	LEU	2.1
33	1b	221	LEU	2.1
39	1h	133	LEU	2.1
50	1s	69	HIS	2.1
51	1t	16	HIS	2.1
51	1t	64	ASP	2.1
3	2D	238	GLY	2.1
32	2a	1042	G	2.1
32	2a	1386	G	2.1
33	1b	101	MET	2.1
4	2E	116	VAL	2.1
7	2H	114	VAL	2.1
8	2I	63	ALA	2.1
31	29	5	ALA	2.1
36	1e	86	ALA	2.1
7	2H	152	ARG	2.1
40	2i	104	ARG	2.1
8	2I	79	ILE	2.1
11	1P	75	ILE	2.1
40	2i	75	ASP	2.1
48	2q	65	ILE	2.1
51	2t	58	LYS	2.1
41	1j	71	LEU	2.1
43	2l	60	LEU	2.1
45	1n	37	PHE	2.1
31	29	29	ASN	2.1
34	2c	22	TRP	2.1
34	2c	63	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
24	22	70	GLN	2.1
40	2i	31	GLN	2.1
20	2Y	5	MET	2.1
1	2A	2807	G	2.1
6	2G	75	LYS	2.1
7	2H	146	ALA	2.1
9	2N	27	ALA	2.1
32	1a	220	G	2.1
10	2O	62	VAL	2.1
36	1e	16	THR	2.1
38	1g	69	VAL	2.1
48	2q	35	VAL	2.1
4	2E	14	ILE	2.1
15	2T	52	ILE	2.1
31	29	32	HIS	2.1
32	1a	101	A	2.1
32	1a	162	A	2.1
40	1i	62	TYR	2.1
48	1q	60	ILE	2.1
50	1s	62	ILE	2.1
6	2G	133	LEU	2.1
36	1e	53	LEU	2.1
44	2m	90	LEU	2.1
31	29	14	CYS	2.1
35	1d	156	GLU	2.1
40	1i	48	GLU	2.1
20	2Y	47	LYS	2.1
21	1Z	80	ARG	2.1
23	21	76	ARG	2.1
41	1j	70	ARG	2.1
1	1A	2103	C	2.0
32	2a	1192	C	2.0
41	1j	20	ALA	2.0
41	2j	100	THR	2.0
48	1q	23	VAL	2.0
21	2Z	121	HIS	2.0
34	1c	124	ILE	2.0
38	1g	151	TYR	2.0
1	1A	899	A	2.0
1	2A	2062	A	2.0
15	1T	123	GLN	2.0
23	11	82	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
33	2b	115	LEU	2.0
40	2i	23	ASN	2.0
32	2a	977	A	2.0
33	2b	66	GLY	2.0
35	1d	75	PHE	2.0
45	1n	47	LEU	2.0
49	1r	85	LEU	2.0
51	1t	53	LEU	2.0
51	2t	10	LEU	2.0
7	2H	62	LYS	2.0
21	2Z	78	LYS	2.0
22	20	74	ARG	2.0
34	1c	11	ARG	2.0
47	1p	5	ARG	2.0
5	2F	39	TRP	2.0
51	1t	32	ALA	2.0
12	2Q	27	VAL	2.0
12	2Q	96	VAL	2.0
34	1c	6	HIS	2.0
34	2c	64	VAL	2.0
35	1d	198	VAL	2.0
44	2m	7	VAL	2.0
52	1u	17	THR	2.0
32	2a	175	C	2.0
32	2a	1226	C	2.0
4	1E	195	LEU	2.0
10	2O	64	ARG	2.0
14	2S	54	LEU	2.0
14	2S	58	LEU	2.0
20	2Y	55	TYR	2.0
21	1Z	171	ILE	2.0
33	1b	41	ILE	2.0
41	2j	99	LYS	2.0
51	1t	21	LYS	2.0
34	2c	80	GLY	2.0
34	2c	145	GLY	2.0
35	1d	73	ARG	2.0
40	1i	42	ARG	2.0
40	1i	111	ARG	2.0
47	2p	74	LEU	2.0
26	14	59	PHE	2.0
52	1u	15	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
32	1a	1353	G	2.0
32	2a	220	G	2.0
32	2a	485	G	2.0
54	1w	69	G	2.0
32	2a	983	A	2.0
51	2t	64	ASP	2.0
7	2H	140	LYS	2.0
34	2c	113	ALA	2.0
40	2i	87	GLN	2.0
7	2H	16	SER	2.0
9	2N	77	GLY	2.0
14	2S	31	SER	2.0
20	2Y	2	ARG	2.0
33	1b	210	SER	2.0
33	2b	219	VAL	2.0
33	2b	229	VAL	2.0
43	1l	43	VAL	2.0
44	2m	98	VAL	2.0
50	2s	53	ASN	2.0
44	2m	71	ARG	2.0
48	2q	38	ARG	2.0
4	2E	197	ILE	2.0
32	1a	307	C	2.0
32	1a	1006	C	2.0
32	1a	1029	C	2.0
32	2a	1129	C	2.0
35	1d	70	ILE	2.0
10	2O	32	TYR	2.0
12	2Q	93	TYR	2.0
21	2Z	9	TYR	2.0
35	2d	110	PHE	2.0
33	1b	129	GLU	2.0
1	1A	1085	A	2.0
32	1a	77	G	2.0
32	2a	1503	A	2.0
21	2Z	98	MET	2.0
40	1i	98	PRO	2.0
42	1k	13	GLN	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
56	4SU	2y	8	20/21	0.62	0.27	98,102,113,128	0
56	G7M	2y	46	24/25	0.65	0.26	86,101,106,121	0
56	PSU	1y	55	20/21	0.66	0.52	96,101,103,114	0
56	5MU	1y	54	21/22	0.70	0.47	89,98,103,112	0
56	5MU	2y	54	21/22	0.70	0.52	94,100,111,124	0
56	MIA	1y	37	22/30	0.71	0.43	88,95,103,115	0
56	PSU	2y	55	20/21	0.72	0.41	92,99,110,115	0
56	MIA	2y	37	22/30	0.76	0.44	88,94,108,126	0
56	PSU	2y	32	20/21	0.76	0.51	89,96,103,113	0
56	4SU	1y	8	20/21	0.77	0.30	97,101,109,117	0
56	G7M	1y	46	24/25	0.77	0.33	90,98,107,113	0
54	G7M	1w	46	24/25	0.79	0.19	79,86,99,118	0
54	G7M	2w	46	24/25	0.79	0.18	87,94,105,120	0
56	PSU	1y	39	20/21	0.80	0.35	88,94,105,106	0
54	4SU	2w	8	20/21	0.81	0.15	89,94,104,105	0
56	PSU	2y	39	20/21	0.85	0.38	88,94,105,111	0
54	MIA	2w	37	25/30	0.85	0.28	56,74,82,100	0
56	PSU	1y	32	20/21	0.86	0.39	90,96,105,109	0
54	PSU	1w	55	20/21	0.89	0.17	59,73,84,87	0
55	PSU	2x	55	20/21	0.89	0.15	69,75,87,90	0
54	4SU	1w	8	20/21	0.89	0.24	83,88,93,95	0
55	4SU	2x	8	20/21	0.90	0.19	71,78,82,83	0
32	PSU	2a	516	20/21	0.90	0.16	53,67,71,74	0
54	PSU	2w	55	20/21	0.90	0.16	85,89,96,99	0
54	MIA	1w	37	29/30	0.91	0.34	51,59,73,87	0
32	2MG	2a	1207	24/25	0.91	0.18	71,81,83,85	0
54	PSU	1w	32	20/21	0.91	0.22	56,62,69,71	0
54	PSU	2w	32	20/21	0.92	0.20	73,78,86,86	0
55	PSU	1x	55	20/21	0.93	0.13	57,63,72,72	0
54	5MU	2w	54	21/22	0.93	0.16	79,84,89,93	0
32	G7M	2a	527	24/25	0.93	0.21	56,64,71,72	0
54	PSU	2w	39	20/21	0.93	0.26	68,78,84,85	0
43	0TD	1l	92	10/11	0.94	0.19	47,52,55,67	0
32	M2G	2a	966	25/26	0.94	0.29	53,62,68,73	0
54	5MU	1w	54	21/22	0.94	0.16	52,63,66,70	0
43	0TD	2l	92	10/11	0.94	0.18	63,65,68,72	0
32	5MC	2a	967	21/22	0.95	0.21	59,66,72,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	M2G	1a	966	25/26	0.95	0.21	39,49,60,63	0
32	2MG	1a	1207	24/25	0.95	0.15	66,70,74,75	0
32	G7M	1a	527	24/25	0.95	0.19	36,49,56,60	0
55	5MU	1x	54	21/22	0.95	0.17	58,63,72,74	0
55	5MU	2x	54	21/22	0.95	0.20	72,77,80,83	0
54	PSU	1w	39	20/21	0.95	0.21	47,61,66,69	0
1	5MU	1A	1915	21/22	0.95	0.18	44,49,57,57	0
1	5MU	2A	1915	21/22	0.95	0.17	53,61,65,67	0
32	5MC	1a	967	21/22	0.96	0.19	45,50,59,62	0
55	31H	2x	76	32/33	0.96	0.23	39,47,57,57	0
55	4SU	1x	8	20/21	0.96	0.17	55,62,66,67	0
55	31H	1x	76	32/33	0.96	0.23	21,27,33,45	10
32	5MC	2a	1400	21/22	0.96	0.23	61,66,74,74	0
32	4OC	2a	1402	22/23	0.96	0.19	53,59,63,66	0
32	5MC	2a	1404	21/22	0.96	0.20	49,52,56,58	0
32	MA6	2a	1518	24/25	0.96	0.22	52,59,64,67	0
32	MA6	2a	1519	24/25	0.96	0.23	48,59,64,66	0
1	PSU	2A	1911	20/21	0.96	0.19	49,53,58,64	0
55	5MC	2x	32	21/22	0.96	0.19	63,68,73,78	0
55	5MC	1x	32	21/22	0.96	0.18	51,56,60,64	0
1	PSU	2A	1917	20/21	0.96	0.17	50,57,63,64	0
1	OMC	2A	1920	21/22	0.96	0.21	51,56,60,62	0
1	5MC	2A	1962	21/22	0.96	0.20	43,48,53,61	0
1	PSU	2A	2605	20/21	0.96	0.20	36,42,47,51	0
32	MA6	1a	1519	24/25	0.97	0.23	33,41,45,49	0
54	F3N	2w	76	33/34	0.97	0.24	36,43,47,50	0
32	5MC	2a	1407	21/22	0.97	0.19	49,56,60,62	0
32	UR3	2a	1498	21/22	0.97	0.21	51,56,59,62	0
32	PSU	1a	516	20/21	0.97	0.14	51,57,62,62	0
1	5MC	2A	1942	21/22	0.97	0.19	50,57,63,73	0
32	5MC	1a	1400	21/22	0.97	0.20	45,51,56,56	0
1	OMG	2A	2251	24/25	0.97	0.21	40,45,50,52	0
1	2MU	2A	2552	21/23	0.97	0.22	44,49,52,58	0
1	PSU	1A	2605	20/21	0.97	0.23	23,29,32,35	0
32	MA6	1a	1518	24/25	0.97	0.23	34,40,47,47	0
1	OMC	1A	1920	21/22	0.98	0.19	38,47,50,52	0
54	F3N	1w	76	33/34	0.98	0.24	19,27,32,33	0
1	5MU	1A	1939	21/22	0.98	0.21	25,31,35,42	0
1	5MU	2A	1939	21/22	0.98	0.21	33,41,46,51	0
1	5MC	1A	1942	21/22	0.98	0.21	35,41,46,50	0
1	PSU	1A	1911	20/21	0.98	0.17	40,51,54,55	0
1	5MC	1A	1962	21/22	0.98	0.19	28,34,37,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	5MC	1a	1407	21/22	0.98	0.18	35,44,46,50	0
32	UR3	1a	1498	21/22	0.98	0.21	37,42,45,48	0
1	8AH	1A	2503	24/25	0.98	0.22	16,25,30,32	0
1	8AH	2A	2503	24/25	0.98	0.22	35,40,43,49	0
32	4OC	1a	1402	22/23	0.98	0.20	36,43,46,50	0
1	PSU	1A	1917	20/21	0.98	0.17	47,51,55,55	0
32	5MC	1a	1404	21/22	0.98	0.18	34,40,45,47	0
1	2MU	1A	2552	21/23	0.99	0.20	24,29,34,35	0
1	OMG	1A	2251	24/25	0.99	0.20	22,26,30,33	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
57	MG	1B	230	1/1	-0.14	0.30	84,84,84,84	0
57	MG	2A	3660	1/1	0.14	0.11	75,75,75,75	0
57	MG	18	105	1/1	0.15	0.40	78,78,78,78	0
57	MG	1A	3092	1/1	0.18	0.25	79,79,79,79	0
57	MG	2A	3592	1/1	0.20	0.47	73,73,73,73	0
57	MG	1A	4022	1/1	0.34	0.21	55,55,55,55	0
57	MG	1A	3099	1/1	0.36	0.32	68,68,68,68	0
57	MG	1A	3072	1/1	0.40	0.43	69,69,69,69	0
57	MG	2A	3018	1/1	0.45	0.27	66,66,66,66	0
57	MG	1A	3291	1/1	0.47	0.24	64,64,64,64	0
57	MG	1A	3918	1/1	0.47	0.08	78,78,78,78	0
57	MG	1A	3479	1/1	0.50	0.28	65,65,65,65	0
57	MG	2A	3252	1/1	0.51	0.13	76,76,76,76	0
57	MG	2A	3369	1/1	0.51	0.25	73,73,73,73	0
57	MG	2y	105	1/1	0.52	0.17	89,89,89,89	0
57	MG	1A	3914	1/1	0.53	0.15	57,57,57,57	0
57	MG	1A	4041	1/1	0.53	0.23	70,70,70,70	0
57	MG	1a	1755	1/1	0.53	0.12	70,70,70,70	0
57	MG	2A	3328	1/1	0.54	0.23	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4051	1/1	0.55	0.13	54,54,54,54	0
57	MG	2A	3176	1/1	0.55	0.23	67,67,67,67	0
57	MG	1a	1656	1/1	0.55	0.27	68,68,68,68	0
57	MG	2A	3674	1/1	0.55	0.16	57,57,57,57	0
57	MG	1A	3554	1/1	0.55	0.39	65,65,65,65	0
57	MG	2A	3404	1/1	0.56	0.25	72,72,72,72	0
57	MG	1A	3976	1/1	0.56	0.29	60,60,60,60	0
57	MG	2A	3287	1/1	0.56	0.12	77,77,77,77	0
57	MG	2A	3108	1/1	0.56	0.23	58,58,58,58	0
57	MG	1A	3908	1/1	0.56	0.17	52,52,52,52	0
57	MG	2A	3062	1/1	0.57	0.16	73,73,73,73	0
57	MG	2A	3708	1/1	0.57	0.26	73,73,73,73	0
57	MG	1A	4113	1/1	0.57	0.30	56,56,56,56	0
57	MG	1a	1711	1/1	0.58	0.15	71,71,71,71	0
57	MG	1a	1725	1/1	0.58	0.15	75,75,75,75	0
57	MG	2A	3235	1/1	0.58	0.09	80,80,80,80	0
57	MG	1A	4010	1/1	0.58	0.06	83,83,83,83	0
57	MG	2A	3269	1/1	0.58	0.33	73,73,73,73	0
57	MG	1a	1655	1/1	0.58	0.55	66,66,66,66	0
57	MG	1A	4003	1/1	0.58	0.23	75,75,75,75	0
57	MG	1x	111	1/1	0.59	0.21	78,78,78,78	0
57	MG	2A	3320	1/1	0.59	0.33	70,70,70,70	0
57	MG	1A	3824	1/1	0.59	0.14	64,64,64,64	0
57	MG	2A	3686	1/1	0.59	0.53	58,58,58,58	0
57	MG	1A	3721	1/1	0.59	0.26	66,66,66,66	0
57	MG	2A	3791	1/1	0.59	0.19	71,71,71,71	0
57	MG	1l	201	1/1	0.59	0.21	82,82,82,82	0
57	MG	2A	3562	1/1	0.60	0.23	56,56,56,56	0
57	MG	1a	1684	1/1	0.60	0.23	61,61,61,61	0
57	MG	1A	3970	1/1	0.60	0.23	33,33,33,33	0
57	MG	1A	3315	1/1	0.60	0.20	57,57,57,57	0
57	MG	1A	4061	1/1	0.61	0.15	28,28,28,28	0
57	MG	2A	3491	1/1	0.61	0.17	82,82,82,82	0
57	MG	1A	3819	1/1	0.61	0.21	70,70,70,70	0
57	MG	1A	3800	1/1	0.61	0.19	64,64,64,64	0
57	MG	1B	237	1/1	0.61	0.20	62,62,62,62	0
57	MG	1A	3329	1/1	0.62	0.78	59,59,59,59	0
57	MG	1A	3939	1/1	0.62	0.38	74,74,74,74	0
57	MG	1a	1744	1/1	0.62	0.11	64,64,64,64	0
57	MG	1A	4050	1/1	0.62	0.17	56,56,56,56	0
57	MG	2A	3580	1/1	0.62	0.16	75,75,75,75	0
57	MG	2x	103	1/1	0.62	0.15	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3332	1/1	0.62	0.38	72,72,72,72	0
57	MG	1A	3909	1/1	0.63	0.08	61,61,61,61	0
57	MG	1A	3887	1/1	0.63	0.12	46,46,46,46	0
57	MG	2A	3160	1/1	0.63	0.37	68,68,68,68	0
57	MG	2A	3161	1/1	0.63	0.23	87,87,87,87	0
57	MG	1a	1785	1/1	0.63	0.17	76,76,76,76	0
57	MG	1A	3895	1/1	0.64	0.21	67,67,67,67	0
57	MG	1A	3884	1/1	0.64	0.32	47,47,47,47	0
57	MG	2A	3620	1/1	0.64	0.23	77,77,77,77	0
57	MG	2A	3042	1/1	0.64	0.26	74,74,74,74	0
57	MG	2A	3365	1/1	0.64	0.31	62,62,62,62	0
57	MG	1A	4073	1/1	0.65	0.15	73,73,73,73	0
57	MG	2A	3363	1/1	0.65	0.24	63,63,63,63	0
57	MG	2A	3082	1/1	0.65	0.54	69,69,69,69	0
57	MG	2A	3673	1/1	0.65	0.18	64,64,64,64	0
57	MG	1A	3436	1/1	0.65	1.02	65,65,65,65	0
57	MG	1a	1692	1/1	0.65	0.12	63,63,63,63	0
57	MG	2A	3317	1/1	0.65	0.48	71,71,71,71	0
57	MG	2A	3507	1/1	0.65	0.16	47,47,47,47	0
57	MG	2w	106	1/1	0.65	0.23	82,82,82,82	0
57	MG	2A	3031	1/1	0.65	0.29	70,70,70,70	0
57	MG	1A	4008	1/1	0.65	0.24	73,73,73,73	0
57	MG	1A	3840	1/1	0.66	0.14	68,68,68,68	0
57	MG	2A	3390	1/1	0.66	0.15	75,75,75,75	0
57	MG	1A	3940	1/1	0.66	0.12	64,64,64,64	0
57	MG	2w	103	1/1	0.66	0.25	93,93,93,93	0
57	MG	1A	3241	1/1	0.66	0.14	61,61,61,61	0
57	MG	2A	3084	1/1	0.66	0.51	57,57,57,57	0
57	MG	2A	3177	1/1	0.66	0.34	70,70,70,70	0
57	MG	1A	3260	1/1	0.67	0.25	56,56,56,56	0
57	MG	1B	214	1/1	0.67	0.39	69,69,69,69	0
57	MG	2A	3327	1/1	0.67	0.14	73,73,73,73	0
57	MG	1A	3444	1/1	0.67	0.17	69,69,69,69	0
57	MG	2A	3560	1/1	0.67	0.22	44,44,44,44	0
57	MG	1A	3302	1/1	0.67	0.33	50,50,50,50	0
57	MG	2B	208	1/1	0.67	0.18	66,66,66,66	0
57	MG	2A	3102	1/1	0.67	0.19	72,72,72,72	0
57	MG	2A	3585	1/1	0.67	0.19	59,59,59,59	0
57	MG	1A	3386	1/1	0.67	0.17	55,55,55,55	0
57	MG	1A	3641	1/1	0.67	0.37	53,53,53,53	0
57	MG	2A	3099	1/1	0.68	0.20	59,59,59,59	0
57	MG	1q	201	1/1	0.68	0.19	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1x	106	1/1	0.68	0.19	58,58,58,58	0
57	MG	1a	1602	1/1	0.68	0.30	62,62,62,62	0
57	MG	1a	1604	1/1	0.68	0.12	68,68,68,68	0
57	MG	1A	3949	1/1	0.68	0.23	49,49,49,49	0
57	MG	1A	3309	1/1	0.68	0.18	48,48,48,48	0
57	MG	2A	3054	1/1	0.68	0.17	66,66,66,66	0
57	MG	2A	3387	1/1	0.68	0.81	79,79,79,79	0
57	MG	1a	1758	1/1	0.68	0.08	77,77,77,77	0
57	MG	10	106	1/1	0.68	0.14	68,68,68,68	0
57	MG	2B	207	1/1	0.68	0.23	61,61,61,61	0
57	MG	2A	3410	1/1	0.68	0.29	73,73,73,73	0
57	MG	1A	4047	1/1	0.68	0.14	43,43,43,43	0
57	MG	2A	3297	1/1	0.68	0.19	74,74,74,74	0
57	MG	2A	3532	1/1	0.68	0.20	52,52,52,52	0
57	MG	2A	3308	1/1	0.68	0.47	65,65,65,65	0
57	MG	2A	3301	1/1	0.69	0.90	55,55,55,55	0
57	MG	1A	3051	1/1	0.69	0.42	54,54,54,54	0
57	MG	2A	3033	1/1	0.69	0.17	56,56,56,56	0
57	MG	2A	3041	1/1	0.69	0.32	71,71,71,71	0
57	MG	1A	4032	1/1	0.69	0.15	48,48,48,48	0
57	MG	1a	1743	1/1	0.69	0.35	87,87,87,87	0
57	MG	1a	1601	1/1	0.69	0.20	59,59,59,59	0
57	MG	2A	3639	1/1	0.69	0.36	88,88,88,88	0
57	MG	2A	3500	1/1	0.69	0.29	84,84,84,84	0
57	MG	2x	107	1/1	0.69	0.23	49,49,49,49	0
57	MG	2A	3071	1/1	0.69	0.20	71,71,71,71	0
57	MG	2A	3360	1/1	0.70	0.24	66,66,66,66	0
57	MG	1A	3953	1/1	0.70	0.49	53,53,53,53	0
57	MG	1A	3762	1/1	0.70	0.12	66,66,66,66	0
57	MG	1A	4018	1/1	0.70	0.37	56,56,56,56	0
57	MG	2A	3138	1/1	0.70	0.27	58,58,58,58	0
57	MG	2A	3139	1/1	0.70	0.64	61,61,61,61	0
57	MG	1A	3448	1/1	0.70	0.22	50,50,50,50	0
57	MG	1A	3560	1/1	0.70	0.25	47,47,47,47	0
57	MG	1A	3711	1/1	0.71	0.21	61,61,61,61	0
57	MG	1N	205	1/1	0.71	0.69	53,53,53,53	0
57	MG	1A	3292	1/1	0.71	0.55	55,55,55,55	0
57	MG	1A	3296	1/1	0.71	0.31	58,58,58,58	0
57	MG	2A	3528	1/1	0.71	0.21	56,56,56,56	0
57	MG	1A	3503	1/1	0.71	0.17	57,57,57,57	0
57	MG	1A	3814	1/1	0.71	0.25	41,41,41,41	0
57	MG	1A	3298	1/1	0.71	0.24	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3277	1/1	0.71	0.20	43,43,43,43	0
57	MG	1A	4102	1/1	0.71	0.10	64,64,64,64	0
57	MG	1A	3929	1/1	0.71	0.13	62,62,62,62	0
57	MG	1A	3938	1/1	0.71	0.12	50,50,50,50	0
57	MG	1A	3242	1/1	0.71	0.26	59,59,59,59	0
57	MG	1A	3788	1/1	0.72	0.11	54,54,54,54	0
57	MG	2A	3093	1/1	0.72	0.12	71,71,71,71	0
57	MG	1A	3653	1/1	0.72	0.24	40,40,40,40	0
57	MG	1a	1814	1/1	0.72	0.21	64,64,64,64	0
57	MG	2A	3608	1/1	0.72	0.14	62,62,62,62	0
57	MG	1a	1629	1/1	0.72	0.13	77,77,77,77	0
57	MG	1l	202	1/1	0.72	0.24	65,65,65,65	0
57	MG	1B	224	1/1	0.72	0.17	59,59,59,59	0
57	MG	1A	3673	1/1	0.72	0.17	61,61,61,61	0
57	MG	1a	1659	1/1	0.72	0.29	80,80,80,80	0
57	MG	2A	3676	1/1	0.72	0.11	60,60,60,60	0
57	MG	1A	3261	1/1	0.72	0.25	49,49,49,49	0
57	MG	1a	1690	1/1	0.72	0.16	58,58,58,58	0
57	MG	2A	3212	1/1	0.72	0.23	52,52,52,52	0
57	MG	1D	311	1/1	0.72	0.23	65,65,65,65	0
57	MG	1G	203	1/1	0.72	0.15	65,65,65,65	0
57	MG	1A	4058	1/1	0.72	0.22	61,61,61,61	0
57	MG	1a	1742	1/1	0.72	0.34	71,71,71,71	0
57	MG	1A	3823	1/1	0.72	0.15	67,67,67,67	0
57	MG	1A	3336	1/1	0.72	0.23	49,49,49,49	0
57	MG	2y	103	1/1	0.72	0.14	80,80,80,80	0
57	MG	1A	3510	1/1	0.72	0.26	64,64,64,64	0
57	MG	2A	3648	1/1	0.73	0.27	68,68,68,68	0
57	MG	2A	3063	1/1	0.73	0.26	67,67,67,67	0
57	MG	2A	3175	1/1	0.73	0.61	68,68,68,68	0
57	MG	1A	3684	1/1	0.73	0.20	41,41,41,41	0
57	MG	1A	3118	1/1	0.73	0.28	37,37,37,37	0
57	MG	2A	3525	1/1	0.73	0.14	65,65,65,65	0
57	MG	1A	3174	1/1	0.73	0.27	63,63,63,63	0
57	MG	2A	3733	1/1	0.73	0.24	57,57,57,57	0
57	MG	2A	3351	1/1	0.73	0.13	62,62,62,62	0
57	MG	2A	3796	1/1	0.73	0.18	70,70,70,70	0
57	MG	1A	4006	1/1	0.73	0.11	70,70,70,70	0
57	MG	1A	3286	1/1	0.73	0.38	60,60,60,60	0
57	MG	2D	303	1/1	0.73	0.56	54,54,54,54	0
57	MG	25	103	1/1	0.73	0.34	76,76,76,76	0
57	MG	1A	3186	1/1	0.73	0.48	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3377	1/1	0.73	0.28	45,45,45,45	0
57	MG	2A	3384	1/1	0.73	0.94	91,91,91,91	0
57	MG	1A	4086	1/1	0.73	0.17	61,61,61,61	0
57	MG	1A	3656	1/1	0.73	0.18	37,37,37,37	0
57	MG	1A	3381	1/1	0.73	0.28	65,65,65,65	0
57	MG	2A	3229	1/1	0.74	0.26	76,76,76,76	0
57	MG	1A	3581	1/1	0.74	0.22	64,64,64,64	0
57	MG	2A	3109	1/1	0.74	0.30	58,58,58,58	0
57	MG	1O	204	1/1	0.74	0.27	67,67,67,67	0
57	MG	2A	3766	1/1	0.74	0.11	49,49,49,49	0
57	MG	1A	3312	1/1	0.74	0.27	59,59,59,59	0
57	MG	2A	3792	1/1	0.74	0.17	78,78,78,78	0
57	MG	1A	3428	1/1	0.74	0.73	61,61,61,61	0
57	MG	2A	3803	1/1	0.74	0.12	59,59,59,59	0
57	MG	1A	3727	1/1	0.74	0.10	58,58,58,58	0
57	MG	2A	3595	1/1	0.74	0.16	52,52,52,52	0
57	MG	2A	3598	1/1	0.74	0.24	57,57,57,57	0
57	MG	1a	1772	1/1	0.74	0.24	86,86,86,86	0
57	MG	1A	3465	1/1	0.74	0.31	50,50,50,50	0
57	MG	1A	4042	1/1	0.74	0.41	40,40,40,40	0
57	MG	2A	3189	1/1	0.74	0.53	67,67,67,67	0
57	MG	2A	3202	1/1	0.74	0.29	53,53,53,53	0
57	MG	1A	3371	1/1	0.74	0.14	54,54,54,54	0
57	MG	2A	3336	1/1	0.74	0.28	55,55,55,55	0
59	ZN	14	102	1/1	0.74	0.06	113,113,113,113	0
57	MG	2A	3318	1/1	0.75	0.41	72,72,72,72	0
57	MG	2A	3091	1/1	0.75	0.11	63,63,63,63	0
57	MG	2A	3182	1/1	0.75	0.16	69,69,69,69	0
57	MG	2A	3023	1/1	0.75	0.11	71,71,71,71	0
57	MG	1A	3587	1/1	0.75	0.23	49,49,49,49	0
57	MG	1A	3461	1/1	0.75	0.26	61,61,61,61	0
57	MG	2A	3349	1/1	0.75	0.14	69,69,69,69	0
57	MG	2A	3218	1/1	0.75	0.20	68,68,68,68	0
57	MG	2A	3221	1/1	0.75	0.14	77,77,77,77	0
57	MG	1A	3238	1/1	0.75	0.17	66,66,66,66	0
57	MG	1A	3556	1/1	0.75	0.22	49,49,49,49	0
57	MG	1A	3399	1/1	0.75	0.65	64,64,64,64	0
57	MG	1A	3090	1/1	0.75	0.16	65,65,65,65	0
57	MG	2A	3142	1/1	0.75	0.29	64,64,64,64	0
57	MG	1A	3963	1/1	0.75	0.19	64,64,64,64	0
57	MG	1S	203	1/1	0.75	0.25	72,72,72,72	0
57	MG	2A	3008	1/1	0.75	0.19	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2y	104	1/1	0.75	0.18	71,71,71,71	0
57	MG	2A	3316	1/1	0.75	0.13	76,76,76,76	0
57	MG	1B	215	1/1	0.75	0.20	71,71,71,71	0
57	MG	1A	3983	1/1	0.76	0.32	43,43,43,43	0
57	MG	2A	3465	1/1	0.76	0.19	59,59,59,59	0
57	MG	1A	3443	1/1	0.76	0.29	55,55,55,55	0
57	MG	1A	3417	1/1	0.76	0.23	48,48,48,48	0
57	MG	2A	3709	1/1	0.76	0.13	52,52,52,52	0
57	MG	1A	3696	1/1	0.76	0.14	54,54,54,54	0
57	MG	2A	3081	1/1	0.76	0.27	58,58,58,58	0
57	MG	2A	3783	1/1	0.76	0.20	75,75,75,75	0
57	MG	1A	3707	1/1	0.76	0.14	55,55,55,55	0
57	MG	1w	102	1/1	0.76	0.13	60,60,60,60	0
57	MG	2A	3553	1/1	0.76	0.37	55,55,55,55	0
57	MG	1A	3361	1/1	0.76	0.18	58,58,58,58	0
57	MG	15	108	1/1	0.76	1.32	60,60,60,60	0
57	MG	1A	3452	1/1	0.76	0.43	55,55,55,55	0
57	MG	2A	3016	1/1	0.76	0.16	67,67,67,67	0
57	MG	1A	3595	1/1	0.76	0.17	35,35,35,35	0
57	MG	2A	3250	1/1	0.76	0.16	74,74,74,74	0
57	MG	1A	3520	1/1	0.76	0.18	71,71,71,71	0
57	MG	1A	3550	1/1	0.76	0.23	48,48,48,48	0
57	MG	1A	3255	1/1	0.76	0.18	57,57,57,57	0
57	MG	2A	3294	1/1	0.76	0.25	63,63,63,63	0
57	MG	1a	1759	1/1	0.76	0.09	70,70,70,70	0
57	MG	2A	3394	1/1	0.76	0.28	58,58,58,58	0
57	MG	1A	3911	1/1	0.76	0.25	29,29,29,29	0
57	MG	1T	203	1/1	0.77	0.49	64,64,64,64	0
57	MG	2A	3362	1/1	0.77	0.44	71,71,71,71	0
57	MG	1V	206	1/1	0.77	0.15	57,57,57,57	0
57	MG	1B	203	1/1	0.77	0.26	60,60,60,60	0
57	MG	1B	213	1/1	0.77	0.33	61,61,61,61	0
57	MG	1A	3283	1/1	0.77	0.23	40,40,40,40	0
57	MG	2A	3661	1/1	0.77	0.18	72,72,72,72	0
57	MG	2A	3279	1/1	0.77	0.55	61,61,61,61	0
57	MG	2A	3388	1/1	0.77	0.22	70,70,70,70	0
57	MG	1A	3306	1/1	0.77	0.18	46,46,46,46	0
57	MG	2A	3677	1/1	0.77	0.20	66,66,66,66	0
57	MG	1A	3018	1/1	0.77	0.16	57,57,57,57	0
57	MG	2A	3400	1/1	0.77	0.18	65,65,65,65	0
57	MG	1A	3347	1/1	0.77	0.28	48,48,48,48	0
57	MG	1A	3467	1/1	0.77	0.28	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3764	1/1	0.77	0.26	57,57,57,57	0
57	MG	2A	3462	1/1	0.77	0.24	41,41,41,41	0
57	MG	1a	1771	1/1	0.77	0.10	69,69,69,69	0
57	MG	2A	3483	1/1	0.77	0.23	38,38,38,38	0
57	MG	2A	3313	1/1	0.77	0.19	73,73,73,73	0
57	MG	1A	3239	1/1	0.77	0.18	59,59,59,59	0
57	MG	2A	3502	1/1	0.77	0.17	70,70,70,70	0
57	MG	2A	3057	1/1	0.77	0.28	72,72,72,72	0
57	MG	1A	3857	1/1	0.77	0.29	38,38,38,38	0
57	MG	1a	1786	1/1	0.77	0.08	71,71,71,71	0
57	MG	1A	4024	1/1	0.77	0.49	74,74,74,74	0
57	MG	28	101	1/1	0.77	0.12	64,64,64,64	0
57	MG	2A	3534	1/1	0.77	0.10	63,63,63,63	0
57	MG	2w	104	1/1	0.77	0.36	80,80,80,80	0
57	MG	1a	1670	1/1	0.77	0.33	49,49,49,49	0
57	MG	2A	3329	1/1	0.77	0.13	73,73,73,73	0
57	MG	2A	3211	1/1	0.77	0.30	67,67,67,67	0
57	MG	1a	1677	1/1	0.77	0.21	63,63,63,63	0
57	MG	1A	3975	1/1	0.77	0.15	32,32,32,32	0
57	MG	1A	3447	1/1	0.77	0.47	57,57,57,57	0
57	MG	2A	3352	1/1	0.77	0.17	65,65,65,65	0
57	MG	2A	3397	1/1	0.78	0.12	57,57,57,57	0
57	MG	1A	3198	1/1	0.78	0.28	58,58,58,58	0
57	MG	1A	3199	1/1	0.78	0.25	70,70,70,70	0
57	MG	1A	4059	1/1	0.78	0.24	55,55,55,55	0
57	MG	2A	3451	1/1	0.78	0.14	68,68,68,68	0
57	MG	1A	3518	1/1	0.78	0.39	60,60,60,60	0
57	MG	1N	202	1/1	0.78	0.44	52,52,52,52	0
57	MG	2A	3701	1/1	0.78	0.14	68,68,68,68	0
57	MG	2A	3703	1/1	0.78	0.17	58,58,58,58	0
57	MG	2A	3706	1/1	0.78	0.10	54,54,54,54	0
57	MG	1A	3113	1/1	0.78	0.26	49,49,49,49	0
57	MG	1A	3945	1/1	0.78	0.09	57,57,57,57	0
57	MG	2A	3499	1/1	0.78	0.10	75,75,75,75	0
57	MG	1a	1815	1/1	0.78	0.11	74,74,74,74	0
57	MG	1A	3545	1/1	0.78	0.21	46,46,46,46	0
57	MG	2A	3772	1/1	0.78	0.20	77,77,77,77	0
57	MG	2A	3331	1/1	0.78	0.23	75,75,75,75	0
57	MG	2A	3789	1/1	0.78	0.09	69,69,69,69	0
57	MG	1A	4104	1/1	0.78	0.15	64,64,64,64	0
57	MG	1A	3786	1/1	0.78	0.10	56,56,56,56	0
57	MG	2A	3346	1/1	0.78	0.43	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3226	1/1	0.78	0.62	69,69,69,69	0
57	MG	2A	3540	1/1	0.78	0.16	77,77,77,77	0
57	MG	1v	101	1/1	0.78	0.19	74,74,74,74	0
57	MG	1A	3101	1/1	0.78	0.58	44,44,44,44	0
57	MG	2D	306	1/1	0.78	0.32	62,62,62,62	0
57	MG	2A	3237	1/1	0.78	0.26	79,79,79,79	0
57	MG	11	104	1/1	0.78	0.10	48,48,48,48	0
57	MG	1x	108	1/1	0.78	0.24	72,72,72,72	0
57	MG	2A	3591	1/1	0.78	0.17	61,61,61,61	0
57	MG	1a	1732	1/1	0.78	0.09	54,54,54,54	0
57	MG	1A	3348	1/1	0.78	0.19	51,51,51,51	0
57	MG	2A	3285	1/1	0.78	0.45	65,65,65,65	0
57	MG	1A	3356	1/1	0.78	0.29	68,68,68,68	0
57	MG	1A	3685	1/1	0.78	0.23	36,36,36,36	0
57	MG	1a	1753	1/1	0.78	0.13	48,48,48,48	0
57	MG	1A	3490	1/1	0.78	0.30	53,53,53,53	0
57	MG	1A	4014	1/1	0.79	0.15	59,59,59,59	0
57	MG	1A	3502	1/1	0.79	0.47	38,38,38,38	0
57	MG	1a	1651	1/1	0.79	0.47	60,60,60,60	0
57	MG	1A	4070	1/1	0.79	0.22	71,71,71,71	0
57	MG	1A	3853	1/1	0.79	0.19	47,47,47,47	0
57	MG	2A	3207	1/1	0.79	0.21	61,61,61,61	0
57	MG	2A	3519	1/1	0.79	0.20	43,43,43,43	0
57	MG	1A	4075	1/1	0.79	0.17	60,60,60,60	0
57	MG	2A	3070	1/1	0.79	0.13	59,59,59,59	0
57	MG	1A	3854	1/1	0.79	0.12	40,40,40,40	0
57	MG	2A	3076	1/1	0.79	0.29	58,58,58,58	0
57	MG	1A	4026	1/1	0.79	0.10	43,43,43,43	0
57	MG	1R	204	1/1	0.79	0.18	53,53,53,53	0
57	MG	1a	1686	1/1	0.79	0.36	76,76,76,76	0
57	MG	1A	3563	1/1	0.79	0.53	45,45,45,45	0
57	MG	1A	3870	1/1	0.79	0.18	25,25,25,25	0
57	MG	2B	201	1/1	0.79	0.15	75,75,75,75	0
57	MG	2A	3097	1/1	0.79	0.26	75,75,75,75	0
57	MG	1a	1700	1/1	0.79	0.15	62,62,62,62	0
57	MG	2A	3380	1/1	0.79	0.29	75,75,75,75	0
57	MG	2A	3278	1/1	0.79	0.28	58,58,58,58	0
57	MG	2E	302	1/1	0.79	0.40	67,67,67,67	0
57	MG	2U	202	1/1	0.79	0.52	62,62,62,62	0
57	MG	20	102	1/1	0.79	0.17	72,72,72,72	0
57	MG	1a	1706	1/1	0.79	0.12	53,53,53,53	0
57	MG	1A	3476	1/1	0.79	0.28	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1602	1/1	0.79	0.31	70,70,70,70	0
57	MG	1B	204	1/1	0.79	0.21	62,62,62,62	0
57	MG	1A	3507	1/1	0.79	0.28	47,47,47,47	0
57	MG	1A	3335	1/1	0.79	0.20	65,65,65,65	0
57	MG	2A	3298	1/1	0.79	0.24	69,69,69,69	0
57	MG	16	101	1/1	0.79	0.24	56,56,56,56	0
57	MG	2A	3147	1/1	0.79	0.08	69,69,69,69	0
57	MG	1A	3903	1/1	0.79	0.17	40,40,40,40	0
57	MG	1A	3294	1/1	0.79	0.39	60,60,60,60	0
57	MG	2y	107	1/1	0.79	0.10	84,84,84,84	0
57	MG	1B	228	1/1	0.79	0.18	54,54,54,54	0
57	MG	1A	3251	1/1	0.80	0.13	49,49,49,49	0
57	MG	2A	3649	1/1	0.80	0.10	67,67,67,67	0
57	MG	1A	3994	1/1	0.80	0.12	32,32,32,32	0
57	MG	1Q	207	1/1	0.80	0.46	54,54,54,54	0
57	MG	2A	3381	1/1	0.80	0.32	56,56,56,56	0
57	MG	1A	3121	1/1	0.80	0.18	44,44,44,44	0
57	MG	1A	3497	1/1	0.80	0.34	61,61,61,61	0
57	MG	1A	3259	1/1	0.80	0.67	54,54,54,54	0
57	MG	1A	3454	1/1	0.80	0.33	40,40,40,40	0
57	MG	1A	4085	1/1	0.80	0.06	61,61,61,61	0
57	MG	11	102	1/1	0.80	0.18	54,54,54,54	0
57	MG	2A	3398	1/1	0.80	0.40	67,67,67,67	0
57	MG	1A	4013	1/1	0.80	0.11	45,45,45,45	0
57	MG	1A	3934	1/1	0.80	0.12	72,72,72,72	0
57	MG	1A	3460	1/1	0.80	0.14	64,64,64,64	0
57	MG	2A	3753	1/1	0.80	0.27	48,48,48,48	0
57	MG	18	101	1/1	0.80	0.34	59,59,59,59	0
57	MG	1A	4109	1/1	0.80	0.25	52,52,52,52	0
57	MG	2A	3098	1/1	0.80	0.14	82,82,82,82	0
57	MG	1a	1794	1/1	0.80	0.24	64,64,64,64	0
57	MG	2A	3786	1/1	0.80	0.10	72,72,72,72	0
57	MG	1A	4021	1/1	0.80	0.27	57,57,57,57	0
57	MG	2A	3790	1/1	0.80	0.13	75,75,75,75	0
57	MG	2A	3106	1/1	0.80	0.16	69,69,69,69	0
57	MG	2A	3302	1/1	0.80	0.41	55,55,55,55	0
57	MG	1A	3301	1/1	0.80	0.37	36,36,36,36	0
57	MG	1A	3588	1/1	0.80	0.18	53,53,53,53	0
57	MG	2A	3135	1/1	0.80	0.26	64,64,64,64	0
57	MG	1B	210	1/1	0.80	0.17	48,48,48,48	0
57	MG	1A	3858	1/1	0.80	0.09	38,38,38,38	0
57	MG	2D	301	1/1	0.80	0.26	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3734	1/1	0.80	0.18	62,62,62,62	0
57	MG	1A	4035	1/1	0.80	0.32	65,65,65,65	0
57	MG	1B	221	1/1	0.80	0.21	46,46,46,46	0
57	MG	2A	3547	1/1	0.80	0.35	49,49,49,49	0
57	MG	1A	4038	1/1	0.80	0.21	69,69,69,69	0
57	MG	1A	3437	1/1	0.80	0.52	44,44,44,44	0
57	MG	1A	3519	1/1	0.80	0.42	61,61,61,61	0
57	MG	2A	3569	1/1	0.80	0.24	55,55,55,55	0
57	MG	1A	4044	1/1	0.80	0.10	42,42,42,42	0
57	MG	2A	3181	1/1	0.80	0.24	64,64,64,64	0
57	MG	2A	3587	1/1	0.80	0.28	62,62,62,62	0
57	MG	1A	3282	1/1	0.80	0.30	45,45,45,45	0
57	MG	1E	308	1/1	0.80	0.18	55,55,55,55	0
57	MG	1a	1693	1/1	0.80	0.20	58,58,58,58	0
57	MG	2A	3353	1/1	0.80	0.29	54,54,54,54	0
57	MG	2A	3206	1/1	0.80	0.42	59,59,59,59	0
57	MG	1A	3394	1/1	0.80	0.23	54,54,54,54	0
57	MG	1A	3802	1/1	0.80	0.27	59,59,59,59	0
57	MG	2A	3599	1/1	0.81	0.16	75,75,75,75	0
57	MG	1a	1621	1/1	0.81	0.15	59,59,59,59	0
57	MG	1a	1623	1/1	0.81	0.15	57,57,57,57	0
57	MG	2A	3624	1/1	0.81	0.15	37,37,37,37	0
57	MG	2A	3634	1/1	0.81	0.23	66,66,66,66	0
57	MG	2A	3167	1/1	0.81	0.14	65,65,65,65	0
57	MG	1A	3222	1/1	0.81	0.28	61,61,61,61	0
57	MG	1w	101	1/1	0.81	0.16	74,74,74,74	0
57	MG	1a	1645	1/1	0.81	0.10	78,78,78,78	0
57	MG	1A	3257	1/1	0.81	0.13	63,63,63,63	0
57	MG	1A	3754	1/1	0.81	0.17	39,39,39,39	0
57	MG	2A	3185	1/1	0.81	0.27	55,55,55,55	0
57	MG	1A	3398	1/1	0.81	0.12	55,55,55,55	0
57	MG	1a	1658	1/1	0.81	0.19	77,77,77,77	0
57	MG	2A	3011	1/1	0.81	0.12	58,58,58,58	0
57	MG	1A	4025	1/1	0.81	0.08	58,58,58,58	0
57	MG	1A	3925	1/1	0.81	0.21	73,73,73,73	0
57	MG	1A	3237	1/1	0.81	0.39	58,58,58,58	0
57	MG	1A	3036	1/1	0.81	0.15	51,51,51,51	0
57	MG	1A	3425	1/1	0.81	0.23	63,63,63,63	0
57	MG	1A	3117	1/1	0.81	0.61	59,59,59,59	0
57	MG	1A	3591	1/1	0.81	0.20	39,39,39,39	0
57	MG	2A	3230	1/1	0.81	0.42	57,57,57,57	0
57	MG	2A	3231	1/1	0.81	0.47	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1E	311	1/1	0.81	0.14	53,53,53,53	0
57	MG	1F	312	1/1	0.81	0.36	56,56,56,56	0
57	MG	2A	3784	1/1	0.81	0.20	56,56,56,56	0
57	MG	2A	3415	1/1	0.81	0.31	66,66,66,66	0
57	MG	1A	3431	1/1	0.81	0.18	51,51,51,51	0
57	MG	1A	3948	1/1	0.81	0.26	59,59,59,59	0
57	MG	2A	3261	1/1	0.81	0.16	69,69,69,69	0
57	MG	2A	3267	1/1	0.81	0.18	61,61,61,61	0
57	MG	1a	1719	1/1	0.81	0.14	58,58,58,58	0
57	MG	2A	3270	1/1	0.81	0.20	76,76,76,76	0
57	MG	1A	3628	1/1	0.81	0.21	23,23,23,23	0
57	MG	1A	3352	1/1	0.81	0.74	64,64,64,64	0
57	MG	1A	3193	1/1	0.81	0.16	63,63,63,63	0
57	MG	1A	3506	1/1	0.81	0.17	65,65,65,65	0
57	MG	1A	3666	1/1	0.81	0.13	63,63,63,63	0
57	MG	1A	3441	1/1	0.81	0.20	54,54,54,54	0
57	MG	1A	3977	1/1	0.81	0.53	49,49,49,49	0
57	MG	2E	307	1/1	0.81	0.14	71,71,71,71	0
57	MG	1A	3680	1/1	0.81	0.10	65,65,65,65	0
57	MG	1A	3360	1/1	0.81	0.18	53,53,53,53	0
57	MG	2A	3546	1/1	0.81	0.14	60,60,60,60	0
57	MG	2A	3305	1/1	0.81	0.25	71,71,71,71	0
57	MG	1A	3997	1/1	0.81	0.11	50,50,50,50	0
57	MG	1A	3877	1/1	0.81	0.19	29,29,29,29	0
57	MG	1A	3080	1/1	0.81	0.41	50,50,50,50	0
57	MG	1A	3246	1/1	0.81	0.32	56,56,56,56	0
57	MG	1a	1791	1/1	0.81	0.12	62,62,62,62	0
57	MG	1A	3247	1/1	0.81	0.22	74,74,74,74	0
57	MG	1a	1798	1/1	0.81	0.12	63,63,63,63	0
57	MG	1A	3030	1/1	0.81	0.16	33,33,33,33	0
57	MG	1A	3383	1/1	0.81	0.20	56,56,56,56	0
57	MG	1B	208	1/1	0.81	0.15	63,63,63,63	0
57	MG	2A	3158	1/1	0.81	0.11	79,79,79,79	0
57	MG	1A	3087	1/1	0.82	0.22	45,45,45,45	0
57	MG	2A	3386	1/1	0.82	0.32	68,68,68,68	0
57	MG	2A	3669	1/1	0.82	0.20	44,44,44,44	0
57	MG	1Q	204	1/1	0.82	0.14	73,73,73,73	0
57	MG	1A	3256	1/1	0.82	0.19	61,61,61,61	0
57	MG	1A	3400	1/1	0.82	0.41	56,56,56,56	0
57	MG	1A	3695	1/1	0.82	0.25	42,42,42,42	0
57	MG	1A	3102	1/1	0.82	0.69	50,50,50,50	0
57	MG	2A	3077	1/1	0.82	0.17	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3699	1/1	0.82	0.19	55,55,55,55	0
57	MG	1A	3561	1/1	0.82	0.26	35,35,35,35	0
57	MG	1A	4103	1/1	0.82	0.14	63,63,63,63	0
57	MG	1A	3499	1/1	0.82	0.29	51,51,51,51	0
57	MG	1A	3299	1/1	0.82	0.37	70,70,70,70	0
57	MG	2A	3749	1/1	0.82	0.27	65,65,65,65	0
57	MG	1A	3725	1/1	0.82	0.17	52,52,52,52	0
57	MG	1A	3189	1/1	0.82	0.18	39,39,39,39	0
57	MG	1A	3732	1/1	0.82	0.32	56,56,56,56	0
57	MG	2A	3771	1/1	0.82	0.16	57,57,57,57	0
57	MG	1A	3430	1/1	0.82	0.16	60,60,60,60	0
57	MG	2A	3494	1/1	0.82	0.20	56,56,56,56	0
57	MG	1A	3359	1/1	0.82	0.13	70,70,70,70	0
57	MG	1a	1793	1/1	0.82	0.10	66,66,66,66	0
57	MG	1A	3509	1/1	0.82	0.30	58,58,58,58	0
57	MG	1A	3770	1/1	0.82	0.10	72,72,72,72	0
57	MG	1a	1799	1/1	0.82	0.07	65,65,65,65	0
57	MG	1A	3774	1/1	0.82	0.12	45,45,45,45	0
57	MG	1B	216	1/1	0.82	0.21	54,54,54,54	0
57	MG	1a	1644	1/1	0.82	0.13	47,47,47,47	0
57	MG	1A	3785	1/1	0.82	0.11	44,44,44,44	0
57	MG	1A	3607	1/1	0.82	0.33	60,60,60,60	0
57	MG	1A	3935	1/1	0.82	0.12	61,61,61,61	0
57	MG	1A	3387	1/1	0.82	0.52	75,75,75,75	0
57	MG	1B	233	1/1	0.82	0.57	61,61,61,61	0
57	MG	2A	3330	1/1	0.82	0.92	60,60,60,60	0
57	MG	1w	109	1/1	0.82	0.45	79,79,79,79	0
57	MG	1A	3789	1/1	0.82	0.11	24,24,24,24	0
57	MG	1a	1660	1/1	0.82	0.20	58,58,58,58	0
57	MG	1a	1665	1/1	0.82	0.19	64,64,64,64	0
57	MG	1A	3633	1/1	0.82	0.14	36,36,36,36	0
57	MG	1D	312	1/1	0.82	0.62	47,47,47,47	0
57	MG	1A	3293	1/1	0.82	0.27	64,64,64,64	0
57	MG	1A	3809	1/1	0.82	0.12	43,43,43,43	0
57	MG	2A	3354	1/1	0.82	0.22	61,61,61,61	0
57	MG	1F	304	1/1	0.82	0.20	42,42,42,42	0
57	MG	1A	3438	1/1	0.82	0.12	69,69,69,69	0
57	MG	2x	104	1/1	0.82	0.36	73,73,73,73	0
57	MG	1A	3471	1/1	0.82	0.22	48,48,48,48	0
57	MG	1a	1696	1/1	0.82	0.12	58,58,58,58	0
57	MG	2A	3367	1/1	0.82	0.36	65,65,65,65	0
57	MG	1A	3542	1/1	0.82	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3049	1/1	0.82	0.33	50,50,50,50	0
57	MG	1A	3473	1/1	0.82	0.13	53,53,53,53	0
57	MG	2A	3275	1/1	0.83	0.10	71,71,71,71	0
57	MG	1A	3216	1/1	0.83	0.18	57,57,57,57	0
57	MG	1A	3114	1/1	0.83	0.57	51,51,51,51	0
57	MG	1A	3795	1/1	0.83	0.18	51,51,51,51	0
57	MG	1A	3324	1/1	0.83	0.33	45,45,45,45	0
57	MG	2A	3691	1/1	0.83	0.29	60,60,60,60	0
57	MG	1A	3801	1/1	0.83	0.15	32,32,32,32	0
57	MG	2A	3425	1/1	0.83	0.17	60,60,60,60	0
57	MG	2A	3705	1/1	0.83	0.28	68,68,68,68	0
57	MG	1A	3224	1/1	0.83	0.58	48,48,48,48	0
57	MG	1a	1727	1/1	0.83	0.15	82,82,82,82	0
57	MG	1A	3712	1/1	0.83	0.10	74,74,74,74	0
57	MG	1a	1741	1/1	0.83	0.12	65,65,65,65	0
57	MG	1A	3367	1/1	0.83	0.26	60,60,60,60	0
57	MG	1A	3002	1/1	0.83	0.29	55,55,55,55	0
57	MG	2A	3760	1/1	0.83	0.16	39,39,39,39	0
57	MG	2A	3495	1/1	0.83	0.21	43,43,43,43	0
57	MG	1A	3651	1/1	0.83	0.13	49,49,49,49	0
57	MG	1a	1746	1/1	0.83	0.24	78,78,78,78	0
57	MG	1a	1748	1/1	0.83	0.17	57,57,57,57	0
57	MG	1A	3148	1/1	0.83	0.45	40,40,40,40	0
57	MG	2A	3188	1/1	0.83	0.36	68,68,68,68	0
57	MG	1A	3830	1/1	0.83	0.09	61,61,61,61	0
57	MG	2A	3198	1/1	0.83	0.10	73,73,73,73	0
57	MG	1A	4101	1/1	0.83	0.21	65,65,65,65	0
57	MG	1A	3339	1/1	0.83	0.14	54,54,54,54	0
57	MG	1a	1769	1/1	0.83	0.12	81,81,81,81	0
57	MG	1A	4019	1/1	0.83	0.10	52,52,52,52	0
57	MG	1A	3849	1/1	0.83	0.14	53,53,53,53	0
57	MG	1N	206	1/1	0.83	0.28	45,45,45,45	0
57	MG	1A	3276	1/1	0.83	0.15	56,56,56,56	0
57	MG	2A	3561	1/1	0.83	0.22	55,55,55,55	0
57	MG	2B	212	1/1	0.83	0.12	73,73,73,73	0
57	MG	2A	3225	1/1	0.83	0.25	64,64,64,64	0
57	MG	1A	3307	1/1	0.83	0.18	63,63,63,63	0
57	MG	1Q	206	1/1	0.83	0.13	51,51,51,51	0
57	MG	1A	3947	1/1	0.83	0.10	45,45,45,45	0
57	MG	1a	1675	1/1	0.83	0.10	61,61,61,61	0
57	MG	1A	3768	1/1	0.83	0.19	57,57,57,57	0
57	MG	2X	102	1/1	0.83	0.16	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3566	1/1	0.83	0.24	57,57,57,57	0
57	MG	25	101	1/1	0.83	0.16	59,59,59,59	0
57	MG	2A	3239	1/1	0.83	0.16	73,73,73,73	0
57	MG	1a	1685	1/1	0.83	0.19	61,61,61,61	0
57	MG	1A	3351	1/1	0.83	0.15	60,60,60,60	0
57	MG	2A	3607	1/1	0.83	0.20	66,66,66,66	0
57	MG	2A	3372	1/1	0.83	0.40	52,52,52,52	0
57	MG	1A	3513	1/1	0.83	1.00	54,54,54,54	0
57	MG	2A	3264	1/1	0.83	0.17	82,82,82,82	0
57	MG	1A	3965	1/1	0.83	0.18	69,69,69,69	0
57	MG	1A	3201	1/1	0.83	0.22	50,50,50,50	0
57	MG	1a	1694	1/1	0.83	0.22	62,62,62,62	0
57	MG	2A	3271	1/1	0.83	0.23	80,80,80,80	0
57	MG	2A	3272	1/1	0.83	0.41	59,59,59,59	0
57	MG	2A	3273	1/1	0.83	0.56	59,59,59,59	0
57	MG	2A	3395	1/1	0.83	0.13	65,65,65,65	0
57	MG	1A	3330	1/1	0.84	0.12	60,60,60,60	0
57	MG	1A	3933	1/1	0.84	0.14	45,45,45,45	0
57	MG	1A	3349	1/1	0.84	0.53	47,47,47,47	0
57	MG	1A	4015	1/1	0.84	0.15	51,51,51,51	0
57	MG	2A	3662	1/1	0.84	0.26	71,71,71,71	0
57	MG	1A	3738	1/1	0.84	0.10	49,49,49,49	0
57	MG	1O	203	1/1	0.84	0.10	62,62,62,62	0
57	MG	1a	1807	1/1	0.84	0.18	61,61,61,61	0
57	MG	1A	3747	1/1	0.84	0.18	44,44,44,44	0
57	MG	1A	3847	1/1	0.84	0.09	43,43,43,43	0
57	MG	2A	3679	1/1	0.84	0.14	71,71,71,71	0
57	MG	2A	3117	1/1	0.84	0.17	58,58,58,58	0
57	MG	1A	3160	1/1	0.84	0.49	68,68,68,68	0
57	MG	1A	3504	1/1	0.84	0.33	55,55,55,55	0
57	MG	1A	3112	1/1	0.84	0.15	42,42,42,42	0
57	MG	2A	3280	1/1	0.84	0.32	57,57,57,57	0
57	MG	1S	201	1/1	0.84	1.12	60,60,60,60	0
57	MG	2A	3427	1/1	0.84	0.11	63,63,63,63	0
57	MG	1B	205	1/1	0.84	0.34	62,62,62,62	0
57	MG	2A	3714	1/1	0.84	0.50	66,66,66,66	0
57	MG	2A	3720	1/1	0.84	0.20	69,69,69,69	0
57	MG	2A	3728	1/1	0.84	0.22	62,62,62,62	0
57	MG	2A	3154	1/1	0.84	0.19	68,68,68,68	0
57	MG	1A	3379	1/1	0.84	0.25	55,55,55,55	0
57	MG	1A	4029	1/1	0.84	0.18	27,27,27,27	0
57	MG	1x	102	1/1	0.84	0.17	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1Z	302	1/1	0.84	0.24	54,54,54,54	0
57	MG	2A	3303	1/1	0.84	0.31	68,68,68,68	0
57	MG	1A	3565	1/1	0.84	0.14	68,68,68,68	0
57	MG	1A	3406	1/1	0.84	0.40	61,61,61,61	0
57	MG	2A	3776	1/1	0.84	0.53	63,63,63,63	0
57	MG	1A	3575	1/1	0.84	0.17	41,41,41,41	0
57	MG	1A	3580	1/1	0.84	0.15	51,51,51,51	0
57	MG	2A	3515	1/1	0.84	0.27	56,56,56,56	0
57	MG	2A	3517	1/1	0.84	0.33	62,62,62,62	0
57	MG	1A	3408	1/1	0.84	0.30	55,55,55,55	0
57	MG	2A	3524	1/1	0.84	0.22	75,75,75,75	0
57	MG	1A	3338	1/1	0.84	0.37	62,62,62,62	0
57	MG	1B	227	1/1	0.84	0.26	67,67,67,67	0
57	MG	2A	3529	1/1	0.84	0.14	70,70,70,70	0
57	MG	2A	3029	1/1	0.84	0.29	68,68,68,68	0
57	MG	2B	202	1/1	0.84	0.27	67,67,67,67	0
57	MG	1A	3798	1/1	0.84	0.19	73,73,73,73	0
57	MG	2A	3536	1/1	0.84	0.21	55,55,55,55	0
57	MG	2A	3200	1/1	0.84	0.42	66,66,66,66	0
57	MG	1A	3423	1/1	0.84	0.31	45,45,45,45	0
57	MG	1A	3175	1/1	0.84	0.12	73,73,73,73	0
57	MG	1a	1619	1/1	0.84	0.15	56,56,56,56	0
57	MG	2A	3333	1/1	0.84	0.22	45,45,45,45	0
57	MG	2A	3334	1/1	0.84	0.17	50,50,50,50	0
57	MG	2G	201	1/1	0.84	0.12	66,66,66,66	0
57	MG	1B	234	1/1	0.84	0.17	56,56,56,56	0
57	MG	2W	203	1/1	0.84	0.94	65,65,65,65	0
57	MG	1a	1747	1/1	0.84	0.16	66,66,66,66	0
57	MG	1A	3492	1/1	0.84	0.33	56,56,56,56	0
57	MG	1A	3521	1/1	0.84	0.17	77,77,77,77	0
57	MG	1A	4002	1/1	0.84	0.16	54,54,54,54	0
57	MG	2A	3590	1/1	0.84	0.16	78,78,78,78	0
57	MG	1A	3493	1/1	0.84	0.27	68,68,68,68	0
57	MG	1a	1646	1/1	0.84	0.10	66,66,66,66	0
57	MG	2A	3593	1/1	0.84	0.41	78,78,78,78	0
57	MG	1a	1649	1/1	0.84	0.11	61,61,61,61	0
57	MG	1A	3922	1/1	0.84	0.14	55,55,55,55	0
57	MG	1a	1654	1/1	0.84	0.10	61,61,61,61	0
57	MG	1a	1773	1/1	0.84	0.19	71,71,71,71	0
57	MG	2A	3366	1/1	0.84	0.40	66,66,66,66	0
57	MG	2A	3238	1/1	0.84	0.23	65,65,65,65	0
57	MG	1A	3179	1/1	0.84	0.37	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3244	1/1	0.84	0.66	72,72,72,72	0
57	MG	2A	3249	1/1	0.84	0.16	75,75,75,75	0
59	ZN	24	501	1/1	0.84	0.05	127,127,127,127	0
57	MG	2A	3487	1/1	0.85	0.25	35,35,35,35	0
57	MG	1A	3525	1/1	0.85	0.24	55,55,55,55	0
57	MG	1W	202	1/1	0.85	0.16	58,58,58,58	0
57	MG	2A	3321	1/1	0.85	0.52	62,62,62,62	0
57	MG	1a	1678	1/1	0.85	0.37	56,56,56,56	0
57	MG	1A	3567	1/1	0.85	0.24	46,46,46,46	0
57	MG	1A	3944	1/1	0.85	0.14	44,44,44,44	0
57	MG	2A	3504	1/1	0.85	0.25	64,64,64,64	0
57	MG	1A	3650	1/1	0.85	0.17	44,44,44,44	0
57	MG	1A	3484	1/1	0.85	0.21	62,62,62,62	0
57	MG	2A	3721	1/1	0.85	0.09	69,69,69,69	0
57	MG	2A	3078	1/1	0.85	0.74	57,57,57,57	0
57	MG	2A	3079	1/1	0.85	0.42	58,58,58,58	0
57	MG	2A	3736	1/1	0.85	0.12	58,58,58,58	0
57	MG	2A	3743	1/1	0.85	0.12	64,64,64,64	0
57	MG	2A	3227	1/1	0.85	0.28	60,60,60,60	0
57	MG	1A	4020	1/1	0.85	0.06	58,58,58,58	0
57	MG	2A	3756	1/1	0.85	0.06	67,67,67,67	0
57	MG	2A	3339	1/1	0.85	0.17	51,51,51,51	0
57	MG	1a	1806	1/1	0.85	0.16	65,65,65,65	0
57	MG	1A	4088	1/1	0.85	0.17	45,45,45,45	0
57	MG	1a	1810	1/1	0.85	0.14	69,69,69,69	0
57	MG	1A	3253	1/1	0.85	0.10	69,69,69,69	0
57	MG	1A	3892	1/1	0.85	0.17	64,64,64,64	0
57	MG	1E	309	1/1	0.85	0.18	29,29,29,29	0
57	MG	1A	3654	1/1	0.85	0.15	30,30,30,30	0
57	MG	1A	3897	1/1	0.85	0.35	40,40,40,40	0
57	MG	1F	310	1/1	0.85	0.28	38,38,38,38	0
57	MG	1a	1722	1/1	0.85	0.10	71,71,71,71	0
57	MG	1a	1620	1/1	0.85	0.34	61,61,61,61	0
57	MG	1A	3466	1/1	0.85	0.41	60,60,60,60	0
57	MG	2A	3124	1/1	0.85	0.13	52,52,52,52	0
57	MG	1x	101	1/1	0.85	0.29	69,69,69,69	0
57	MG	1A	4112	1/1	0.85	0.18	55,55,55,55	0
57	MG	1A	3736	1/1	0.85	0.26	45,45,45,45	0
57	MG	1A	3215	1/1	0.85	0.22	56,56,56,56	0
57	MG	1x	109	1/1	0.85	0.18	32,32,32,32	0
57	MG	1A	3745	1/1	0.85	0.21	24,24,24,24	0
57	MG	2A	3156	1/1	0.85	0.14	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3002	1/1	0.85	0.45	63,63,63,63	0
57	MG	2A	3007	1/1	0.85	0.08	54,54,54,54	0
57	MG	1A	3089	1/1	0.85	0.23	65,65,65,65	0
57	MG	1A	3343	1/1	0.85	0.30	50,50,50,50	0
57	MG	2A	3616	1/1	0.85	0.14	62,62,62,62	0
57	MG	2R	201	1/1	0.85	0.26	64,64,64,64	0
57	MG	2A	3172	1/1	0.85	0.21	59,59,59,59	0
57	MG	2A	3622	1/1	0.85	0.20	66,66,66,66	0
57	MG	1Q	201	1/1	0.85	0.51	41,41,41,41	0
57	MG	2A	3632	1/1	0.85	0.17	69,69,69,69	0
57	MG	23	101	1/1	0.85	0.36	70,70,70,70	0
57	MG	1A	3593	1/1	0.85	0.20	30,30,30,30	0
57	MG	2A	3635	1/1	0.85	0.21	64,64,64,64	0
57	MG	2A	3407	1/1	0.85	0.12	54,54,54,54	0
57	MG	2A	3644	1/1	0.85	0.28	63,63,63,63	0
57	MG	1A	3422	1/1	0.85	0.19	56,56,56,56	0
57	MG	2A	3413	1/1	0.85	0.50	68,68,68,68	0
57	MG	2A	3659	1/1	0.85	0.09	60,60,60,60	0
57	MG	1A	3596	1/1	0.85	0.19	57,57,57,57	0
57	MG	2A	3422	1/1	0.85	0.08	67,67,67,67	0
57	MG	1a	1756	1/1	0.85	0.21	55,55,55,55	0
57	MG	1A	3433	1/1	0.85	0.29	57,57,57,57	0
57	MG	1R	206	1/1	0.85	0.30	44,44,44,44	0
57	MG	2A	3459	1/1	0.85	0.16	69,69,69,69	0
57	MG	2y	106	1/1	0.85	0.11	71,71,71,71	0
57	MG	1A	3776	1/1	0.85	0.20	84,84,84,84	0
57	MG	1A	3622	1/1	0.85	0.15	34,34,34,34	0
57	MG	1A	3480	1/1	0.85	0.20	45,45,45,45	0
57	MG	1A	3562	1/1	0.86	0.12	70,70,70,70	0
57	MG	1A	4055	1/1	0.86	0.15	38,38,38,38	0
57	MG	2A	3436	1/1	0.86	0.17	47,47,47,47	0
57	MG	2A	3442	1/1	0.86	0.25	65,65,65,65	0
57	MG	2A	3445	1/1	0.86	0.14	47,47,47,47	0
57	MG	2A	3447	1/1	0.86	0.13	42,42,42,42	0
57	MG	2A	3157	1/1	0.86	0.10	53,53,53,53	0
57	MG	1A	3091	1/1	0.86	0.20	56,56,56,56	0
57	MG	2A	3460	1/1	0.86	0.26	46,46,46,46	0
57	MG	2A	3299	1/1	0.86	0.68	64,64,64,64	0
57	MG	2A	3300	1/1	0.86	0.34	67,67,67,67	0
57	MG	1a	1726	1/1	0.86	0.11	60,60,60,60	0
57	MG	1x	113	1/1	0.86	0.23	66,66,66,66	0
57	MG	1x	114	1/1	0.86	0.16	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1B	236	1/1	0.86	0.17	71,71,71,71	0
57	MG	1A	3464	1/1	0.86	0.37	56,56,56,56	0
57	MG	1A	3522	1/1	0.86	0.18	60,60,60,60	0
57	MG	1A	4064	1/1	0.86	0.10	54,54,54,54	0
57	MG	1A	3483	1/1	0.86	0.30	56,56,56,56	0
57	MG	1A	4071	1/1	0.86	0.31	56,56,56,56	0
57	MG	1A	3719	1/1	0.86	0.12	69,69,69,69	0
57	MG	1a	1635	1/1	0.86	0.17	62,62,62,62	0
57	MG	2A	3323	1/1	0.86	0.21	62,62,62,62	0
57	MG	2A	3518	1/1	0.86	0.14	69,69,69,69	0
57	MG	1A	3720	1/1	0.86	0.10	69,69,69,69	0
57	MG	2A	3192	1/1	0.86	0.15	57,57,57,57	0
57	MG	1A	3643	1/1	0.86	0.24	46,46,46,46	0
57	MG	1A	3570	1/1	0.86	0.24	50,50,50,50	0
57	MG	1A	3537	1/1	0.86	0.20	54,54,54,54	0
57	MG	1a	1650	1/1	0.86	0.09	74,74,74,74	0
57	MG	2A	3050	1/1	0.86	0.54	73,73,73,73	0
57	MG	1A	4100	1/1	0.86	0.17	53,53,53,53	0
57	MG	1a	1761	1/1	0.86	0.10	66,66,66,66	0
57	MG	2A	3213	1/1	0.86	0.22	59,59,59,59	0
57	MG	2A	3344	1/1	0.86	0.29	53,53,53,53	0
57	MG	1A	3920	1/1	0.86	0.14	39,39,39,39	0
57	MG	2A	3794	1/1	0.86	0.24	63,63,63,63	0
57	MG	2A	3555	1/1	0.86	0.17	44,44,44,44	0
57	MG	1A	3541	1/1	0.86	0.46	59,59,59,59	0
57	MG	1A	3337	1/1	0.86	0.19	59,59,59,59	0
57	MG	1A	3488	1/1	0.86	0.91	43,43,43,43	0
57	MG	2A	3564	1/1	0.86	0.13	70,70,70,70	0
57	MG	1a	1776	1/1	0.86	0.08	50,50,50,50	0
57	MG	1A	3004	1/1	0.86	0.22	34,34,34,34	0
57	MG	1A	3836	1/1	0.86	0.36	41,41,41,41	0
57	MG	1A	3671	1/1	0.86	0.17	43,43,43,43	0
57	MG	2A	3233	1/1	0.86	0.25	64,64,64,64	0
57	MG	2E	301	1/1	0.86	0.09	70,70,70,70	0
57	MG	1a	1667	1/1	0.86	0.23	64,64,64,64	0
57	MG	1A	3746	1/1	0.86	0.17	52,52,52,52	0
57	MG	1A	3848	1/1	0.86	0.13	42,42,42,42	0
57	MG	2A	3087	1/1	0.86	0.41	55,55,55,55	0
57	MG	1A	3589	1/1	0.86	0.14	42,42,42,42	0
57	MG	2A	3374	1/1	0.86	0.29	69,69,69,69	0
57	MG	1A	3674	1/1	0.86	0.13	30,30,30,30	0
57	MG	1a	1682	1/1	0.86	0.12	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3677	1/1	0.86	0.22	30,30,30,30	0
57	MG	1B	211	1/1	0.86	0.49	50,50,50,50	0
57	MG	1A	3015	1/1	0.86	0.27	51,51,51,51	0
57	MG	1A	3354	1/1	0.86	0.45	37,37,37,37	0
57	MG	1A	3867	1/1	0.86	0.14	39,39,39,39	0
57	MG	1A	3869	1/1	0.86	0.19	48,48,48,48	0
57	MG	1A	3085	1/1	0.86	0.25	37,37,37,37	0
57	MG	2A	3123	1/1	0.86	0.19	52,52,52,52	0
57	MG	2x	102	1/1	0.86	0.18	76,76,76,76	0
57	MG	1A	3872	1/1	0.86	0.23	32,32,32,32	0
57	MG	2A	3274	1/1	0.86	0.14	76,76,76,76	0
57	MG	2x	105	1/1	0.86	0.17	56,56,56,56	0
57	MG	12	102	1/1	0.86	0.18	50,50,50,50	0
57	MG	2y	101	1/1	0.86	0.12	57,57,57,57	0
57	MG	2A	3650	1/1	0.86	0.26	61,61,61,61	0
57	MG	2A	3657	1/1	0.86	0.11	68,68,68,68	0
57	MG	2A	3277	1/1	0.86	0.56	69,69,69,69	0
57	MG	1A	3693	1/1	0.86	0.22	35,35,35,35	0
57	MG	1A	3220	1/1	0.86	0.51	54,54,54,54	0
57	MG	1a	1714	1/1	0.86	0.18	78,78,78,78	0
57	MG	1x	103	1/1	0.86	0.15	55,55,55,55	0
57	MG	1Y	201	1/1	0.87	0.22	69,69,69,69	0
57	MG	1Z	301	1/1	0.87	0.15	61,61,61,61	0
57	MG	2A	3383	1/1	0.87	0.82	58,58,58,58	0
57	MG	1A	3235	1/1	0.87	0.30	52,52,52,52	0
57	MG	2A	3653	1/1	0.87	0.17	76,76,76,76	0
57	MG	10	104	1/1	0.87	0.20	57,57,57,57	0
57	MG	1B	201	1/1	0.87	0.14	54,54,54,54	0
57	MG	2A	3044	1/1	0.87	0.09	71,71,71,71	0
57	MG	1A	3557	1/1	0.87	0.55	47,47,47,47	0
57	MG	1A	3882	1/1	0.87	0.10	64,64,64,64	0
57	MG	1a	1733	1/1	0.87	0.11	57,57,57,57	0
57	MG	1A	3391	1/1	0.87	0.09	58,58,58,58	0
57	MG	15	106	1/1	0.87	0.80	46,46,46,46	0
57	MG	2A	3241	1/1	0.87	0.34	50,50,50,50	0
57	MG	1A	3284	1/1	0.87	0.46	66,66,66,66	0
57	MG	1A	3395	1/1	0.87	0.23	63,63,63,63	0
57	MG	2A	3681	1/1	0.87	0.18	57,57,57,57	0
57	MG	1A	3769	1/1	0.87	0.19	31,31,31,31	0
57	MG	1B	212	1/1	0.87	0.48	58,58,58,58	0
57	MG	2A	3257	1/1	0.87	0.36	64,64,64,64	0
57	MG	1A	3182	1/1	0.87	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3423	1/1	0.87	0.39	69,69,69,69	0
57	MG	1A	3214	1/1	0.87	0.24	45,45,45,45	0
57	MG	1A	3322	1/1	0.87	0.23	60,60,60,60	0
57	MG	1a	1606	1/1	0.87	0.08	67,67,67,67	0
57	MG	1A	3006	1/1	0.87	0.15	38,38,38,38	0
57	MG	2A	3715	1/1	0.87	0.17	62,62,62,62	0
57	MG	1A	3325	1/1	0.87	0.18	44,44,44,44	0
57	MG	2A	3086	1/1	0.87	0.39	44,44,44,44	0
57	MG	1A	3679	1/1	0.87	0.17	31,31,31,31	0
57	MG	1A	3086	1/1	0.87	0.23	42,42,42,42	0
57	MG	1a	1626	1/1	0.87	0.27	51,51,51,51	0
57	MG	1A	3682	1/1	0.87	0.19	51,51,51,51	0
57	MG	2A	3747	1/1	0.87	0.08	63,63,63,63	0
57	MG	1a	1632	1/1	0.87	0.17	70,70,70,70	0
57	MG	2A	3467	1/1	0.87	0.21	55,55,55,55	0
57	MG	1a	1634	1/1	0.87	0.14	74,74,74,74	0
57	MG	1A	4030	1/1	0.87	0.21	40,40,40,40	0
57	MG	1a	1639	1/1	0.87	0.12	56,56,56,56	0
57	MG	1A	3797	1/1	0.87	0.34	53,53,53,53	0
57	MG	2A	3767	1/1	0.87	0.11	51,51,51,51	0
57	MG	1A	3579	1/1	0.87	0.20	48,48,48,48	0
57	MG	1A	3017	1/1	0.87	0.22	33,33,33,33	0
57	MG	1a	1647	1/1	0.87	0.54	59,59,59,59	0
57	MG	1A	3688	1/1	0.87	0.23	28,28,28,28	0
57	MG	1A	3515	1/1	0.87	0.28	60,60,60,60	0
57	MG	1A	3295	1/1	0.87	0.18	47,47,47,47	0
57	MG	2A	3511	1/1	0.87	0.24	74,74,74,74	0
57	MG	2A	3514	1/1	0.87	0.19	69,69,69,69	0
57	MG	1a	1808	1/1	0.87	0.18	67,67,67,67	0
57	MG	1A	4045	1/1	0.87	0.22	64,64,64,64	0
57	MG	2A	3144	1/1	0.87	0.20	62,62,62,62	0
57	MG	1A	3470	1/1	0.87	0.28	30,30,30,30	0
57	MG	2A	3310	1/1	0.87	0.15	61,61,61,61	0
57	MG	2A	3149	1/1	0.87	0.32	61,61,61,61	0
57	MG	1A	3369	1/1	0.87	0.62	44,44,44,44	0
57	MG	1a	1817	1/1	0.87	0.10	66,66,66,66	0
57	MG	1a	1818	1/1	0.87	0.13	54,54,54,54	0
57	MG	1d	301	1/1	0.87	0.39	61,61,61,61	0
57	MG	2B	215	1/1	0.87	0.11	73,73,73,73	0
57	MG	1A	3700	1/1	0.87	0.07	48,48,48,48	0
57	MG	2A	3322	1/1	0.87	0.29	70,70,70,70	0
57	MG	1A	3943	1/1	0.87	0.13	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3166	1/1	0.87	0.28	74,74,74,74	0
57	MG	1A	3701	1/1	0.87	0.43	69,69,69,69	0
57	MG	1A	3084	1/1	0.87	0.47	44,44,44,44	0
57	MG	2F	302	1/1	0.87	0.25	65,65,65,65	0
57	MG	1a	1666	1/1	0.87	0.13	73,73,73,73	0
57	MG	1G	204	1/1	0.87	0.22	50,50,50,50	0
57	MG	1A	3831	1/1	0.87	0.18	57,57,57,57	0
57	MG	1A	3372	1/1	0.87	0.24	68,68,68,68	0
57	MG	1a	1676	1/1	0.87	0.21	61,61,61,61	0
57	MG	2A	3578	1/1	0.87	0.23	65,65,65,65	0
57	MG	2A	3183	1/1	0.87	0.19	54,54,54,54	0
57	MG	1A	3268	1/1	0.87	0.23	40,40,40,40	0
57	MG	1A	3845	1/1	0.87	0.35	33,33,33,33	0
57	MG	1A	3956	1/1	0.87	0.12	69,69,69,69	0
57	MG	1A	3535	1/1	0.87	0.40	56,56,56,56	0
57	MG	2w	102	1/1	0.87	0.17	86,86,86,86	0
57	MG	1A	3599	1/1	0.87	0.17	37,37,37,37	0
57	MG	2A	3199	1/1	0.87	0.14	52,52,52,52	0
57	MG	2A	3594	1/1	0.87	0.26	49,49,49,49	0
57	MG	2x	101	1/1	0.87	0.20	71,71,71,71	0
57	MG	1A	3145	1/1	0.87	0.23	45,45,45,45	0
57	MG	1A	3380	1/1	0.87	0.24	54,54,54,54	0
57	MG	2A	3355	1/1	0.87	0.23	63,63,63,63	0
57	MG	2A	3204	1/1	0.87	0.85	55,55,55,55	0
57	MG	1A	3626	1/1	0.87	0.20	40,40,40,40	0
57	MG	1A	3228	1/1	0.87	0.23	46,46,46,46	0
57	MG	2A	3364	1/1	0.87	0.27	46,46,46,46	0
57	MG	2A	3209	1/1	0.87	0.25	59,59,59,59	0
57	MG	1A	3278	1/1	0.87	0.54	66,66,66,66	0
57	MG	1A	3859	1/1	0.87	0.29	42,42,42,42	0
57	MG	1A	3252	1/1	0.87	0.12	66,66,66,66	0
57	MG	1A	3442	1/1	0.87	0.14	59,59,59,59	0
57	MG	1A	3649	1/1	0.87	0.23	27,27,27,27	0
59	ZN	2n	501	1/1	0.87	0.10	96,96,96,96	0
57	MG	1A	3088	1/1	0.88	1.03	57,57,57,57	0
57	MG	1A	3161	1/1	0.88	0.43	43,43,43,43	0
57	MG	2A	3651	1/1	0.88	0.52	62,62,62,62	0
57	MG	2A	3248	1/1	0.88	0.17	60,60,60,60	0
57	MG	1A	3289	1/1	0.88	0.21	52,52,52,52	0
57	MG	1a	1795	1/1	0.88	0.07	68,68,68,68	0
57	MG	1A	3350	1/1	0.88	0.28	67,67,67,67	0
57	MG	1A	3389	1/1	0.88	0.14	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3399	1/1	0.88	0.12	56,56,56,56	0
57	MG	2A	3667	1/1	0.88	0.12	69,69,69,69	0
57	MG	2A	3258	1/1	0.88	0.20	67,67,67,67	0
57	MG	1A	3775	1/1	0.88	0.23	23,23,23,23	0
57	MG	1A	3162	1/1	0.88	0.35	41,41,41,41	0
57	MG	2A	3266	1/1	0.88	0.51	49,49,49,49	0
57	MG	1A	3781	1/1	0.88	0.19	26,26,26,26	0
57	MG	1A	3317	1/1	0.88	0.19	54,54,54,54	0
57	MG	1A	3318	1/1	0.88	0.30	62,62,62,62	0
57	MG	1A	3027	1/1	0.88	0.17	51,51,51,51	0
57	MG	2A	3118	1/1	0.88	0.21	68,68,68,68	0
57	MG	2A	3692	1/1	0.88	0.21	55,55,55,55	0
57	MG	1A	3904	1/1	0.88	0.21	55,55,55,55	0
57	MG	2A	3428	1/1	0.88	0.23	52,52,52,52	0
57	MG	1A	3905	1/1	0.88	0.12	40,40,40,40	0
57	MG	1A	3455	1/1	0.88	0.27	41,41,41,41	0
57	MG	1a	1689	1/1	0.88	0.22	57,57,57,57	0
57	MG	1A	3794	1/1	0.88	0.15	69,69,69,69	0
57	MG	2A	3710	1/1	0.88	0.23	85,85,85,85	0
57	MG	1A	3457	1/1	0.88	0.15	49,49,49,49	0
57	MG	2A	3453	1/1	0.88	0.14	55,55,55,55	0
57	MG	11	106	1/1	0.88	0.15	54,54,54,54	0
57	MG	2A	3283	1/1	0.88	0.09	59,59,59,59	0
57	MG	2A	3727	1/1	0.88	0.07	56,56,56,56	0
57	MG	1A	3205	1/1	0.88	0.28	57,57,57,57	0
57	MG	2A	3148	1/1	0.88	0.20	61,61,61,61	0
57	MG	2A	3735	1/1	0.88	0.19	38,38,38,38	0
57	MG	2A	3288	1/1	0.88	0.10	78,78,78,78	0
57	MG	2A	3471	1/1	0.88	0.21	34,34,34,34	0
57	MG	2A	3482	1/1	0.88	0.21	56,56,56,56	0
57	MG	1A	3207	1/1	0.88	0.19	41,41,41,41	0
57	MG	2A	3752	1/1	0.88	0.16	56,56,56,56	0
57	MG	2A	3295	1/1	0.88	0.21	59,59,59,59	0
57	MG	2A	3488	1/1	0.88	0.14	49,49,49,49	0
57	MG	1w	104	1/1	0.88	0.22	65,65,65,65	0
57	MG	2A	3761	1/1	0.88	0.29	85,85,85,85	0
57	MG	1A	3698	1/1	0.88	0.18	64,64,64,64	0
57	MG	1a	1705	1/1	0.88	0.15	57,57,57,57	0
57	MG	1A	3921	1/1	0.88	0.16	37,37,37,37	0
57	MG	1a	1709	1/1	0.88	0.13	36,36,36,36	0
57	MG	1a	1710	1/1	0.88	0.06	68,68,68,68	0
57	MG	2A	3773	1/1	0.88	0.10	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3130	1/1	0.88	0.47	46,46,46,46	0
57	MG	2A	3780	1/1	0.88	0.12	63,63,63,63	0
57	MG	2A	3782	1/1	0.88	0.16	50,50,50,50	0
57	MG	1A	4031	1/1	0.88	0.13	49,49,49,49	0
57	MG	2A	3306	1/1	0.88	0.13	55,55,55,55	0
57	MG	1A	3176	1/1	0.88	0.15	45,45,45,45	0
57	MG	1A	3927	1/1	0.88	0.15	30,30,30,30	0
57	MG	1a	1723	1/1	0.88	0.14	53,53,53,53	0
57	MG	1A	3805	1/1	0.88	0.12	48,48,48,48	0
57	MG	2A	3178	1/1	0.88	0.23	59,59,59,59	0
57	MG	2A	3004	1/1	0.88	0.48	67,67,67,67	0
57	MG	1A	3416	1/1	0.88	0.32	44,44,44,44	0
57	MG	1a	1608	1/1	0.88	0.35	70,70,70,70	0
57	MG	1a	1731	1/1	0.88	0.25	57,57,57,57	0
57	MG	2A	3531	1/1	0.88	0.14	42,42,42,42	0
57	MG	2A	3187	1/1	0.88	0.25	49,49,49,49	0
57	MG	1a	1618	1/1	0.88	0.14	54,54,54,54	0
57	MG	1A	3703	1/1	0.88	0.12	58,58,58,58	0
57	MG	2A	3190	1/1	0.88	0.21	57,57,57,57	0
57	MG	1a	1735	1/1	0.88	0.13	68,68,68,68	0
57	MG	2A	3195	1/1	0.88	0.28	68,68,68,68	0
57	MG	2A	3197	1/1	0.88	0.34	56,56,56,56	0
57	MG	1A	3605	1/1	0.88	0.22	39,39,39,39	0
57	MG	1A	3297	1/1	0.88	0.24	50,50,50,50	0
57	MG	1A	3419	1/1	0.88	0.26	43,43,43,43	0
57	MG	1E	306	1/1	0.88	0.26	58,58,58,58	0
57	MG	2A	3340	1/1	0.88	0.41	58,58,58,58	0
57	MG	2A	3203	1/1	0.88	0.28	52,52,52,52	0
57	MG	2U	201	1/1	0.88	0.45	54,54,54,54	0
57	MG	1A	3829	1/1	0.88	0.08	69,69,69,69	0
57	MG	1A	3370	1/1	0.88	0.18	58,58,58,58	0
57	MG	1A	3141	1/1	0.88	0.20	49,49,49,49	0
57	MG	2Z	301	1/1	0.88	0.19	80,80,80,80	0
57	MG	2A	3586	1/1	0.88	0.22	63,63,63,63	0
57	MG	1A	3058	1/1	0.88	0.30	59,59,59,59	0
57	MG	2A	3053	1/1	0.88	0.19	58,58,58,58	0
57	MG	1F	308	1/1	0.88	0.34	59,59,59,59	0
57	MG	1A	3373	1/1	0.88	0.12	69,69,69,69	0
57	MG	2a	1601	1/1	0.88	0.24	55,55,55,55	0
57	MG	2A	3357	1/1	0.88	0.34	59,59,59,59	0
57	MG	2A	3216	1/1	0.88	0.22	56,56,56,56	0
57	MG	2A	3060	1/1	0.88	0.13	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3429	1/1	0.88	0.64	47,47,47,47	0
57	MG	1A	3648	1/1	0.88	0.19	23,23,23,23	0
57	MG	2A	3604	1/1	0.88	0.24	61,61,61,61	0
57	MG	1A	3376	1/1	0.88	0.31	37,37,37,37	0
57	MG	1A	3281	1/1	0.88	0.16	77,77,77,77	0
57	MG	2A	3610	1/1	0.88	0.24	49,49,49,49	0
57	MG	2A	3228	1/1	0.88	0.27	56,56,56,56	0
57	MG	2A	3072	1/1	0.88	0.18	47,47,47,47	0
57	MG	2A	3371	1/1	0.88	0.22	59,59,59,59	0
57	MG	1A	3378	1/1	0.88	0.39	49,49,49,49	0
57	MG	2A	3631	1/1	0.88	0.22	49,49,49,49	0
57	MG	1A	3741	1/1	0.88	0.19	30,30,30,30	0
57	MG	1A	3435	1/1	0.88	0.13	60,60,60,60	0
57	MG	1A	3147	1/1	0.88	0.32	45,45,45,45	0
57	MG	1a	1778	1/1	0.88	0.10	67,67,67,67	0
57	MG	1A	3068	1/1	0.88	0.17	54,54,54,54	0
57	MG	1A	3495	1/1	0.88	0.17	68,68,68,68	0
57	MG	1A	3128	1/1	0.89	0.58	48,48,48,48	0
57	MG	2A	3245	1/1	0.89	0.42	72,72,72,72	0
57	MG	2A	3247	1/1	0.89	0.21	76,76,76,76	0
57	MG	1A	3737	1/1	0.89	0.14	48,48,48,48	0
57	MG	1a	1764	1/1	0.89	0.15	77,77,77,77	0
57	MG	1A	3076	1/1	0.89	0.41	53,53,53,53	0
57	MG	2A	3666	1/1	0.89	0.11	75,75,75,75	0
57	MG	1A	3930	1/1	0.89	0.14	67,67,67,67	0
57	MG	1A	3219	1/1	0.89	0.46	37,37,37,37	0
57	MG	1A	3835	1/1	0.89	0.32	68,68,68,68	0
57	MG	2A	3420	1/1	0.89	0.28	60,60,60,60	0
57	MG	1A	3743	1/1	0.89	0.27	44,44,44,44	0
57	MG	2A	3092	1/1	0.89	0.20	60,60,60,60	0
57	MG	1A	3937	1/1	0.89	0.13	75,75,75,75	0
57	MG	1A	3839	1/1	0.89	0.16	61,61,61,61	0
57	MG	1A	3744	1/1	0.89	0.21	59,59,59,59	0
57	MG	2A	3689	1/1	0.89	0.12	73,73,73,73	0
57	MG	2A	3430	1/1	0.89	0.10	71,71,71,71	0
57	MG	2A	3435	1/1	0.89	0.31	51,51,51,51	0
57	MG	1a	1653	1/1	0.89	0.18	61,61,61,61	0
57	MG	2A	3440	1/1	0.89	0.09	69,69,69,69	0
57	MG	1a	1792	1/1	0.89	0.10	66,66,66,66	0
57	MG	1A	3137	1/1	0.89	0.23	38,38,38,38	0
57	MG	1A	3321	1/1	0.89	0.15	58,58,58,58	0
57	MG	1A	3597	1/1	0.89	0.16	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1657	1/1	0.89	0.19	67,67,67,67	0
57	MG	2A	3454	1/1	0.89	0.21	62,62,62,62	0
57	MG	1A	3750	1/1	0.89	0.18	27,27,27,27	0
57	MG	1A	4053	1/1	0.89	0.21	74,74,74,74	0
57	MG	2A	3461	1/1	0.89	0.16	62,62,62,62	0
57	MG	1A	3172	1/1	0.89	0.35	39,39,39,39	0
57	MG	2A	3125	1/1	0.89	0.24	65,65,65,65	0
57	MG	2A	3126	1/1	0.89	0.19	47,47,47,47	0
57	MG	1A	3066	1/1	0.89	0.19	32,32,32,32	0
57	MG	2A	3479	1/1	0.89	0.25	37,37,37,37	0
57	MG	1A	3766	1/1	0.89	0.20	28,28,28,28	0
57	MG	1A	3689	1/1	0.89	0.14	31,31,31,31	0
57	MG	2A	3292	1/1	0.89	0.33	62,62,62,62	0
57	MG	2A	3141	1/1	0.89	0.30	74,74,74,74	0
57	MG	1A	3042	1/1	0.89	0.14	47,47,47,47	0
57	MG	1P	204	1/1	0.89	0.10	40,40,40,40	0
57	MG	1A	3618	1/1	0.89	0.16	21,21,21,21	0
57	MG	1b	301	1/1	0.89	0.18	86,86,86,86	0
57	MG	2A	3763	1/1	0.89	0.14	42,42,42,42	0
57	MG	1A	3384	1/1	0.89	0.16	51,51,51,51	0
57	MG	1e	201	1/1	0.89	0.15	69,69,69,69	0
57	MG	1Q	205	1/1	0.89	0.39	55,55,55,55	0
57	MG	2A	3506	1/1	0.89	0.22	69,69,69,69	0
57	MG	1A	3967	1/1	0.89	0.29	71,71,71,71	0
57	MG	1A	3229	1/1	0.89	0.30	33,33,33,33	0
57	MG	1t	201	1/1	0.89	0.11	55,55,55,55	0
57	MG	1A	3971	1/1	0.89	0.12	39,39,39,39	0
57	MG	1A	3357	1/1	0.89	0.37	58,58,58,58	0
57	MG	2A	3312	1/1	0.89	0.23	75,75,75,75	0
57	MG	1A	3047	1/1	0.89	0.17	31,31,31,31	0
57	MG	2A	3169	1/1	0.89	0.28	54,54,54,54	0
57	MG	2A	3788	1/1	0.89	0.10	65,65,65,65	0
57	MG	1A	3880	1/1	0.89	0.14	25,25,25,25	0
57	MG	2A	3173	1/1	0.89	0.30	61,61,61,61	0
57	MG	1A	3331	1/1	0.89	0.18	67,67,67,67	0
57	MG	1A	3989	1/1	0.89	0.09	68,68,68,68	0
57	MG	1V	207	1/1	0.89	0.26	53,53,53,53	0
57	MG	1A	3991	1/1	0.89	0.20	50,50,50,50	0
57	MG	1a	1698	1/1	0.89	0.10	46,46,46,46	0
57	MG	1A	3993	1/1	0.89	0.18	25,25,25,25	0
57	MG	1A	4106	1/1	0.89	0.19	53,53,53,53	0
57	MG	2B	205	1/1	0.89	0.28	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1x	110	1/1	0.89	0.19	67,67,67,67	0
57	MG	1A	4108	1/1	0.89	0.10	59,59,59,59	0
57	MG	2B	210	1/1	0.89	0.22	68,68,68,68	0
57	MG	10	101	1/1	0.89	0.22	47,47,47,47	0
57	MG	2B	214	1/1	0.89	0.21	69,69,69,69	0
57	MG	1A	3122	1/1	0.89	0.35	33,33,33,33	0
57	MG	1A	3885	1/1	0.89	0.06	46,46,46,46	0
57	MG	1A	4001	1/1	0.89	0.17	54,54,54,54	0
57	MG	2A	3005	1/1	0.89	0.11	71,71,71,71	0
57	MG	1a	1716	1/1	0.89	0.11	37,37,37,37	0
57	MG	1A	3704	1/1	0.89	0.17	47,47,47,47	0
57	MG	2A	3579	1/1	0.89	0.14	68,68,68,68	0
57	MG	1A	3287	1/1	0.89	0.28	62,62,62,62	0
57	MG	2A	3581	1/1	0.89	0.11	64,64,64,64	0
57	MG	2Q	204	1/1	0.89	0.31	59,59,59,59	0
57	MG	1A	4004	1/1	0.89	0.08	76,76,76,76	0
57	MG	1A	3710	1/1	0.89	0.18	59,59,59,59	0
57	MG	2A	3020	1/1	0.89	0.27	62,62,62,62	0
57	MG	1A	4007	1/1	0.89	0.20	77,77,77,77	0
57	MG	2A	3205	1/1	0.89	0.35	58,58,58,58	0
57	MG	1A	3474	1/1	0.89	0.17	52,52,52,52	0
57	MG	1A	3568	1/1	0.89	0.17	64,64,64,64	0
57	MG	21	103	1/1	0.89	0.21	54,54,54,54	0
57	MG	1A	4012	1/1	0.89	0.20	49,49,49,49	0
57	MG	2A	3040	1/1	0.89	0.26	58,58,58,58	0
57	MG	2A	3596	1/1	0.89	0.09	64,64,64,64	0
57	MG	1A	3516	1/1	0.89	0.27	51,51,51,51	0
57	MG	1A	3211	1/1	0.89	0.17	45,45,45,45	0
57	MG	1a	1736	1/1	0.89	0.12	76,76,76,76	0
57	MG	2A	3047	1/1	0.89	0.21	68,68,68,68	0
57	MG	1A	3152	1/1	0.89	0.14	46,46,46,46	0
57	MG	1A	3722	1/1	0.89	0.11	49,49,49,49	0
57	MG	1A	3310	1/1	0.89	0.20	42,42,42,42	0
57	MG	1B	222	1/1	0.89	0.11	61,61,61,61	0
57	MG	1A	3402	1/1	0.89	0.25	40,40,40,40	0
57	MG	2A	3375	1/1	0.89	0.15	72,72,72,72	0
57	MG	2A	3626	1/1	0.89	0.29	56,56,56,56	0
57	MG	1B	226	1/1	0.89	0.17	62,62,62,62	0
57	MG	2x	106	1/1	0.89	0.15	66,66,66,66	0
57	MG	1A	3812	1/1	0.89	0.10	42,42,42,42	0
57	MG	1a	1750	1/1	0.89	0.14	78,78,78,78	0
57	MG	1A	3729	1/1	0.89	0.37	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1754	1/1	0.89	0.09	64,64,64,64	0
57	MG	2A	3642	1/1	0.89	0.11	69,69,69,69	0
57	MG	1A	3340	1/1	0.89	0.26	51,51,51,51	0
57	MG	2A	3074	1/1	0.89	0.20	53,53,53,53	0
57	MG	1B	231	1/1	0.89	0.47	67,67,67,67	0
57	MG	1A	3486	1/1	0.89	0.42	37,37,37,37	0
57	MG	2A	3242	1/1	0.89	0.60	56,56,56,56	0
57	MG	1a	1671	1/1	0.90	0.27	54,54,54,54	0
57	MG	1a	1673	1/1	0.90	0.22	60,60,60,60	0
57	MG	2A	3633	1/1	0.90	0.27	74,74,74,74	0
57	MG	1A	3658	1/1	0.90	0.16	51,51,51,51	0
57	MG	1w	107	1/1	0.90	0.24	68,68,68,68	0
57	MG	1O	202	1/1	0.90	0.16	61,61,61,61	0
57	MG	1A	3266	1/1	0.90	0.33	42,42,42,42	0
57	MG	1A	3667	1/1	0.90	0.10	51,51,51,51	0
57	MG	1a	1679	1/1	0.90	0.14	58,58,58,58	0
57	MG	1a	1680	1/1	0.90	0.21	59,59,59,59	0
57	MG	1A	3196	1/1	0.90	0.13	50,50,50,50	0
57	MG	1A	3243	1/1	0.90	0.26	65,65,65,65	0
57	MG	1Q	203	1/1	0.90	0.26	50,50,50,50	0
57	MG	2A	3654	1/1	0.90	0.14	62,62,62,62	0
57	MG	1A	3106	1/1	0.90	0.62	33,33,33,33	0
57	MG	1A	3477	1/1	0.90	0.40	53,53,53,53	0
57	MG	1A	3960	1/1	0.90	0.42	76,76,76,76	0
57	MG	1A	3961	1/1	0.90	0.15	42,42,42,42	0
57	MG	1A	3107	1/1	0.90	0.64	34,34,34,34	0
57	MG	1A	4084	1/1	0.90	0.10	47,47,47,47	0
57	MG	2A	3006	1/1	0.90	0.13	59,59,59,59	0
57	MG	1A	3749	1/1	0.90	0.16	47,47,47,47	0
57	MG	1a	1697	1/1	0.90	0.11	59,59,59,59	0
57	MG	2A	3396	1/1	0.90	0.23	39,39,39,39	0
57	MG	1A	3856	1/1	0.90	0.12	38,38,38,38	0
57	MG	2A	3014	1/1	0.90	0.22	46,46,46,46	0
57	MG	1A	3413	1/1	0.90	0.17	66,66,66,66	0
57	MG	1a	1701	1/1	0.90	0.19	58,58,58,58	0
57	MG	1a	1703	1/1	0.90	0.16	67,67,67,67	0
57	MG	1A	4091	1/1	0.90	0.11	68,68,68,68	0
57	MG	2A	3408	1/1	0.90	0.72	81,81,81,81	0
57	MG	1A	4095	1/1	0.90	0.24	65,65,65,65	0
57	MG	2A	3697	1/1	0.90	0.20	74,74,74,74	0
57	MG	2A	3030	1/1	0.90	0.08	50,50,50,50	0
57	MG	1A	3590	1/1	0.90	0.15	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3032	1/1	0.90	0.33	47,47,47,47	0
57	MG	1X	102	1/1	0.90	0.27	40,40,40,40	0
57	MG	2A	3039	1/1	0.90	0.30	53,53,53,53	0
57	MG	1X	106	1/1	0.90	0.21	42,42,42,42	0
57	MG	1A	3974	1/1	0.90	0.18	30,30,30,30	0
57	MG	1A	3757	1/1	0.90	0.17	22,22,22,22	0
57	MG	1A	3866	1/1	0.90	0.10	66,66,66,66	0
57	MG	1Z	303	1/1	0.90	0.24	59,59,59,59	0
57	MG	1A	3683	1/1	0.90	0.13	33,33,33,33	0
57	MG	1A	3764	1/1	0.90	0.15	33,33,33,33	0
57	MG	1A	3482	1/1	0.90	0.45	49,49,49,49	0
57	MG	2A	3729	1/1	0.90	0.14	62,62,62,62	0
57	MG	2A	3730	1/1	0.90	0.09	79,79,79,79	0
57	MG	2A	3731	1/1	0.90	0.24	52,52,52,52	0
57	MG	1A	3767	1/1	0.90	0.13	54,54,54,54	0
57	MG	1A	3992	1/1	0.90	0.17	33,33,33,33	0
57	MG	2A	3449	1/1	0.90	0.23	43,43,43,43	0
57	MG	2A	3740	1/1	0.90	0.16	56,56,56,56	0
57	MG	1A	3874	1/1	0.90	0.17	39,39,39,39	0
57	MG	1A	3414	1/1	0.90	0.14	62,62,62,62	0
57	MG	2A	3748	1/1	0.90	0.10	69,69,69,69	0
57	MG	2A	3256	1/1	0.90	0.96	68,68,68,68	0
57	MG	1A	3995	1/1	0.90	0.23	41,41,41,41	0
57	MG	2A	3066	1/1	0.90	0.18	42,42,42,42	0
57	MG	2A	3260	1/1	0.90	0.49	65,65,65,65	0
57	MG	2A	3068	1/1	0.90	0.32	52,52,52,52	0
57	MG	2A	3262	1/1	0.90	0.19	62,62,62,62	0
57	MG	2A	3263	1/1	0.90	0.24	70,70,70,70	0
57	MG	1A	3110	1/1	0.90	0.25	39,39,39,39	0
57	MG	1A	3149	1/1	0.90	0.52	48,48,48,48	0
57	MG	16	102	1/1	0.90	0.13	51,51,51,51	0
57	MG	1A	3449	1/1	0.90	0.41	51,51,51,51	0
57	MG	1A	3598	1/1	0.90	0.15	62,62,62,62	0
57	MG	1a	1745	1/1	0.90	0.06	67,67,67,67	0
57	MG	2A	3774	1/1	0.90	0.19	58,58,58,58	0
57	MG	1A	3328	1/1	0.90	0.36	40,40,40,40	0
57	MG	1A	3601	1/1	0.90	0.14	45,45,45,45	0
57	MG	1A	3893	1/1	0.90	0.14	45,45,45,45	0
57	MG	1A	3782	1/1	0.90	0.17	32,32,32,32	0
57	MG	1A	4009	1/1	0.90	0.24	61,61,61,61	0
57	MG	1a	1613	1/1	0.90	0.13	63,63,63,63	0
57	MG	1A	3206	1/1	0.90	0.26	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3090	1/1	0.90	0.12	69,69,69,69	0
57	MG	1A	3016	1/1	0.90	0.13	51,51,51,51	0
57	MG	2A	3510	1/1	0.90	0.30	71,71,71,71	0
57	MG	1A	3456	1/1	0.90	0.14	61,61,61,61	0
57	MG	2A	3793	1/1	0.90	0.20	64,64,64,64	0
57	MG	1A	3619	1/1	0.90	0.18	30,30,30,30	0
57	MG	1A	3496	1/1	0.90	0.13	87,87,87,87	0
57	MG	2A	3797	1/1	0.90	0.18	72,72,72,72	0
57	MG	2A	3802	1/1	0.90	0.15	59,59,59,59	0
57	MG	1a	1624	1/1	0.90	0.10	60,60,60,60	0
57	MG	2A	3805	1/1	0.90	0.23	58,58,58,58	0
57	MG	1a	1765	1/1	0.90	0.06	62,62,62,62	0
57	MG	2A	3101	1/1	0.90	0.23	48,48,48,48	0
57	MG	1a	1767	1/1	0.90	0.29	74,74,74,74	0
57	MG	1a	1768	1/1	0.90	0.13	59,59,59,59	0
57	MG	1a	1625	1/1	0.90	0.15	63,63,63,63	0
57	MG	1A	3305	1/1	0.90	0.35	60,60,60,60	0
57	MG	2A	3113	1/1	0.90	0.16	73,73,73,73	0
57	MG	1A	3458	1/1	0.90	0.65	53,53,53,53	0
57	MG	1a	1630	1/1	0.90	0.11	56,56,56,56	0
57	MG	2A	3122	1/1	0.90	0.34	73,73,73,73	0
57	MG	2D	302	1/1	0.90	0.52	72,72,72,72	0
57	MG	2A	3538	1/1	0.90	0.08	75,75,75,75	0
57	MG	1A	3913	1/1	0.90	0.15	44,44,44,44	0
57	MG	2A	3542	1/1	0.90	0.14	39,39,39,39	0
57	MG	1a	1633	1/1	0.90	0.22	66,66,66,66	0
57	MG	1A	3631	1/1	0.90	0.32	72,72,72,72	0
57	MG	2A	3552	1/1	0.90	0.18	40,40,40,40	0
57	MG	2F	303	1/1	0.90	0.23	45,45,45,45	0
57	MG	1B	232	1/1	0.90	0.12	72,72,72,72	0
57	MG	2Q	201	1/1	0.90	0.10	64,64,64,64	0
57	MG	1a	1637	1/1	0.90	0.14	63,63,63,63	0
57	MG	1A	3155	1/1	0.90	0.17	64,64,64,64	0
57	MG	1a	1643	1/1	0.90	0.23	60,60,60,60	0
57	MG	1A	3713	1/1	0.90	0.21	54,54,54,54	0
57	MG	1A	3635	1/1	0.90	0.14	25,25,25,25	0
57	MG	1A	3059	1/1	0.90	0.26	47,47,47,47	0
57	MG	2A	3146	1/1	0.90	0.35	58,58,58,58	0
57	MG	1A	3808	1/1	0.90	0.14	29,29,29,29	0
57	MG	2A	3325	1/1	0.90	0.16	77,77,77,77	0
57	MG	1A	3308	1/1	0.90	0.30	47,47,47,47	0
57	MG	1A	3928	1/1	0.90	0.19	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3063	1/1	0.90	0.39	56,56,56,56	0
57	MG	1A	3724	1/1	0.90	0.06	54,54,54,54	0
57	MG	1A	3818	1/1	0.90	0.25	62,62,62,62	0
57	MG	1A	3432	1/1	0.90	0.27	39,39,39,39	0
57	MG	1F	305	1/1	0.90	0.17	43,43,43,43	0
57	MG	1A	3240	1/1	0.90	0.21	40,40,40,40	0
57	MG	1a	1819	1/1	0.90	0.12	76,76,76,76	0
57	MG	2A	3338	1/1	0.90	0.28	51,51,51,51	0
57	MG	1a	1820	1/1	0.90	0.14	45,45,45,45	0
57	MG	1A	3023	1/1	0.90	0.27	39,39,39,39	0
57	MG	1A	3569	1/1	0.90	0.39	48,48,48,48	0
57	MG	2A	3600	1/1	0.90	0.11	71,71,71,71	0
57	MG	1G	202	1/1	0.90	0.20	64,64,64,64	0
57	MG	1f	202	1/1	0.90	0.15	70,70,70,70	0
57	MG	1a	1664	1/1	0.90	0.13	73,73,73,73	0
57	MG	1A	4046	1/1	0.90	0.21	44,44,44,44	0
57	MG	2y	102	1/1	0.90	0.10	87,87,87,87	0
57	MG	2A	3613	1/1	0.90	0.13	60,60,60,60	0
57	MG	2A	3615	1/1	0.90	0.26	63,63,63,63	0
57	MG	1m	3001	1/1	0.90	0.13	61,61,61,61	0
57	MG	2A	3619	1/1	0.90	0.09	81,81,81,81	0
57	MG	1A	3512	1/1	0.90	0.28	46,46,46,46	0
57	MG	1A	3735	1/1	0.90	0.29	45,45,45,45	0
59	ZN	2Y	501	1/1	0.90	0.11	105,105,105,105	0
57	MG	1A	3573	1/1	0.90	0.25	57,57,57,57	0
57	MG	2A	3184	1/1	0.90	0.29	57,57,57,57	0
57	MG	1A	3896	1/1	0.91	0.18	42,42,42,42	0
57	MG	1A	3204	1/1	0.91	0.15	52,52,52,52	0
57	MG	1A	3900	1/1	0.91	0.14	33,33,33,33	0
57	MG	2A	3046	1/1	0.91	0.37	63,63,63,63	0
57	MG	1A	3901	1/1	0.91	0.25	23,23,23,23	0
57	MG	1A	3902	1/1	0.91	0.17	46,46,46,46	0
57	MG	1A	3462	1/1	0.91	0.27	50,50,50,50	0
57	MG	2A	3051	1/1	0.91	0.11	51,51,51,51	0
57	MG	1A	3041	1/1	0.91	0.32	68,68,68,68	0
57	MG	1a	1614	1/1	0.91	0.13	73,73,73,73	0
57	MG	1A	3508	1/1	0.91	0.25	44,44,44,44	0
57	MG	1A	3249	1/1	0.91	0.21	43,43,43,43	0
57	MG	1A	3250	1/1	0.91	0.17	44,44,44,44	0
57	MG	2A	3234	1/1	0.91	0.23	72,72,72,72	0
57	MG	1A	3806	1/1	0.91	0.13	25,25,25,25	0
57	MG	1A	4017	1/1	0.91	0.21	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3067	1/1	0.91	0.61	65,65,65,65	0
57	MG	1A	3173	1/1	0.91	0.22	54,54,54,54	0
57	MG	2A	3680	1/1	0.91	0.10	66,66,66,66	0
57	MG	1A	3657	1/1	0.91	0.12	30,30,30,30	0
57	MG	1A	3811	1/1	0.91	0.11	39,39,39,39	0
57	MG	1A	3129	1/1	0.91	0.21	37,37,37,37	0
57	MG	2A	3690	1/1	0.91	0.21	71,71,71,71	0
57	MG	1A	3661	1/1	0.91	0.12	27,27,27,27	0
57	MG	1A	3514	1/1	0.91	0.17	62,62,62,62	0
57	MG	2A	3695	1/1	0.91	0.19	49,49,49,49	0
57	MG	1A	3923	1/1	0.91	0.16	46,46,46,46	0
57	MG	2A	3698	1/1	0.91	0.11	60,60,60,60	0
57	MG	1A	3332	1/1	0.91	0.15	64,64,64,64	0
57	MG	2A	3431	1/1	0.91	0.25	47,47,47,47	0
57	MG	1A	3820	1/1	0.91	0.41	45,45,45,45	0
57	MG	2A	3251	1/1	0.91	0.13	54,54,54,54	0
57	MG	1E	301	1/1	0.91	0.42	31,31,31,31	0
57	MG	2A	3441	1/1	0.91	0.22	46,46,46,46	0
57	MG	2A	3255	1/1	0.91	0.34	62,62,62,62	0
57	MG	2A	3712	1/1	0.91	0.11	66,66,66,66	0
57	MG	1E	302	1/1	0.91	0.23	40,40,40,40	0
57	MG	1a	1642	1/1	0.91	0.10	58,58,58,58	0
57	MG	2A	3085	1/1	0.91	0.25	64,64,64,64	0
57	MG	1A	3669	1/1	0.91	0.23	70,70,70,70	0
57	MG	2A	3723	1/1	0.91	0.11	80,80,80,80	0
57	MG	1A	3392	1/1	0.91	0.18	48,48,48,48	0
57	MG	1A	3826	1/1	0.91	0.10	40,40,40,40	0
57	MG	2A	3456	1/1	0.91	0.23	64,64,64,64	0
57	MG	1a	1788	1/1	0.91	0.23	68,68,68,68	0
57	MG	1a	1790	1/1	0.91	0.11	56,56,56,56	0
57	MG	1A	3584	1/1	0.91	0.11	41,41,41,41	0
57	MG	1A	4036	1/1	0.91	0.10	49,49,49,49	0
57	MG	2A	3464	1/1	0.91	0.23	39,39,39,39	0
57	MG	2A	3737	1/1	0.91	0.24	66,66,66,66	0
57	MG	1A	3230	1/1	0.91	0.15	41,41,41,41	0
57	MG	2A	3466	1/1	0.91	0.16	55,55,55,55	0
57	MG	2A	3744	1/1	0.91	0.10	46,46,46,46	0
57	MG	1A	3209	1/1	0.91	0.40	41,41,41,41	0
57	MG	1F	309	1/1	0.91	0.13	51,51,51,51	0
57	MG	1a	1652	1/1	0.91	0.09	69,69,69,69	0
57	MG	2A	3105	1/1	0.91	0.09	65,65,65,65	0
57	MG	1A	3936	1/1	0.91	0.14	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3107	1/1	0.91	0.19	69,69,69,69	0
57	MG	1A	3397	1/1	0.91	0.35	48,48,48,48	0
57	MG	2A	3490	1/1	0.91	0.19	55,55,55,55	0
57	MG	1A	3236	1/1	0.91	0.25	48,48,48,48	0
57	MG	2A	3112	1/1	0.91	0.29	49,49,49,49	0
57	MG	1A	3748	1/1	0.91	0.19	23,23,23,23	0
57	MG	2A	3114	1/1	0.91	0.23	61,61,61,61	0
57	MG	2A	3116	1/1	0.91	0.14	56,56,56,56	0
57	MG	2A	3286	1/1	0.91	0.18	69,69,69,69	0
57	MG	1A	3210	1/1	0.91	0.47	46,46,46,46	0
57	MG	1H	201	1/1	0.91	0.22	54,54,54,54	0
57	MG	2A	3119	1/1	0.91	0.25	61,61,61,61	0
57	MG	1N	201	1/1	0.91	0.24	40,40,40,40	0
57	MG	1A	3844	1/1	0.91	0.15	63,63,63,63	0
57	MG	2A	3296	1/1	0.91	0.12	65,65,65,65	0
57	MG	1N	204	1/1	0.91	0.28	40,40,40,40	0
57	MG	1A	3592	1/1	0.91	0.23	58,58,58,58	0
57	MG	1A	3751	1/1	0.91	0.18	37,37,37,37	0
57	MG	2A	3129	1/1	0.91	0.35	59,59,59,59	0
57	MG	2A	3130	1/1	0.91	0.18	49,49,49,49	0
57	MG	2A	3132	1/1	0.91	0.24	49,49,49,49	0
57	MG	2A	3526	1/1	0.91	0.19	63,63,63,63	0
57	MG	1A	4054	1/1	0.91	0.22	46,46,46,46	0
57	MG	1a	1668	1/1	0.91	0.37	70,70,70,70	0
57	MG	1A	3753	1/1	0.91	0.24	32,32,32,32	0
57	MG	1f	201	1/1	0.91	0.30	52,52,52,52	0
57	MG	1A	4057	1/1	0.91	0.16	47,47,47,47	0
57	MG	2A	3311	1/1	0.91	0.25	69,69,69,69	0
57	MG	1A	3524	1/1	0.91	0.25	34,34,34,34	0
57	MG	1A	3156	1/1	0.91	0.35	31,31,31,31	0
57	MG	2A	3314	1/1	0.91	0.18	77,77,77,77	0
57	MG	1A	3530	1/1	0.91	0.72	50,50,50,50	0
57	MG	1A	4062	1/1	0.91	0.25	37,37,37,37	0
57	MG	1A	3955	1/1	0.91	0.10	49,49,49,49	0
57	MG	2A	3319	1/1	0.91	0.15	75,75,75,75	0
57	MG	2A	3150	1/1	0.91	0.39	46,46,46,46	0
57	MG	2A	3558	1/1	0.91	0.65	59,59,59,59	0
57	MG	1A	3763	1/1	0.91	0.13	40,40,40,40	0
57	MG	1A	3533	1/1	0.91	0.10	60,60,60,60	0
57	MG	1A	3534	1/1	0.91	0.18	60,60,60,60	0
57	MG	1w	103	1/1	0.91	0.22	75,75,75,75	0
57	MG	2D	305	1/1	0.91	0.54	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3159	1/1	0.91	0.12	71,71,71,71	0
57	MG	2A	3571	1/1	0.91	0.24	84,84,84,84	0
57	MG	2A	3577	1/1	0.91	0.09	60,60,60,60	0
57	MG	1R	205	1/1	0.91	0.21	34,34,34,34	0
57	MG	1A	3096	1/1	0.91	0.14	55,55,55,55	0
57	MG	1A	4083	1/1	0.91	0.20	58,58,58,58	0
57	MG	2F	304	1/1	0.91	0.20	55,55,55,55	0
57	MG	1A	3404	1/1	0.91	0.16	49,49,49,49	0
57	MG	2A	3582	1/1	0.91	0.21	59,59,59,59	0
57	MG	2Q	202	1/1	0.91	0.20	57,57,57,57	0
57	MG	1T	202	1/1	0.91	0.20	59,59,59,59	0
57	MG	1A	3446	1/1	0.91	0.12	55,55,55,55	0
57	MG	2T	201	1/1	0.91	0.20	62,62,62,62	0
57	MG	1U	202	1/1	0.91	0.48	36,36,36,36	0
57	MG	2A	3588	1/1	0.91	0.13	59,59,59,59	0
57	MG	2A	3335	1/1	0.91	0.34	46,46,46,46	0
57	MG	1A	3341	1/1	0.91	0.16	55,55,55,55	0
57	MG	1A	3407	1/1	0.91	0.16	52,52,52,52	0
57	MG	20	101	1/1	0.91	0.23	67,67,67,67	0
57	MG	1A	3973	1/1	0.91	0.21	21,21,21,21	0
57	MG	21	101	1/1	0.91	0.25	68,68,68,68	0
57	MG	1W	205	1/1	0.91	0.17	42,42,42,42	0
57	MG	1A	4093	1/1	0.91	0.11	43,43,43,43	0
57	MG	2A	3345	1/1	0.91	0.47	65,65,65,65	0
57	MG	1X	105	1/1	0.91	0.25	51,51,51,51	0
57	MG	27	102	1/1	0.91	0.76	67,67,67,67	0
57	MG	1A	3546	1/1	0.91	0.41	41,41,41,41	0
57	MG	28	102	1/1	0.91	0.19	62,62,62,62	0
57	MG	1A	3342	1/1	0.91	0.48	54,54,54,54	0
57	MG	1A	3409	1/1	0.91	0.13	41,41,41,41	0
57	MG	1A	3878	1/1	0.91	0.22	30,30,30,30	0
57	MG	1A	3982	1/1	0.91	0.19	47,47,47,47	0
57	MG	1A	3374	1/1	0.91	0.44	40,40,40,40	0
57	MG	1A	3056	1/1	0.91	0.17	50,50,50,50	0
57	MG	10	105	1/1	0.91	0.10	34,34,34,34	0
57	MG	2A	3194	1/1	0.91	0.24	65,65,65,65	0
57	MG	2A	3618	1/1	0.91	0.18	59,59,59,59	0
57	MG	1A	3345	1/1	0.91	0.27	41,41,41,41	0
57	MG	2A	3017	1/1	0.91	0.34	54,54,54,54	0
57	MG	1A	3787	1/1	0.91	0.16	47,47,47,47	0
57	MG	2A	3019	1/1	0.91	0.20	44,44,44,44	0
57	MG	1A	3200	1/1	0.91	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
57	MG	1A	3889	1/1	0.91	0.15	55,55,55,55	0
57	MG	1A	3891	1/1	0.91	0.17	42,42,42,42	0
57	MG	15	104	1/1	0.91	0.56	44,44,44,44	0
57	MG	1A	3996	1/1	0.91	0.17	29,29,29,29	0
57	MG	1A	3139	1/1	0.91	0.18	49,49,49,49	0
57	MG	2A	3376	1/1	0.91	0.25	60,60,60,60	0
57	MG	1A	3998	1/1	0.91	0.10	40,40,40,40	0
57	MG	1A	3714	1/1	0.91	0.22	50,50,50,50	0
57	MG	2A	3647	1/1	0.91	0.18	54,54,54,54	0
57	MG	1A	3203	1/1	0.91	0.17	45,45,45,45	0
57	MG	1A	3950	1/1	0.92	0.09	33,33,33,33	0
57	MG	2A	3489	1/1	0.92	0.20	39,39,39,39	0
57	MG	1A	3421	1/1	0.92	0.40	40,40,40,40	0
57	MG	2A	3699	1/1	0.92	0.09	56,56,56,56	0
57	MG	1A	4033	1/1	0.92	0.11	50,50,50,50	0
57	MG	2A	3493	1/1	0.92	0.14	77,77,77,77	0
57	MG	2A	3704	1/1	0.92	0.12	68,68,68,68	0
57	MG	1A	3157	1/1	0.92	0.25	33,33,33,33	0
57	MG	1B	217	1/1	0.92	0.10	54,54,54,54	0
57	MG	1Y	202	1/1	0.92	0.69	53,53,53,53	0
57	MG	1A	3334	1/1	0.92	0.17	60,60,60,60	0
57	MG	1A	3459	1/1	0.92	0.14	60,60,60,60	0
57	MG	1A	3043	1/1	0.92	0.44	31,31,31,31	0
57	MG	1a	1796	1/1	0.92	0.11	66,66,66,66	0
57	MG	1A	3888	1/1	0.92	0.16	48,48,48,48	0
57	MG	2A	3508	1/1	0.92	0.06	54,54,54,54	0
57	MG	10	103	1/1	0.92	0.50	47,47,47,47	0
57	MG	1A	4043	1/1	0.92	0.14	25,25,25,25	0
57	MG	2A	3724	1/1	0.92	0.16	56,56,56,56	0
57	MG	2A	3513	1/1	0.92	0.09	51,51,51,51	0
57	MG	1A	3426	1/1	0.92	0.24	50,50,50,50	0
57	MG	2A	3208	1/1	0.92	0.13	66,66,66,66	0
57	MG	1A	3600	1/1	0.92	0.19	46,46,46,46	0
57	MG	1a	1681	1/1	0.92	0.06	70,70,70,70	0
57	MG	1A	3111	1/1	0.92	0.25	41,41,41,41	0
57	MG	1A	3393	1/1	0.92	0.14	64,64,64,64	0
57	MG	2A	3083	1/1	0.92	0.29	63,63,63,63	0
57	MG	1a	1816	1/1	0.92	0.13	67,67,67,67	0
57	MG	2A	3738	1/1	0.92	0.12	46,46,46,46	0
57	MG	1A	3123	1/1	0.92	0.55	41,41,41,41	0
57	MG	2A	3347	1/1	0.92	0.41	61,61,61,61	0
57	MG	1A	3223	1/1	0.92	0.27	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3745	1/1	0.92	0.15	59,59,59,59	0
57	MG	2A	3746	1/1	0.92	0.25	60,60,60,60	0
57	MG	2A	3350	1/1	0.92	0.37	58,58,58,58	0
57	MG	1A	3815	1/1	0.92	0.38	53,53,53,53	0
57	MG	1A	3898	1/1	0.92	0.30	37,37,37,37	0
57	MG	2A	3750	1/1	0.92	0.18	63,63,63,63	0
57	MG	1A	3311	1/1	0.92	0.15	56,56,56,56	0
57	MG	1A	3469	1/1	0.92	0.37	31,31,31,31	0
57	MG	2A	3755	1/1	0.92	0.15	83,83,83,83	0
57	MG	1A	3192	1/1	0.92	0.29	39,39,39,39	0
57	MG	1A	3752	1/1	0.92	0.19	26,26,26,26	0
57	MG	2A	3359	1/1	0.92	0.18	67,67,67,67	0
57	MG	1A	3314	1/1	0.92	0.36	57,57,57,57	0
57	MG	1A	3265	1/1	0.92	0.15	51,51,51,51	0
57	MG	2A	3100	1/1	0.92	0.28	57,57,57,57	0
57	MG	2A	3236	1/1	0.92	0.26	61,61,61,61	0
57	MG	1A	3907	1/1	0.92	0.14	51,51,51,51	0
57	MG	1A	4066	1/1	0.92	0.20	56,56,56,56	0
57	MG	1p	101	1/1	0.92	0.08	57,57,57,57	0
57	MG	1E	314	1/1	0.92	0.10	36,36,36,36	0
57	MG	2A	3568	1/1	0.92	0.30	50,50,50,50	0
57	MG	2A	3370	1/1	0.92	0.16	63,63,63,63	0
57	MG	1A	3225	1/1	0.92	0.29	52,52,52,52	0
57	MG	2A	3573	1/1	0.92	0.17	65,65,65,65	0
57	MG	2A	3575	1/1	0.92	0.25	61,61,61,61	0
57	MG	2A	3576	1/1	0.92	0.24	76,76,76,76	0
57	MG	2A	3787	1/1	0.92	0.16	60,60,60,60	0
57	MG	1A	3403	1/1	0.92	0.21	46,46,46,46	0
57	MG	1A	3517	1/1	0.92	0.47	58,58,58,58	0
57	MG	1A	3049	1/1	0.92	0.19	40,40,40,40	0
57	MG	1A	4077	1/1	0.92	0.21	57,57,57,57	0
57	MG	1A	4078	1/1	0.92	0.06	34,34,34,34	0
57	MG	2A	3115	1/1	0.92	0.11	67,67,67,67	0
57	MG	1A	4081	1/1	0.92	0.37	53,53,53,53	0
57	MG	2A	3795	1/1	0.92	0.15	62,62,62,62	0
57	MG	1a	1717	1/1	0.92	0.09	61,61,61,61	0
57	MG	2A	3385	1/1	0.92	1.12	59,59,59,59	0
57	MG	2A	3253	1/1	0.92	0.26	64,64,64,64	0
57	MG	2A	3589	1/1	0.92	0.12	47,47,47,47	0
57	MG	2A	3804	1/1	0.92	0.09	79,79,79,79	0
57	MG	1A	3574	1/1	0.92	0.63	43,43,43,43	0
57	MG	1A	3708	1/1	0.92	0.32	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3050	1/1	0.92	0.18	24,24,24,24	0
57	MG	2B	203	1/1	0.92	0.20	68,68,68,68	0
57	MG	2A	3393	1/1	0.92	0.27	44,44,44,44	0
57	MG	1A	3197	1/1	0.92	0.16	47,47,47,47	0
57	MG	1a	1627	1/1	0.92	0.18	46,46,46,46	0
57	MG	1a	1628	1/1	0.92	0.18	58,58,58,58	0
57	MG	1A	3105	1/1	0.92	0.72	44,44,44,44	0
57	MG	1A	4005	1/1	0.92	0.12	64,64,64,64	0
57	MG	1a	1631	1/1	0.92	0.10	51,51,51,51	0
57	MG	2A	3601	1/1	0.92	0.20	43,43,43,43	0
57	MG	1A	3846	1/1	0.92	0.10	53,53,53,53	0
57	MG	2A	3403	1/1	0.92	0.27	76,76,76,76	0
57	MG	2A	3001	1/1	0.92	0.27	68,68,68,68	0
57	MG	2A	3609	1/1	0.92	0.18	54,54,54,54	0
57	MG	1A	3772	1/1	0.92	0.17	42,42,42,42	0
57	MG	2A	3611	1/1	0.92	0.10	66,66,66,66	0
57	MG	2E	303	1/1	0.92	0.16	52,52,52,52	0
57	MG	2E	305	1/1	0.92	0.14	60,60,60,60	0
57	MG	2A	3003	1/1	0.92	0.20	49,49,49,49	0
57	MG	1a	1738	1/1	0.92	0.14	63,63,63,63	0
57	MG	2A	3411	1/1	0.92	0.62	54,54,54,54	0
57	MG	1A	4096	1/1	0.92	0.15	69,69,69,69	0
57	MG	1A	3280	1/1	0.92	0.12	44,44,44,44	0
57	MG	2O	201	1/1	0.92	0.15	55,55,55,55	0
57	MG	1a	1636	1/1	0.92	0.15	69,69,69,69	0
57	MG	1A	3582	1/1	0.92	0.38	47,47,47,47	0
57	MG	1A	3717	1/1	0.92	0.18	28,28,28,28	0
57	MG	2A	3625	1/1	0.92	0.10	72,72,72,72	0
57	MG	2A	3424	1/1	0.92	0.21	41,41,41,41	0
57	MG	2A	3629	1/1	0.92	0.14	40,40,40,40	0
57	MG	1A	3583	1/1	0.92	0.23	36,36,36,36	0
57	MG	2W	201	1/1	0.92	0.31	72,72,72,72	0
57	MG	1A	3062	1/1	0.92	0.38	54,54,54,54	0
57	MG	1A	3784	1/1	0.92	0.19	42,42,42,42	0
57	MG	2A	3155	1/1	0.92	0.19	64,64,64,64	0
57	MG	1A	4107	1/1	0.92	0.14	47,47,47,47	0
57	MG	1A	3382	1/1	0.92	0.16	50,50,50,50	0
57	MG	1A	3487	1/1	0.92	0.44	42,42,42,42	0
57	MG	1A	3662	1/1	0.92	0.22	22,22,22,22	0
57	MG	2A	3645	1/1	0.92	0.16	68,68,68,68	0
57	MG	2A	3024	1/1	0.92	0.21	60,60,60,60	0
57	MG	1A	3665	1/1	0.92	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
57	MG	2A	3443	1/1	0.92	0.18	35,35,35,35	0
57	MG	2A	3164	1/1	0.92	0.20	50,50,50,50	0
57	MG	2A	3165	1/1	0.92	0.33	66,66,66,66	0
57	MG	2A	3448	1/1	0.92	0.15	47,47,47,47	0
57	MG	1A	3045	1/1	0.92	0.13	46,46,46,46	0
57	MG	2w	101	1/1	0.92	0.21	75,75,75,75	0
57	MG	1B	202	1/1	0.92	0.26	59,59,59,59	0
57	MG	1A	3790	1/1	0.92	0.18	25,25,25,25	0
57	MG	2A	3171	1/1	0.92	0.08	61,61,61,61	0
57	MG	2w	105	1/1	0.92	0.17	79,79,79,79	0
57	MG	1A	3303	1/1	0.92	0.32	40,40,40,40	0
57	MG	2A	3458	1/1	0.92	0.34	57,57,57,57	0
57	MG	2A	3034	1/1	0.92	0.45	53,53,53,53	0
57	MG	1A	3873	1/1	0.92	0.18	31,31,31,31	0
57	MG	1A	3418	1/1	0.92	0.33	50,50,50,50	0
57	MG	1V	201	1/1	0.92	0.35	40,40,40,40	0
57	MG	2A	3463	1/1	0.92	0.31	59,59,59,59	0
57	MG	1A	3796	1/1	0.92	0.15	44,44,44,44	0
57	MG	1A	3254	1/1	0.92	0.17	65,65,65,65	0
57	MG	2A	3678	1/1	0.92	0.09	61,61,61,61	0
57	MG	2A	3045	1/1	0.92	0.29	48,48,48,48	0
57	MG	1A	3879	1/1	0.92	0.16	26,26,26,26	0
57	MG	1a	1661	1/1	0.92	0.10	66,66,66,66	0
57	MG	1a	1662	1/1	0.92	0.15	48,48,48,48	0
57	MG	2A	3687	1/1	0.92	0.26	69,69,69,69	0
58	K	2A	3377	1/1	0.92	0.07	65,65,65,65	0
57	MG	2A	3480	1/1	0.92	0.26	55,55,55,55	0
57	MG	1a	1663	1/1	0.92	0.17	77,77,77,77	0
57	MG	1a	1779	1/1	0.92	0.08	62,62,62,62	0
57	MG	1a	1782	1/1	0.92	0.10	85,85,85,85	0
57	MG	1A	3910	1/1	0.93	0.12	56,56,56,56	0
57	MG	1A	3558	1/1	0.93	0.26	41,41,41,41	0
57	MG	1a	1774	1/1	0.93	0.08	61,61,61,61	0
57	MG	2A	3180	1/1	0.93	0.38	56,56,56,56	0
57	MG	1A	3489	1/1	0.93	0.45	38,38,38,38	0
57	MG	1A	3221	1/1	0.93	0.34	47,47,47,47	0
57	MG	2A	3496	1/1	0.93	0.14	44,44,44,44	0
57	MG	2A	3498	1/1	0.93	0.16	52,52,52,52	0
57	MG	1A	3915	1/1	0.93	0.18	43,43,43,43	0
57	MG	1A	3075	1/1	0.93	0.53	44,44,44,44	0
57	MG	2A	3501	1/1	0.93	0.19	38,38,38,38	0
57	MG	1A	3108	1/1	0.93	0.22	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3326	1/1	0.93	0.10	61,61,61,61	0
57	MG	1D	306	1/1	0.93	0.39	41,41,41,41	0
57	MG	2A	3052	1/1	0.93	0.16	61,61,61,61	0
57	MG	2A	3716	1/1	0.93	0.15	70,70,70,70	0
57	MG	2A	3717	1/1	0.93	0.19	54,54,54,54	0
57	MG	1a	1787	1/1	0.93	0.08	74,74,74,74	0
57	MG	1D	307	1/1	0.93	0.49	45,45,45,45	0
57	MG	2A	3055	1/1	0.93	0.21	64,64,64,64	0
57	MG	2A	3056	1/1	0.93	0.08	66,66,66,66	0
57	MG	1a	1674	1/1	0.93	0.18	64,64,64,64	0
57	MG	2A	3196	1/1	0.93	0.38	65,65,65,65	0
57	MG	2A	3516	1/1	0.93	0.20	62,62,62,62	0
57	MG	1A	3668	1/1	0.93	0.13	27,27,27,27	0
57	MG	1A	3728	1/1	0.93	0.22	21,21,21,21	0
57	MG	11	105	1/1	0.93	0.23	78,78,78,78	0
57	MG	2A	3520	1/1	0.93	0.34	67,67,67,67	0
57	MG	2A	3521	1/1	0.93	0.28	67,67,67,67	0
57	MG	2A	3064	1/1	0.93	0.34	62,62,62,62	0
57	MG	1A	4072	1/1	0.93	0.17	49,49,49,49	0
57	MG	2A	3341	1/1	0.93	0.17	40,40,40,40	0
57	MG	2A	3527	1/1	0.93	0.22	48,48,48,48	0
57	MG	1A	3564	1/1	0.93	0.36	54,54,54,54	0
57	MG	13	103	1/1	0.93	0.11	51,51,51,51	0
57	MG	1E	305	1/1	0.93	0.32	38,38,38,38	0
57	MG	1A	3730	1/1	0.93	0.18	28,28,28,28	0
57	MG	1A	3127	1/1	0.93	0.16	66,66,66,66	0
57	MG	1A	3791	1/1	0.93	0.10	46,46,46,46	0
57	MG	2A	3075	1/1	0.93	0.27	40,40,40,40	0
57	MG	1A	3863	1/1	0.93	0.21	42,42,42,42	0
57	MG	2A	3541	1/1	0.93	0.21	46,46,46,46	0
57	MG	1a	1809	1/1	0.93	0.16	66,66,66,66	0
57	MG	2A	3543	1/1	0.93	0.31	65,65,65,65	0
57	MG	2A	3757	1/1	0.93	0.11	64,64,64,64	0
57	MG	2A	3759	1/1	0.93	0.13	63,63,63,63	0
57	MG	17	106	1/1	0.93	0.16	45,45,45,45	0
57	MG	1a	1813	1/1	0.93	0.09	57,57,57,57	0
57	MG	2A	3762	1/1	0.93	0.25	78,78,78,78	0
57	MG	2A	3356	1/1	0.93	0.33	53,53,53,53	0
57	MG	1A	3424	1/1	0.93	0.16	67,67,67,67	0
57	MG	2A	3220	1/1	0.93	0.28	62,62,62,62	0
57	MG	1a	1691	1/1	0.93	0.10	68,68,68,68	0
57	MG	2A	3769	1/1	0.93	0.26	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3559	1/1	0.93	0.36	72,72,72,72	0
57	MG	2A	3361	1/1	0.93	0.10	44,44,44,44	0
57	MG	1F	301	1/1	0.93	0.27	30,30,30,30	0
57	MG	1F	302	1/1	0.93	0.31	35,35,35,35	0
57	MG	1A	3932	1/1	0.93	0.10	49,49,49,49	0
57	MG	1a	1603	1/1	0.93	0.10	62,62,62,62	0
57	MG	1A	3603	1/1	0.93	0.16	34,34,34,34	0
57	MG	2A	3088	1/1	0.93	0.21	47,47,47,47	0
57	MG	1A	3604	1/1	0.93	0.18	16,16,16,16	0
57	MG	2A	3574	1/1	0.93	0.21	68,68,68,68	0
57	MG	1A	4087	1/1	0.93	0.12	58,58,58,58	0
57	MG	1A	3279	1/1	0.93	0.24	49,49,49,49	0
57	MG	1A	4011	1/1	0.93	0.11	59,59,59,59	0
57	MG	2A	3094	1/1	0.93	0.17	76,76,76,76	0
57	MG	2A	3095	1/1	0.93	0.18	37,37,37,37	0
57	MG	1a	1616	1/1	0.93	0.09	67,67,67,67	0
57	MG	1F	313	1/1	0.93	0.09	57,57,57,57	0
57	MG	1a	1708	1/1	0.93	0.19	34,34,34,34	0
57	MG	2A	3382	1/1	0.93	0.18	65,65,65,65	0
57	MG	1A	3097	1/1	0.93	0.24	62,62,62,62	0
57	MG	1A	3610	1/1	0.93	0.23	29,29,29,29	0
57	MG	1A	3472	1/1	0.93	0.47	39,39,39,39	0
57	MG	1a	1712	1/1	0.93	0.15	55,55,55,55	0
57	MG	1A	3532	1/1	0.93	0.26	41,41,41,41	0
57	MG	1a	1715	1/1	0.93	0.26	44,44,44,44	0
57	MG	1A	3621	1/1	0.93	0.13	59,59,59,59	0
57	MG	1A	3572	1/1	0.93	0.20	54,54,54,54	0
57	MG	2A	3110	1/1	0.93	0.09	73,73,73,73	0
57	MG	1A	3427	1/1	0.93	0.35	60,60,60,60	0
57	MG	2A	3254	1/1	0.93	0.16	66,66,66,66	0
57	MG	2A	3597	1/1	0.93	0.38	65,65,65,65	0
57	MG	1A	3627	1/1	0.93	0.23	47,47,47,47	0
57	MG	1A	3451	1/1	0.93	0.15	48,48,48,48	0
57	MG	1O	201	1/1	0.93	0.57	51,51,51,51	0
57	MG	1A	3177	1/1	0.93	0.12	49,49,49,49	0
57	MG	2B	216	1/1	0.93	0.13	74,74,74,74	0
57	MG	2A	3401	1/1	0.93	0.22	67,67,67,67	0
57	MG	2A	3605	1/1	0.93	0.17	67,67,67,67	0
57	MG	1A	3697	1/1	0.93	0.18	59,59,59,59	0
57	MG	2D	304	1/1	0.93	0.23	35,35,35,35	0
57	MG	1a	1728	1/1	0.93	0.10	55,55,55,55	0
57	MG	1x	107	1/1	0.93	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
57	MG	2A	3121	1/1	0.93	0.22	47,47,47,47	0
57	MG	1A	3578	1/1	0.93	0.10	49,49,49,49	0
57	MG	2A	3265	1/1	0.93	0.09	56,56,56,56	0
57	MG	1A	3951	1/1	0.93	0.15	55,55,55,55	0
57	MG	1P	205	1/1	0.93	0.20	45,45,45,45	0
57	MG	1a	1734	1/1	0.93	0.15	66,66,66,66	0
57	MG	1A	3816	1/1	0.93	0.21	64,64,64,64	0
57	MG	1A	3954	1/1	0.93	0.15	51,51,51,51	0
57	MG	2A	3621	1/1	0.93	0.22	65,65,65,65	0
57	MG	1a	1737	1/1	0.93	0.10	60,60,60,60	0
57	MG	2P	201	1/1	0.93	0.19	57,57,57,57	0
57	MG	1A	3817	1/1	0.93	0.23	66,66,66,66	0
57	MG	2A	3134	1/1	0.93	0.25	59,59,59,59	0
57	MG	1A	3634	1/1	0.93	0.09	37,37,37,37	0
57	MG	1A	3146	1/1	0.93	0.38	37,37,37,37	0
57	MG	1A	3539	1/1	0.93	0.19	23,23,23,23	0
57	MG	1A	3010	1/1	0.93	0.16	49,49,49,49	0
57	MG	1B	209	1/1	0.93	0.16	54,54,54,54	0
57	MG	2V	201	1/1	0.93	0.09	65,65,65,65	0
57	MG	2A	3437	1/1	0.93	0.09	57,57,57,57	0
57	MG	2A	3438	1/1	0.93	0.22	57,57,57,57	0
57	MG	2X	101	1/1	0.93	0.32	61,61,61,61	0
57	MG	2A	3281	1/1	0.93	0.13	70,70,70,70	0
57	MG	2A	3282	1/1	0.93	0.22	54,54,54,54	0
57	MG	2A	3643	1/1	0.93	0.18	38,38,38,38	0
57	MG	1A	3964	1/1	0.93	0.09	37,37,37,37	0
57	MG	2A	3284	1/1	0.93	0.25	58,58,58,58	0
57	MG	2A	3010	1/1	0.93	0.10	56,56,56,56	0
57	MG	1A	3645	1/1	0.93	0.16	40,40,40,40	0
57	MG	2A	3012	1/1	0.93	0.12	55,55,55,55	0
57	MG	1a	1648	1/1	0.93	0.17	79,79,79,79	0
57	MG	2A	3291	1/1	0.93	0.27	65,65,65,65	0
57	MG	2A	3452	1/1	0.93	0.13	40,40,40,40	0
57	MG	2A	3015	1/1	0.93	0.30	41,41,41,41	0
57	MG	2A	3656	1/1	0.93	0.14	49,49,49,49	0
57	MG	2A	3293	1/1	0.93	0.15	63,63,63,63	0
57	MG	2A	3658	1/1	0.93	0.14	68,68,68,68	0
57	MG	1a	1749	1/1	0.93	0.08	59,59,59,59	0
57	MG	1S	202	1/1	0.93	0.18	52,52,52,52	0
57	MG	1A	3411	1/1	0.93	0.56	39,39,39,39	0
57	MG	1A	3544	1/1	0.93	0.42	40,40,40,40	0
57	MG	2A	3663	1/1	0.93	0.36	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3664	1/1	0.93	0.11	62,62,62,62	0
57	MG	1A	3100	1/1	0.93	0.15	41,41,41,41	0
57	MG	1A	3264	1/1	0.93	0.43	44,44,44,44	0
57	MG	1A	3834	1/1	0.93	0.12	51,51,51,51	0
57	MG	2A	3028	1/1	0.93	1.09	62,62,62,62	0
57	MG	1A	3415	1/1	0.93	0.45	45,45,45,45	0
57	MG	1A	3319	1/1	0.93	0.81	47,47,47,47	0
57	MG	1A	3555	1/1	0.93	0.14	40,40,40,40	0
57	MG	1B	223	1/1	0.93	0.20	60,60,60,60	0
57	MG	2A	3477	1/1	0.93	0.24	54,54,54,54	0
57	MG	2A	3478	1/1	0.93	0.18	55,55,55,55	0
57	MG	2A	3168	1/1	0.93	0.31	64,64,64,64	0
57	MG	2A	3684	1/1	0.93	0.15	46,46,46,46	0
57	MG	1A	3979	1/1	0.93	0.11	52,52,52,52	0
57	MG	1A	3163	1/1	0.93	0.18	63,63,63,63	0
57	MG	2A	3036	1/1	0.93	0.15	56,56,56,56	0
59	ZN	1n	102	1/1	0.93	0.14	68,68,68,68	0
57	MG	2A	3484	1/1	0.93	0.25	62,62,62,62	0
57	MG	1A	3133	1/1	0.93	0.40	35,35,35,35	0
57	MG	1A	4056	1/1	0.93	0.11	51,51,51,51	0
57	MG	1A	3716	1/1	0.94	0.06	49,49,49,49	0
57	MG	2A	3688	1/1	0.94	0.10	69,69,69,69	0
57	MG	1A	3131	1/1	0.94	0.20	45,45,45,45	0
57	MG	10	107	1/1	0.94	0.09	59,59,59,59	0
57	MG	1A	3941	1/1	0.94	0.14	39,39,39,39	0
57	MG	11	103	1/1	0.94	0.09	45,45,45,45	0
57	MG	1B	225	1/1	0.94	0.26	57,57,57,57	0
57	MG	1A	3594	1/1	0.94	0.27	36,36,36,36	0
57	MG	1a	1704	1/1	0.94	0.14	51,51,51,51	0
57	MG	1x	104	1/1	0.94	0.13	67,67,67,67	0
57	MG	1x	105	1/1	0.94	0.28	53,53,53,53	0
57	MG	2A	3702	1/1	0.94	0.06	46,46,46,46	0
57	MG	1A	4034	1/1	0.94	0.17	29,29,29,29	0
57	MG	1A	3862	1/1	0.94	0.35	35,35,35,35	0
57	MG	1A	3057	1/1	0.94	0.15	38,38,38,38	0
57	MG	14	101	1/1	0.94	0.07	74,74,74,74	0
57	MG	2A	3151	1/1	0.94	0.47	67,67,67,67	0
57	MG	2A	3497	1/1	0.94	0.12	49,49,49,49	0
57	MG	2A	3153	1/1	0.94	0.32	53,53,53,53	0
57	MG	1A	4037	1/1	0.94	0.15	17,17,17,17	0
57	MG	15	105	1/1	0.94	0.24	40,40,40,40	0
57	MG	1x	112	1/1	0.94	0.26	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3659	1/1	0.94	0.16	27,27,27,27	0
57	MG	1A	3660	1/1	0.94	0.22	27,27,27,27	0
57	MG	2A	3718	1/1	0.94	0.23	57,57,57,57	0
57	MG	2A	3719	1/1	0.94	0.12	65,65,65,65	0
57	MG	1A	3868	1/1	0.94	0.18	30,30,30,30	0
57	MG	1A	3135	1/1	0.94	0.37	47,47,47,47	0
57	MG	17	103	1/1	0.94	0.22	37,37,37,37	0
57	MG	1a	1718	1/1	0.94	0.11	68,68,68,68	0
57	MG	2A	3726	1/1	0.94	0.09	54,54,54,54	0
57	MG	17	105	1/1	0.94	0.23	46,46,46,46	0
57	MG	1a	1720	1/1	0.94	0.09	47,47,47,47	0
57	MG	1A	3170	1/1	0.94	0.17	22,22,22,22	0
57	MG	1A	3952	1/1	0.94	0.05	50,50,50,50	0
57	MG	1a	1724	1/1	0.94	0.19	59,59,59,59	0
57	MG	1A	3046	1/1	0.94	0.20	34,34,34,34	0
57	MG	19	101	1/1	0.94	0.23	42,42,42,42	0
57	MG	1D	309	1/1	0.94	0.31	46,46,46,46	0
57	MG	1A	3792	1/1	0.94	0.14	27,27,27,27	0
57	MG	1a	1729	1/1	0.94	0.15	50,50,50,50	0
57	MG	1a	1730	1/1	0.94	0.14	61,61,61,61	0
57	MG	1A	3226	1/1	0.94	0.28	30,30,30,30	0
57	MG	1A	3012	1/1	0.94	0.24	27,27,27,27	0
57	MG	1a	1605	1/1	0.94	0.09	60,60,60,60	0
57	MG	1A	3055	1/1	0.94	0.13	53,53,53,53	0
57	MG	1E	303	1/1	0.94	0.15	36,36,36,36	0
57	MG	1A	3731	1/1	0.94	0.14	24,24,24,24	0
57	MG	1A	3962	1/1	0.94	0.12	74,74,74,74	0
57	MG	2A	3533	1/1	0.94	0.15	51,51,51,51	0
57	MG	2A	3751	1/1	0.94	0.18	41,41,41,41	0
57	MG	2A	3343	1/1	0.94	0.23	59,59,59,59	0
57	MG	2A	3186	1/1	0.94	0.16	57,57,57,57	0
57	MG	1A	3120	1/1	0.94	0.24	44,44,44,44	0
57	MG	1a	1739	1/1	0.94	0.14	58,58,58,58	0
57	MG	1a	1617	1/1	0.94	0.10	50,50,50,50	0
57	MG	2A	3758	1/1	0.94	0.21	58,58,58,58	0
57	MG	1A	3799	1/1	0.94	0.12	56,56,56,56	0
57	MG	2A	3191	1/1	0.94	0.14	66,66,66,66	0
57	MG	1E	310	1/1	0.94	0.20	33,33,33,33	0
57	MG	2A	3193	1/1	0.94	0.17	56,56,56,56	0
57	MG	2A	3550	1/1	0.94	0.23	61,61,61,61	0
57	MG	1A	3733	1/1	0.94	0.22	58,58,58,58	0
57	MG	2A	3037	1/1	0.94	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3038	1/1	0.94	0.19	31,31,31,31	0
57	MG	1A	3966	1/1	0.94	0.12	73,73,73,73	0
57	MG	2A	3770	1/1	0.94	0.22	62,62,62,62	0
57	MG	1A	4060	1/1	0.94	0.22	43,43,43,43	0
57	MG	1A	3028	1/1	0.94	0.13	60,60,60,60	0
57	MG	1A	3968	1/1	0.94	0.13	65,65,65,65	0
57	MG	2A	3043	1/1	0.94	0.16	56,56,56,56	0
57	MG	2A	3563	1/1	0.94	0.14	36,36,36,36	0
57	MG	1A	3353	1/1	0.94	0.25	51,51,51,51	0
57	MG	2A	3566	1/1	0.94	0.07	60,60,60,60	0
57	MG	1F	306	1/1	0.94	0.31	33,33,33,33	0
57	MG	1a	1751	1/1	0.94	0.11	71,71,71,71	0
57	MG	1a	1752	1/1	0.94	0.17	61,61,61,61	0
57	MG	1A	3804	1/1	0.94	0.10	55,55,55,55	0
57	MG	1A	3078	1/1	0.94	0.25	40,40,40,40	0
57	MG	2A	3368	1/1	0.94	0.36	57,57,57,57	0
57	MG	1A	3675	1/1	0.94	0.23	32,32,32,32	0
57	MG	1A	3523	1/1	0.94	0.36	42,42,42,42	0
57	MG	1A	3612	1/1	0.94	0.15	55,55,55,55	0
57	MG	1G	201	1/1	0.94	0.19	39,39,39,39	0
57	MG	1A	4074	1/1	0.94	0.15	62,62,62,62	0
57	MG	1A	3390	1/1	0.94	0.35	49,49,49,49	0
57	MG	1A	3978	1/1	0.94	0.30	66,66,66,66	0
57	MG	2A	3583	1/1	0.94	0.10	64,64,64,64	0
57	MG	2A	3798	1/1	0.94	0.12	73,73,73,73	0
57	MG	2A	3799	1/1	0.94	0.27	58,58,58,58	0
57	MG	2A	3059	1/1	0.94	0.10	56,56,56,56	0
57	MG	2A	3222	1/1	0.94	0.07	72,72,72,72	0
57	MG	1A	3355	1/1	0.94	0.12	41,41,41,41	0
57	MG	1A	3980	1/1	0.94	0.32	43,43,43,43	0
57	MG	1a	1641	1/1	0.94	0.25	53,53,53,53	0
57	MG	1A	3813	1/1	0.94	0.16	50,50,50,50	0
57	MG	1A	3491	1/1	0.94	0.51	36,36,36,36	0
57	MG	1A	3986	1/1	0.94	0.18	24,24,24,24	0
57	MG	1A	3064	1/1	0.94	0.21	38,38,38,38	0
57	MG	1A	3125	1/1	0.94	0.17	59,59,59,59	0
57	MG	2B	209	1/1	0.94	0.14	78,78,78,78	0
57	MG	1a	1777	1/1	0.94	0.17	58,58,58,58	0
57	MG	1A	3577	1/1	0.94	0.42	62,62,62,62	0
57	MG	1A	3494	1/1	0.94	0.29	59,59,59,59	0
57	MG	1A	3691	1/1	0.94	0.21	58,58,58,58	0
57	MG	1a	1783	1/1	0.94	0.06	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1784	1/1	0.94	0.19	57,57,57,57	0
57	MG	1A	3126	1/1	0.94	0.19	45,45,45,45	0
57	MG	1A	3212	1/1	0.94	0.16	42,42,42,42	0
57	MG	2A	3243	1/1	0.94	0.11	49,49,49,49	0
57	MG	1A	4099	1/1	0.94	0.10	64,64,64,64	0
57	MG	1A	3269	1/1	0.94	0.56	41,41,41,41	0
57	MG	2A	3405	1/1	0.94	0.13	42,42,42,42	0
57	MG	2A	3246	1/1	0.94	0.19	72,72,72,72	0
57	MG	1a	1789	1/1	0.94	0.17	48,48,48,48	0
57	MG	2E	304	1/1	0.94	0.16	40,40,40,40	0
57	MG	1A	3825	1/1	0.94	0.15	51,51,51,51	0
57	MG	2A	3614	1/1	0.94	0.19	58,58,58,58	0
57	MG	1A	3362	1/1	0.94	0.22	71,71,71,71	0
57	MG	2A	3412	1/1	0.94	0.23	48,48,48,48	0
57	MG	2A	3617	1/1	0.94	0.08	76,76,76,76	0
57	MG	1A	3640	1/1	0.94	0.13	50,50,50,50	0
57	MG	1A	3912	1/1	0.94	0.13	50,50,50,50	0
57	MG	2A	3418	1/1	0.94	0.50	60,60,60,60	0
57	MG	1A	4105	1/1	0.94	0.09	68,68,68,68	0
57	MG	2A	3089	1/1	0.94	0.20	72,72,72,72	0
57	MG	1A	3758	1/1	0.94	0.14	56,56,56,56	0
57	MG	1A	3213	1/1	0.94	0.18	30,30,30,30	0
57	MG	1A	3832	1/1	0.94	0.09	60,60,60,60	0
57	MG	2T	203	1/1	0.94	0.05	72,72,72,72	0
57	MG	2A	3426	1/1	0.94	0.20	57,57,57,57	0
57	MG	1A	3187	1/1	0.94	0.19	43,43,43,43	0
57	MG	1a	1801	1/1	0.94	0.20	47,47,47,47	0
57	MG	2A	3429	1/1	0.94	0.33	46,46,46,46	0
57	MG	1A	3644	1/1	0.94	0.18	46,46,46,46	0
57	MG	1T	201	1/1	0.94	0.08	50,50,50,50	0
57	MG	2A	3636	1/1	0.94	0.22	53,53,53,53	0
57	MG	2A	3637	1/1	0.94	0.13	56,56,56,56	0
57	MG	1A	3765	1/1	0.94	0.18	23,23,23,23	0
57	MG	2A	3641	1/1	0.94	0.26	45,45,45,45	0
57	MG	1A	4114	1/1	0.94	0.18	61,61,61,61	0
57	MG	1A	3837	1/1	0.94	0.26	21,21,21,21	0
57	MG	1A	3586	1/1	0.94	0.14	47,47,47,47	0
57	MG	2A	3439	1/1	0.94	0.10	49,49,49,49	0
57	MG	1V	203	1/1	0.94	0.25	30,30,30,30	0
57	MG	27	101	1/1	0.94	0.20	52,52,52,52	0
57	MG	2A	3103	1/1	0.94	0.09	55,55,55,55	0
57	MG	1V	204	1/1	0.94	0.25	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3647	1/1	0.94	0.17	27,27,27,27	0
57	MG	1A	3926	1/1	0.94	0.05	51,51,51,51	0
57	MG	1W	201	1/1	0.94	0.27	51,51,51,51	0
57	MG	1A	3081	1/1	0.94	0.17	41,41,41,41	0
57	MG	2A	3655	1/1	0.94	0.20	54,54,54,54	0
57	MG	1A	3244	1/1	0.94	0.31	55,55,55,55	0
57	MG	1A	3709	1/1	0.94	0.17	23,23,23,23	0
57	MG	1X	103	1/1	0.94	0.18	44,44,44,44	0
57	MG	1X	104	1/1	0.94	0.54	45,45,45,45	0
57	MG	1e	202	1/1	0.94	0.53	64,64,64,64	0
57	MG	1A	3083	1/1	0.94	0.39	31,31,31,31	0
57	MG	2A	3457	1/1	0.94	0.10	59,59,59,59	0
57	MG	1A	3931	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3773	1/1	0.94	0.12	38,38,38,38	0
57	MG	1A	3551	1/1	0.94	0.41	42,42,42,42	0
57	MG	1A	3851	1/1	0.94	0.12	68,68,68,68	0
57	MG	1n	101	1/1	0.94	0.11	50,50,50,50	0
57	MG	2A	3671	1/1	0.94	0.14	65,65,65,65	0
57	MG	1A	3065	1/1	0.94	0.26	57,57,57,57	0
57	MG	1A	3098	1/1	0.94	0.28	53,53,53,53	0
57	MG	2A	3675	1/1	0.94	0.20	58,58,58,58	0
57	MG	1A	3855	1/1	0.94	0.20	39,39,39,39	0
57	MG	2A	3289	1/1	0.94	0.10	64,64,64,64	0
57	MG	2A	3290	1/1	0.94	0.14	65,65,65,65	0
57	MG	2A	3468	1/1	0.94	0.13	45,45,45,45	0
57	MG	1B	219	1/1	0.94	0.17	57,57,57,57	0
57	MG	2A	3474	1/1	0.94	0.15	65,65,65,65	0
57	MG	2A	3475	1/1	0.94	0.16	48,48,48,48	0
57	MG	1A	3655	1/1	0.94	0.16	23,23,23,23	0
57	MG	1A	3054	1/1	0.95	0.81	49,49,49,49	0
57	MG	2A	3713	1/1	0.95	0.17	53,53,53,53	0
57	MG	2A	3358	1/1	0.95	0.34	48,48,48,48	0
57	MG	2A	3530	1/1	0.95	0.15	61,61,61,61	0
57	MG	1A	3300	1/1	0.95	0.44	35,35,35,35	0
57	MG	1W	203	1/1	0.95	0.49	43,43,43,43	0
57	MG	1W	204	1/1	0.95	0.26	38,38,38,38	0
57	MG	2A	3217	1/1	0.95	0.26	58,58,58,58	0
57	MG	1B	220	1/1	0.95	0.35	53,53,53,53	0
57	MG	1W	206	1/1	0.95	0.26	27,27,27,27	0
57	MG	2A	3722	1/1	0.95	0.19	69,69,69,69	0
57	MG	1X	101	1/1	0.95	0.45	41,41,41,41	0
57	MG	1A	3119	1/1	0.95	0.50	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3224	1/1	0.95	0.17	53,53,53,53	0
57	MG	1A	3142	1/1	0.95	0.37	36,36,36,36	0
57	MG	1A	3144	1/1	0.95	0.12	30,30,30,30	0
57	MG	1a	1672	1/1	0.95	0.18	49,49,49,49	0
57	MG	1A	3410	1/1	0.95	0.26	47,47,47,47	0
57	MG	1A	3450	1/1	0.95	0.13	42,42,42,42	0
57	MG	1A	3959	1/1	0.95	0.13	47,47,47,47	0
57	MG	2A	3734	1/1	0.95	0.25	44,44,44,44	0
57	MG	1A	3375	1/1	0.95	0.21	38,38,38,38	0
57	MG	2A	3556	1/1	0.95	0.13	48,48,48,48	0
57	MG	2A	3557	1/1	0.95	0.15	46,46,46,46	0
57	MG	2A	3232	1/1	0.95	0.21	52,52,52,52	0
57	MG	1a	1800	1/1	0.95	0.19	32,32,32,32	0
57	MG	1A	3304	1/1	0.95	0.15	51,51,51,51	0
57	MG	1a	1805	1/1	0.95	0.13	59,59,59,59	0
57	MG	1A	3883	1/1	0.95	0.13	37,37,37,37	0
57	MG	1A	3272	1/1	0.95	0.43	35,35,35,35	0
57	MG	1A	3022	1/1	0.95	0.14	18,18,18,18	0
57	MG	10	102	1/1	0.95	0.35	50,50,50,50	0
57	MG	2A	3567	1/1	0.95	0.23	73,73,73,73	0
57	MG	1A	4052	1/1	0.95	0.18	22,22,22,22	0
57	MG	1a	1812	1/1	0.95	0.43	73,73,73,73	0
57	MG	2A	3570	1/1	0.95	0.15	59,59,59,59	0
57	MG	2A	3389	1/1	0.95	0.16	37,37,37,37	0
57	MG	1a	1683	1/1	0.95	0.10	41,41,41,41	0
57	MG	2A	3392	1/1	0.95	0.16	65,65,65,65	0
57	MG	1A	3007	1/1	0.95	0.15	25,25,25,25	0
57	MG	1A	3103	1/1	0.95	0.38	42,42,42,42	0
57	MG	1A	3501	1/1	0.95	0.43	40,40,40,40	0
57	MG	2A	3096	1/1	0.95	0.08	57,57,57,57	0
57	MG	1a	1687	1/1	0.95	0.15	55,55,55,55	0
57	MG	1a	1688	1/1	0.95	0.17	49,49,49,49	0
57	MG	1B	238	1/1	0.95	0.16	37,37,37,37	0
57	MG	11	101	1/1	0.95	0.52	42,42,42,42	0
57	MG	1D	302	1/1	0.95	0.28	49,49,49,49	0
57	MG	2A	3402	1/1	0.95	0.16	56,56,56,56	0
57	MG	2A	3768	1/1	0.95	0.09	45,45,45,45	0
57	MG	1D	304	1/1	0.95	0.15	21,21,21,21	0
57	MG	1A	3344	1/1	0.95	0.16	42,42,42,42	0
57	MG	1A	3070	1/1	0.95	0.57	35,35,35,35	0
57	MG	1a	1695	1/1	0.95	0.22	51,51,51,51	0
57	MG	1A	3559	1/1	0.95	0.28	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3409	1/1	0.95	0.36	55,55,55,55	0
57	MG	12	101	1/1	0.95	0.21	51,51,51,51	0
57	MG	2A	3779	1/1	0.95	0.12	59,59,59,59	0
57	MG	1A	3972	1/1	0.95	0.20	38,38,38,38	0
57	MG	2A	3781	1/1	0.95	0.21	75,75,75,75	0
57	MG	1a	1699	1/1	0.95	0.22	59,59,59,59	0
57	MG	1A	3810	1/1	0.95	0.18	44,44,44,44	0
57	MG	1A	3740	1/1	0.95	0.14	16,16,16,16	0
57	MG	2A	3416	1/1	0.95	0.24	53,53,53,53	0
57	MG	1A	3676	1/1	0.95	0.29	35,35,35,35	0
57	MG	1A	3742	1/1	0.95	0.19	52,52,52,52	0
57	MG	2A	3421	1/1	0.95	0.12	62,62,62,62	0
57	MG	1A	4065	1/1	0.95	0.26	44,44,44,44	0
57	MG	1A	3033	1/1	0.95	0.44	32,32,32,32	0
57	MG	2A	3268	1/1	0.95	0.11	58,58,58,58	0
57	MG	2A	3606	1/1	0.95	0.05	64,64,64,64	0
57	MG	1a	1707	1/1	0.95	0.13	32,32,32,32	0
57	MG	1A	4067	1/1	0.95	0.16	52,52,52,52	0
57	MG	1A	3248	1/1	0.95	0.40	32,32,32,32	0
57	MG	1w	105	1/1	0.95	0.16	63,63,63,63	0
57	MG	1A	3385	1/1	0.95	0.86	49,49,49,49	0
57	MG	2A	3612	1/1	0.95	0.24	30,30,30,30	0
57	MG	1A	3681	1/1	0.95	0.23	29,29,29,29	0
57	MG	1E	313	1/1	0.95	0.18	48,48,48,48	0
57	MG	2A	3434	1/1	0.95	0.42	55,55,55,55	0
57	MG	1A	3614	1/1	0.95	0.21	28,28,28,28	0
57	MG	2A	3127	1/1	0.95	0.12	68,68,68,68	0
57	MG	1A	3150	1/1	0.95	0.19	36,36,36,36	0
57	MG	1A	3985	1/1	0.95	0.52	43,43,43,43	0
57	MG	2A	3131	1/1	0.95	0.19	44,44,44,44	0
57	MG	2B	206	1/1	0.95	0.15	71,71,71,71	0
57	MG	1F	303	1/1	0.95	0.44	40,40,40,40	0
57	MG	2A	3133	1/1	0.95	0.14	70,70,70,70	0
57	MG	1A	3906	1/1	0.95	0.09	65,65,65,65	0
57	MG	1A	3074	1/1	0.95	0.13	30,30,30,30	0
57	MG	1A	3822	1/1	0.95	0.09	59,59,59,59	0
57	MG	2A	3627	1/1	0.95	0.18	60,60,60,60	0
57	MG	1a	1721	1/1	0.95	0.18	59,59,59,59	0
57	MG	2A	3630	1/1	0.95	0.23	34,34,34,34	0
57	MG	1A	4082	1/1	0.95	0.17	49,49,49,49	0
57	MG	1A	3620	1/1	0.95	0.19	22,22,22,22	0
57	MG	1a	1607	1/1	0.95	0.42	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3388	1/1	0.95	0.14	59,59,59,59	0
57	MG	1a	1611	1/1	0.95	0.11	74,74,74,74	0
57	MG	1F	311	1/1	0.95	0.22	64,64,64,64	0
57	MG	1A	3511	1/1	0.95	0.18	24,24,24,24	0
57	MG	1a	1615	1/1	0.95	0.17	53,53,53,53	0
57	MG	2A	3640	1/1	0.95	0.22	42,42,42,42	0
57	MG	1A	3025	1/1	0.95	0.39	59,59,59,59	0
57	MG	1A	3692	1/1	0.95	0.15	33,33,33,33	0
57	MG	1A	3109	1/1	0.95	0.42	34,34,34,34	0
57	MG	1A	3048	1/1	0.95	0.12	43,43,43,43	0
57	MG	1A	4092	1/1	0.95	0.21	32,32,32,32	0
57	MG	1A	4000	1/1	0.95	0.16	36,36,36,36	0
57	MG	2F	306	1/1	0.95	0.36	53,53,53,53	0
57	MG	1a	1622	1/1	0.95	0.13	53,53,53,53	0
57	MG	1A	4094	1/1	0.95	0.11	63,63,63,63	0
57	MG	1A	3917	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	3761	1/1	0.95	0.12	41,41,41,41	0
57	MG	2A	3162	1/1	0.95	0.20	65,65,65,65	0
57	MG	2Q	203	1/1	0.95	0.41	58,58,58,58	0
57	MG	1a	1740	1/1	0.95	0.19	56,56,56,56	0
57	MG	1A	4097	1/1	0.95	0.15	55,55,55,55	0
57	MG	2R	202	1/1	0.95	0.26	52,52,52,52	0
57	MG	1A	3630	1/1	0.95	0.27	66,66,66,66	0
57	MG	1A	3060	1/1	0.95	0.37	34,34,34,34	0
57	MG	1A	3290	1/1	0.95	0.35	48,48,48,48	0
57	MG	2A	3022	1/1	0.95	0.40	47,47,47,47	0
57	MG	1A	3079	1/1	0.95	0.22	36,36,36,36	0
57	MG	1A	3040	1/1	0.95	0.56	33,33,33,33	0
57	MG	2W	202	1/1	0.95	0.15	54,54,54,54	0
57	MG	2A	3027	1/1	0.95	0.22	40,40,40,40	0
57	MG	1P	201	1/1	0.95	0.57	29,29,29,29	0
57	MG	1P	202	1/1	0.95	0.26	31,31,31,31	0
57	MG	1A	3639	1/1	0.95	0.25	48,48,48,48	0
57	MG	1A	3841	1/1	0.95	0.24	21,21,21,21	0
57	MG	2A	3324	1/1	0.95	0.11	78,78,78,78	0
57	MG	2A	3670	1/1	0.95	0.10	52,52,52,52	0
57	MG	21	102	1/1	0.95	1.20	59,59,59,59	0
57	MG	1A	3475	1/1	0.95	0.17	65,65,65,65	0
57	MG	2A	3672	1/1	0.95	0.23	43,43,43,43	0
57	MG	1A	3026	1/1	0.95	0.47	42,42,42,42	0
57	MG	1A	3705	1/1	0.95	0.09	58,58,58,58	0
57	MG	1a	1640	1/1	0.95	0.13	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3706	1/1	0.95	0.36	48,48,48,48	0
57	MG	1A	3642	1/1	0.95	0.16	46,46,46,46	0
57	MG	1A	3168	1/1	0.95	0.31	43,43,43,43	0
57	MG	1R	201	1/1	0.95	0.16	45,45,45,45	0
57	MG	1a	1760	1/1	0.95	0.07	57,57,57,57	0
57	MG	1A	3478	1/1	0.95	0.16	40,40,40,40	0
57	MG	2A	3683	1/1	0.95	0.20	66,66,66,66	0
57	MG	1a	1762	1/1	0.95	0.11	62,62,62,62	0
57	MG	1a	1763	1/1	0.95	0.13	43,43,43,43	0
57	MG	1A	3136	1/1	0.95	0.49	48,48,48,48	0
57	MG	1A	3777	1/1	0.95	0.14	52,52,52,52	0
57	MG	1A	3778	1/1	0.95	0.18	50,50,50,50	0
57	MG	1A	3779	1/1	0.95	0.09	39,39,39,39	0
57	MG	1A	3019	1/1	0.95	0.19	49,49,49,49	0
57	MG	2A	3512	1/1	0.95	0.15	43,43,43,43	0
57	MG	2A	3693	1/1	0.95	0.13	64,64,64,64	0
57	MG	2A	3694	1/1	0.95	0.04	68,68,68,68	0
57	MG	1A	3440	1/1	0.95	0.20	50,50,50,50	0
57	MG	1A	3783	1/1	0.95	0.18	23,23,23,23	0
57	MG	1A	3942	1/1	0.95	0.09	56,56,56,56	0
57	MG	1A	3526	1/1	0.95	0.24	41,41,41,41	0
57	MG	2A	3700	1/1	0.95	0.14	62,62,62,62	0
57	MG	2A	3348	1/1	0.95	0.32	64,64,64,64	0
57	MG	1A	3263	1/1	0.95	0.20	48,48,48,48	0
57	MG	1V	202	1/1	0.95	0.51	34,34,34,34	0
57	MG	1A	3715	1/1	0.95	0.13	49,49,49,49	0
57	MG	2A	3058	1/1	0.95	0.21	61,61,61,61	0
57	MG	1A	3585	1/1	0.95	0.50	32,32,32,32	0
57	MG	1a	1781	1/1	0.95	0.08	60,60,60,60	0
57	MG	1A	3138	1/1	0.95	0.14	23,23,23,23	0
59	ZN	29	501	1/1	0.95	0.07	84,84,84,84	0
57	MG	1A	3485	1/1	0.95	0.23	69,69,69,69	0
57	MG	2A	3419	1/1	0.96	0.12	64,64,64,64	0
57	MG	1A	3273	1/1	0.96	0.29	44,44,44,44	0
57	MG	1A	3275	1/1	0.96	0.17	34,34,34,34	0
57	MG	1A	3498	1/1	0.96	0.20	45,45,45,45	0
57	MG	1A	3021	1/1	0.96	0.23	51,51,51,51	0
57	MG	2A	3741	1/1	0.96	0.18	47,47,47,47	0
57	MG	1A	3549	1/1	0.96	0.18	44,44,44,44	0
57	MG	1A	3232	1/1	0.96	0.54	37,37,37,37	0
57	MG	1A	3850	1/1	0.96	0.13	48,48,48,48	0
57	MG	1A	3463	1/1	0.96	0.35	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	15	107	1/1	0.96	0.08	49,49,49,49	0
57	MG	1A	3852	1/1	0.96	0.21	25,25,25,25	0
57	MG	1A	3553	1/1	0.96	0.20	38,38,38,38	0
57	MG	2A	3170	1/1	0.96	0.21	44,44,44,44	0
57	MG	1A	3358	1/1	0.96	0.49	27,27,27,27	0
57	MG	17	101	1/1	0.96	0.18	35,35,35,35	0
57	MG	1A	3233	1/1	0.96	0.76	42,42,42,42	0
57	MG	2A	3754	1/1	0.96	0.21	33,33,33,33	0
57	MG	2A	3174	1/1	0.96	0.09	51,51,51,51	0
57	MG	17	104	1/1	0.96	0.17	57,57,57,57	0
57	MG	1A	3505	1/1	0.96	0.23	57,57,57,57	0
57	MG	1A	3663	1/1	0.96	0.16	28,28,28,28	0
57	MG	2A	3304	1/1	0.96	0.31	65,65,65,65	0
57	MG	1A	3726	1/1	0.96	0.06	68,68,68,68	0
57	MG	2A	3179	1/1	0.96	0.13	67,67,67,67	0
57	MG	2A	3444	1/1	0.96	0.10	64,64,64,64	0
57	MG	2A	3603	1/1	0.96	0.13	65,65,65,65	0
57	MG	1A	3664	1/1	0.96	0.19	28,28,28,28	0
57	MG	2A	3765	1/1	0.96	0.21	66,66,66,66	0
57	MG	2A	3446	1/1	0.96	0.27	53,53,53,53	0
57	MG	2A	3309	1/1	0.96	0.32	53,53,53,53	0
57	MG	1G	205	1/1	0.96	0.23	57,57,57,57	0
57	MG	1A	3234	1/1	0.96	0.18	47,47,47,47	0
57	MG	1a	1802	1/1	0.96	0.15	75,75,75,75	0
57	MG	1a	1804	1/1	0.96	0.52	56,56,56,56	0
57	MG	1A	3602	1/1	0.96	0.21	26,26,26,26	0
57	MG	2A	3315	1/1	0.96	0.09	67,67,67,67	0
57	MG	1A	3333	1/1	0.96	0.14	35,35,35,35	0
57	MG	1A	3468	1/1	0.96	0.51	48,48,48,48	0
57	MG	1A	4023	1/1	0.96	0.11	34,34,34,34	0
57	MG	1A	4110	1/1	0.96	0.11	36,36,36,36	0
57	MG	1A	4111	1/1	0.96	0.14	49,49,49,49	0
57	MG	1A	3124	1/1	0.96	0.41	37,37,37,37	0
57	MG	1a	1609	1/1	0.96	0.24	61,61,61,61	0
57	MG	1a	1610	1/1	0.96	0.18	45,45,45,45	0
57	MG	2A	3785	1/1	0.96	0.22	51,51,51,51	0
57	MG	1A	3670	1/1	0.96	0.21	22,22,22,22	0
57	MG	2A	3073	1/1	0.96	0.36	49,49,49,49	0
57	MG	1A	3946	1/1	0.96	0.12	32,32,32,32	0
57	MG	1A	4027	1/1	0.96	0.13	50,50,50,50	0
57	MG	1A	4028	1/1	0.96	0.26	32,32,32,32	0
57	MG	1a	1713	1/1	0.96	0.18	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3472	1/1	0.96	0.23	34,34,34,34	0
57	MG	1P	203	1/1	0.96	0.52	33,33,33,33	0
57	MG	1A	3363	1/1	0.96	0.68	44,44,44,44	0
57	MG	2A	3476	1/1	0.96	0.25	33,33,33,33	0
57	MG	2A	3080	1/1	0.96	0.27	59,59,59,59	0
57	MG	1A	3871	1/1	0.96	0.18	24,24,24,24	0
57	MG	1A	3672	1/1	0.96	0.21	32,32,32,32	0
57	MG	1Q	202	1/1	0.96	0.20	34,34,34,34	0
57	MG	2A	3800	1/1	0.96	0.07	65,65,65,65	0
57	MG	1B	206	1/1	0.96	0.12	54,54,54,54	0
57	MG	2A	3638	1/1	0.96	0.17	49,49,49,49	0
57	MG	1B	207	1/1	0.96	0.37	51,51,51,51	0
57	MG	1A	3608	1/1	0.96	0.26	31,31,31,31	0
57	MG	2A	3485	1/1	0.96	0.20	37,37,37,37	0
57	MG	2A	3486	1/1	0.96	0.17	45,45,45,45	0
57	MG	2A	3210	1/1	0.96	0.14	45,45,45,45	0
57	MG	2B	204	1/1	0.96	0.24	71,71,71,71	0
57	MG	1A	3609	1/1	0.96	0.10	44,44,44,44	0
57	MG	2A	3342	1/1	0.96	0.19	48,48,48,48	0
57	MG	2A	3646	1/1	0.96	0.12	39,39,39,39	0
57	MG	1A	3876	1/1	0.96	0.09	50,50,50,50	0
57	MG	1A	3365	1/1	0.96	0.25	25,25,25,25	0
57	MG	2A	3492	1/1	0.96	0.14	40,40,40,40	0
57	MG	2B	211	1/1	0.96	0.21	71,71,71,71	0
57	MG	2A	3214	1/1	0.96	0.17	63,63,63,63	0
57	MG	1R	203	1/1	0.96	0.47	39,39,39,39	0
57	MG	2A	3652	1/1	0.96	0.13	70,70,70,70	0
57	MG	1A	3739	1/1	0.96	0.22	41,41,41,41	0
57	MG	1A	3434	1/1	0.96	0.16	44,44,44,44	0
57	MG	1A	3613	1/1	0.96	0.14	48,48,48,48	0
57	MG	1A	3957	1/1	0.96	0.09	62,62,62,62	0
57	MG	1A	3366	1/1	0.96	0.19	27,27,27,27	0
57	MG	1A	3615	1/1	0.96	0.15	51,51,51,51	0
57	MG	1A	3617	1/1	0.96	0.15	39,39,39,39	0
57	MG	1A	3014	1/1	0.96	0.39	44,44,44,44	0
57	MG	1w	106	1/1	0.96	0.19	82,82,82,82	0
57	MG	2A	3505	1/1	0.96	0.20	48,48,48,48	0
57	MG	1A	3067	1/1	0.96	0.17	30,30,30,30	0
57	MG	1w	108	1/1	0.96	0.34	66,66,66,66	0
57	MG	2E	306	1/1	0.96	0.23	56,56,56,56	0
57	MG	2A	3665	1/1	0.96	0.27	61,61,61,61	0
57	MG	1A	3217	1/1	0.96	0.14	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1638	1/1	0.96	0.10	48,48,48,48	0
57	MG	1U	204	1/1	0.96	0.84	46,46,46,46	0
57	MG	1U	205	1/1	0.96	0.54	40,40,40,40	0
57	MG	1U	206	1/1	0.96	0.67	32,32,32,32	0
57	MG	1A	4049	1/1	0.96	0.20	28,28,28,28	0
57	MG	1A	3178	1/1	0.96	0.31	41,41,41,41	0
57	MG	1A	3285	1/1	0.96	0.12	31,31,31,31	0
57	MG	1A	3082	1/1	0.96	0.18	36,36,36,36	0
57	MG	1A	3104	1/1	0.96	0.14	25,25,25,25	0
57	MG	1A	3183	1/1	0.96	0.43	39,39,39,39	0
57	MG	1B	229	1/1	0.96	0.21	43,43,43,43	0
57	MG	1A	3445	1/1	0.96	0.15	55,55,55,55	0
57	MG	2A	3523	1/1	0.96	0.06	73,73,73,73	0
57	MG	1A	3044	1/1	0.96	0.17	35,35,35,35	0
57	MG	2A	3682	1/1	0.96	0.20	60,60,60,60	0
57	MG	1A	3755	1/1	0.96	0.16	31,31,31,31	0
57	MG	2A	3373	1/1	0.96	0.26	71,71,71,71	0
57	MG	2A	3685	1/1	0.96	0.24	45,45,45,45	0
57	MG	1A	3821	1/1	0.96	0.13	38,38,38,38	0
57	MG	2A	3120	1/1	0.96	0.09	54,54,54,54	0
57	MG	1A	3576	1/1	0.96	0.22	35,35,35,35	0
57	MG	1B	235	1/1	0.96	0.38	60,60,60,60	0
57	MG	1A	3166	1/1	0.96	0.29	32,32,32,32	0
57	MG	1A	3760	1/1	0.96	0.19	26,26,26,26	0
57	MG	1A	3316	1/1	0.96	0.32	50,50,50,50	0
57	MG	1D	301	1/1	0.96	0.19	35,35,35,35	0
57	MG	2A	3535	1/1	0.96	0.25	46,46,46,46	0
57	MG	1a	1757	1/1	0.96	0.12	53,53,53,53	0
57	MG	2A	3696	1/1	0.96	0.24	82,82,82,82	0
57	MG	23	102	1/1	0.96	0.08	59,59,59,59	0
57	MG	2A	3537	1/1	0.96	0.32	54,54,54,54	0
57	MG	2A	3128	1/1	0.96	0.30	47,47,47,47	0
57	MG	1A	3346	1/1	0.96	0.20	57,57,57,57	0
57	MG	1A	3827	1/1	0.96	0.36	68,68,68,68	0
57	MG	1A	3528	1/1	0.96	0.28	40,40,40,40	0
57	MG	1A	3140	1/1	0.96	0.20	58,58,58,58	0
57	MG	1A	3267	1/1	0.96	0.45	30,30,30,30	0
57	MG	1A	3151	1/1	0.96	0.16	36,36,36,36	0
57	MG	2A	3549	1/1	0.96	0.20	40,40,40,40	0
57	MG	1A	3833	1/1	0.96	0.12	68,68,68,68	0
57	MG	2A	3551	1/1	0.96	0.19	63,63,63,63	0
57	MG	2A	3136	1/1	0.96	0.30	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3005	1/1	0.96	0.24	39,39,39,39	0
57	MG	1a	1766	1/1	0.96	0.09	48,48,48,48	0
57	MG	2A	3140	1/1	0.96	0.16	60,60,60,60	0
57	MG	1A	3271	1/1	0.96	0.66	38,38,38,38	0
57	MG	1A	3646	1/1	0.96	0.18	30,30,30,30	0
57	MG	2A	3143	1/1	0.96	0.32	72,72,72,72	0
57	MG	1A	4076	1/1	0.96	0.28	60,60,60,60	0
57	MG	2A	3145	1/1	0.96	0.27	40,40,40,40	0
57	MG	1a	1770	1/1	0.96	0.07	76,76,76,76	0
57	MG	2A	3026	1/1	0.96	0.56	56,56,56,56	0
57	MG	2A	3406	1/1	0.96	0.20	52,52,52,52	0
57	MG	2A	3565	1/1	0.96	0.20	62,62,62,62	0
57	MG	1A	3420	1/1	0.96	0.47	32,32,32,32	0
57	MG	2A	3276	1/1	0.96	0.10	52,52,52,52	0
57	MG	1A	3538	1/1	0.96	0.20	33,33,33,33	0
57	MG	1A	3323	1/1	0.96	0.58	38,38,38,38	0
58	K	1A	3536	1/1	0.96	0.09	42,42,42,42	0
57	MG	1A	3919	1/1	0.96	0.16	30,30,30,30	0
57	MG	1a	1775	1/1	0.96	0.06	70,70,70,70	0
57	MG	1A	3153	1/1	0.96	0.63	37,37,37,37	0
57	MG	1A	3842	1/1	0.96	0.25	26,26,26,26	0
57	MG	2A	3732	1/1	0.96	0.22	36,36,36,36	0
57	MG	1A	3843	1/1	0.96	0.13	29,29,29,29	0
57	MG	2A	3035	1/1	0.96	0.13	33,33,33,33	0
57	MG	1U	203	1/1	0.97	0.16	37,37,37,37	0
57	MG	2A	3545	1/1	0.97	0.13	42,42,42,42	0
57	MG	1A	3231	1/1	0.97	0.84	35,35,35,35	0
57	MG	2A	3432	1/1	0.97	0.33	57,57,57,57	0
57	MG	2A	3548	1/1	0.97	0.14	68,68,68,68	0
57	MG	1a	1797	1/1	0.97	0.07	57,57,57,57	0
57	MG	1A	4079	1/1	0.97	0.10	29,29,29,29	0
57	MG	1A	4080	1/1	0.97	0.12	46,46,46,46	0
57	MG	1A	3875	1/1	0.97	0.20	50,50,50,50	0
57	MG	2A	3668	1/1	0.97	0.29	61,61,61,61	0
57	MG	1D	303	1/1	0.97	0.21	40,40,40,40	0
57	MG	1A	3009	1/1	0.97	0.14	36,36,36,36	0
57	MG	1a	1803	1/1	0.97	0.14	62,62,62,62	0
57	MG	1D	305	1/1	0.97	0.21	39,39,39,39	0
57	MG	2A	3137	1/1	0.97	0.17	41,41,41,41	0
57	MG	1V	205	1/1	0.97	0.18	34,34,34,34	0
57	MG	1A	3094	1/1	0.97	0.16	38,38,38,38	0
57	MG	1A	3481	1/1	0.97	0.18	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3240	1/1	0.97	0.24	66,66,66,66	0
57	MG	1A	3313	1/1	0.97	0.11	49,49,49,49	0
57	MG	2A	3801	1/1	0.97	0.16	56,56,56,56	0
57	MG	1A	3029	1/1	0.97	0.52	37,37,37,37	0
57	MG	1A	3020	1/1	0.97	0.15	30,30,30,30	0
57	MG	1A	3184	1/1	0.97	0.52	30,30,30,30	0
57	MG	1A	4089	1/1	0.97	0.13	17,17,17,17	0
57	MG	1A	3262	1/1	0.97	0.29	36,36,36,36	0
57	MG	1E	304	1/1	0.97	0.23	32,32,32,32	0
57	MG	2A	3455	1/1	0.97	0.24	72,72,72,72	0
57	MG	1A	3069	1/1	0.97	0.17	27,27,27,27	0
57	MG	2A	3572	1/1	0.97	0.33	56,56,56,56	0
57	MG	1A	3886	1/1	0.97	0.26	32,32,32,32	0
57	MG	1E	307	1/1	0.97	0.23	32,32,32,32	0
57	MG	1A	3718	1/1	0.97	0.12	24,24,24,24	0
57	MG	2A	3152	1/1	0.97	0.20	55,55,55,55	0
57	MG	1A	3032	1/1	0.97	0.19	31,31,31,31	0
57	MG	1A	3828	1/1	0.97	0.28	33,33,33,33	0
57	MG	1A	3890	1/1	0.97	0.13	38,38,38,38	0
57	MG	2B	213	1/1	0.97	0.16	60,60,60,60	0
57	MG	1E	312	1/1	0.97	0.37	48,48,48,48	0
57	MG	1A	4098	1/1	0.97	0.10	43,43,43,43	0
57	MG	1A	3320	1/1	0.97	0.16	46,46,46,46	0
57	MG	1A	3453	1/1	0.97	0.23	48,48,48,48	0
57	MG	1A	3531	1/1	0.97	0.25	46,46,46,46	0
57	MG	2A	3469	1/1	0.97	0.13	47,47,47,47	0
57	MG	2A	3470	1/1	0.97	0.23	39,39,39,39	0
57	MG	1A	3723	1/1	0.97	0.10	55,55,55,55	0
57	MG	1A	3003	1/1	0.97	0.20	25,25,25,25	0
57	MG	2A	3473	1/1	0.97	0.25	48,48,48,48	0
57	MG	1A	3164	1/1	0.97	0.19	17,17,17,17	0
57	MG	1A	3624	1/1	0.97	0.08	61,61,61,61	0
57	MG	2A	3707	1/1	0.97	0.14	56,56,56,56	0
57	MG	1F	307	1/1	0.97	0.19	31,31,31,31	0
57	MG	1A	3165	1/1	0.97	0.13	48,48,48,48	0
57	MG	1A	3218	1/1	0.97	0.26	29,29,29,29	0
57	MG	1A	3838	1/1	0.97	0.18	52,52,52,52	0
57	MG	1A	3061	1/1	0.97	0.09	53,53,53,53	0
57	MG	1A	3326	1/1	0.97	0.44	40,40,40,40	0
57	MG	1A	3678	1/1	0.97	0.18	28,28,28,28	0
57	MG	1A	3327	1/1	0.97	0.45	46,46,46,46	0
57	MG	1A	3632	1/1	0.97	0.20	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3602	1/1	0.97	0.27	57,57,57,57	0
57	MG	1A	4039	1/1	0.97	0.29	69,69,69,69	0
57	MG	1A	4040	1/1	0.97	0.19	52,52,52,52	0
57	MG	1A	3540	1/1	0.97	0.24	33,33,33,33	0
57	MG	1a	1669	1/1	0.97	0.14	47,47,47,47	0
57	MG	1A	3115	1/1	0.97	0.28	27,27,27,27	0
57	MG	1A	3245	1/1	0.97	0.29	29,29,29,29	0
57	MG	2A	3725	1/1	0.97	0.13	59,59,59,59	0
57	MG	1A	3636	1/1	0.97	0.09	28,28,28,28	0
57	MG	1N	203	1/1	0.97	0.17	37,37,37,37	0
57	MG	1A	3637	1/1	0.97	0.12	59,59,59,59	0
57	MG	1A	3686	1/1	0.97	0.15	24,24,24,24	0
57	MG	1A	3687	1/1	0.97	0.19	45,45,45,45	0
57	MG	1A	3543	1/1	0.97	0.31	38,38,38,38	0
57	MG	1A	3916	1/1	0.97	0.12	16,16,16,16	0
57	MG	1A	3169	1/1	0.97	0.19	31,31,31,31	0
57	MG	2A	3391	1/1	0.97	0.32	48,48,48,48	0
57	MG	1A	3274	1/1	0.97	0.25	51,51,51,51	0
57	MG	1A	3052	1/1	0.97	0.15	26,26,26,26	0
57	MG	18	102	1/1	0.97	0.36	47,47,47,47	0
57	MG	18	103	1/1	0.97	0.39	44,44,44,44	0
57	MG	2A	3739	1/1	0.97	0.19	55,55,55,55	0
57	MG	1A	3548	1/1	0.97	0.33	29,29,29,29	0
57	MG	2A	3623	1/1	0.97	0.14	62,62,62,62	0
57	MG	1A	3053	1/1	0.97	0.20	29,29,29,29	0
57	MG	1A	3988	1/1	0.97	0.12	60,60,60,60	0
57	MG	25	102	1/1	0.97	0.17	53,53,53,53	0
57	MG	1A	3396	1/1	0.97	0.32	62,62,62,62	0
57	MG	1B	218	1/1	0.97	0.22	46,46,46,46	0
57	MG	2A	3628	1/1	0.97	0.16	55,55,55,55	0
57	MG	1A	3990	1/1	0.97	0.24	75,75,75,75	0
57	MG	2A	3104	1/1	0.97	0.20	42,42,42,42	0
57	MG	1A	3803	1/1	0.97	0.18	26,26,26,26	0
57	MG	2A	3009	1/1	0.97	0.20	39,39,39,39	0
57	MG	1A	3924	1/1	0.97	0.14	54,54,54,54	0
57	MG	1A	3134	1/1	0.97	0.46	41,41,41,41	0
57	MG	1A	3860	1/1	0.97	0.16	37,37,37,37	0
57	MG	2A	3013	1/1	0.97	0.15	55,55,55,55	0
57	MG	2A	3111	1/1	0.97	0.17	40,40,40,40	0
57	MG	2A	3307	1/1	0.97	0.11	58,58,58,58	0
57	MG	1a	1780	1/1	0.97	0.15	66,66,66,66	0
57	MG	1A	3202	1/1	0.97	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
57	MG	1A	3077	1/1	0.97	0.20	30,30,30,30	0
57	MG	2A	3414	1/1	0.97	0.21	50,50,50,50	0
57	MG	1A	3865	1/1	0.97	0.30	36,36,36,36	0
57	MG	1a	1612	1/1	0.97	0.15	26,26,26,26	0
57	MG	2A	3417	1/1	0.97	0.17	57,57,57,57	0
57	MG	1A	3368	1/1	0.97	0.69	44,44,44,44	0
57	MG	1A	4069	1/1	0.97	0.18	47,47,47,47	0
57	MG	1A	3999	1/1	0.97	0.18	46,46,46,46	0
57	MG	1A	3401	1/1	0.97	0.31	39,39,39,39	0
57	MG	1A	3011	1/1	0.97	0.20	36,36,36,36	0
57	MG	2A	3219	1/1	0.97	0.14	71,71,71,71	0
57	MG	1A	3037	1/1	0.97	0.17	37,37,37,37	0
57	MG	1A	3439	1/1	0.97	0.22	37,37,37,37	0
57	MG	1A	3756	1/1	0.97	0.17	32,32,32,32	0
59	ZN	1Y	203	1/1	0.97	0.14	72,72,72,72	0
57	MG	2A	3539	1/1	0.97	0.12	54,54,54,54	0
57	MG	2A	3775	1/1	0.97	0.15	65,65,65,65	0
57	MG	2A	3223	1/1	0.97	0.08	65,65,65,65	0
57	MG	2A	3778	1/1	0.97	0.06	61,61,61,61	0
57	MG	1A	3154	1/1	0.97	0.16	42,42,42,42	0
57	MG	1A	3405	1/1	0.97	0.29	50,50,50,50	0
57	MG	17	102	1/1	0.98	0.37	38,38,38,38	0
57	MG	1A	3195	1/1	0.98	0.20	36,36,36,36	0
57	MG	1A	3258	1/1	0.98	0.29	35,35,35,35	0
57	MG	1U	201	1/1	0.98	0.27	28,28,28,28	0
57	MG	1A	4068	1/1	0.98	0.10	44,44,44,44	0
57	MG	1A	4016	1/1	0.98	0.14	23,23,23,23	0
57	MG	2A	3742	1/1	0.98	0.21	37,37,37,37	0
57	MG	1A	3638	1/1	0.98	0.11	44,44,44,44	0
57	MG	2A	3061	1/1	0.98	0.16	51,51,51,51	0
57	MG	1A	3116	1/1	0.98	0.32	33,33,33,33	0
57	MG	18	104	1/1	0.98	0.21	43,43,43,43	0
57	MG	1A	3034	1/1	0.98	0.36	29,29,29,29	0
57	MG	2A	3584	1/1	0.98	0.13	37,37,37,37	0
57	MG	2A	3503	1/1	0.98	0.32	58,58,58,58	0
57	MG	2A	3065	1/1	0.98	0.19	54,54,54,54	0
57	MG	2F	301	1/1	0.98	0.16	60,60,60,60	0
57	MG	1A	3969	1/1	0.98	0.14	67,67,67,67	0
57	MG	1A	3073	1/1	0.98	0.12	28,28,28,28	0
57	MG	1A	3606	1/1	0.98	0.17	32,32,32,32	0
57	MG	2F	305	1/1	0.98	0.64	50,50,50,50	0
57	MG	2A	3069	1/1	0.98	0.12	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3509	1/1	0.98	0.20	65,65,65,65	0
57	MG	1A	3547	1/1	0.98	0.32	27,27,27,27	0
57	MG	1A	3881	1/1	0.98	0.13	19,19,19,19	0
57	MG	1A	3035	1/1	0.98	0.27	40,40,40,40	0
57	MG	1A	3180	1/1	0.98	0.25	33,33,33,33	0
57	MG	1A	3759	1/1	0.98	0.17	19,19,19,19	0
57	MG	2A	3215	1/1	0.98	0.16	52,52,52,52	0
57	MG	1A	3181	1/1	0.98	0.59	39,39,39,39	0
57	MG	1A	3611	1/1	0.98	0.13	46,46,46,46	0
57	MG	1A	3167	1/1	0.98	0.36	34,34,34,34	0
57	MG	2T	202	1/1	0.98	0.14	52,52,52,52	0
57	MG	1A	3552	1/1	0.98	0.16	49,49,49,49	0
57	MG	1A	3981	1/1	0.98	0.19	28,28,28,28	0
57	MG	1A	3001	1/1	0.98	0.14	38,38,38,38	0
57	MG	2A	3522	1/1	0.98	0.16	66,66,66,66	0
57	MG	1A	3807	1/1	0.98	0.19	33,33,33,33	0
57	MG	1A	3984	1/1	0.98	0.16	15,15,15,15	0
57	MG	1A	3008	1/1	0.98	0.17	23,23,23,23	0
57	MG	1A	4090	1/1	0.98	0.18	28,28,28,28	0
57	MG	1A	3652	1/1	0.98	0.15	38,38,38,38	0
57	MG	1A	3616	1/1	0.98	0.13	28,28,28,28	0
57	MG	2A	3450	1/1	0.98	0.12	62,62,62,62	0
57	MG	1A	3894	1/1	0.98	0.16	43,43,43,43	0
57	MG	2A	3777	1/1	0.98	0.08	58,58,58,58	0
57	MG	1a	1811	1/1	0.98	0.20	53,53,53,53	0
57	MG	1A	3500	1/1	0.98	0.43	38,38,38,38	0
57	MG	1A	3158	1/1	0.98	0.33	29,29,29,29	0
57	MG	2A	3379	1/1	0.98	0.23	25,25,25,25	0
57	MG	2A	3021	1/1	0.98	0.19	32,32,32,32	0
57	MG	1A	3527	1/1	0.98	0.30	37,37,37,37	0
57	MG	1A	3694	1/1	0.98	0.17	41,41,41,41	0
57	MG	2A	3163	1/1	0.98	0.29	35,35,35,35	0
57	MG	1A	3899	1/1	0.98	0.17	24,24,24,24	0
57	MG	2A	3025	1/1	0.98	0.45	54,54,54,54	0
57	MG	1A	3159	1/1	0.98	0.30	34,34,34,34	0
57	MG	1A	3529	1/1	0.98	0.39	38,38,38,38	0
57	MG	1A	3227	1/1	0.98	0.15	28,28,28,28	0
57	MG	1A	3188	1/1	0.98	0.43	34,34,34,34	0
57	MG	1A	3625	1/1	0.98	0.10	55,55,55,55	0
57	MG	1A	3208	1/1	0.98	0.14	49,49,49,49	0
57	MG	1A	3861	1/1	0.98	0.28	39,39,39,39	0
57	MG	2A	3711	1/1	0.98	0.10	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3038	1/1	0.98	0.18	25,25,25,25	0
57	MG	1D	308	1/1	0.98	0.33	44,44,44,44	0
57	MG	1A	3702	1/1	0.98	0.17	18,18,18,18	0
57	MG	1D	310	1/1	0.98	0.35	27,27,27,27	0
57	MG	1A	3864	1/1	0.98	0.28	30,30,30,30	0
57	MG	2A	3554	1/1	0.98	0.22	54,54,54,54	0
57	MG	1A	3364	1/1	0.98	0.34	28,28,28,28	0
57	MG	13	102	1/1	0.98	0.32	39,39,39,39	0
57	MG	1A	3629	1/1	0.98	0.15	17,17,17,17	0
57	MG	1R	202	1/1	0.98	0.23	35,35,35,35	0
57	MG	15	101	1/1	0.98	0.56	44,44,44,44	0
57	MG	15	102	1/1	0.98	0.42	32,32,32,32	0
57	MG	15	103	1/1	0.98	0.52	32,32,32,32	0
57	MG	2A	3481	1/1	0.98	0.26	57,57,57,57	0
57	MG	1A	3190	1/1	0.98	0.17	29,29,29,29	0
57	MG	1A	3958	1/1	0.98	0.11	59,59,59,59	0
57	MG	2A	3259	1/1	0.98	0.19	58,58,58,58	0
57	MG	1A	3412	1/1	0.98	0.20	42,42,42,42	0
57	MG	1A	3191	1/1	0.98	0.24	36,36,36,36	0
59	ZN	15	109	1/1	0.98	0.18	43,43,43,43	0
59	ZN	16	103	1/1	0.98	0.20	42,42,42,42	0
57	MG	1A	3013	1/1	0.98	0.20	29,29,29,29	0
57	MG	1A	4063	1/1	0.98	0.32	40,40,40,40	0
57	MG	1A	3132	1/1	0.98	0.14	47,47,47,47	0
59	ZN	25	104	1/1	0.98	0.22	60,60,60,60	0
59	ZN	26	501	1/1	0.98	0.16	60,60,60,60	0
57	MG	2A	3337	1/1	0.98	0.34	45,45,45,45	0
57	MG	1A	3194	1/1	0.98	0.19	25,25,25,25	0
57	MG	1A	3093	1/1	0.99	0.23	40,40,40,40	0
57	MG	2A	3378	1/1	0.99	0.20	53,53,53,53	0
57	MG	1A	3690	1/1	0.99	0.13	15,15,15,15	0
57	MG	2A	3048	1/1	0.99	0.25	39,39,39,39	0
57	MG	1A	3288	1/1	0.99	0.31	40,40,40,40	0
57	MG	1A	3793	1/1	0.99	0.48	24,24,24,24	0
57	MG	2A	3433	1/1	0.99	0.23	25,25,25,25	0
57	MG	1A	3039	1/1	0.99	0.22	31,31,31,31	0
57	MG	1A	3171	1/1	0.99	0.12	35,35,35,35	0
57	MG	1A	3270	1/1	0.99	0.30	31,31,31,31	0
57	MG	1A	3780	1/1	0.99	0.18	22,22,22,22	0
57	MG	1A	3143	1/1	0.99	0.20	30,30,30,30	0
57	MG	1A	3095	1/1	0.99	0.19	19,19,19,19	0
57	MG	2A	3544	1/1	0.99	0.24	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3987	1/1	0.99	0.10	40,40,40,40	0
57	MG	1A	3031	1/1	0.99	0.25	26,26,26,26	0
57	MG	1A	3571	1/1	0.99	0.18	30,30,30,30	0
57	MG	1A	3071	1/1	0.99	0.20	15,15,15,15	0
57	MG	1A	3024	1/1	0.99	0.31	29,29,29,29	0
57	MG	1A	3771	1/1	0.99	0.18	49,49,49,49	0
57	MG	2A	3201	1/1	0.99	0.14	67,67,67,67	0
59	ZN	19	102	1/1	0.99	0.19	46,46,46,46	0
57	MG	1A	3185	1/1	0.99	0.36	36,36,36,36	0
57	MG	1X	107	1/1	0.99	0.15	65,65,65,65	0
57	MG	13	101	1/1	0.99	0.12	32,32,32,32	0
57	MG	1a	1702	1/1	0.99	0.19	61,61,61,61	0
57	MG	1A	4048	1/1	0.99	0.24	14,14,14,14	0
57	MG	1A	3623	1/1	0.99	0.12	24,24,24,24	0
57	MG	2U	203	1/1	0.99	0.08	68,68,68,68	0
60	SF4	1d	302	8/8	0.99	0.16	58,66,72,72	0
60	SF4	2d	501	8/8	0.99	0.14	61,68,76,83	0

6.5 Other polymers (i)

There are no such residues in this entry.