Full wwPDB X-ray Structure Validation Report (i)

Mar 16, 2026 – 09:16 PM UTC

PDB ID	:	8G2A / pdb_00008g2a
Title	:	Crystal structure of the A2503-C2,C8-dimethylated Thermus thermophilus 70S ribosome in complex with mRNA, aminoacylated A-site Phe-tRNAphe, peptidyl P-site fMTHSMRC-tRNAmet, and deacylated E-site tRNAphe at 2.45A 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	:	2.45 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:

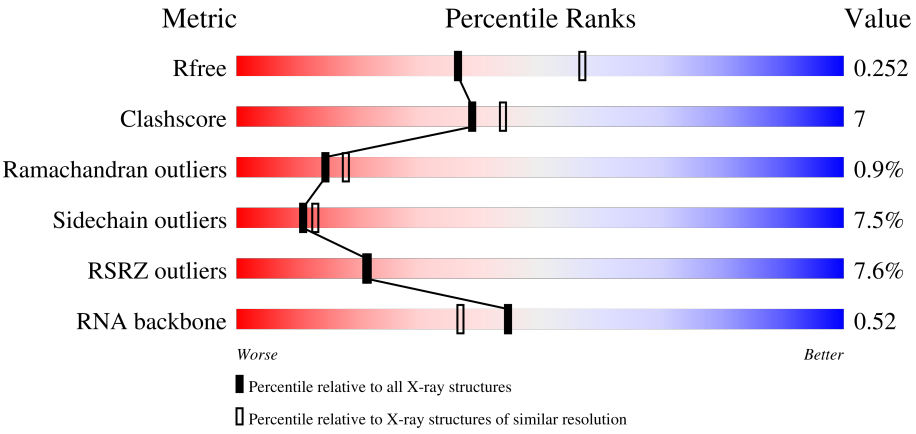
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 2.45 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}	164625	1096 (2.46-2.46)
Clashscore	180529	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)
RSRZ outliers	164620	1096 (2.46-2.46)
RNA backbone	3690	1040 (2.76-2.16)

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% 71% 22% 5% •
1	2A	2915	5% 64% 26% 6% •

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.48.1

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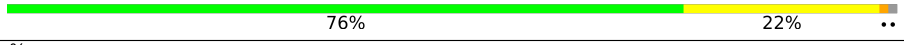
Mol	Chain	Length	Quality of chain
2	1B	121	
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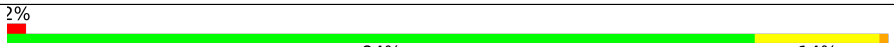
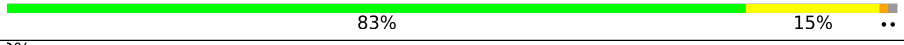
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	

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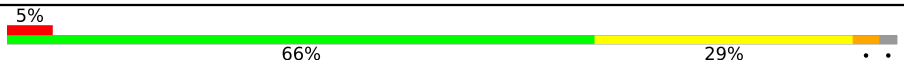
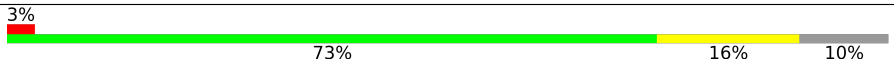
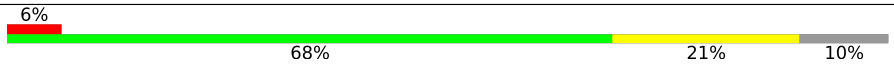
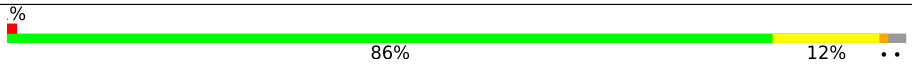
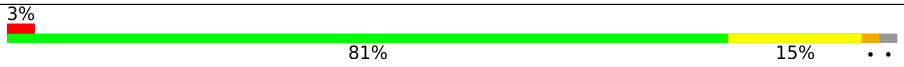
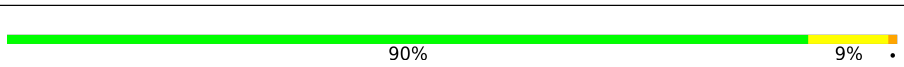
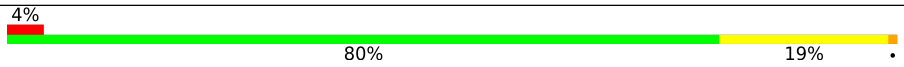
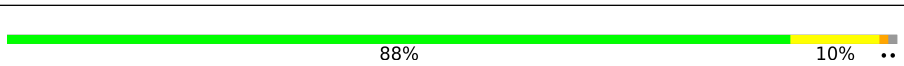
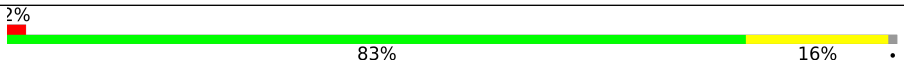
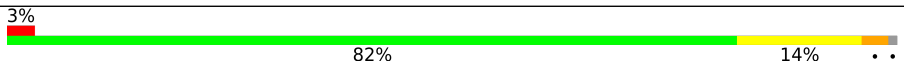
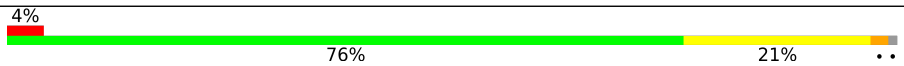
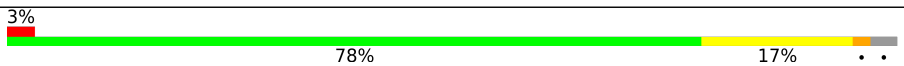
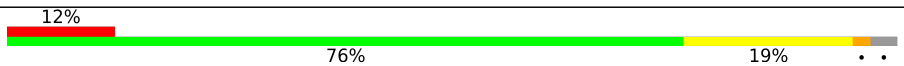
Mol	Chain	Length	Quality of chain
14	2S	112	
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
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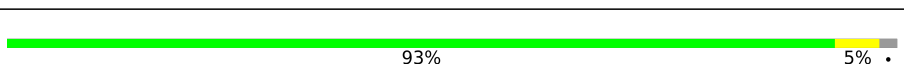
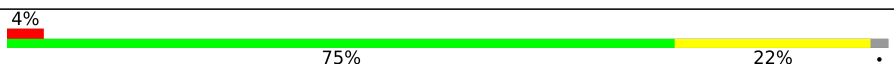
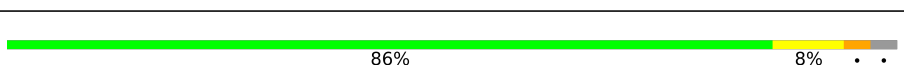
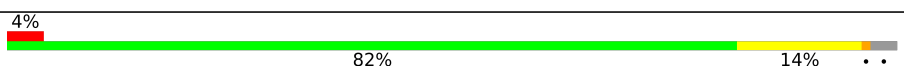
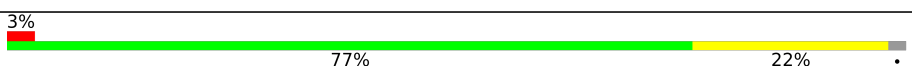
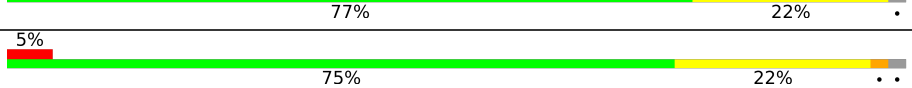
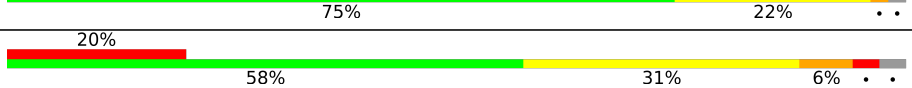
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	

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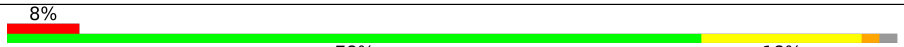
Mol	Chain	Length	Quality of chain
27	15	60	
27	25	60	
28	16	54	
28	26	54	
29	17	49	
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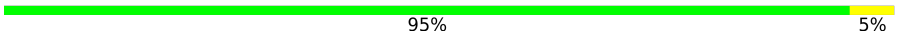
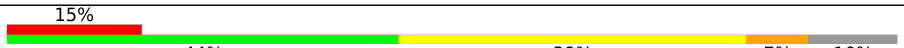
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
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34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	

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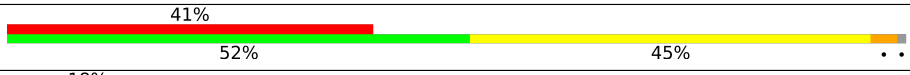
Mol	Chain	Length	Quality of chain
39	2h	138	
40	1i	128	
40	2i	128	
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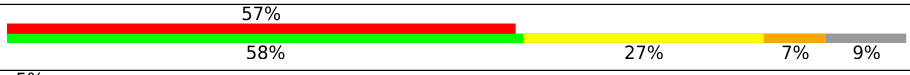
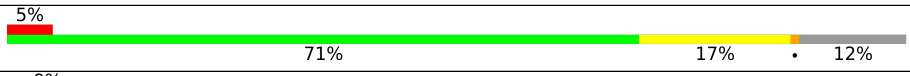
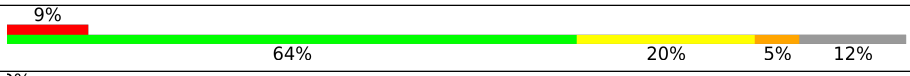
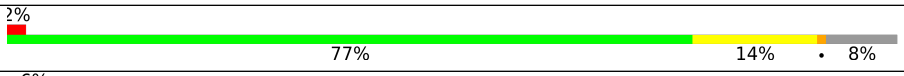
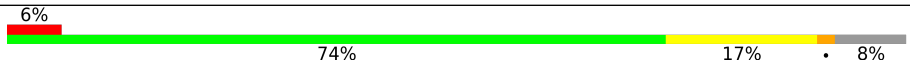
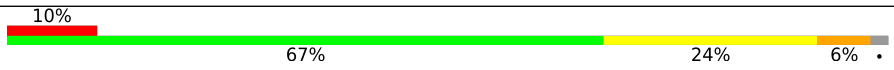
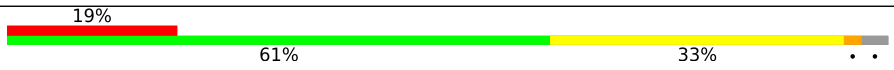
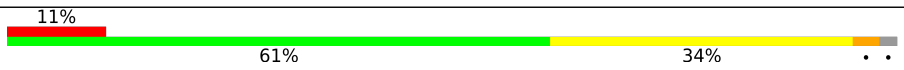
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
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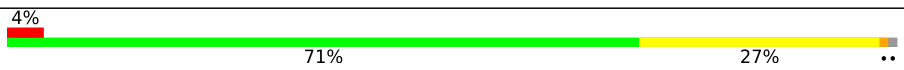
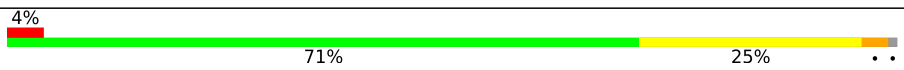
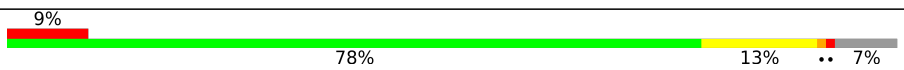
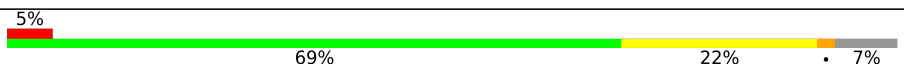
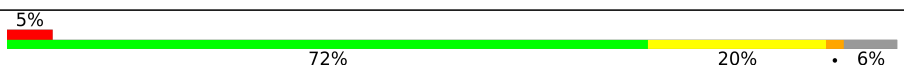
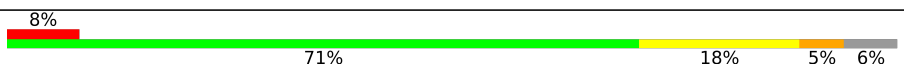
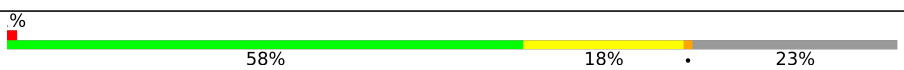
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
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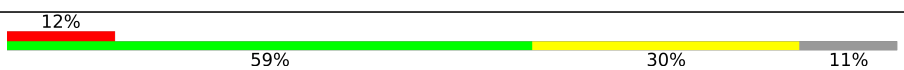
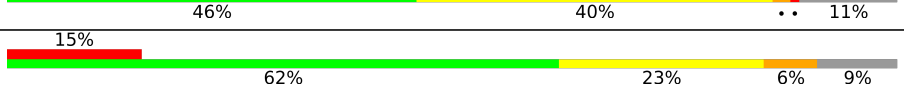
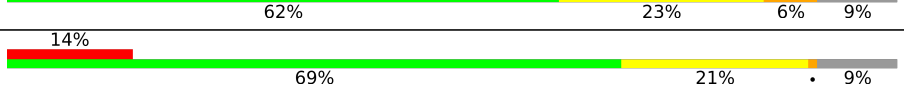
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	

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Mol	Chain	Length	Quality of chain
52	1u	27	15% 70% 15% 15%
52	2u	27	37% 59% 22% 15%
53	1v	24	8% 38% 12% 46%
53	2v	24	17% 42% 8% 46%
54	1w	76	21% 42% 46% 8%
54	2w	76	17% 42% 39% 12% 5%
55	1x	77	5% 77% 19%
55	2x	77	% 68% 25% 8%
56	1z	7	29% 43% 43% 14%
56	2z	7	29% 43% 29% 29%
57	1y	76	38% 21% 49% 26%
57	2y	76	46% 36% 39% 21%

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
58	MG	1A	3260	-	-	-	X
58	MG	2A	3217	-	-	-	X
58	MG	2A	3265	-	-	-	X
58	MG	2a	1721	-	-	-	X
58	MG	2x	106	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 300665 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 Peptidyl-tRNA fMTHSMRC-tRNAmet RNA-part.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			

- Molecule 56 is a protein called P-site Peptidyl-tRNA fMTHSMRC-tRNAmet Peptide-part.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1z	7	Total	C	N	O	S	0	0	0
			58	33	12	10	3			
56	2z	7	Total	C	N	O	S	0	0	0
			58	33	12	10	3			

- Molecule 57 is a RNA chain called E-site Deacylated tRNAphe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
57	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
57	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1111	Total	Mg	0	0
			1111	1111		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1B	37	Total Mg 37 37	0	0
58	1D	11	Total Mg 11 11	0	0
58	1E	13	Total Mg 13 13	0	0
58	1F	15	Total Mg 15 15	0	0
58	1G	4	Total Mg 4 4	0	0
58	1H	1	Total Mg 1 1	0	0
58	1I	1	Total Mg 1 1	0	0
58	1N	4	Total Mg 4 4	0	0
58	1O	6	Total Mg 6 6	0	0
58	1P	6	Total Mg 6 6	0	0
58	1Q	7	Total Mg 7 7	0	0
58	1R	6	Total Mg 6 6	0	0
58	1S	3	Total Mg 3 3	0	0
58	1T	4	Total Mg 4 4	0	0
58	1U	14	Total Mg 14 14	0	0
58	1V	8	Total Mg 8 8	0	0
58	1W	6	Total Mg 6 6	0	0
58	1X	6	Total Mg 6 6	0	0
58	1Y	2	Total Mg 2 2	0	0
58	1Z	3	Total Mg 3 3	0	0
58	10	12	Total Mg 12 12	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	11	5	Total Mg 5 5	0	0
58	12	2	Total Mg 2 2	0	0
58	13	3	Total Mg 3 3	0	0
58	14	1	Total Mg 1 1	0	0
58	15	8	Total Mg 8 8	0	0
58	16	2	Total Mg 2 2	0	0
58	17	4	Total Mg 4 4	0	0
58	18	4	Total Mg 4 4	0	0
58	19	1	Total Mg 1 1	0	0
58	1a	226	Total Mg 226 226	0	0
58	1b	1	Total Mg 1 1	0	0
58	1d	1	Total Mg 1 1	0	0
58	1e	2	Total Mg 2 2	0	0
58	1f	1	Total Mg 1 1	0	0
58	1k	1	Total Mg 1 1	0	0
58	1l	2	Total Mg 2 2	0	0
58	1m	1	Total Mg 1 1	0	0
58	1n	3	Total Mg 3 3	0	0
58	1r	1	Total Mg 1 1	0	0
58	1t	1	Total Mg 1 1	0	0
58	1v	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1w	8	Total Mg 8 8	0	0
58	1x	14	Total Mg 14 14	0	0
58	2A	826	Total Mg 826 826	0	0
58	2B	20	Total Mg 20 20	0	0
58	2D	6	Total Mg 6 6	0	0
58	2E	9	Total Mg 9 9	0	0
58	2F	8	Total Mg 8 8	0	0
58	2G	1	Total Mg 1 1	0	0
58	2O	1	Total Mg 1 1	0	0
58	2P	2	Total Mg 2 2	0	0
58	2Q	2	Total Mg 2 2	0	0
58	2R	2	Total Mg 2 2	0	0
58	2T	4	Total Mg 4 4	0	0
58	2U	2	Total Mg 2 2	0	0
58	2V	2	Total Mg 2 2	0	0
58	2W	2	Total Mg 2 2	0	0
58	2X	2	Total Mg 2 2	0	0
58	2Y	1	Total Mg 1 1	0	0
58	20	2	Total Mg 2 2	0	0
58	21	1	Total Mg 1 1	0	0
58	23	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	25	2	Total Mg 2 2	0	0
58	26	2	Total Mg 2 2	0	0
58	27	4	Total Mg 4 4	0	0
58	28	3	Total Mg 3 3	0	0
58	2a	241	Total Mg 241 241	0	0
58	2d	2	Total Mg 2 2	0	0
58	2e	2	Total Mg 2 2	0	0
58	2f	2	Total Mg 2 2	0	0
58	2j	1	Total Mg 1 1	0	0
58	2l	4	Total Mg 4 4	0	0
58	2n	2	Total Mg 2 2	0	0
58	2p	1	Total Mg 1 1	0	0
58	2q	1	Total Mg 1 1	0	0
58	2t	1	Total Mg 1 1	0	0
58	2v	3	Total Mg 3 3	0	0
58	2w	3	Total Mg 3 3	0	0
58	2x	8	Total Mg 8 8	0	0

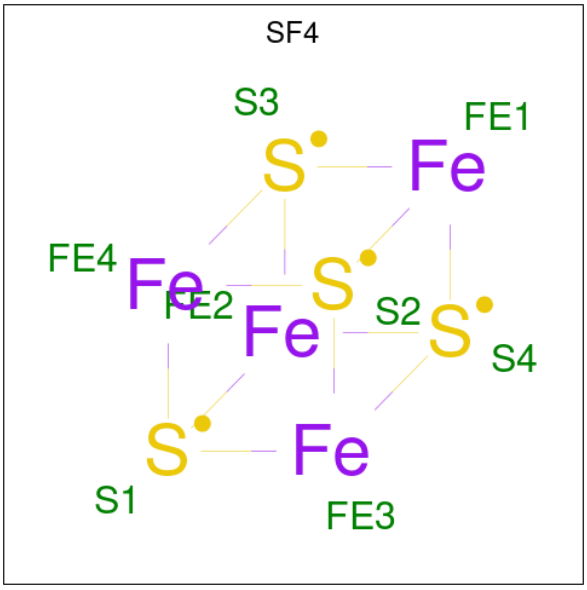
- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1	Total K 1 1	0	0
59	2A	1	Total K 1 1	0	0

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1Y	1	Total Zn 1 1	0	0
60	14	1	Total Zn 1 1	0	0
60	15	1	Total Zn 1 1	0	0
60	16	1	Total Zn 1 1	0	0
60	19	1	Total Zn 1 1	0	0
60	1n	1	Total Zn 1 1	0	0
60	2Y	1	Total Zn 1 1	0	0
60	24	1	Total Zn 1 1	0	0
60	25	1	Total Zn 1 1	0	0
60	26	1	Total Zn 1 1	0	0
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1d	1	Total Fe S 8 4 4	0	0
61	2d	1	Total Fe S 8 4 4	0	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1A	2181	Total O 2181 2181	0	0
62	1B	62	Total O 62 62	0	0
62	1D	28	Total O 28 28	0	0
62	1E	27	Total O 27 27	0	0
62	1F	16	Total O 16 16	0	0
62	1G	2	Total O 2 2	0	0
62	1H	2	Total O 2 2	0	0
62	1N	7	Total O 7 7	0	0
62	1O	5	Total O 5 5	0	0
62	1P	21	Total O 21 21	0	0
62	1Q	12	Total O 12 12	0	0
62	1R	12	Total O 12 12	0	0
62	1S	4	Total O 4 4	0	0
62	1T	11	Total O 11 11	0	0
62	1U	13	Total O 13 13	0	0
62	1V	9	Total O 9 9	0	0
62	1W	9	Total O 9 9	0	0
62	1X	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1Y	3	Total O 3 3	0	0
62	1Z	2	Total O 2 2	0	0
62	10	17	Total O 17 17	0	0
62	11	8	Total O 8 8	0	0
62	12	3	Total O 3 3	0	0
62	13	4	Total O 4 4	0	0
62	14	1	Total O 1 1	0	0
62	15	6	Total O 6 6	0	0
62	16	3	Total O 3 3	0	0
62	17	9	Total O 9 9	0	0
62	18	11	Total O 11 11	0	0
62	1a	436	Total O 436 436	0	0
62	1b	1	Total O 1 1	0	0
62	1d	3	Total O 3 3	0	0
62	1f	3	Total O 3 3	0	0
62	1g	1	Total O 1 1	0	0
62	1j	3	Total O 3 3	0	0
62	1l	5	Total O 5 5	0	0
62	1m	1	Total O 1 1	0	0
62	1n	2	Total O 2 2	0	0
62	1o	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1p	1	Total O 1 1	0	0
62	1q	2	Total O 2 2	0	0
62	1r	2	Total O 2 2	0	0
62	1t	1	Total O 1 1	0	0
62	1v	4	Total O 4 4	0	0
62	1w	12	Total O 12 12	0	0
62	1x	12	Total O 12 12	0	0
62	1z	5	Total O 5 5	0	0
62	1y	1	Total O 1 1	0	0
62	2A	1216	Total O 1216 1216	0	0
62	2B	20	Total O 20 20	0	0
62	2D	18	Total O 18 18	0	0
62	2E	18	Total O 18 18	0	0
62	2F	14	Total O 14 14	0	0
62	2N	1	Total O 1 1	0	0
62	2O	2	Total O 2 2	0	0
62	2P	12	Total O 12 12	0	0
62	2Q	2	Total O 2 2	0	0
62	2R	2	Total O 2 2	0	0
62	2T	6	Total O 6 6	0	0
62	2U	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2W	2	Total O 2 2	0	0
62	2X	1	Total O 1 1	0	0
62	2Y	2	Total O 2 2	0	0
62	20	1	Total O 1 1	0	0
62	21	4	Total O 4 4	0	0
62	23	1	Total O 1 1	0	0
62	27	3	Total O 3 3	0	0
62	28	3	Total O 3 3	0	0
62	29	1	Total O 1 1	0	0
62	2a	357	Total O 357 357	0	0
62	2c	1	Total O 1 1	0	0
62	2d	4	Total O 4 4	0	0
62	2e	3	Total O 3 3	0	0
62	2f	3	Total O 3 3	0	0
62	2j	2	Total O 2 2	0	0
62	2l	4	Total O 4 4	0	0
62	2n	2	Total O 2 2	0	0
62	2o	1	Total O 1 1	0	0
62	2p	2	Total O 2 2	0	0
62	2q	1	Total O 1 1	0	0
62	2r	2	Total O 2 2	0	0

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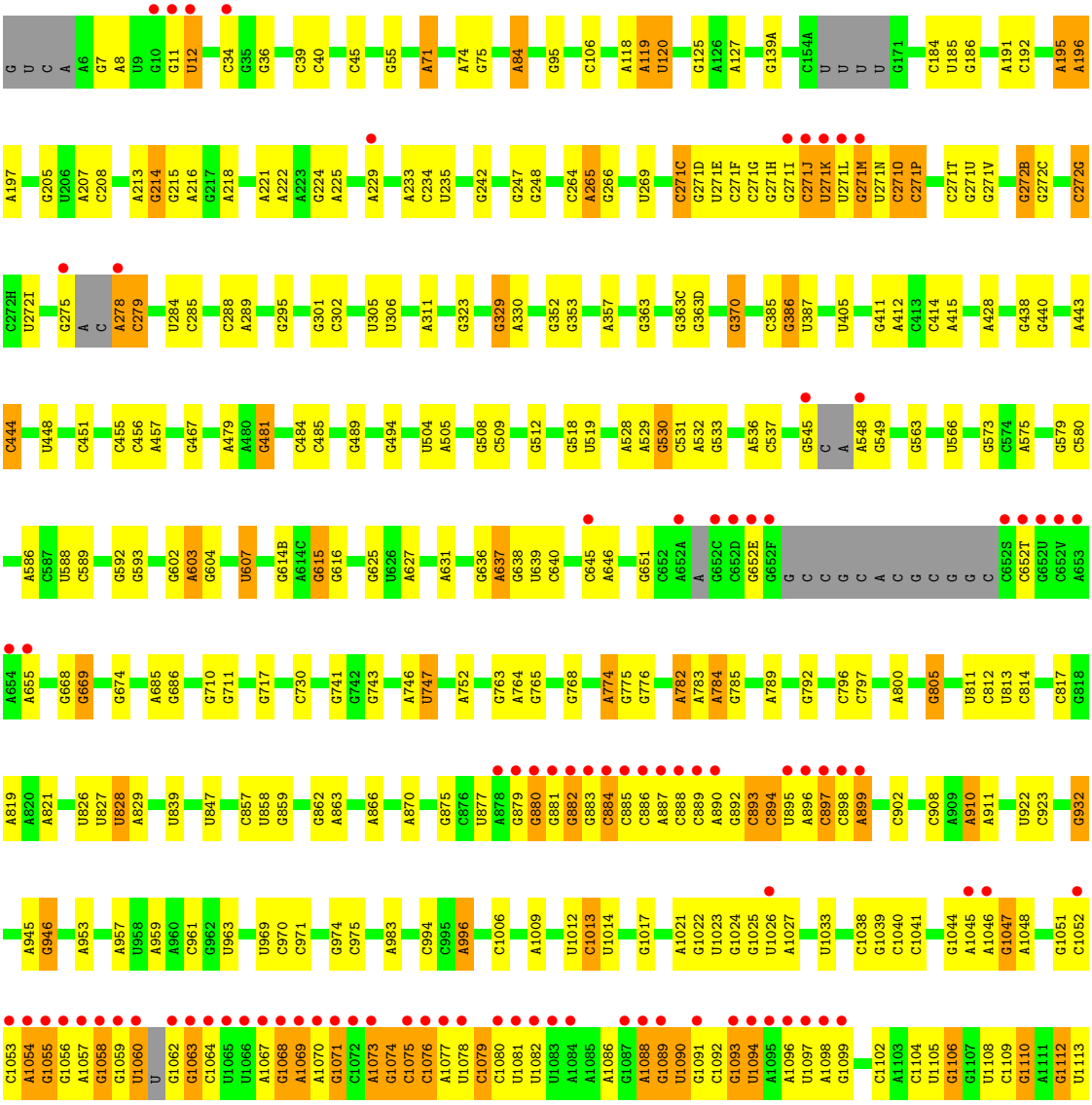
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2t	4	Total O 4 4	0	0
62	2v	3	Total O 3 3	0	0
62	2w	8	Total O 8 8	0	0
62	2x	3	Total O 3 3	0	0
62	2z	1	Total O 1 1	0	0

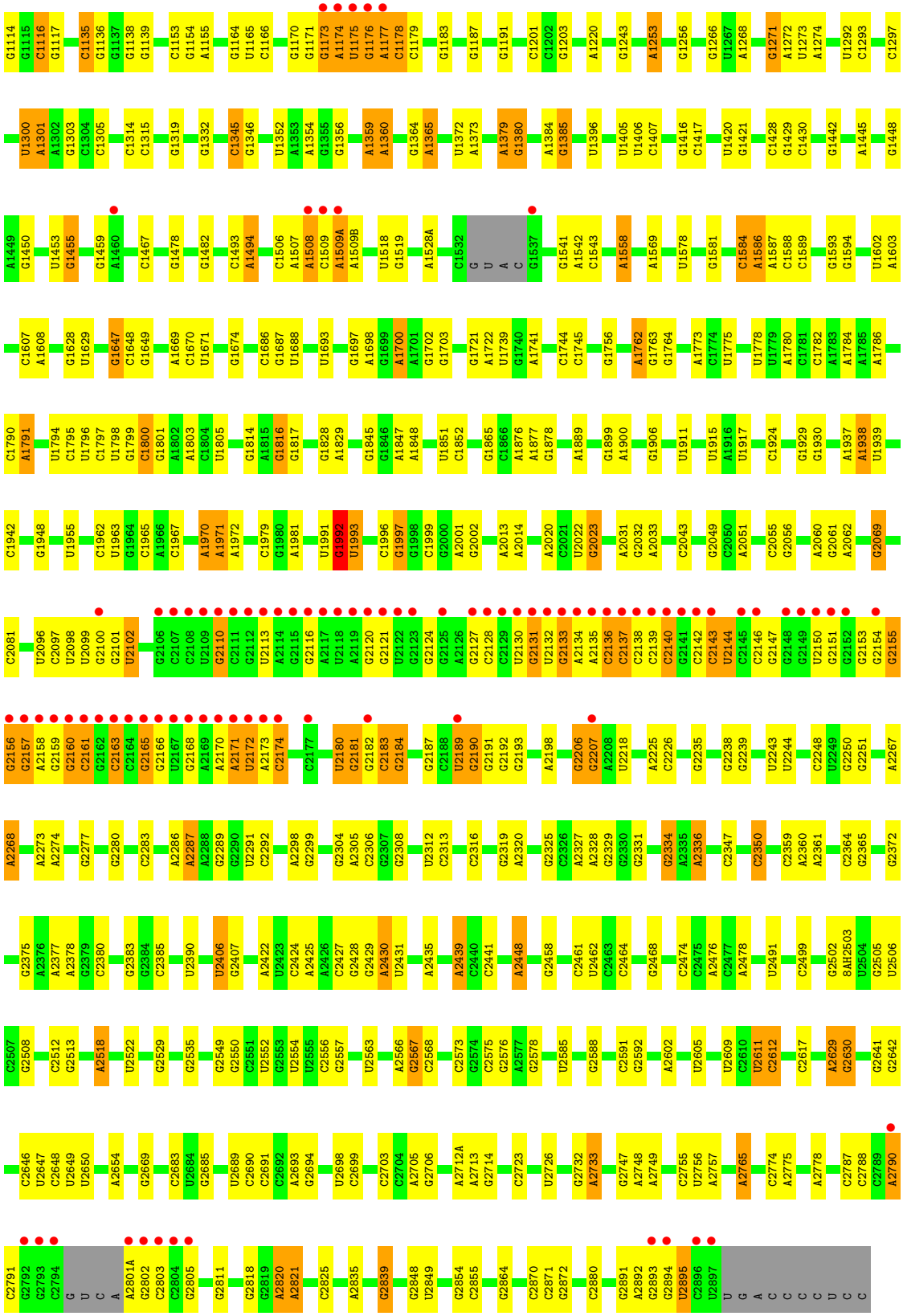
3 Residue-property plots (i)

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

- Molecule 1: 23S Ribosomal RNA

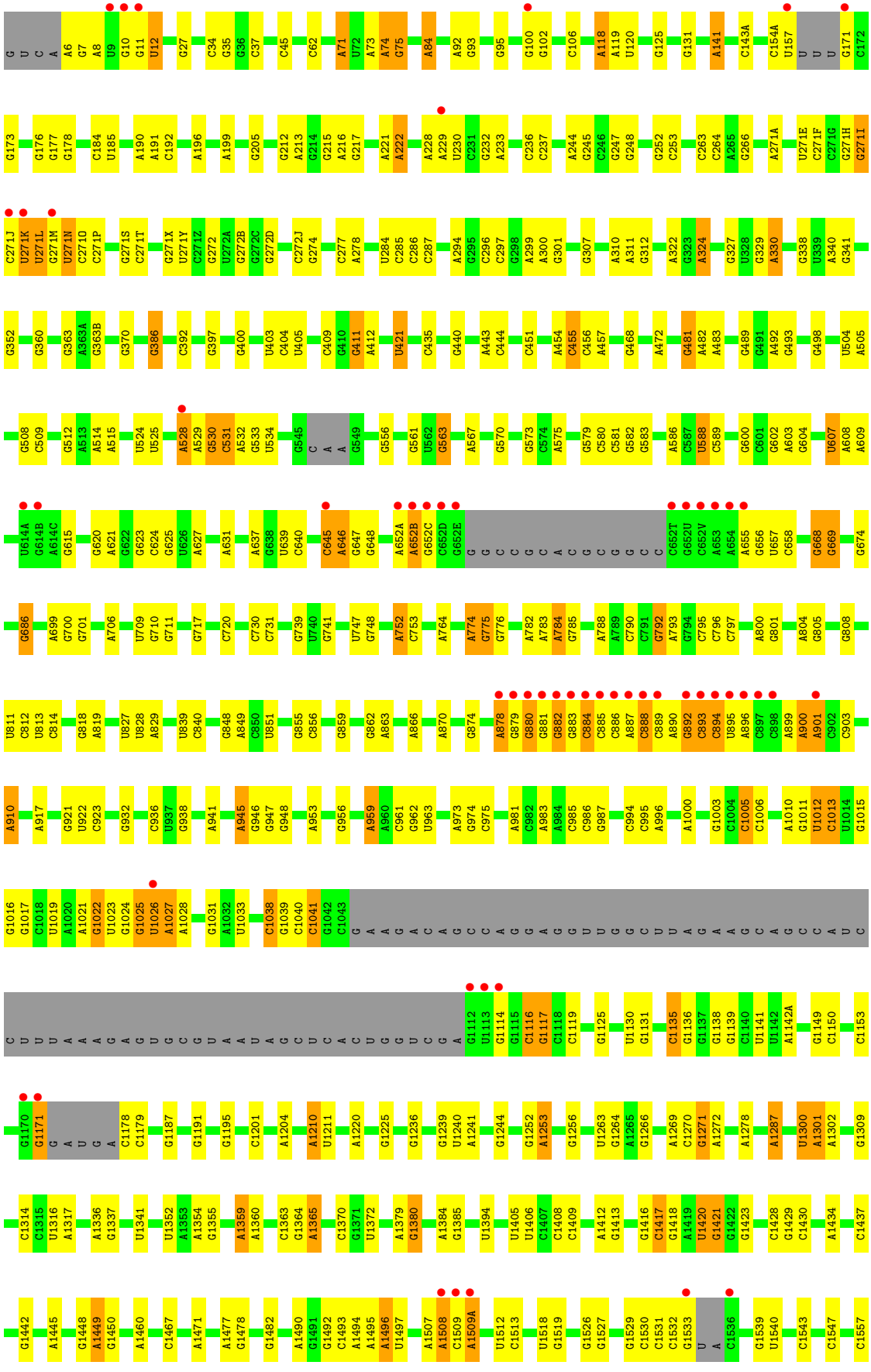
Chain 1A:

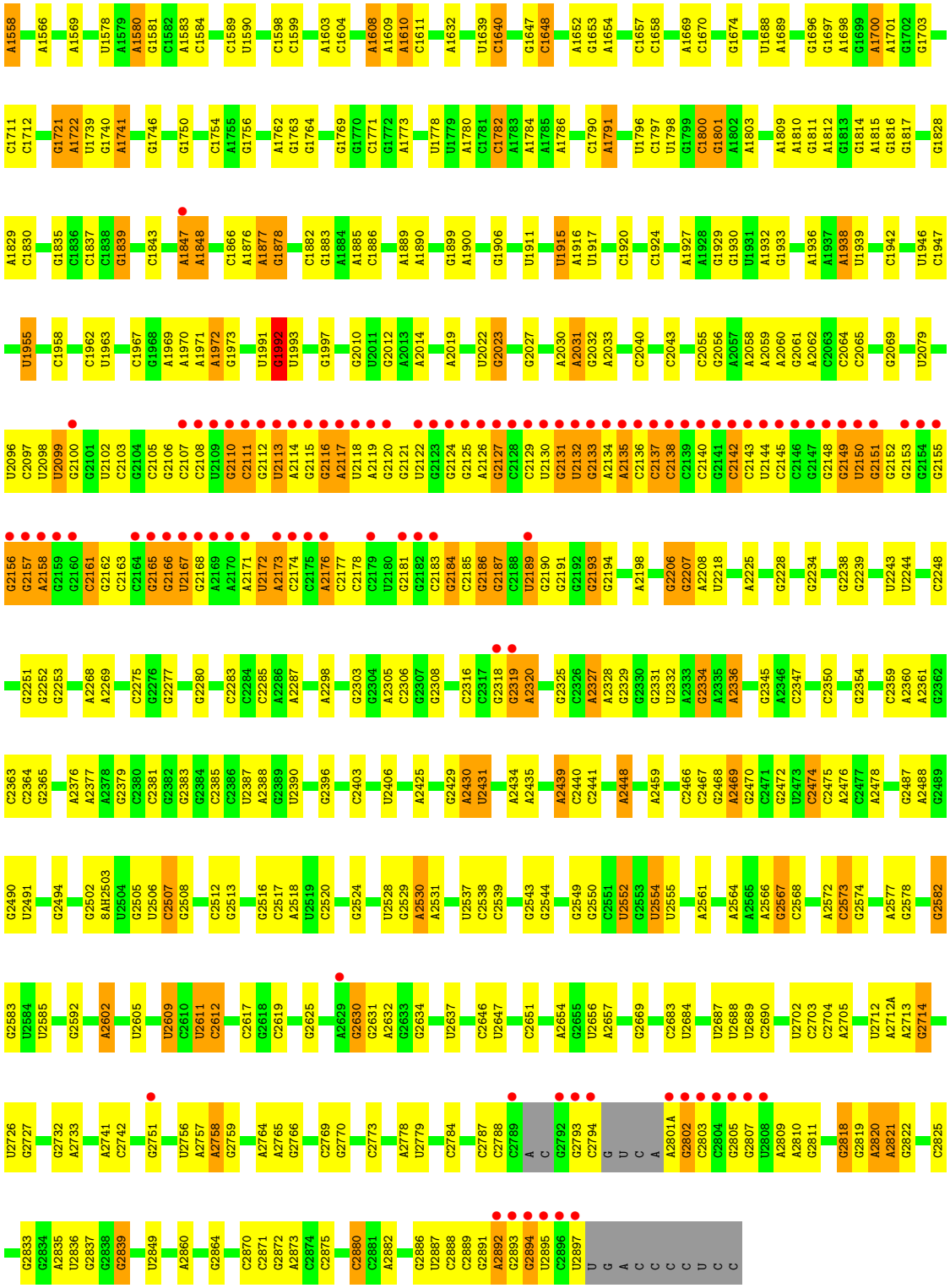




• Molecule 1: 23S Ribosomal RNA

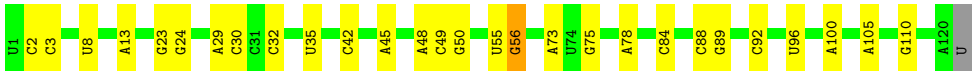
Chain 2A:


G U C A A6 G7 A8 U9 G10 G11 U12 G27 C34 G35 G36 C37 C45 C62 A71 U72 A73 A74 G75 A84 A92 G93 G95 G100 G102 C106 A118 A119 U120 G125 G131 A141 C143A C154A U157 U U U G171 C172
G173 G176 G177 G178 C184 U185 A190 A191 C192 A196 A199 G205 G212 A213 G214 G215 A216 G217 A221 A222 A228 A229 U230 C231 G232 A233 C236 C237 A244 G245 C246 G247 G248 G252 C253 C263 C264 A265 G266 A271A U271E C271F C271G G271H G271I
C271J U271K U271L G271M U271N C271O C271P G271S C271T G271X U271Y C271Z G272 U272A G272B G272C G272D C272J G274 C277 A278 U284 C285 C286 C287 A294 G295 C296 C297 G298 A299 A300 G301 G307 A310 A311 G312 A322 G323 A324 G327 U328 G329 A330 G338 U339 A340 G341
G352 G360 G363 A363A G363B G370 G386 C392 G397 G400 U403 C404 U405 G409 G410 G411 A412 U421 C435 G440 A443 C444 C451 A454 C455 C456 A457 G468 A472 G481 A482 A483 G489 G491 A492 G493 G498 U504 A505
G508 C509 G512 A513 A514 A515 U524 U525 A528 A529 G530 C531 A532 G533 U534 G545 C A A G549 G556 G561 U562 G563 A567 G570 G573 C574 A575 G579 C580 C581 G582 G583 A586 C587 U588 C589 G600 C601 G602 A603 G604 G498 U607 A608 A609
U614A G614B A614C G615 G620 A621 G622 G623 C624 G625 U626 A627 A631 A637 G638 U639 C640 C645 A646 G647 G648 A652A A652B G652C C652D G652E G G C C G C A C G C G C C C652T G652U C652V A653 A654 A655 G656 U657 C658 G668 G669 G674
G686 A699 G700 G701 A706 U709 G710 G711 G717 C720 C730 C731 G739 U740 G741 U747 G748 A752 C753 A764 A774 G775 G776 A782 A783 A784 G785 A788 A789 C790 C791 G792 A793 G794 C795 C796 C797 A800 G801 A804 G805 G808
U811 C812 U813 C814 G818 A819 U827 U828 A829 U839 C840 G848 A849 C850 U851 G855 C856 G859 G862 A863 A866 A870 G874 A878 G879 G880 G881 G882 G883 C884 C885 C886 A887 C888 C889 A890 G892 C893 C894 U895 A896 C897 C898 A899 A900 A901 C902 C903
A910 A917 G921 U922 C923 G932 C936 U937 G938 A941 A945 G946 G947 G948 A953 G956 A959 A960 C961 G962 U963 A973 G974 C975 A981 C982 A983 A984 C985 C986 G987 C994 C995 A996 A1000 G1003 C1004 C1005 C1006 A1010 G1011 U1012 C1013 U1014 G1015
G1016 G1017 C1018 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 G1031 A1032 U1033 C1038 G1039 C1040 C1041 G1042 C1043 G A A G A C A G C C A G G C G U U G G C U C U U A G C C A U C
C U U U A A A G A G U C G G U A A U A G C C A C A C U G U A G A A G C C U C U G A C G A G1112 G1113 G1114 G1115 C1116 G1117 C1118 C1119 G1125 U1130 G1131 C1135 G1136 G1137 G1138 G1139 C1140 U1141 U1142 A1142A G1149 C1150 C1153
G1170 G1171 G A U G A C1178 C1179 G1187 G1191 G1195 C1201 A1204 A1210 U1211 A1220 G1225 G1236 G1239 U1240 A1241 G1244 G1252 A1253 G1256 U1263 G1264 A1265 G1266 A1269 C1270 G1271 A1272 A1278 A1287 U1300 A1301 A1302 G1309
C1314 C1315 U1316 A1317 A1336 G1337 U1341 U1352 A1353 A1354 G1355 A1359 A1360 C1363 G1364 A1365 C1370 G1371 U1372 A1379 G1380 A1384 G1385 U1394 U1405 U1406 C1407 C1408 C1409 A1412 G1413 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 C1428 G1429 C1430 A1434 C1437
G1442 A1445 G1448 A1449 G1450 A1460 C1467 A1471 A1477 G1478 G1482 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 A1507 A1508 C1509 A1509A U1512 C1513 U1518 G1519 G1526 G1527 G1529 C1530 C1531 C1532 G1533 U A C1536 G1539 U1540 C1543 C1547 C1557



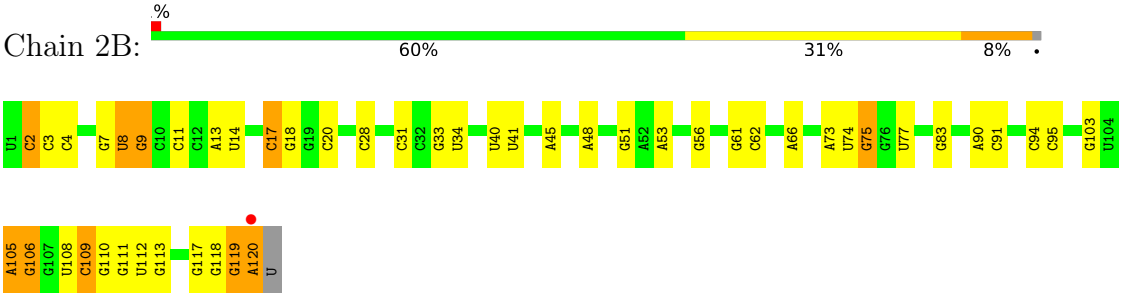
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



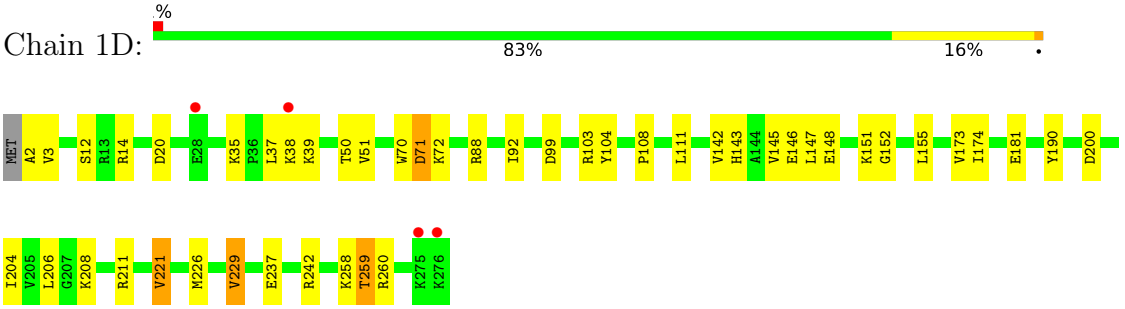
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



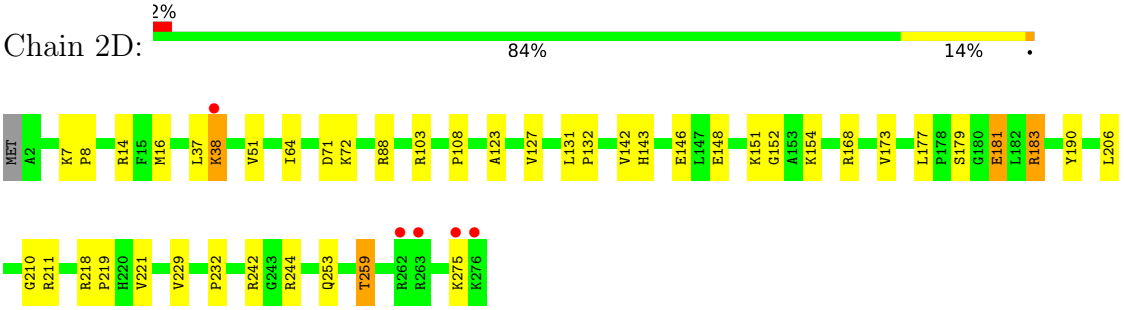
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



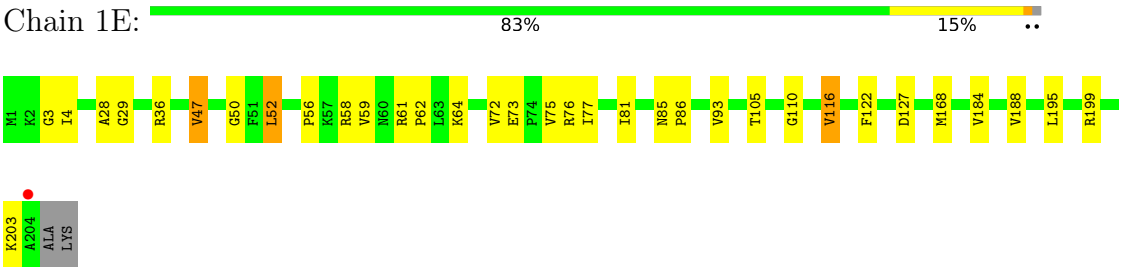
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



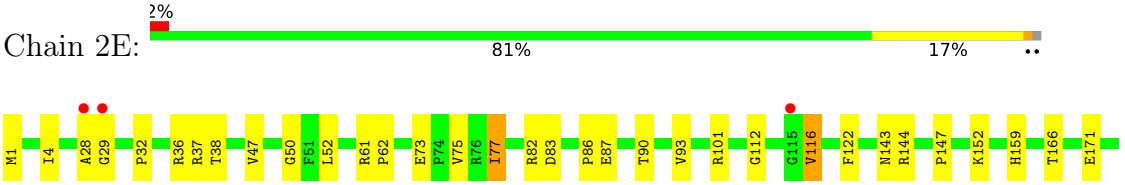
• Molecule 4: 50S ribosomal protein L3

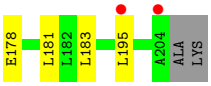
Chain 1E:



• Molecule 4: 50S ribosomal protein L3

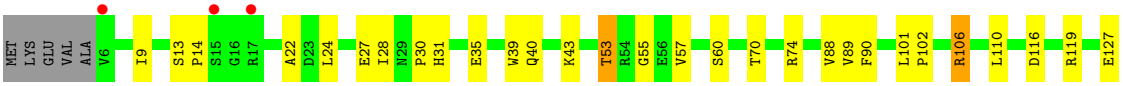
Chain 2E:

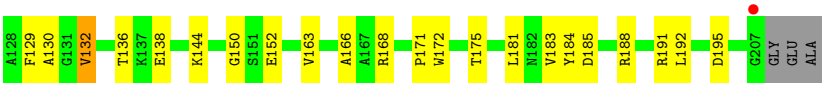




• Molecule 5: 50S ribosomal protein L4

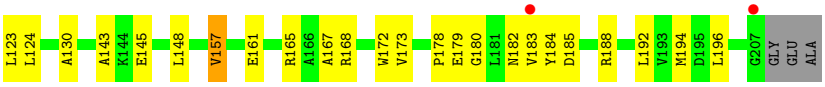
Chain 1F:





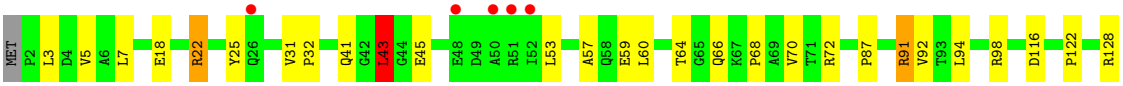
• Molecule 5: 50S ribosomal protein L4

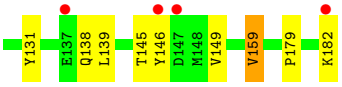
Chain 2F:



• Molecule 6: 50S ribosomal protein L5

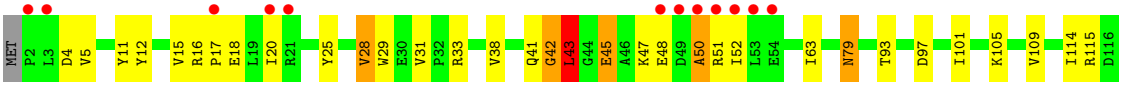
Chain 1G:

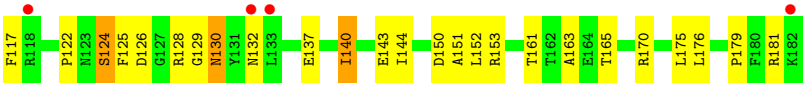




• Molecule 6: 50S ribosomal protein L5

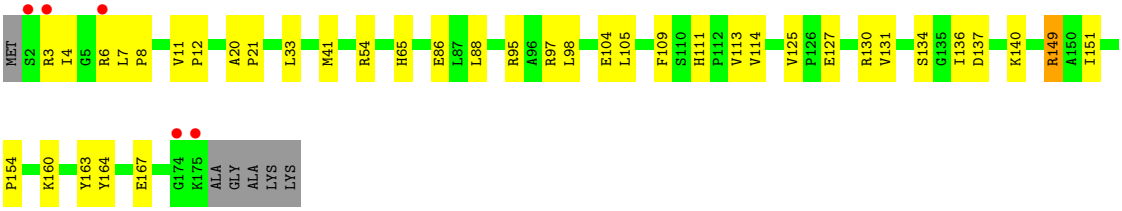
Chain 2G:



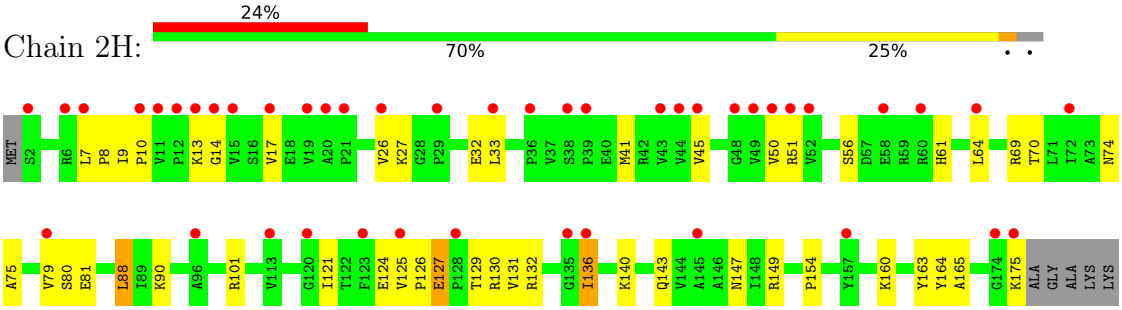


• Molecule 7: 50S ribosomal protein L6

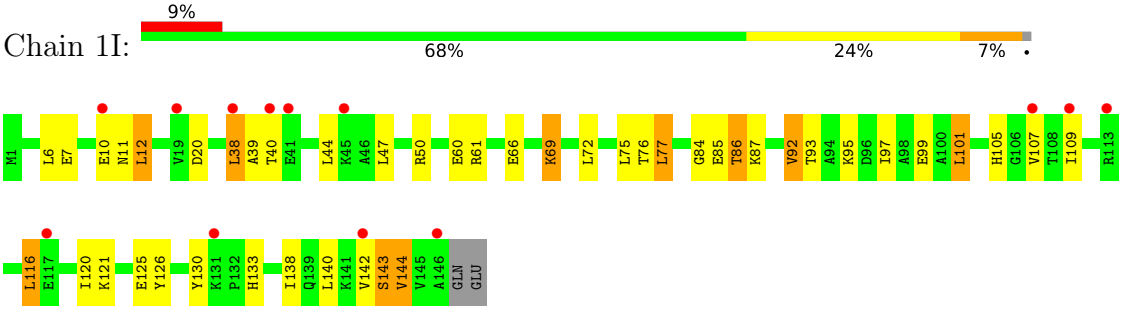
Chain 1H:



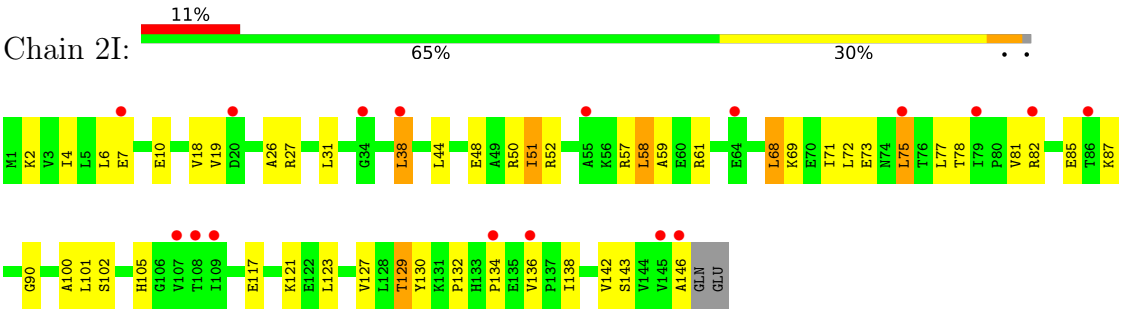
• Molecule 7: 50S ribosomal protein L6



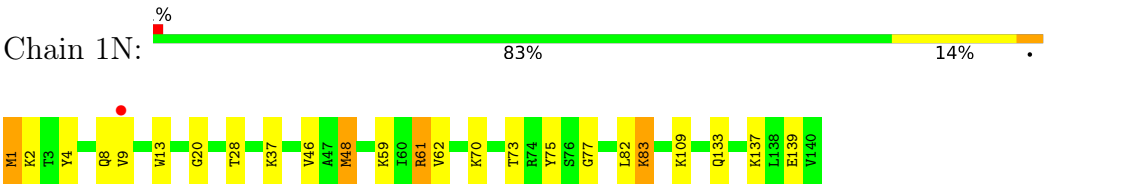
• Molecule 8: 50S ribosomal protein L9



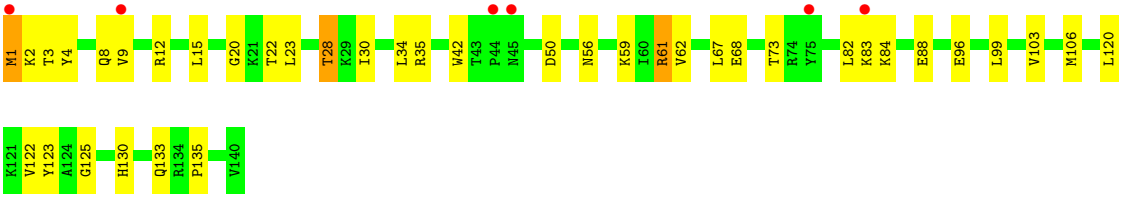
• Molecule 8: 50S ribosomal protein L9



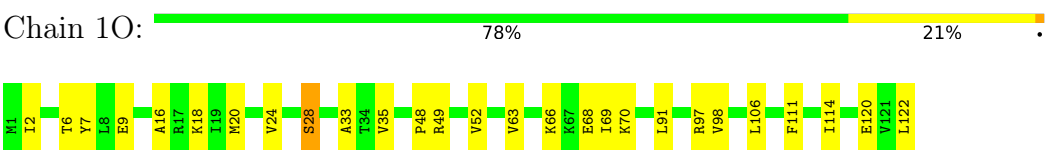
• Molecule 9: 50S ribosomal protein L13



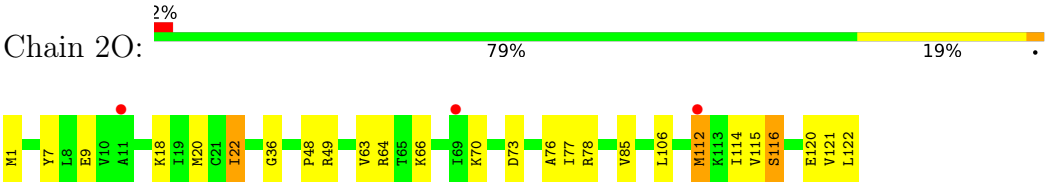
• Molecule 9: 50S ribosomal protein L13



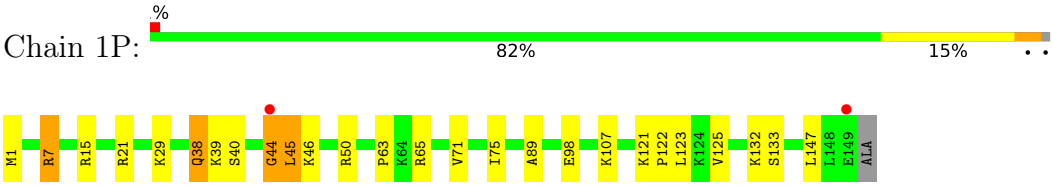
• Molecule 10: 50S ribosomal protein L14



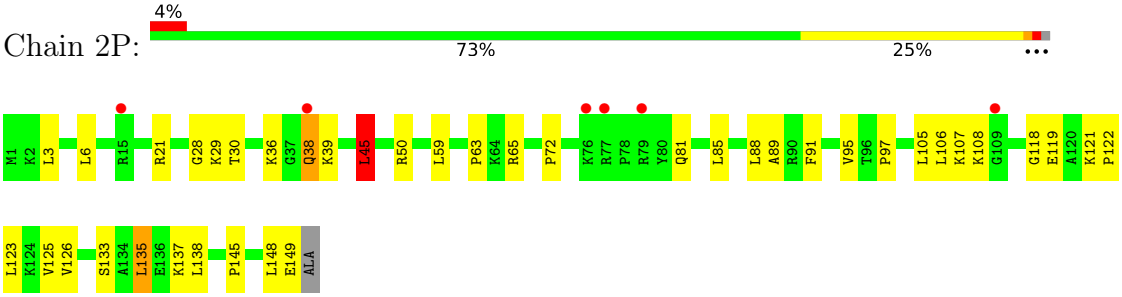
• Molecule 10: 50S ribosomal protein L14



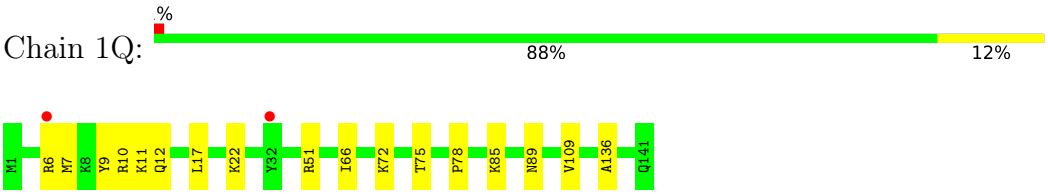
• Molecule 11: 50S ribosomal protein L15



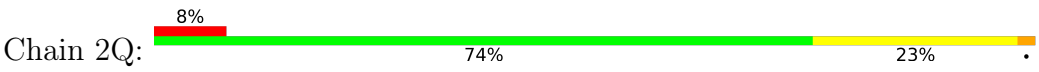
• Molecule 11: 50S ribosomal protein L15

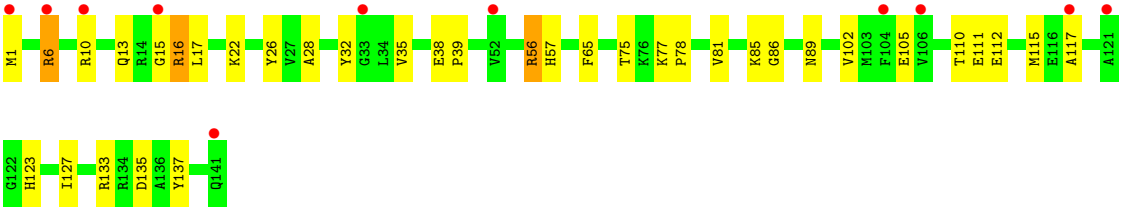


• Molecule 12: 50S ribosomal protein L16



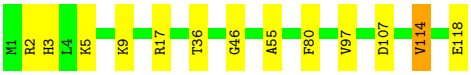
• Molecule 12: 50S ribosomal protein L16





• Molecule 13: 50S ribosomal protein L17

Chain 1R:



• Molecule 13: 50S ribosomal protein L17

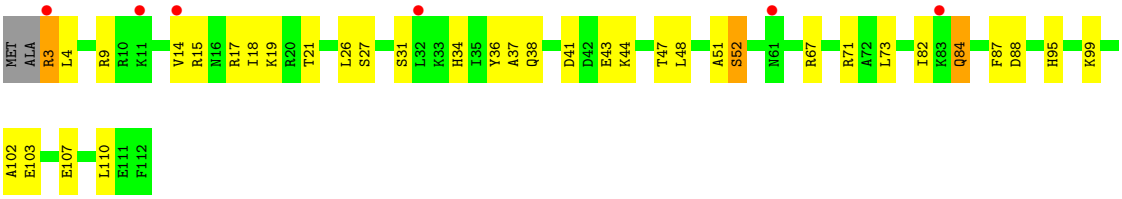
Chain 2R:

• Molecule 14: 50S ribosomal protein L18

Chain 1S:

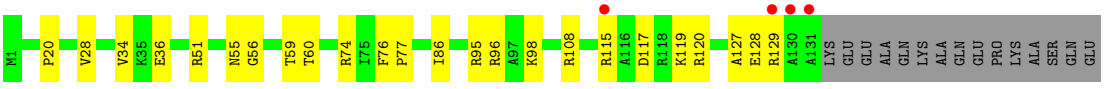
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



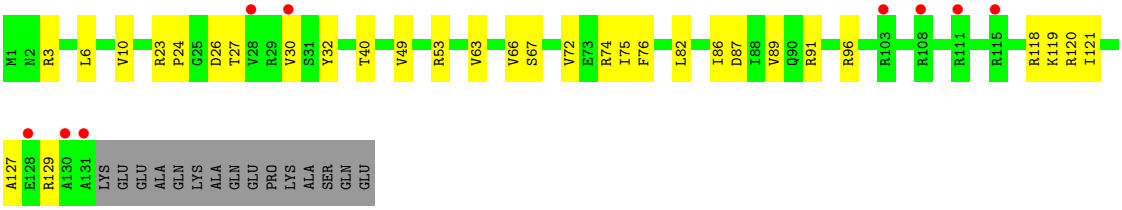
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



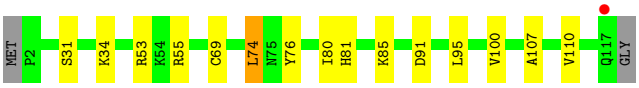
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



• Molecule 16: 50S ribosomal protein L20

Chain 1U:

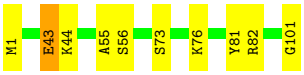


• Molecule 16: 50S ribosomal protein L20

Chain 2U:

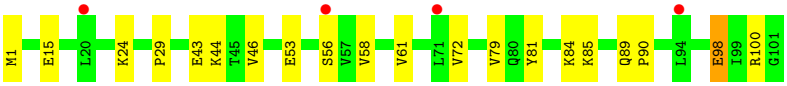
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



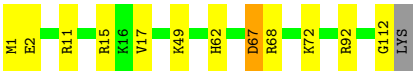
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



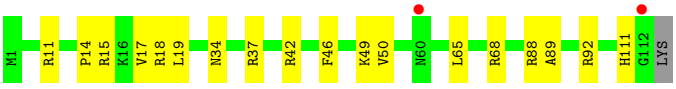
• Molecule 18: 50S ribosomal protein L22

Chain 1W:



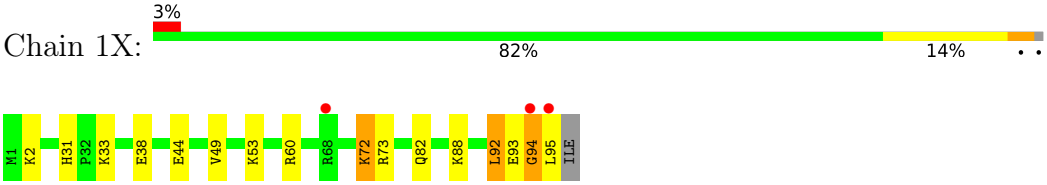
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



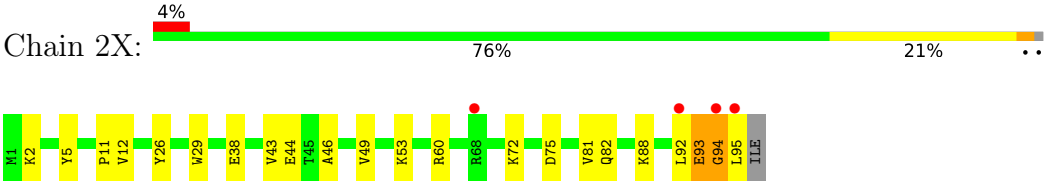
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



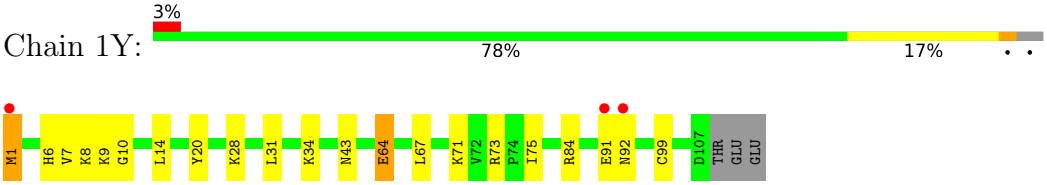
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



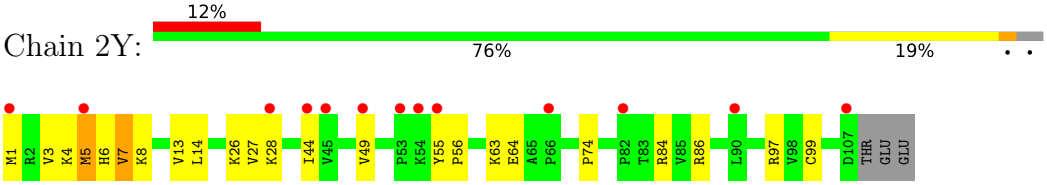
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



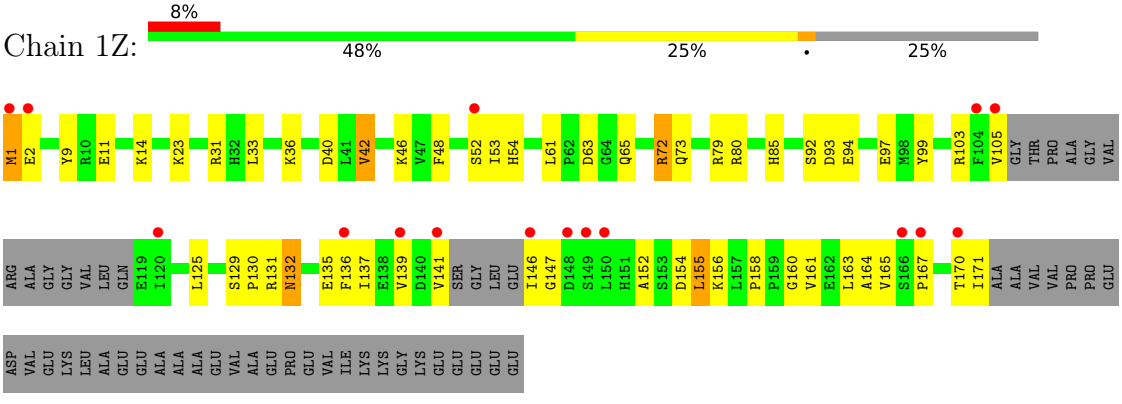
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



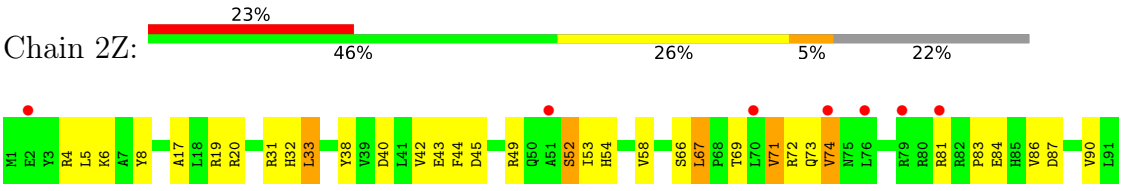
• Molecule 21: 50S ribosomal protein L25

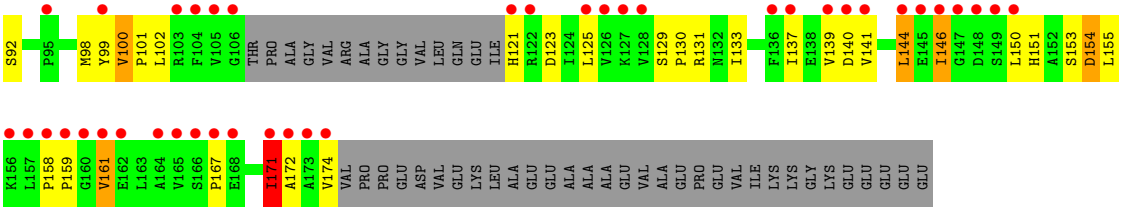
Chain 1Z:



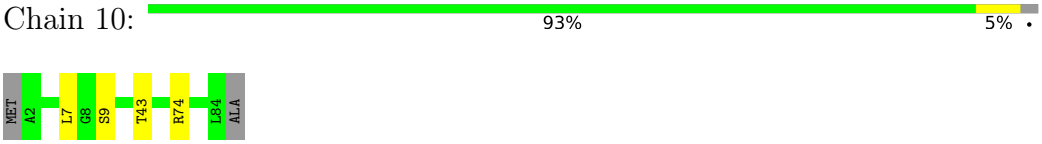
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:

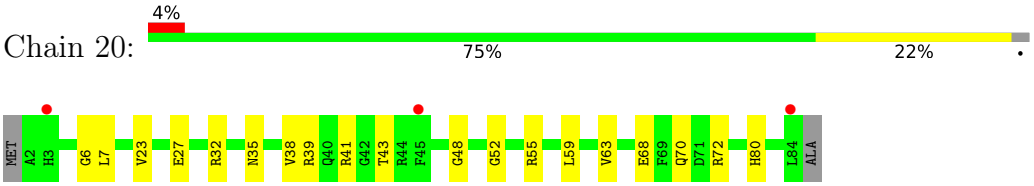




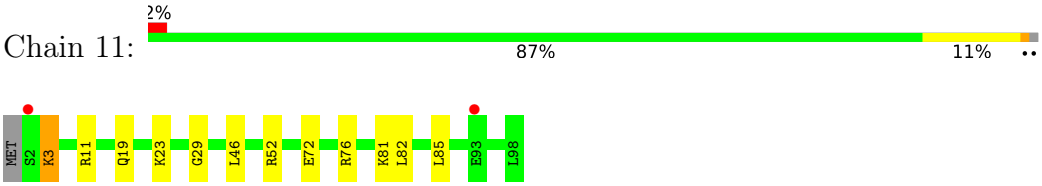
• Molecule 22: 50S ribosomal protein L27



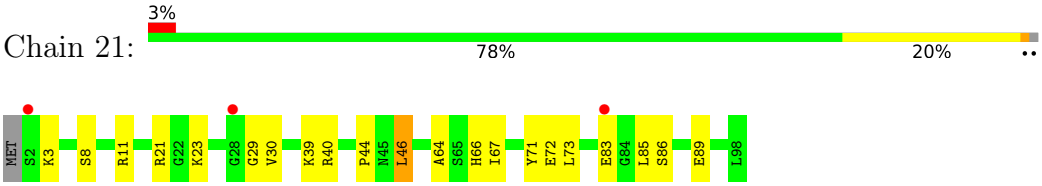
• Molecule 22: 50S ribosomal protein L27



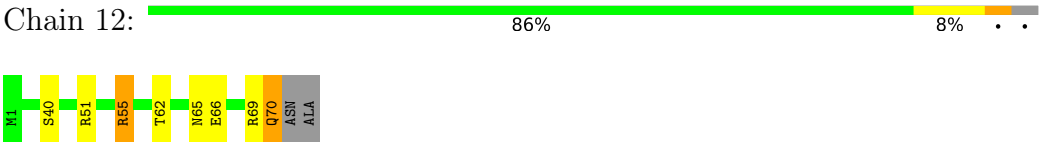
• Molecule 23: 50S ribosomal protein L28



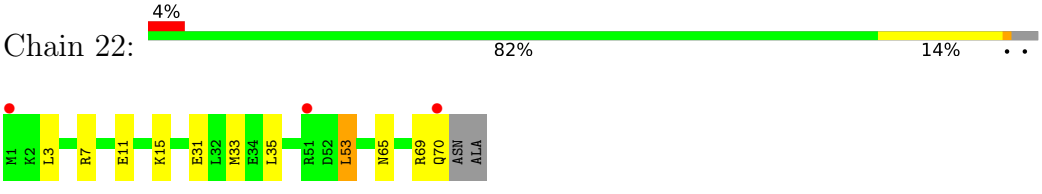
• Molecule 23: 50S ribosomal protein L28



• Molecule 24: 50S ribosomal protein L29

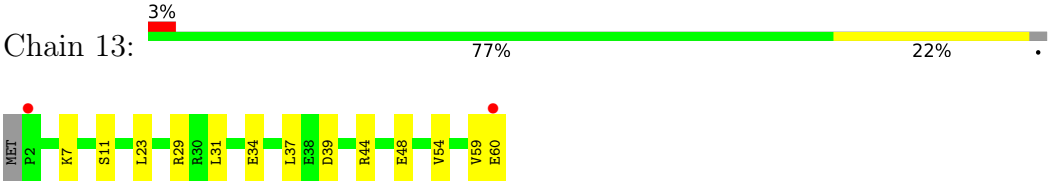


• Molecule 24: 50S ribosomal protein L29



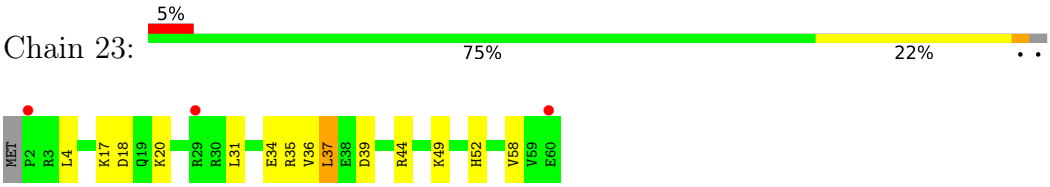
• Molecule 25: 50S ribosomal protein L30

Chain 13:



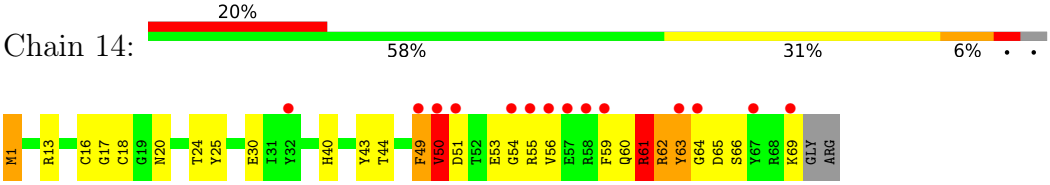
• Molecule 25: 50S ribosomal protein L30

Chain 23:



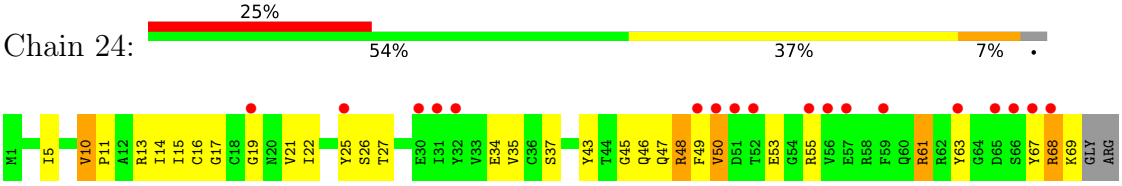
• Molecule 26: 50S ribosomal protein L31

Chain 14:



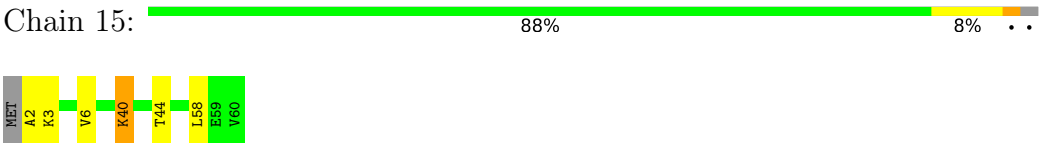
• Molecule 26: 50S ribosomal protein L31

Chain 24:



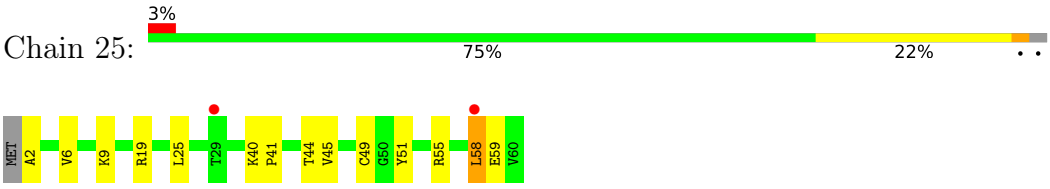
• Molecule 27: 50S ribosomal protein L32

Chain 15:



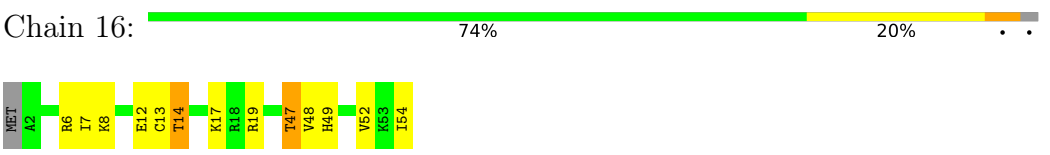
• Molecule 27: 50S ribosomal protein L32

Chain 25:



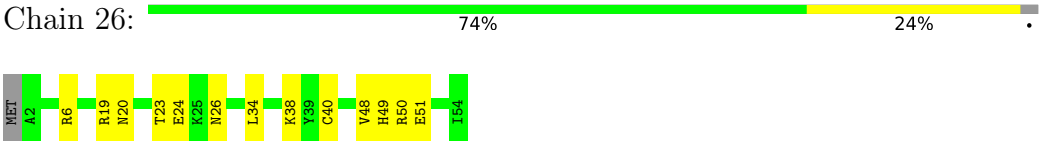
• Molecule 28: 50S ribosomal protein L33

Chain 16:



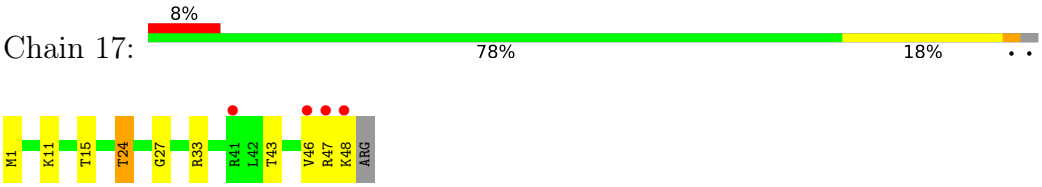
• Molecule 28: 50S ribosomal protein L33

Chain 26:



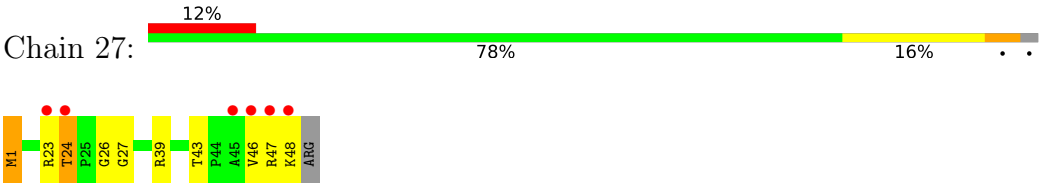
• Molecule 29: 50S ribosomal protein L34

Chain 17:



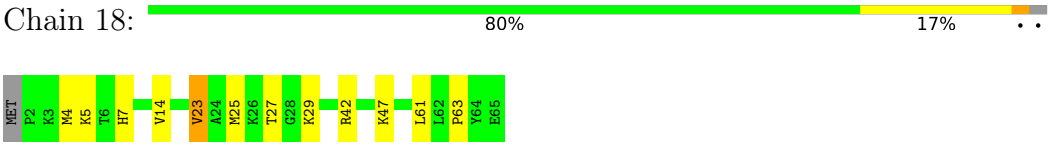
• Molecule 29: 50S ribosomal protein L34

Chain 27:



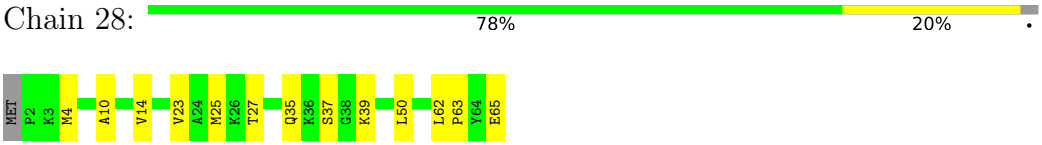
• Molecule 30: 50S ribosomal protein L35

Chain 18:



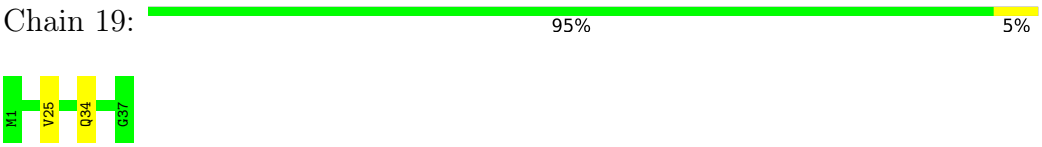
• Molecule 30: 50S ribosomal protein L35

Chain 28:



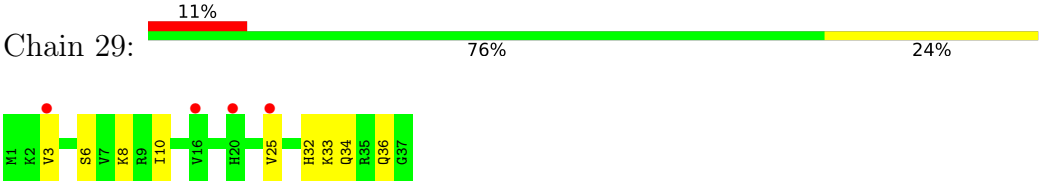
• Molecule 31: 50S ribosomal protein L36

Chain 19:



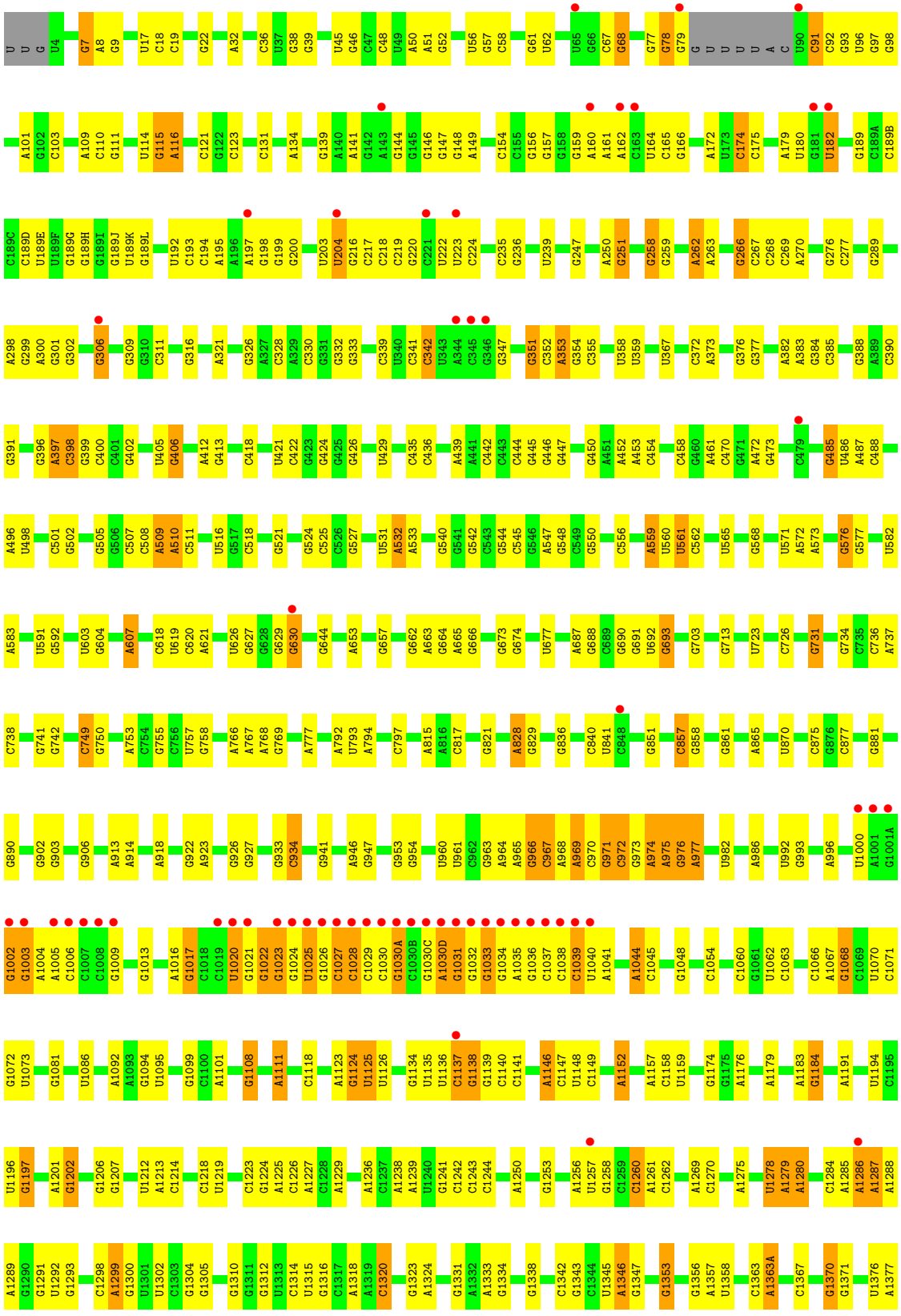
• Molecule 31: 50S ribosomal protein L36

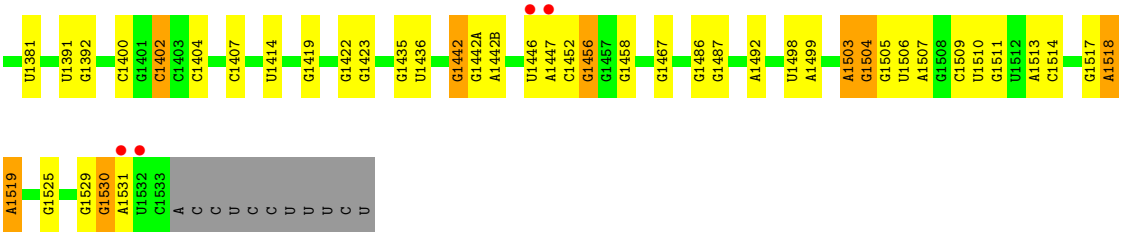
Chain 29:



• Molecule 32: 16S Ribosomal RNA

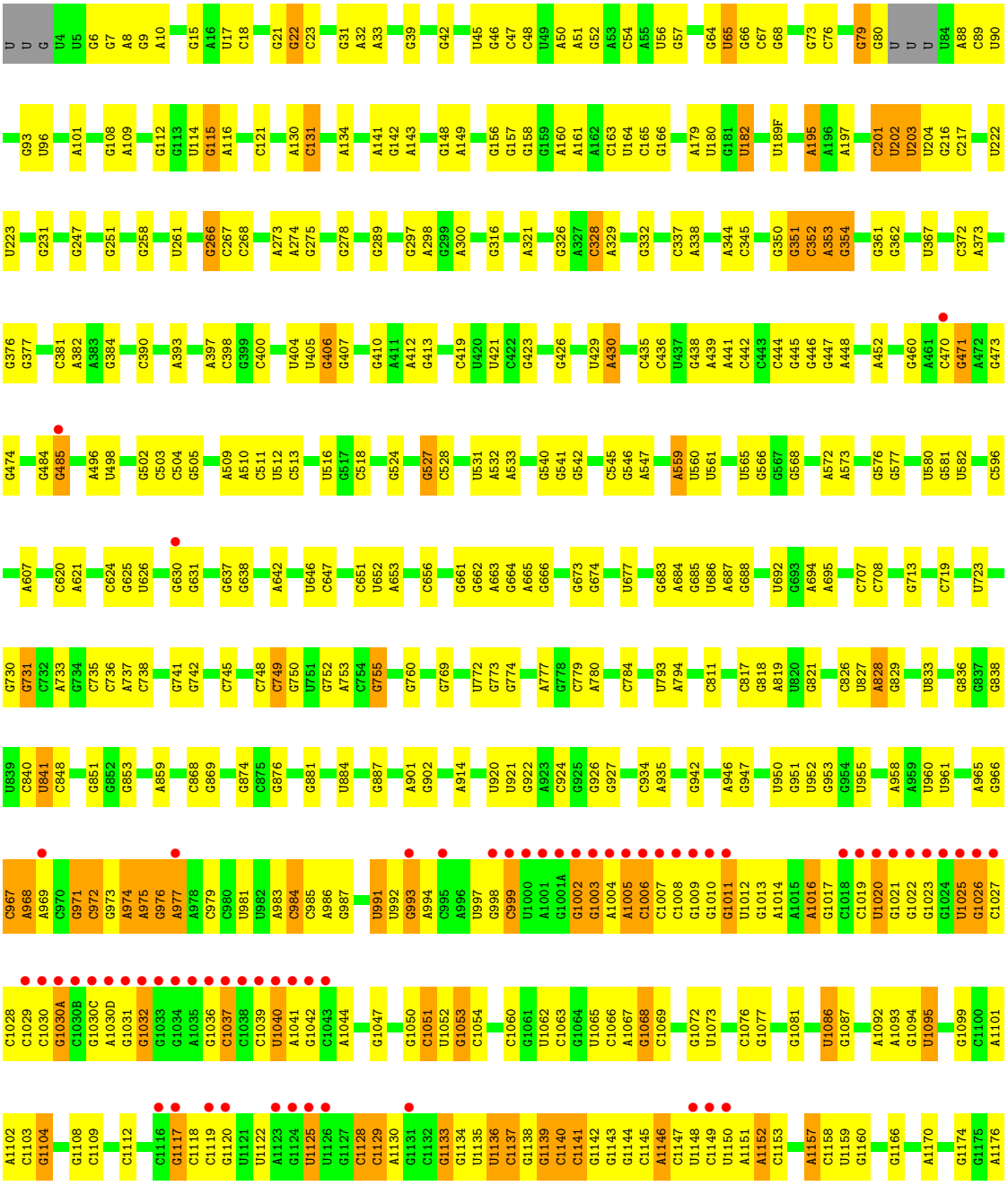
Chain 1a:

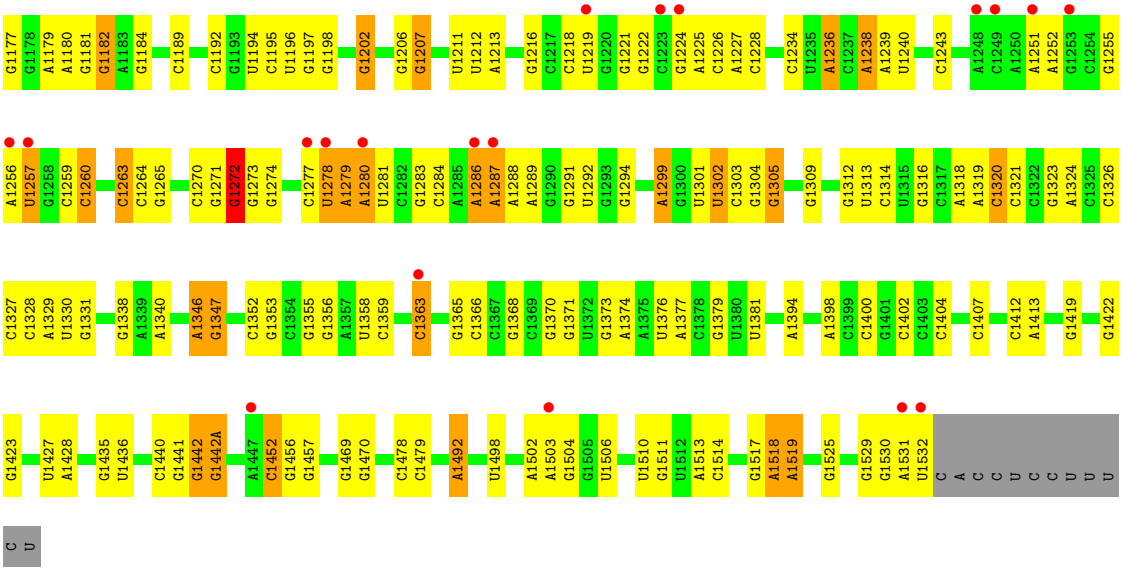




• Molecule 32: 16S Ribosomal RNA

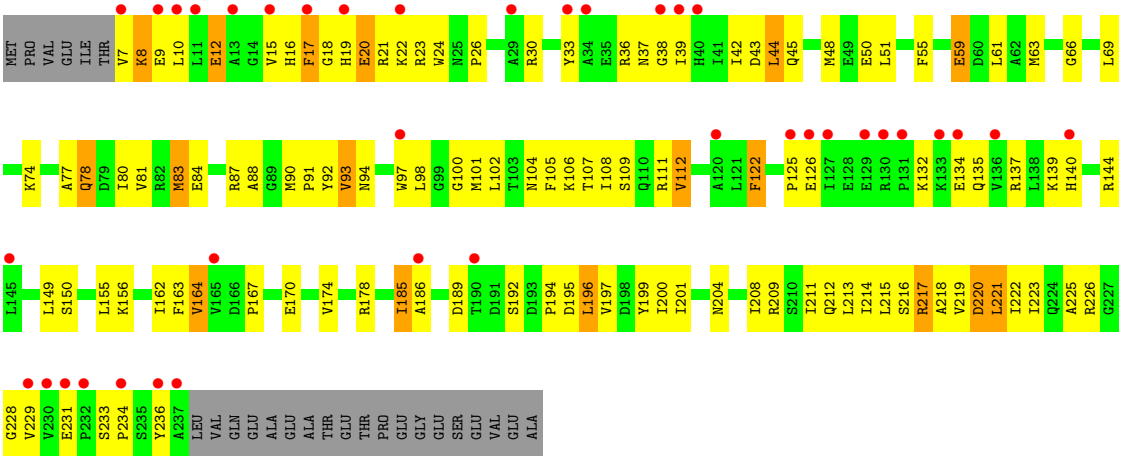
Chain 2a:





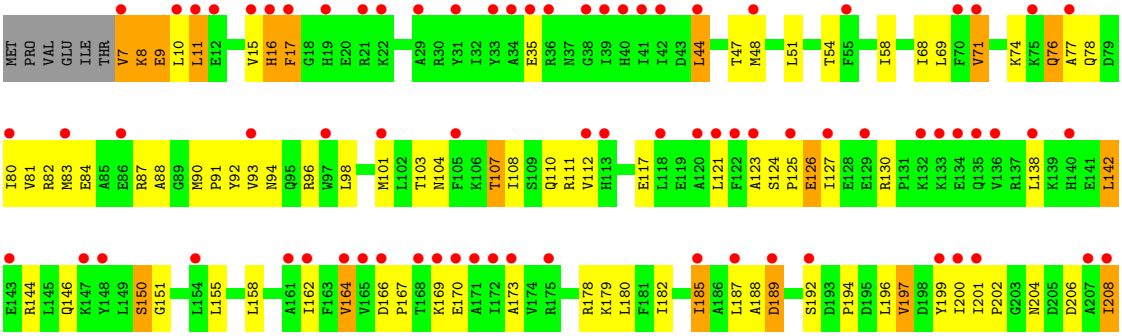
• Molecule 33: 30S ribosomal protein S2

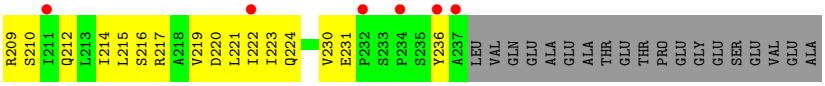
Chain 1b:



• Molecule 33: 30S ribosomal protein S2

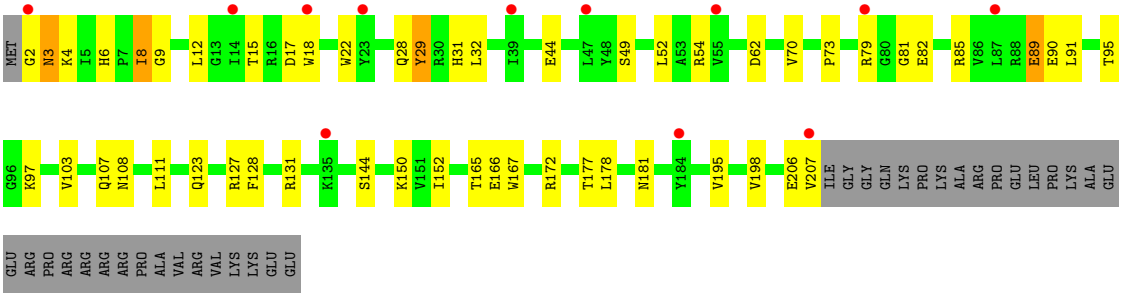
Chain 2b:





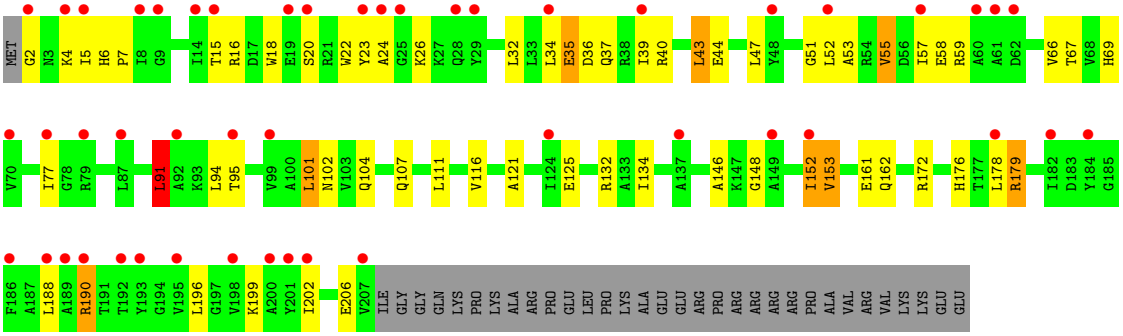
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



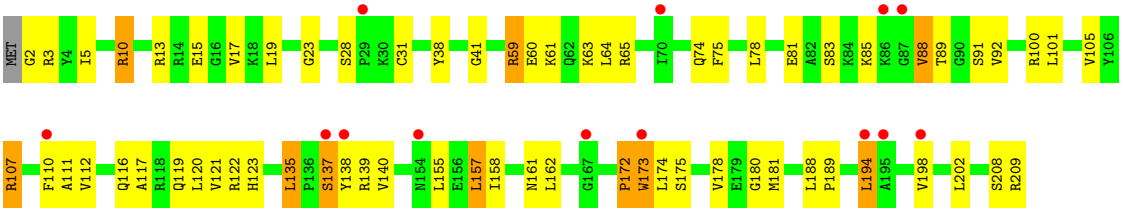
• Molecule 34: 30S ribosomal protein S3

Chain 2c:



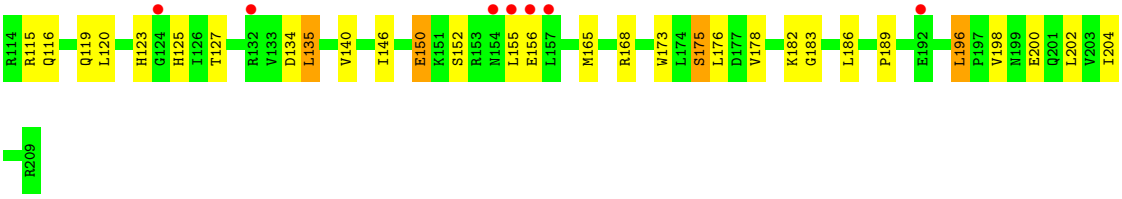
• Molecule 35: 30S ribosomal protein S4

Chain 1d:

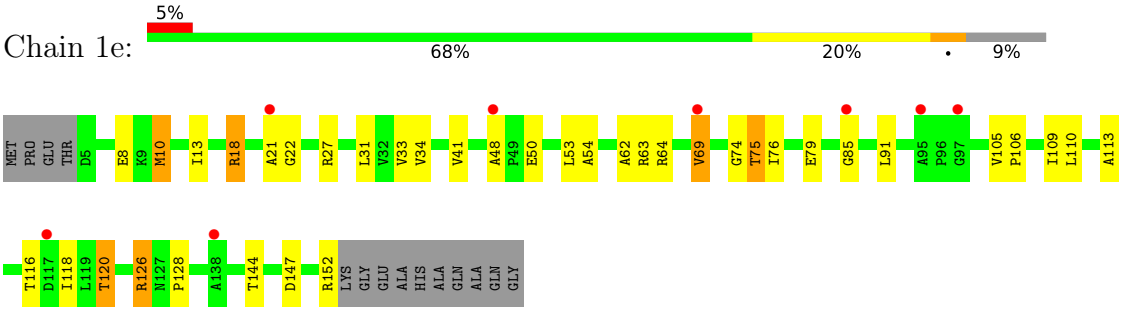


• Molecule 35: 30S ribosomal protein S4

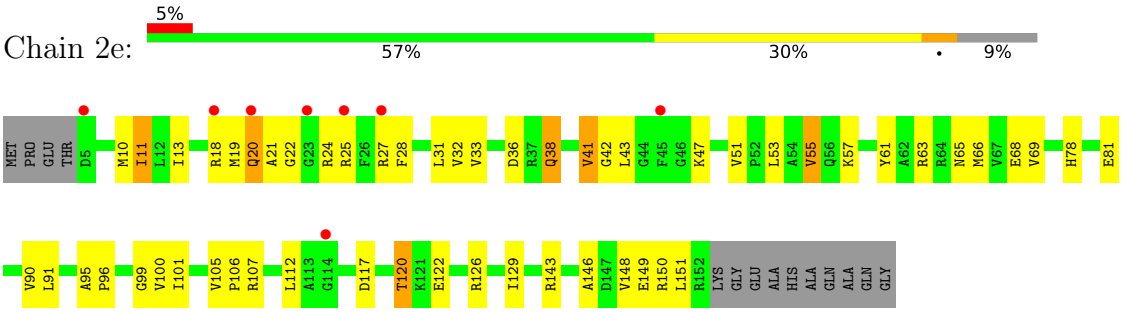
Chain 2d:



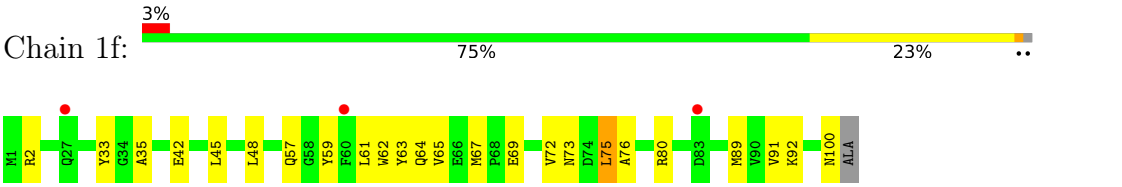
• Molecule 36: 30S ribosomal protein S5



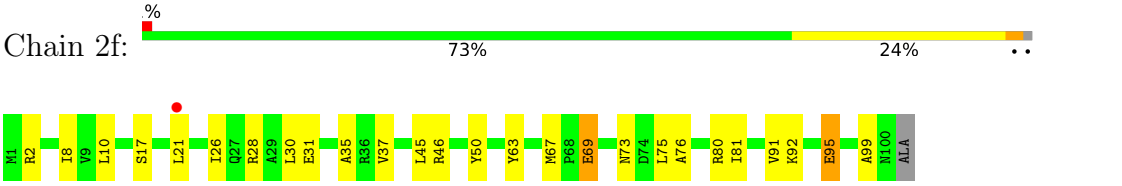
• Molecule 36: 30S ribosomal protein S5



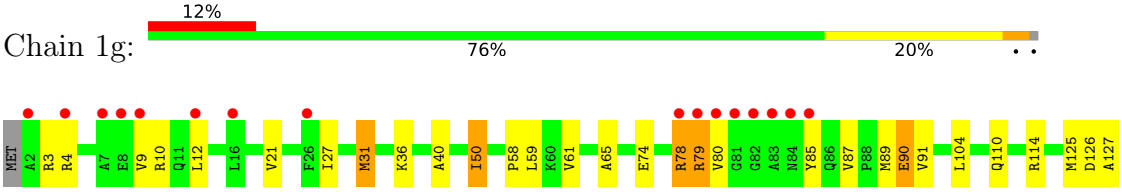
• Molecule 37: 30S ribosomal protein S6



• Molecule 37: 30S ribosomal protein S6

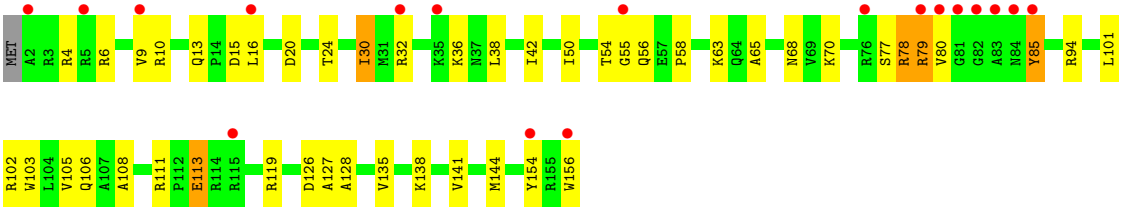


• Molecule 38: 30S ribosomal protein S7



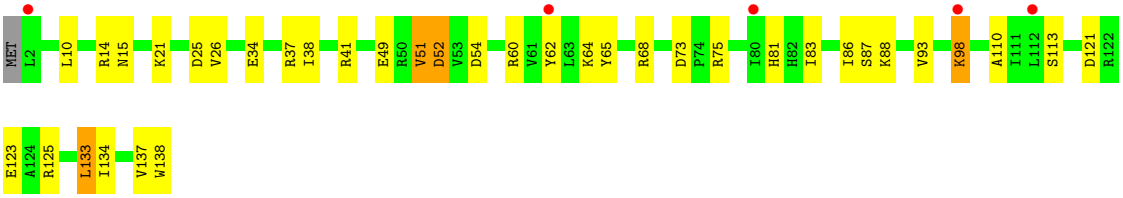
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



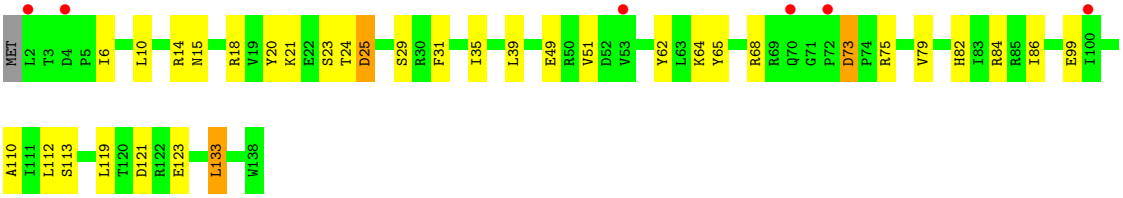
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



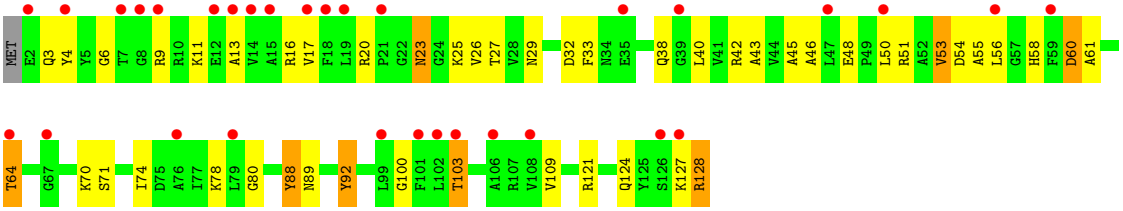
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



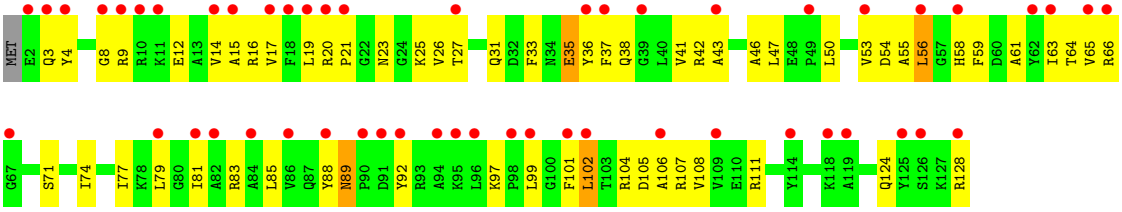
• Molecule 40: 30S ribosomal protein S9

Chain 1i:



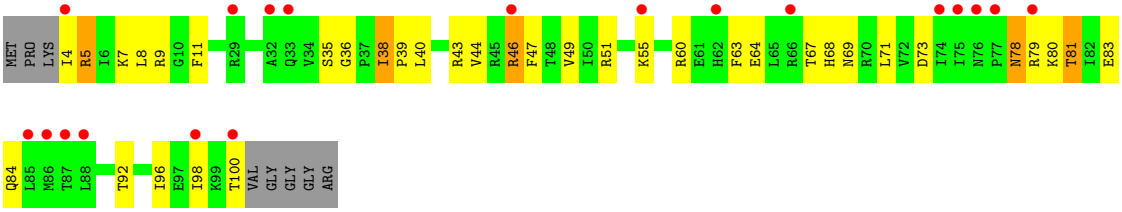
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



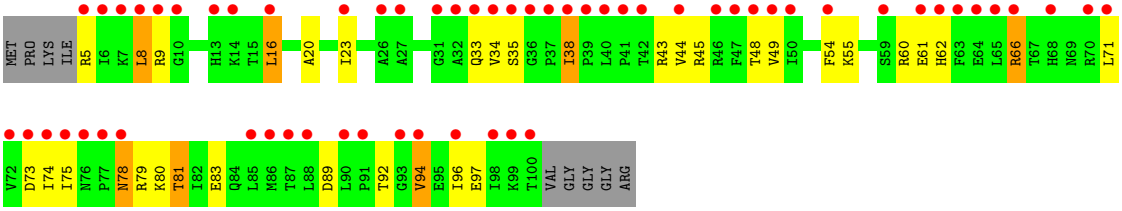
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



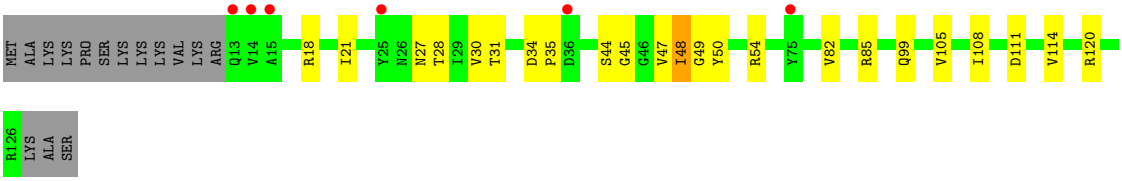
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



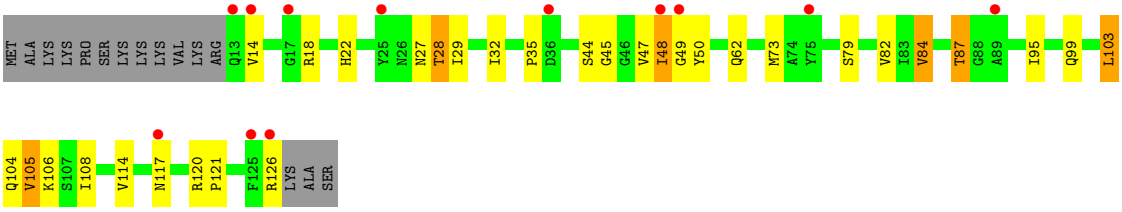
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



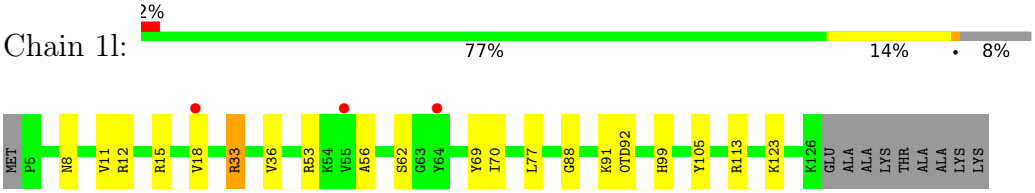
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



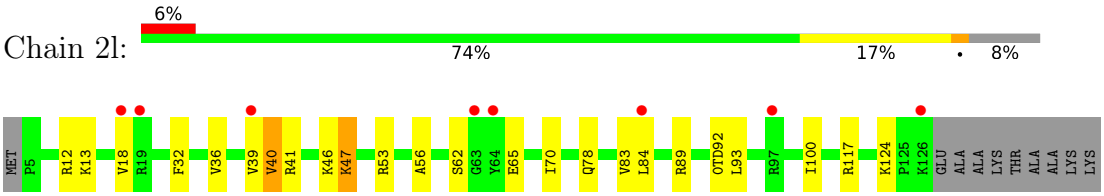
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



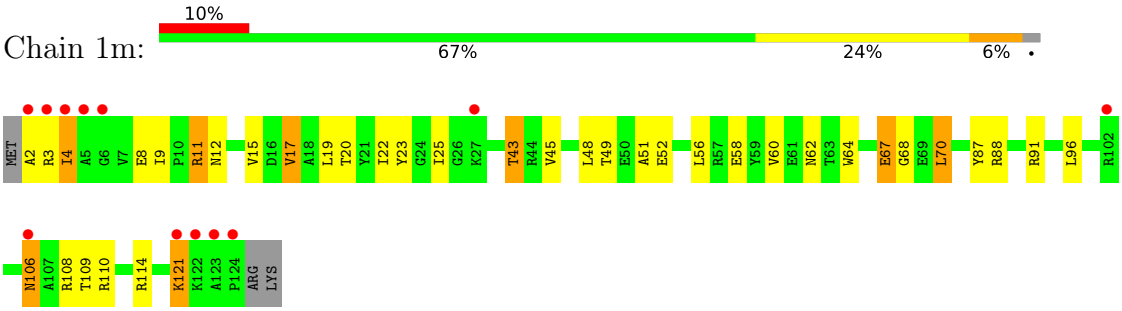
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



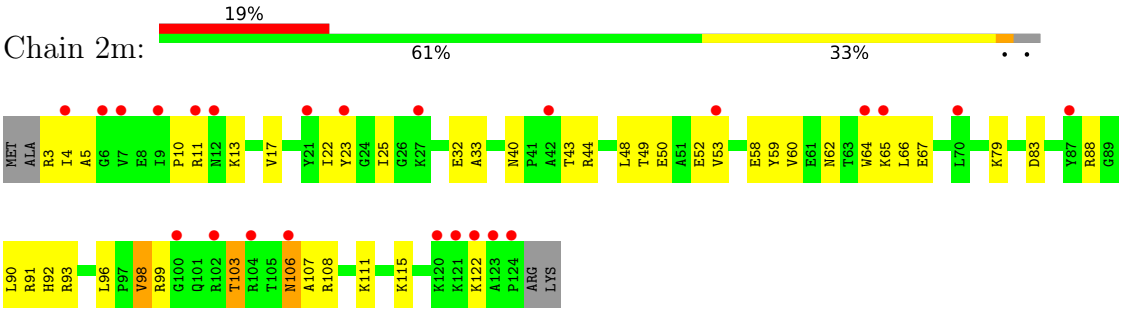
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



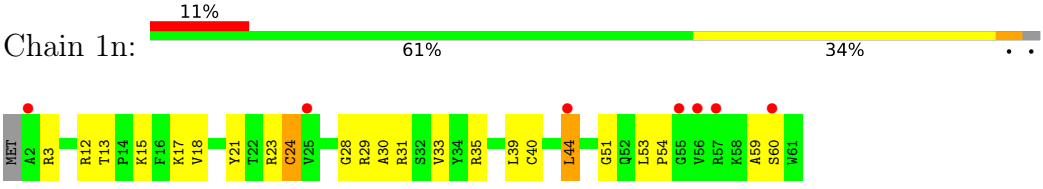
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



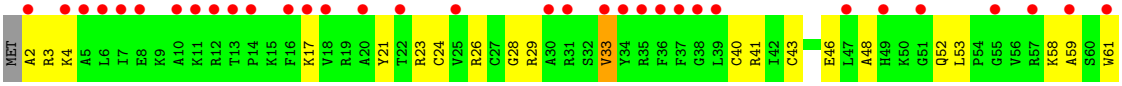
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



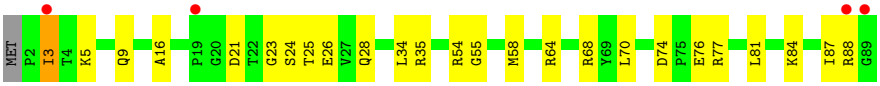
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



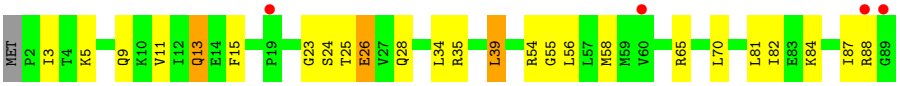
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



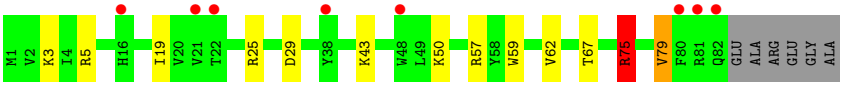
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



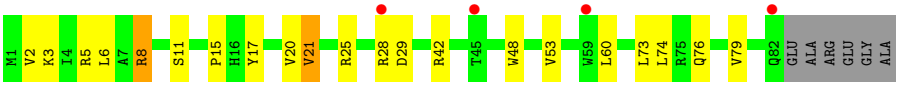
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



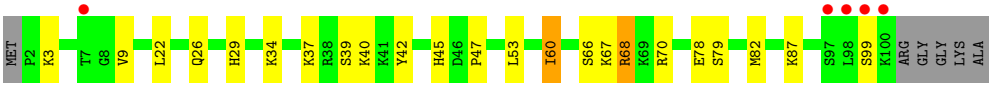
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



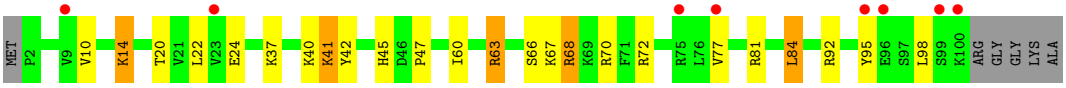
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



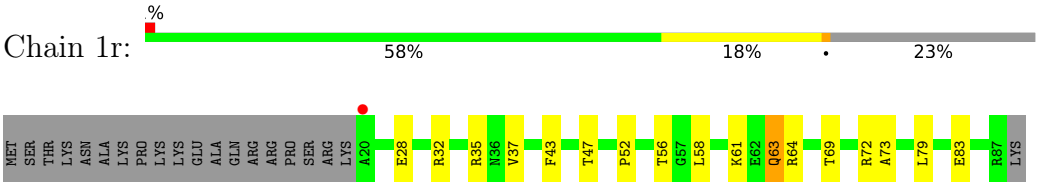
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



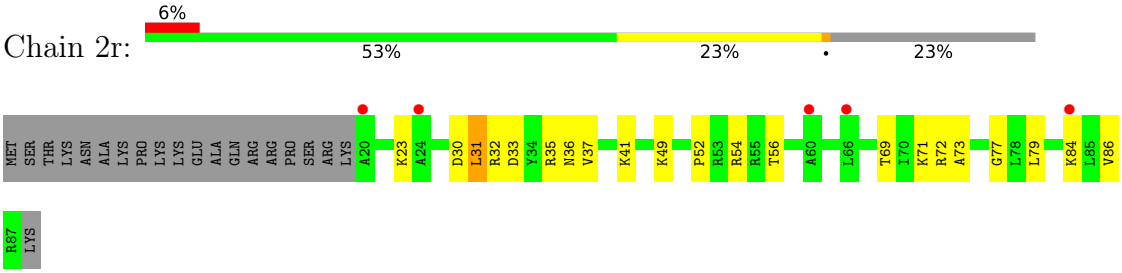
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



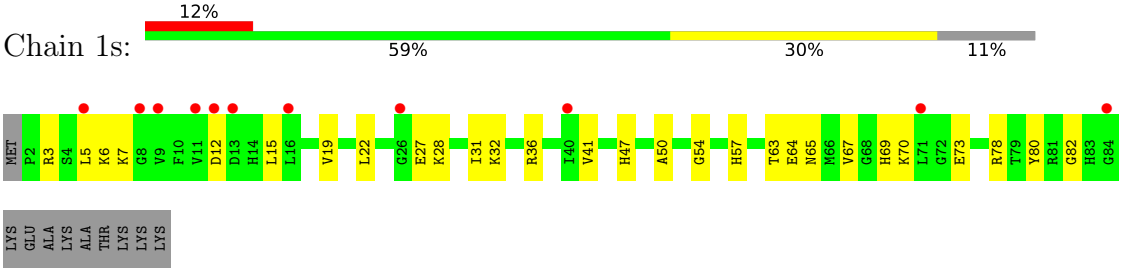
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



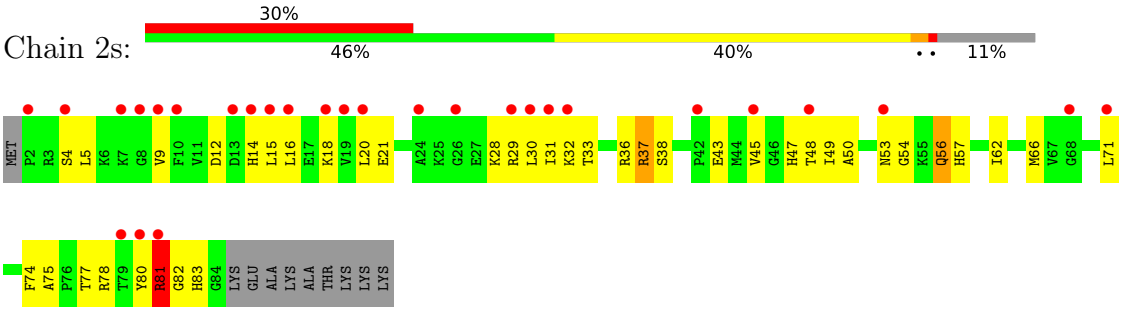
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



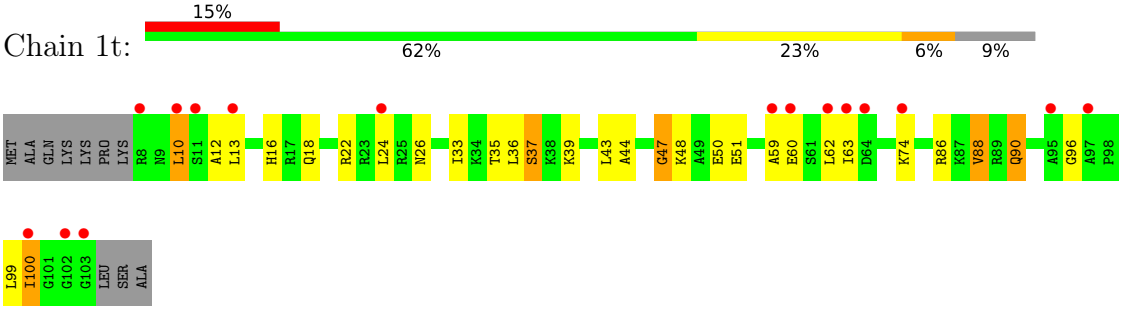
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



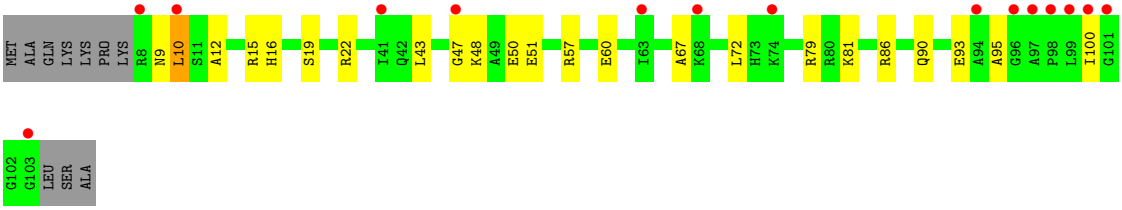
• Molecule 51: 30S ribosomal protein S20

Chain 1t:

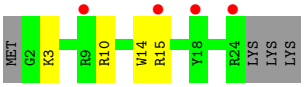


• Molecule 51: 30S ribosomal protein S20

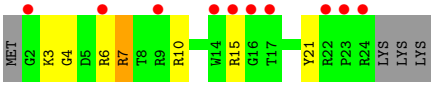
Chain 2t:



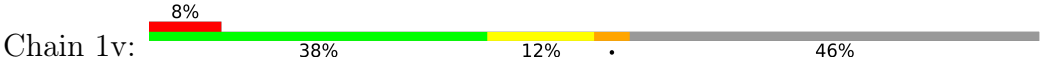
• Molecule 52: 30S ribosomal protein Thx



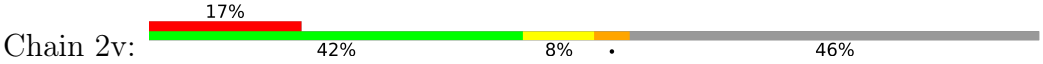
• Molecule 52: 30S ribosomal protein Thx



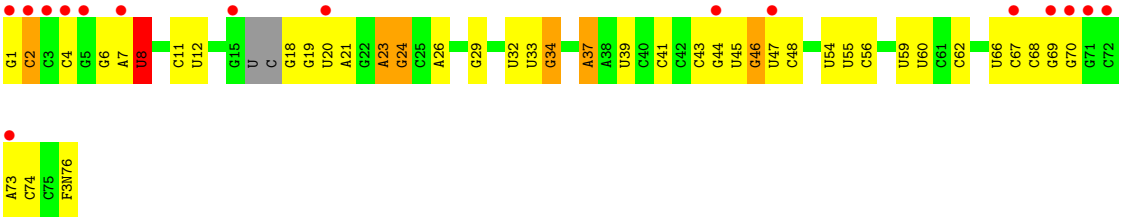
• Molecule 53: MF-mRNA



• Molecule 53: MF-mRNA

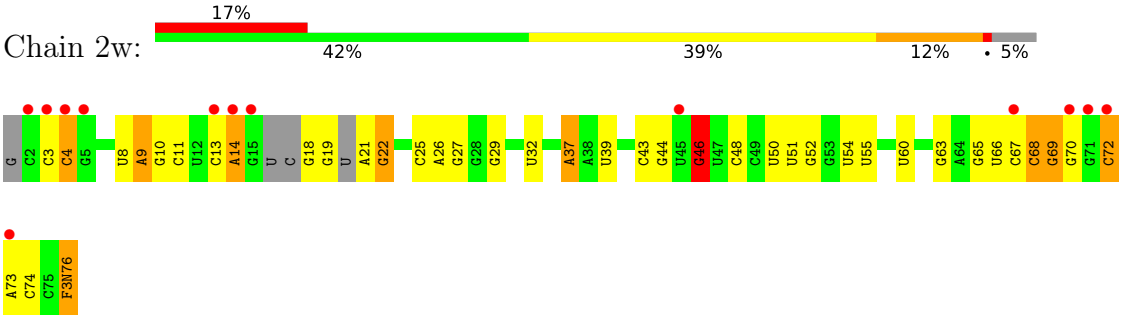


• Molecule 54: A-site Aminoacylated Phe-tRNAphe



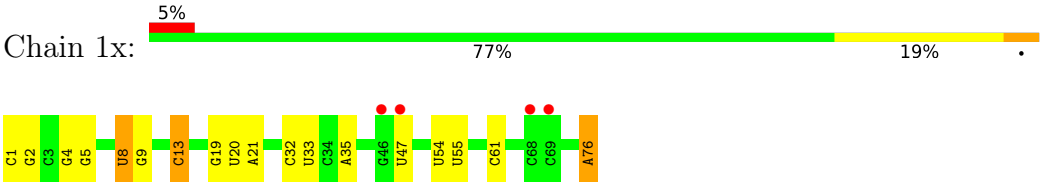
• Molecule 54: A-site Aminoacylated Phe-tRNAphe

Chain 2w:



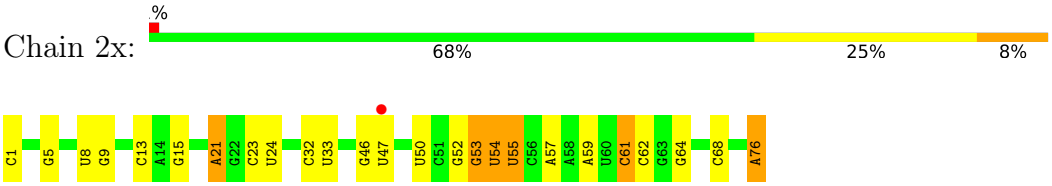
• Molecule 55: P-site Peptidyl-tRNA fMTHSMRC-tRNAmet RNA-part

Chain 1x:



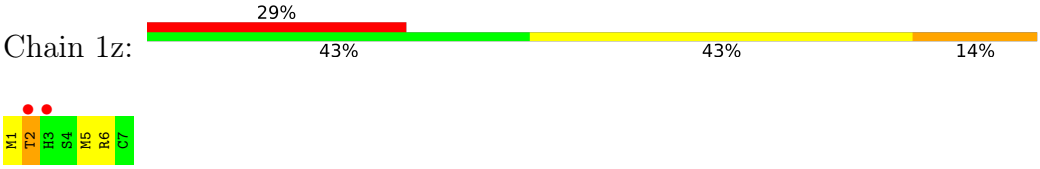
• Molecule 55: P-site Peptidyl-tRNA fMTHSMRC-tRNAmet RNA-part

Chain 2x:



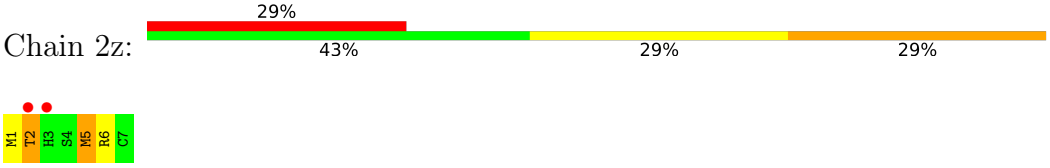
• Molecule 56: P-site Peptidyl-tRNA fMTHSMRC-tRNAmet Peptide-part

Chain 1z:



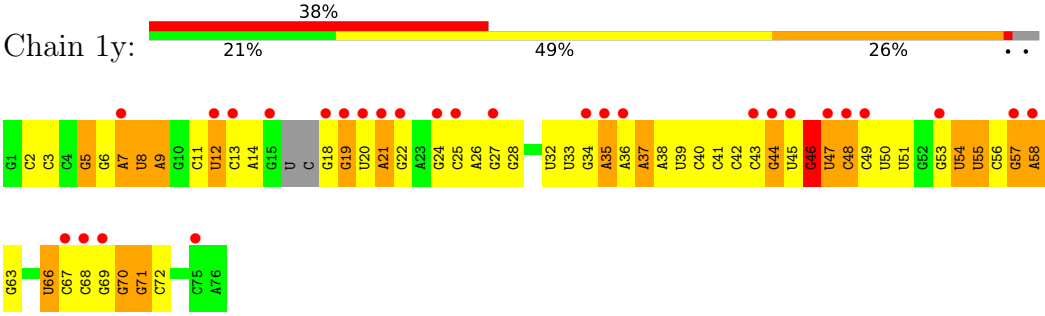
• Molecule 56: P-site Peptidyl-tRNA fMTHSMRC-tRNAmet Peptide-part

Chain 2z:



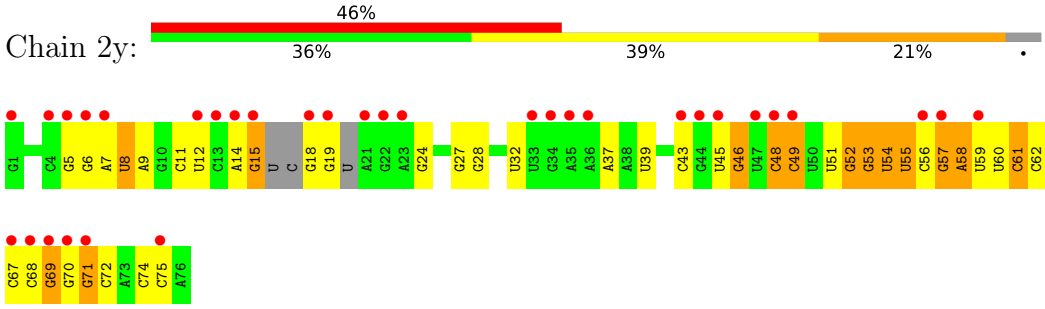
• Molecule 57: E-site Deacylated tRNAphe

Chain 1y:



• Molecule 57: E-site Deacylated tRNAphe

Chain 2y:


46%
36%
39%
21%
G1 C4 G5 G6 A7 U8 A9 G10 C11 U12 C13 A14 G15 U C G18 G19 U A21 G22 A23 G24 G27 G28 U32 U33 G34 A35 A36 A37 A38 U39 C43 G44 U45 G46 U47 C48 C49 U50 U51 G52 G53 U54 U55 C56 G57 A58 U59 U60 C61 C62 G63 A64 G65 U66
C67 C68 G69 G70 G71 C72 A73 C74 C75 A76

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.01Å 450.38Å 625.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	125.46 – 2.45 125.46 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.2 (125.46-2.45) 99.2 (125.46-2.45)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.212 , 0.249 0.215 , 0.252	Depositor DCC
R_{free} test set	106589 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	56.8	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	300665	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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: SF4, 2MU, 4SU, PSU, 5MC, 5MU, K, MG, OMG, MIA, ZN, 0TD, 8AN, 4OC, F3N, G7M, OMC, UR3, M2G, FME, MA6, 2MG, 8AH

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	0.28	0/69010	0.47	2/107716 (0.0%)
1	2A	0.21	0/67294	0.40	1/105038 (0.0%)
2	1B	0.21	0/2882	0.38	0/4494
2	2B	0.18	0/2879	0.35	0/4487
3	1D	0.27	0/2186	0.51	0/2944
3	2D	0.22	0/2186	0.45	0/2944
4	1E	0.27	0/1592	0.50	0/2149
4	2E	0.19	0/1592	0.43	0/2149
5	1F	0.25	0/1618	0.47	0/2191
5	2F	0.21	0/1614	0.45	2/2186 (0.1%)
6	1G	0.22	0/1448	0.44	0/1957
6	2G	0.19	0/1453	0.40	0/1963
7	1H	0.23	0/1356	0.43	0/1834
7	2H	0.20	0/1356	0.38	0/1834
8	1I	0.21	0/1112	0.43	0/1514
8	2I	0.19	0/1079	0.42	0/1475
9	1N	0.25	0/1144	0.45	0/1543
9	2N	0.19	0/1144	0.40	0/1543
10	1O	0.26	0/943	0.44	0/1269
10	2O	0.20	0/943	0.41	0/1269
11	1P	0.25	0/1152	0.55	0/1533
11	2P	0.20	0/1152	0.47	0/1533
12	1Q	0.27	0/1143	0.48	0/1527
12	2Q	0.20	0/1143	0.44	0/1527
13	1R	0.28	0/982	0.51	0/1312
13	2R	0.20	0/982	0.42	0/1312
14	1S	0.21	0/883	0.49	0/1176
14	2S	0.20	0/880	0.42	0/1172
15	1T	0.24	0/1105	0.45	0/1477
15	2T	0.20	0/1097	0.43	0/1468
16	1U	0.27	0/977	0.47	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	2U	0.18	0/977	0.39	0/1301
17	1V	0.25	0/782	0.47	0/1049
17	2V	0.18	0/782	0.37	0/1049
18	1W	0.28	0/897	0.47	0/1205
18	2W	0.21	0/897	0.39	0/1205
19	1X	0.26	0/764	0.53	2/1025 (0.2%)
19	2X	0.21	0/764	0.48	2/1025 (0.2%)
20	1Y	0.23	0/819	0.46	0/1095
20	2Y	0.20	0/819	0.42	0/1095
21	1Z	0.24	0/1267	0.50	1/1717 (0.1%)
21	2Z	0.22	0/1299	0.43	0/1763
22	10	0.25	0/662	0.48	0/881
22	20	0.19	0/662	0.43	0/881
23	11	0.25	0/762	0.43	0/1014
23	21	0.23	0/762	0.41	0/1014
24	12	0.27	0/590	0.47	0/781
24	22	0.18	0/590	0.40	0/781
25	13	0.27	0/474	0.50	0/635
25	23	0.17	0/469	0.38	0/630
26	14	0.27	0/565	0.66	1/761 (0.1%)
26	24	0.25	0/545	0.55	0/737
27	15	0.25	0/469	0.51	0/635
27	25	0.22	0/469	0.42	0/635
28	16	0.23	0/460	0.46	0/613
28	26	0.20	0/456	0.44	0/608
29	17	0.32	0/426	0.54	0/561
29	27	0.28	0/426	0.51	0/561
30	18	0.25	0/525	0.48	0/691
30	28	0.21	0/525	0.39	0/691
31	19	0.27	0/310	0.51	0/407
31	29	0.18	0/310	0.40	0/407
32	1a	0.20	1/35795 (0.0%)	0.39	0/55864
32	2a	0.19	0/35886	0.37	3/56005 (0.0%)
33	1b	0.23	0/1881	0.49	1/2542 (0.0%)
33	2b	0.21	0/1860	0.44	0/2518
34	1c	0.19	0/1572	0.39	0/2126
34	2c	0.21	0/1566	0.40	0/2119
35	1d	0.20	0/1685	0.43	0/2262
35	2d	0.20	0/1704	0.44	0/2284
36	1e	0.20	0/1145	0.46	0/1543
36	2e	0.20	0/1149	0.45	0/1548
37	1f	0.19	0/823	0.39	0/1115
37	2f	0.20	0/829	0.40	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.20	0/1250	0.41	0/1679
38	2g	0.19	0/1254	0.42	0/1683
39	1h	0.20	0/1108	0.43	0/1494
39	2h	0.18	0/1108	0.41	0/1494
40	1i	0.20	0/1002	0.47	0/1346
40	2i	0.20	0/997	0.45	0/1343
41	1j	0.21	0/722	0.41	0/982
41	2j	0.21	0/727	0.49	0/988
42	1k	0.19	0/844	0.41	0/1145
42	2k	0.18	0/848	0.37	0/1149
43	1l	0.21	0/937	0.43	0/1260
43	2l	0.18	0/937	0.38	0/1260
44	1m	0.19	0/969	0.47	0/1302
44	2m	0.22	0/961	0.45	0/1291
45	1n	0.20	0/501	0.53	0/664
45	2n	0.20	0/501	0.47	0/664
46	1o	0.19	0/739	0.35	0/985
46	2o	0.17	0/739	0.37	0/985
47	1p	0.25	0/697	0.52	0/939
47	2p	0.21	0/693	0.44	0/935
48	1q	0.20	0/836	0.44	0/1117
48	2q	0.17	0/836	0.42	0/1117
49	1r	0.20	0/560	0.41	0/746
49	2r	0.17	0/560	0.38	0/746
50	1s	0.20	0/667	0.49	0/900
50	2s	0.25	0/661	0.58	0/893
51	1t	0.18	0/730	0.44	0/965
51	2t	0.21	0/729	0.44	0/965
52	1u	0.22	0/203	0.44	0/266
52	2u	0.22	0/203	0.54	0/266
53	1v	0.22	0/310	0.35	0/480
53	2v	0.21	0/310	0.35	0/480
54	1w	0.28	0/1581	0.41	0/2458
54	2w	0.29	2/1531 (0.1%)	0.38	0/2379
55	1x	0.28	0/1723	0.45	0/2684
55	2x	0.25	0/1723	0.38	0/2684
56	1z	0.36	0/48	0.52	0/62
56	2z	0.24	0/48	0.53	0/62
57	1y	0.32	2/1606 (0.1%)	0.40	0/2497
57	2y	0.31	1/1583 (0.1%)	0.39	0/2459
All	All	0.23	6/316728 (0.0%)	0.43	15/474153 (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
33	1b	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2y	46	G7M	O3'-P	5.41	1.61	1.56
54	2w	46	G7M	O3'-P	5.35	1.61	1.56
32	1a	1498	UR3	O3'-P	5.32	1.61	1.56
57	1y	8	4SU	O3'-P	5.18	1.61	1.56
57	1y	46	G7M	O3'-P	5.17	1.61	1.56
54	2w	8	4SU	O3'-P	5.03	1.61	1.56

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	1Z	135	GLU	N-CA-C	-8.25	105.22	114.62
1	1A	1992	G	C2'-C3'-O3'	6.98	119.97	109.50
26	14	65	ASP	N-CA-C	-6.85	105.71	112.97
32	2a	1272	G	N1-C2-N2	-6.28	97.36	116.20
1	2A	1992	G	C2'-C3'-O3'	6.19	118.79	109.50
32	2a	1263	C	N1-C2-O2	6.09	137.17	118.90
32	2a	1272	G	N3-C2-N2	5.50	136.40	119.90
33	1b	217	ARG	N-CA-C	-5.43	106.96	113.21
19	2X	94	GLY	CA-C-N	5.38	131.39	121.70
19	2X	94	GLY	C-N-CA	5.38	131.39	121.70
5	2F	21	ALA	CA-C-N	5.14	130.95	121.70
5	2F	21	ALA	C-N-CA	5.14	130.95	121.70
19	1X	94	GLY	CA-C-N	5.02	130.73	121.70
19	1X	94	GLY	C-N-CA	5.02	130.73	121.70
1	1A	512	G	O4'-C1'-N9	5.00	115.70	108.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	122	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61853	0	31182	447	0
1	2A	60323	0	30413	536	0
2	1B	2577	0	1305	16	0
2	2B	2575	0	1303	31	0
3	1D	2136	0	2218	29	0
3	2D	2136	0	2218	29	0
4	1E	1559	0	1618	20	0
4	2E	1559	0	1618	23	0
5	1F	1583	0	1625	27	0
5	2F	1579	0	1619	42	0
6	1G	1423	0	1436	21	0
6	2G	1428	0	1438	39	0
7	1H	1330	0	1407	22	0
7	2H	1330	0	1407	27	0
8	1I	1097	0	1140	26	0
8	2I	1064	0	1082	30	0
9	1N	1117	0	1184	13	0
9	2N	1117	0	1184	21	0
10	1O	933	0	996	16	0
10	2O	933	0	996	20	0
11	1P	1135	0	1212	18	0
11	2P	1135	0	1212	27	0
12	1Q	1122	0	1179	16	0
12	2Q	1122	0	1179	22	0
13	1R	968	0	1033	11	0
13	2R	968	0	1033	18	0
14	1S	873	0	927	15	0
14	2S	870	0	923	30	0
15	1T	1091	0	1151	13	0
15	2T	1083	0	1136	20	0
16	1U	959	0	1019	10	0
16	2U	959	0	1018	15	0
17	1V	771	0	830	8	0
17	2V	771	0	830	13	0
18	1W	886	0	940	9	0
18	2W	886	0	940	11	0
19	1X	750	0	814	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2X	750	0	814	14	0
20	1Y	806	0	881	13	0
20	2Y	806	0	881	15	0
21	1Z	1240	0	1240	37	0
21	2Z	1271	0	1273	45	0
22	10	653	0	674	6	0
22	20	653	0	674	15	0
23	11	755	0	826	8	0
23	21	755	0	826	14	0
24	12	588	0	643	6	0
24	22	588	0	643	7	0
25	13	469	0	518	6	0
25	23	464	0	514	6	0
26	14	552	0	533	23	0
26	24	532	0	503	21	0
27	15	455	0	465	3	0
27	25	455	0	465	9	0
28	16	453	0	473	6	0
28	26	449	0	469	5	0
29	17	418	0	467	7	0
29	27	418	0	467	6	0
30	18	517	0	582	10	0
30	28	517	0	582	8	0
31	19	307	0	335	1	0
31	29	307	0	335	6	0
32	1a	32246	0	16295	334	0
32	2a	32327	0	16338	356	0
33	1b	1846	0	1867	69	0
33	2b	1825	0	1828	68	0
34	1c	1548	0	1535	30	0
34	2c	1542	0	1517	35	0
35	1d	1655	0	1672	46	0
35	2d	1674	0	1714	35	0
36	1e	1129	0	1185	22	0
36	2e	1133	0	1191	35	0
37	1f	810	0	804	11	0
37	2f	816	0	808	14	0
38	1g	1231	0	1238	19	0
38	2g	1235	0	1249	24	0
39	1h	1088	0	1126	24	0
39	2h	1088	0	1126	19	0
40	1i	983	0	986	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	2i	978	0	966	39	0
41	1j	709	0	650	23	0
41	2j	714	0	672	24	0
42	1k	829	0	825	12	0
42	2k	833	0	834	16	0
43	1l	932	0	981	11	0
43	2l	932	0	981	11	0
44	1m	958	0	1002	25	0
44	2m	950	0	988	32	0
45	1n	492	0	529	12	0
45	2n	492	0	529	19	0
46	1o	728	0	760	14	0
46	2o	728	0	760	17	0
47	1p	681	0	697	10	0
47	2p	677	0	686	12	0
48	1q	823	0	891	15	0
48	2q	823	0	891	18	0
49	1r	555	0	618	11	0
49	2r	555	0	618	14	0
50	1s	652	0	662	21	0
50	2s	646	0	644	29	0
51	1t	728	0	798	20	0
51	2t	727	0	796	15	0
52	1u	199	0	208	2	0
52	2u	199	0	208	6	0
53	1v	277	0	140	3	0
53	2v	277	0	140	1	0
54	1w	1603	0	828	18	0
54	2w	1555	0	797	23	0
55	1x	1646	0	839	12	0
55	2x	1646	0	839	15	0
56	1z	58	0	56	4	0
56	2z	58	0	56	4	0
57	1y	1585	0	803	36	0
57	2y	1565	0	793	37	0
58	10	12	0	0	0	0
58	11	5	0	0	0	0
58	12	2	0	0	0	0
58	13	3	0	0	0	0
58	14	1	0	0	0	0
58	15	8	0	0	0	0
58	16	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	17	4	0	0	0	0
58	18	4	0	0	0	0
58	19	1	0	0	0	0
58	1A	1111	0	0	0	0
58	1B	37	0	0	0	0
58	1D	11	0	0	0	0
58	1E	13	0	0	0	0
58	1F	15	0	0	0	0
58	1G	4	0	0	0	0
58	1H	1	0	0	0	0
58	1I	1	0	0	0	0
58	1N	4	0	0	0	0
58	1O	6	0	0	0	0
58	1P	6	0	0	0	0
58	1Q	7	0	0	0	0
58	1R	6	0	0	0	0
58	1S	3	0	0	0	0
58	1T	4	0	0	0	0
58	1U	14	0	0	0	0
58	1V	8	0	0	0	0
58	1W	6	0	0	0	0
58	1X	6	0	0	0	0
58	1Y	2	0	0	0	0
58	1Z	3	0	0	0	0
58	1a	226	0	0	0	0
58	1b	1	0	0	0	0
58	1d	1	0	0	0	0
58	1e	2	0	0	0	0
58	1f	1	0	0	0	0
58	1k	1	0	0	0	0
58	1l	2	0	0	0	0
58	1m	1	0	0	0	0
58	1n	3	0	0	0	0
58	1r	1	0	0	0	0
58	1t	1	0	0	0	0
58	1v	1	0	0	0	0
58	1w	8	0	0	0	0
58	1x	14	0	0	0	0
58	20	2	0	0	0	0
58	21	1	0	0	0	0
58	23	1	0	0	0	0
58	25	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	26	2	0	0	0	0
58	27	4	0	0	0	0
58	28	3	0	0	0	0
58	2A	826	0	0	0	0
58	2B	20	0	0	0	0
58	2D	6	0	0	0	0
58	2E	9	0	0	0	0
58	2F	8	0	0	0	0
58	2G	1	0	0	0	0
58	2O	1	0	0	0	0
58	2P	2	0	0	0	0
58	2Q	2	0	0	0	0
58	2R	2	0	0	0	0
58	2T	4	0	0	0	0
58	2U	2	0	0	0	0
58	2V	2	0	0	0	0
58	2W	2	0	0	0	0
58	2X	2	0	0	0	0
58	2Y	1	0	0	0	0
58	2a	241	0	0	0	0
58	2d	2	0	0	0	0
58	2e	2	0	0	0	0
58	2f	2	0	0	0	0
58	2j	1	0	0	0	0
58	2l	4	0	0	0	0
58	2n	2	0	0	0	0
58	2p	1	0	0	0	0
58	2q	1	0	0	0	0
58	2t	1	0	0	0	0
58	2v	3	0	0	0	0
58	2w	3	0	0	0	0
58	2x	8	0	0	0	0
59	1A	1	0	0	0	0
59	2A	1	0	0	0	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0
60	25	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0
61	2d	8	0	0	0	0
62	10	17	0	0	1	0
62	11	8	0	0	0	0
62	12	3	0	0	0	0
62	13	4	0	0	0	0
62	14	1	0	0	0	0
62	15	6	0	0	0	0
62	16	3	0	0	0	0
62	17	9	0	0	0	0
62	18	11	0	0	1	0
62	1A	2181	0	0	71	0
62	1B	62	0	0	1	0
62	1D	28	0	0	1	0
62	1E	27	0	0	2	0
62	1F	16	0	0	1	0
62	1G	2	0	0	0	0
62	1H	2	0	0	0	0
62	1N	7	0	0	1	0
62	1O	5	0	0	0	0
62	1P	21	0	0	0	0
62	1Q	12	0	0	0	0
62	1R	12	0	0	1	0
62	1S	4	0	0	0	0
62	1T	11	0	0	1	0
62	1U	13	0	0	0	0
62	1V	9	0	0	0	0
62	1W	9	0	0	2	0
62	1X	6	0	0	0	0
62	1Y	3	0	0	1	0
62	1Z	2	0	0	0	0
62	1a	436	0	0	33	0
62	1b	1	0	0	0	0
62	1d	3	0	0	1	0
62	1f	3	0	0	0	0
62	1g	1	0	0	0	0
62	1j	3	0	0	0	0
62	1l	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	1m	1	0	0	0	0
62	1n	2	0	0	0	0
62	1o	1	0	0	0	0
62	1p	1	0	0	0	0
62	1q	2	0	0	0	0
62	1r	2	0	0	0	0
62	1t	1	0	0	0	0
62	1v	4	0	0	0	0
62	1w	12	0	0	0	0
62	1x	12	0	0	1	0
62	1y	1	0	0	0	0
62	1z	5	0	0	1	0
62	20	1	0	0	0	0
62	21	4	0	0	0	0
62	23	1	0	0	0	0
62	27	3	0	0	0	0
62	28	3	0	0	0	0
62	29	1	0	0	0	0
62	2A	1216	0	0	64	0
62	2B	20	0	0	0	0
62	2D	18	0	0	0	0
62	2E	18	0	0	0	0
62	2F	14	0	0	0	0
62	2N	1	0	0	0	0
62	2O	2	0	0	0	0
62	2P	12	0	0	0	0
62	2Q	2	0	0	0	0
62	2R	2	0	0	0	0
62	2T	6	0	0	0	0
62	2U	1	0	0	0	0
62	2W	2	0	0	0	0
62	2X	1	0	0	0	0
62	2Y	2	0	0	0	0
62	2a	357	0	0	17	0
62	2c	1	0	0	0	0
62	2d	4	0	0	0	0
62	2e	3	0	0	1	0
62	2f	3	0	0	0	0
62	2j	2	0	0	2	0
62	2l	4	0	0	1	0
62	2n	2	0	0	1	0
62	2o	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	2p	2	0	0	0	0
62	2q	1	0	0	0	0
62	2r	2	0	0	0	0
62	2t	4	0	0	1	0
62	2v	3	0	0	0	0
62	2w	8	0	0	0	0
62	2x	3	0	0	0	0
62	2z	1	0	0	0	0
All	All	300665	0	196812	3255	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (3255) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.27	1.29
1:1A:1082:U:O4	1:1A:1086:A:N1	1.92	1.03
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.48	0.95
1:1A:2427:C:OP1	62:1A:4203:HOH:O	1.85	0.94
32:2a:406:G:H21	35:2d:119:GLN:HE22	1.05	0.93
1:1A:2100:G:H1	1:1A:2189:U:H3	1.17	0.93
29:17:24:THR:HG22	29:17:27:GLY:H	1.34	0.92
1:1A:1082:U:N3	1:1A:1086:A:N6	2.10	0.91
32:2a:1286:A:H8	32:2a:1287:A:H4'	1.35	0.91
32:2a:1086:U:H3	32:2a:1099:G:H22	1.17	0.90
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.20	0.90
26:24:53:GLU:HG2	26:24:55:ARG:H	1.37	0.88
32:1a:376:G:H5"	47:1p:5:ARG:HG2	1.57	0.86
1:1A:1082:U:H3	1:1A:1086:A:H61	0.88	0.86
1:1A:1062:G:H1	1:1A:1077:A:H61	1.24	0.86
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.58	0.86
1:2A:1603:A:OP1	62:2A:3905:HOH:O	1.95	0.85
32:2a:1198:G:OP1	62:2a:1902:HOH:O	1.94	0.84
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.60	0.84
32:1a:1027:C:C2	32:1a:1034:G:N2	2.46	0.83
33:1b:21:ARG:HB3	33:1b:39:ILE:HG22	1.57	0.83
32:1a:1505:G:OP2	62:1a:1904:HOH:O	1.95	0.82
1:2A:1689:A:H62	1:2A:1698:A:H2	1.25	0.82
32:2a:1133:G:H1	32:2a:1141:C:H42	1.27	0.82
1:1A:1647:G:OP1	62:1A:4205:HOH:O	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1346:G:OP2	62:1A:4204:HOH:O	1.97	0.81
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.27	0.81
44:2m:58:GLU:O	44:2m:62:ASN:ND2	2.14	0.81
36:1e:18:ARG:HD3	36:1e:27:ARG:HH12	1.46	0.81
34:2c:58:GLU:HB3	41:2j:92:THR:HG21	1.63	0.80
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.14	0.80
32:1a:509:A:OP2	62:1a:1905:HOH:O	1.98	0.80
32:1a:576:G:OP1	62:1a:1906:HOH:O	1.99	0.80
1:1A:271(K):U:H1'	8:1I:50:ARG:HD2	1.63	0.80
33:1b:33:TYR:HB2	33:1b:43:ASP:HB2	1.64	0.80
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.15	0.80
1:1A:1059:G:H1	1:1A:1079:C:H42	1.30	0.79
8:2I:69:LYS:HG3	8:2I:138:ILE:HG12	1.64	0.79
32:1a:1224:G:OP1	62:1a:1907:HOH:O	2.01	0.79
32:2a:1134:G:H1	32:2a:1140:C:H42	1.31	0.79
1:1A:1014:U:OP2	62:1A:4207:HOH:O	2.01	0.79
10:2O:48:PRO:HB3	32:2a:1422:G:H5"	1.63	0.79
1:2A:2079:U:OP1	23:21:21:ARG:NH2	2.15	0.78
28:16:13:CYS:SG	28:16:47:THR:HG21	2.24	0.78
32:1a:1086:U:H3	32:1a:1099:G:H22	1.28	0.78
1:2A:1812:A:OP2	62:2A:3906:HOH:O	2.00	0.78
54:2w:27:G:H1	54:2w:43:C:H42	1.32	0.78
32:1a:1030(A):G:H1'	32:1a:1031:G:H22	1.45	0.78
33:1b:15:VAL:HG13	33:1b:209:ARG:HG3	1.66	0.78
57:1y:7:A:O2'	57:1y:49:C:OP2	2.02	0.78
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.15	0.78
1:1A:1981:A:OP1	62:1A:4206:HOH:O	2.01	0.77
1:2A:2524:G:N7	62:2A:3933:HOH:O	2.17	0.77
32:2a:1029:C:C4	32:2a:1032:G:N1	2.52	0.77
1:2A:1253:A:OP1	62:2A:3909:HOH:O	2.02	0.77
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.18	0.76
1:2A:2319:G:H22	14:2S:3:ARG:HH11	1.31	0.76
9:2N:20:GLY:HA2	9:2N:61:ARG:HE	1.50	0.76
1:1A:2136:C:N3	1:1A:2155:G:C2	2.53	0.76
1:2A:1647:G:OP1	62:2A:3911:HOH:O	2.03	0.76
1:2A:2592:G:OP1	62:2A:3907:HOH:O	2.02	0.76
54:2w:4:C:H42	54:2w:69:G:H1	1.33	0.76
32:2a:975:A:H4'	32:2a:976:G:H5"	1.66	0.76
36:2e:20:GLN:NE2	36:2e:21:ALA:O	2.18	0.76
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.21	0.76
36:1e:144:THR:H	36:1e:147:ASP:HB2	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1058:G:H1	1:1A:1080:C:H42	1.31	0.76
22:10:9:SER:O	62:10:202:HOH:O	2.04	0.76
18:1W:92:ARG:NH2	62:1W:301:HOH:O	2.18	0.75
32:1a:1108:G:O6	62:1a:1910:HOH:O	2.04	0.75
32:1a:1467:G:O6	62:1a:1909:HOH:O	2.04	0.75
1:2A:2130:U:H2'	1:2A:2158:A:H61	1.51	0.75
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.68	0.75
1:2A:1670:C:OP1	62:2A:3908:HOH:O	2.02	0.75
32:2a:179:A:OP2	62:2a:1903:HOH:O	2.03	0.75
32:1a:934:C:OP1	62:1a:1908:HOH:O	2.04	0.75
46:1o:87:ILE:HG22	46:1o:88:ARG:H	1.52	0.75
50:1s:27:GLU:HB2	50:1s:28:LYS:HA	1.67	0.75
1:2A:528:A:OP1	62:2A:3912:HOH:O	2.04	0.75
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.68	0.75
32:1a:875:C:H1'	39:1h:15:ASN:HD21	1.52	0.75
32:1a:402:G:N7	62:1a:1929:HOH:O	2.20	0.75
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.69	0.74
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.20	0.74
57:2y:18:G:N2	57:2y:55:PSU:N3	2.30	0.74
32:2a:1181:G:O2'	32:2a:1182:G:N7	2.20	0.74
1:1A:1054:A:H61	1:1A:1105:U:H3	1.36	0.74
32:1a:953:G:H5'	32:1a:965:A:H61	1.53	0.74
32:1a:1318:A:H5"	50:1s:3:ARG:HH12	1.52	0.74
32:1a:975:A:H4'	32:1a:976:G:H5"	1.68	0.74
2:2B:103:G:H21	21:2Z:73:GLN:HE22	1.36	0.74
1:1A:2124:G:H1	1:1A:2174:C:H42	1.36	0.74
1:1A:2550:G:OP1	62:1A:4208:HOH:O	2.04	0.74
57:1y:8:4SU:O2'	57:1y:21:A:N1	2.20	0.74
1:2A:2228:G:O6	62:2A:3910:HOH:O	2.02	0.73
21:1Z:105:VAL:N	21:1Z:139:VAL:O	2.21	0.73
1:2A:481:G:N7	62:2A:3953:HOH:O	2.21	0.73
38:2g:111:ARG:NH1	38:2g:113:GLU:OE2	2.21	0.73
1:1A:1024:G:OP2	62:1A:4210:HOH:O	2.05	0.73
32:1a:38:G:H22	32:1a:397:A:H5"	1.53	0.73
32:1a:550:G:OP1	62:1a:1911:HOH:O	2.06	0.73
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.69	0.73
7:1H:86:GLU:OE2	7:1H:130:ARG:NH1	2.22	0.73
40:1i:50:LEU:HD13	40:1i:56:LEU:HA	1.69	0.73
32:2a:266:G:H5"	32:2a:268:C:H41	1.52	0.73
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.71	0.73
33:2b:189:ASP:N	33:2b:189:ASP:OD1	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.22	0.73
1:2A:2127:G:H1	1:2A:2161:C:N4	1.85	0.73
32:1a:559:A:OP1	36:1e:126:ARG:NH2	2.19	0.73
1:2A:244:A:OP1	62:2A:3914:HOH:O	2.07	0.73
1:1A:1970:A:OP1	62:1A:4209:HOH:O	2.04	0.73
1:1A:2306:C:O2	62:1A:4211:HOH:O	2.06	0.73
1:2A:981:A:OP1	62:2A:3913:HOH:O	2.06	0.73
1:1A:1602:U:O4	62:1A:4213:HOH:O	2.06	0.72
1:1A:1603:A:OP1	62:1A:4215:HOH:O	2.07	0.72
32:1a:1035:A:H2'	32:1a:1036:G:H21	1.52	0.72
1:2A:921:G:O6	62:2A:3915:HOH:O	2.07	0.72
1:1A:2128:C:N4	1:1A:2160:G:H1	1.87	0.72
1:2A:1225:G:H4'	17:2V:84:LYS:HG2	1.71	0.72
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.70	0.72
1:1A:1023:U:OP2	62:1A:4210:HOH:O	2.05	0.72
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.21	0.72
32:1a:116:A:OP1	62:1a:1912:HOH:O	2.07	0.72
1:2A:2133:G:O2'	1:2A:2157:G:N2	2.22	0.72
33:2b:74:LYS:NZ	33:2b:206:ASP:OD1	2.21	0.72
4:1E:110:GLY:O	62:1R:301:HOH:O	2.07	0.72
26:14:55:ARG:N	26:14:56:VAL:HA	2.05	0.72
1:2A:1024:G:OP2	62:2A:3916:HOH:O	2.08	0.72
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.70	0.72
33:2b:15:VAL:HG13	33:2b:209:ARG:HB3	1.71	0.72
1:1A:387:U:O4	62:1A:4212:HOH:O	2.06	0.72
1:1A:2499:C:OP1	62:1A:4214:HOH:O	2.06	0.72
1:1A:1013:C:OP2	62:1A:4207:HOH:O	2.07	0.72
1:2A:1204:A:H2	1:2A:1241:A:H62	1.37	0.72
1:1A:2319:G:H22	14:1S:3:ARG:HD3	1.54	0.72
21:2Z:146:ILE:HG12	21:2Z:174:VAL:HG13	1.72	0.72
1:2A:2110:G:OP1	1:2A:2118:U:N3	2.15	0.71
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.53	0.71
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.08	0.71
5:2F:120:GLU:HG3	5:2F:122:LYS:HG2	1.72	0.71
1:1A:1669:A:OP2	62:1A:4208:HOH:O	2.08	0.71
38:2g:78:ARG:HH21	38:2g:79:ARG:HE	1.35	0.71
4:2E:77:ILE:HD12	4:2E:195:LEU:HD13	1.70	0.71
10:1O:63:VAL:HG12	10:1O:106:LEU:HD11	1.72	0.71
32:2a:1272:G:N2	32:2a:1273:G:C5	2.59	0.71
34:2c:47:LEU:HB2	34:2c:52:LEU:HD22	1.72	0.71
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:16:CYS:SG	26:14:17:GLY:N	2.63	0.71
1:1A:1305:C:OP2	62:1A:4216:HOH:O	2.07	0.71
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.23	0.71
32:1a:664:G:H22	32:1a:741:G:H1	1.38	0.71
1:2A:1434:A:H61	1:2A:1558:A:H62	1.39	0.71
38:2g:111:ARG:NH2	38:2g:126:ASP:OD2	2.24	0.71
44:1m:3:ARG:HD2	44:1m:9:ILE:HG12	1.72	0.71
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.72	0.71
21:2Z:154:ASP:N	21:2Z:154:ASP:OD1	2.23	0.71
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.24	0.71
1:1A:1271:G:OP2	62:1A:4205:HOH:O	2.09	0.71
1:1A:2390:U:O4	62:1A:4217:HOH:O	2.09	0.71
32:2a:664:G:H22	32:2a:741:G:H1	1.39	0.71
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.24	0.70
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.25	0.70
33:2b:81:VAL:HB	33:2b:94:ASN:HD21	1.54	0.70
32:1a:933:G:O6	38:1g:3:ARG:NH2	2.23	0.70
51:1t:86:ARG:O	51:1t:90:GLN:NE2	2.25	0.70
1:1A:826:U:OP1	62:1A:4203:HOH:O	2.07	0.70
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.72	0.70
1:2A:1830:C:OP2	62:2A:3917:HOH:O	2.08	0.70
32:2a:1029:C:N3	32:2a:1032:G:N2	2.39	0.70
1:1A:602:G:O2'	1:1A:655:A:N6	2.24	0.70
32:2a:953:G:H5'	32:2a:965:A:H61	1.56	0.70
33:2b:17:PHE:HA	33:2b:44:LEU:HD21	1.74	0.70
1:2A:2625:G:O6	62:2A:3918:HOH:O	2.10	0.70
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.22	0.70
1:1A:1243:G:O2'	11:1P:7:ARG:NH2	2.24	0.70
32:1a:405:U:O4	35:1d:2:GLY:N	2.25	0.70
32:1a:964:A:OP1	62:1a:1913:HOH:O	2.09	0.70
1:2A:1271:G:OP2	62:2A:3911:HOH:O	2.10	0.70
29:27:24:THR:HG22	29:27:27:GLY:H	1.57	0.70
37:2f:76:ALA:HB1	37:2f:80:ARG:HH22	1.55	0.70
1:2A:948:G:OP1	62:2A:3919:HOH:O	2.10	0.70
33:2b:71:VAL:HB	33:2b:164:VAL:HG13	1.73	0.70
40:2i:16:ARG:HB2	40:2i:64:THR:HG22	1.72	0.70
32:2a:1272:G:N2	32:2a:1273:G:N7	2.39	0.70
42:2k:99:GLN:HG2	42:2k:105:VAL:HG21	1.72	0.70
32:1a:1030(D):A:H2'	32:1a:1031:G:H4'	1.74	0.69
1:2A:2127:G:N2	1:2A:2161:C:N3	2.40	0.69
57:2y:58:A:O2'	57:2y:60:U:OP2	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2350:C:OP2	62:1A:4218:HOH:O	2.09	0.69
6:1G:59:GLU:OE2	6:1G:138:GLN:NE2	2.26	0.69
5:2F:103:LYS:HA	5:2F:106:ARG:HD3	1.73	0.69
1:1A:1332:G:OP1	62:1A:4219:HOH:O	2.10	0.69
7:2H:88:LEU:HD11	7:2H:165:ALA:HA	1.75	0.69
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.25	0.69
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.26	0.69
32:1a:836:G:OP1	49:1r:61:LYS:NZ	2.20	0.69
1:2A:741:G:OP2	62:2A:3921:HOH:O	2.11	0.69
21:2Z:52:SER:OG	21:2Z:54:HIS:ND1	2.26	0.69
1:1A:278:A:P	1:1A:278:A:H8	2.16	0.69
1:1A:1092:C:H2'	1:1A:1093:G:H5'	1.75	0.69
62:1A:4211:HOH:O	6:1G:45:GLU:OE2	2.10	0.69
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.73	0.69
57:2y:15:G:H22	57:2y:48:C:H42	1.41	0.69
1:1A:2508:G:OP1	62:1A:4221:HOH:O	2.11	0.68
32:1a:544:G:OP1	35:1d:59:ARG:NH2	2.22	0.68
32:1a:677:U:H3	32:1a:713:G:H22	1.39	0.68
6:2G:79:ASN:OD1	6:2G:79:ASN:N	2.25	0.68
1:1A:1702:G:N7	62:1A:4253:HOH:O	2.25	0.68
32:1a:934:C:OP1	62:1a:1914:HOH:O	2.11	0.68
1:2A:2125:G:N3	1:2A:2173:A:N6	2.41	0.68
1:2A:1508:A:H4'	1:2A:1509(A):A:C5	2.29	0.68
34:1c:15:THR:HG21	34:1c:181:ASN:HA	1.75	0.68
47:2p:15:PRO:HD2	47:2p:42:ARG:HD3	1.75	0.68
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.27	0.68
1:2A:775:G:O3'	62:2A:3920:HOH:O	2.10	0.68
1:2A:2150:U:H2'	1:2A:2151:G:H8	1.58	0.68
32:2a:504:C:OP1	62:2a:1905:HOH:O	2.12	0.68
1:1A:1058:G:H1	1:1A:1080:C:N4	1.91	0.68
41:1j:4:ILE:N	41:1j:100:THR:O	2.26	0.68
40:2i:3:GLN:HE21	40:2i:20:ARG:HE	1.42	0.68
50:2s:77:THR:HG23	50:2s:78:ARG:HG3	1.75	0.68
1:1A:2235:G:N7	62:1A:4256:HOH:O	2.26	0.67
32:2a:446:G:O6	62:2a:1904:HOH:O	2.11	0.67
32:1a:644:G:OP1	62:1a:1915:HOH:O	2.11	0.67
1:2A:2448:A:OP1	62:2A:3922:HOH:O	2.12	0.67
14:2S:99:LYS:NZ	14:2S:103:GLU:OE2	2.28	0.67
40:2i:128:ARG:NH2	55:2x:33:U:OP2	2.28	0.67
26:14:61:ARG:HH12	50:1s:41:VAL:HG23	1.60	0.67
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:737:A:H1'	37:2f:73:ASN:HD21	1.60	0.67
32:2a:1134:G:H1	32:2a:1140:C:N4	1.92	0.67
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.76	0.67
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.77	0.67
1:1A:2375:G:N7	62:1A:4262:HOH:O	2.27	0.67
34:1c:44:GLU:HA	34:1c:52:LEU:HD23	1.76	0.67
36:1e:8:GLU:OE2	36:1e:63:ARG:NH2	2.28	0.67
32:2a:1102:A:O3'	33:2b:96:ARG:NH2	2.28	0.67
32:2a:1257:U:O4	45:2n:17:LYS:NZ	2.27	0.67
1:2A:106:C:H1'	20:2Y:1:MET:HE2	1.77	0.67
1:2A:2127:G:N1	1:2A:2161:C:N4	2.43	0.67
16:2U:50:ARG:HH22	17:2V:72:VAL:HG22	1.60	0.66
1:1A:2629:A:O2'	1:1A:2630:G:OP2	2.12	0.66
49:2r:31:LEU:HD23	49:2r:31:LEU:H	1.60	0.66
57:2y:55:PSU:HN1	57:2y:57:G:H5"	1.60	0.66
33:1b:8:LYS:O	33:1b:217:ARG:NH2	2.27	0.66
1:2A:793:A:O2'	62:2A:3926:HOH:O	2.14	0.66
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.28	0.66
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.78	0.66
40:1i:23:ASN:OD1	40:1i:23:ASN:N	2.27	0.66
40:1i:20:ARG:O	40:1i:60:ASP:N	2.25	0.66
57:1y:57:G:H2'	57:1y:58:A:H5'	1.78	0.66
1:2A:2133:G:HO2'	1:2A:2157:G:N2	1.94	0.66
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.78	0.66
35:1d:105:VAL:HG13	35:1d:110:PHE:HB2	1.77	0.66
55:1x:1:C:O2	62:1x:201:HOH:O	2.11	0.66
44:2m:13:LYS:HA	44:2m:44:ARG:HH11	1.61	0.66
1:2A:1648:C:OP1	62:2A:3911:HOH:O	2.12	0.66
32:1a:1197:G:OP2	62:1a:1917:HOH:O	2.12	0.66
32:2a:1029:C:N4	32:2a:1032:G:N1	2.43	0.66
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.27	0.66
32:1a:1499:A:OP2	62:1a:1904:HOH:O	2.14	0.66
51:1t:33:ILE:O	51:1t:37:SER:OG	2.14	0.66
1:2A:2431:U:OP2	62:2A:3923:HOH:O	2.12	0.66
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.61	0.66
32:2a:1002:G:C2	32:2a:1003:G:H1'	2.31	0.66
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.11	0.66
32:2a:1318:A:H1'	50:2s:37:ARG:HH21	1.61	0.66
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.76	0.65
44:1m:58:GLU:O	44:1m:62:ASN:ND2	2.24	0.65
1:2A:962:G:OP1	62:2A:3919:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1315:C:OP2	62:1A:4219:HOH:O	2.14	0.65
32:1a:1318:A:OP1	50:1s:7:LYS:NZ	2.25	0.65
1:2A:1031:G:H5"	31:29:8:LYS:HE3	1.79	0.65
1:2A:1604:C:OP2	62:2A:3924:HOH:O	2.13	0.65
32:2a:1316:G:H22	32:2a:1319:A:H5"	1.60	0.65
34:2c:35:GLU:OE2	34:2c:59:ARG:NH1	2.27	0.65
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.77	0.65
32:1a:1414:U:O4	62:1a:1916:HOH:O	2.12	0.65
1:2A:253:C:O2'	62:2A:3925:HOH:O	2.14	0.65
12:2Q:78:PRO:HG2	12:2Q:81:VAL:HG11	1.79	0.65
32:2a:1151:A:HO2'	32:2a:1152:A:H8	1.45	0.65
1:2A:400:G:N7	62:2A:3992:HOH:O	2.29	0.65
32:2a:742:G:OP2	46:2o:35:ARG:NH2	2.28	0.65
32:2a:1271:G:N2	32:2a:1272:G:N7	2.45	0.65
1:2A:1762:A:N1	62:2A:3989:HOH:O	2.29	0.65
6:2G:12:TYR:HA	6:2G:16:ARG:HG3	1.77	0.65
1:1A:1356:G:OP2	62:1A:4225:HOH:O	2.15	0.65
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	1.78	0.65
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.30	0.65
1:2A:963:U:OP2	62:2A:3919:HOH:O	2.15	0.65
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.28	0.65
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.77	0.65
32:2a:56:U:H2'	32:2a:57:G:C8	2.32	0.65
32:2a:1255:G:N7	41:2j:43:ARG:NH2	2.44	0.65
1:1A:1506:C:H2'	1:1A:1507:A:H8	1.61	0.64
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.06	0.64
32:1a:1244:C:H42	32:1a:1293:G:H1	1.45	0.64
7:2H:125:VAL:HG22	7:2H:131:VAL:HG22	1.77	0.64
32:2a:1099:G:OP2	33:2b:144:ARG:NH2	2.31	0.64
44:1m:23:TYR:HB3	44:1m:67:GLU:HA	1.79	0.64
1:2A:271(L):U:H5'	8:2I:50:ARG:HH22	1.63	0.64
6:2G:63:ILE:HD11	6:2G:144:ILE:HG13	1.79	0.64
1:1A:1055:G:H1	1:1A:1104:C:H42	1.45	0.64
21:1Z:52:SER:O	21:1Z:54:HIS:N	2.30	0.64
36:1e:10:MET:HE2	36:1e:13:ILE:HD11	1.79	0.64
42:1k:48:ILE:O	42:1k:50:TYR:N	2.30	0.64
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.14	0.64
21:2Z:140:ASP:OD1	21:2Z:141:VAL:N	2.31	0.64
26:24:50:VAL:HB	44:2m:65:LYS:HB3	1.78	0.64
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.29	0.64
1:1A:971:C:OP2	62:1A:4226:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1253:A:OP1	62:1A:4222:HOH:O	2.13	0.64
1:1A:1993:U:OP2	62:1A:4223:HOH:O	2.14	0.64
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.29	0.64
32:1a:1009:G:O6	32:1a:1020:U:O2	2.14	0.64
16:2U:49:HIS:HA	16:2U:52:ARG:HB2	1.78	0.64
25:23:35:ARG:HG2	25:23:37:LEU:HD21	1.80	0.64
1:1A:2575:C:OP2	62:1A:4224:HOH:O	2.14	0.64
32:2a:79:G:H1	32:2a:90:U:H3	1.45	0.64
50:2s:28:LYS:HB3	50:2s:29:ARG:HA	1.79	0.64
32:1a:1530:G:H2'	32:1a:1531:A:C8	2.32	0.64
32:2a:195:A:OP2	62:2a:1906:HOH:O	2.15	0.64
1:1A:1359:A:H2'	1:1A:1360:A:H5'	1.79	0.64
1:1A:1607:C:O2	62:1A:4220:HOH:O	2.11	0.64
1:1A:1721:G:H1'	1:1A:1741:A:H61	1.63	0.64
10:1O:48:PRO:HB3	32:1a:1422:G:H5"	1.80	0.64
32:1a:236:G:OP1	48:1q:40:LYS:NZ	2.31	0.64
1:2A:890:A:H2'	1:2A:892:G:C8	2.33	0.64
1:2A:2319:G:H22	14:2S:3:ARG:NH1	1.96	0.64
18:1W:92:ARG:NH1	62:1W:303:HOH:O	2.31	0.64
32:1a:165:C:H2'	32:1a:166:G:H8	1.62	0.64
32:1a:1334:G:OP2	62:1a:1919:HOH:O	2.15	0.64
35:1d:64:LEU:HB2	35:1d:198:VAL:HG11	1.80	0.64
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	1.79	0.64
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.63	0.64
1:2A:2138:C:H42	1:2A:2153:G:H1	1.44	0.64
34:1c:89:GLU:OE1	34:1c:90:GLU:N	2.31	0.64
1:2A:1023:U:OP2	62:2A:3916:HOH:O	2.15	0.64
57:2y:51:U:H3	57:2y:63:G:H1	1.45	0.64
32:1a:306:G:O3'	62:1a:1918:HOH:O	2.15	0.64
32:1a:533:A:OP1	62:1a:1920:HOH:O	2.15	0.63
36:1e:74:GLY:HA3	36:1e:116:THR:HG22	1.80	0.63
40:2i:42:ARG:NH2	40:2i:71:SER:OG	2.32	0.63
46:2o:87:ILE:HG22	46:2o:88:ARG:H	1.63	0.63
32:1a:376:G:O3'	47:1p:5:ARG:HD2	1.98	0.63
33:1b:122:PHE:HE2	33:1b:139:LYS:HB2	1.63	0.63
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.80	0.63
44:2m:107:ALA:HB3	44:2m:111:LYS:HE2	1.79	0.63
1:1A:1063:G:H2'	1:1A:1064:C:H5	1.64	0.63
20:1Y:28:LYS:NZ	20:1Y:64:GLU:OE1	2.30	0.63
1:2A:2779:U:OP1	62:2A:3927:HOH:O	2.15	0.63
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:175:SER:HB3	35:2d:186:LEU:HD21	1.80	0.63
1:1A:1069:A:H1'	1:1A:1096:A:H4'	1.80	0.63
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.15	0.63
48:2q:95:TYR:HA	48:2q:98:LEU:HD12	1.80	0.63
8:1I:101:LEU:HD12	8:1I:107:VAL:HB	1.80	0.63
1:2A:1287:A:H8	13:2R:104:ARG:HD3	1.62	0.63
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.28	0.63
1:1A:2153:G:H2'	1:1A:2154:G:H8	1.64	0.63
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.32	0.63
1:2A:1119:C:N4	62:2A:4007:HOH:O	2.32	0.63
1:2A:2657:A:O2'	7:2H:160:LYS:NZ	2.26	0.63
11:2P:89:ALA:HA	11:2P:121:LYS:HD3	1.81	0.63
35:2d:111:ALA:HB2	35:2d:120:LEU:HD12	1.81	0.63
1:1A:1816:G:O6	3:1D:35:LYS:NZ	2.27	0.63
32:1a:532:A:N6	32:1a:1206:G:O2'	2.32	0.63
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.80	0.63
32:2a:165:C:H2'	32:2a:166:G:H8	1.63	0.63
50:2s:49:ILE:HG22	50:2s:62:ILE:HD11	1.81	0.63
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.81	0.62
34:2c:179:ARG:NH1	34:2c:206:GLU:OE1	2.23	0.62
32:1a:560:U:O2'	32:1a:561:U:OP2	2.17	0.62
33:1b:48:MET:HA	33:1b:51:LEU:HD12	1.81	0.62
37:1f:89:MET:HE1	49:1r:72:ARG:HB3	1.80	0.62
32:2a:407:G:H5"	35:2d:115:ARG:HB3	1.80	0.62
32:2a:979:C:N4	62:2a:1927:HOH:O	2.32	0.62
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.81	0.62
26:14:61:ARG:HD3	50:1s:67:VAL:HG12	1.81	0.62
44:1m:49:THR:HG22	44:1m:51:ALA:H	1.64	0.62
1:2A:2156:G:H2'	1:2A:2157:G:C2	2.35	0.62
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.31	0.62
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.34	0.62
1:2A:1021:A:H62	1:2A:1141:U:H3	1.48	0.62
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.17	0.62
1:2A:1508:A:H4'	1:2A:1509(A):A:C6	2.34	0.62
10:2O:7:TYR:HE2	10:2O:20:MET:HE3	1.65	0.62
34:2c:44:GLU:HA	34:2c:52:LEU:HD23	1.79	0.62
1:1A:1093:G:H3'	1:1A:1094:U:H5"	1.81	0.62
32:2a:677:U:H3	32:2a:713:G:H22	1.47	0.62
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	1.99	0.62
26:24:46:GLN:O	26:24:48:ARG:N	2.31	0.62
1:1A:884:C:H42	1:1A:892:G:H1	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2506:U:H1'	54:2w:76:F3N:HD2	1.82	0.62
30:28:62:LEU:HB3	30:28:65:GLU:HG2	1.81	0.62
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.15	0.62
10:1O:7:TYR:HE2	10:1O:20:MET:HE3	1.65	0.62
14:1S:83:LYS:HB3	14:1S:111:GLU:HG3	1.81	0.62
1:2A:489:G:N7	18:2W:49:LYS:NZ	2.48	0.62
1:2A:625:G:O6	11:2P:107:LYS:NZ	2.33	0.62
43:2l:70:ILE:HG12	43:2l:100:ILE:HD12	1.82	0.62
32:1a:200:G:H1	32:1a:217:C:H42	1.48	0.61
1:2A:1771:C:OP1	62:2A:3928:HOH:O	2.16	0.61
7:2H:33:LEU:HD21	7:2H:136:ILE:HB	1.80	0.61
23:21:86:SER:HB3	23:21:89:GLU:HG3	1.81	0.61
32:2a:1305:G:H22	32:2a:1331:G:H1'	1.65	0.61
33:2b:74:LYS:O	33:2b:78:GLN:HG2	2.00	0.61
39:2h:21:LYS:O	39:2h:65:TYR:OH	2.15	0.61
43:2l:53:ARG:HG3	43:2l:93:LEU:HD21	1.80	0.61
57:1y:37:MIA:H2'	57:1y:38:A:C8	2.35	0.61
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.34	0.61
1:2A:2269:A:OP1	62:2A:3929:HOH:O	2.16	0.61
1:2A:2306:C:N4	6:2G:42:GLY:O	2.33	0.61
1:1A:2069:G:OP2	62:1A:4227:HOH:O	2.16	0.61
32:2a:1026:G:O6	32:2a:1036:G:N2	2.33	0.61
32:2a:1133:G:H1	32:2a:1141:C:N4	1.96	0.61
32:2a:1314:C:OP2	50:2s:4:SER:OG	2.11	0.61
45:2n:26:ARG:HD3	45:2n:43:CYS:HB3	1.82	0.61
50:2s:18:LYS:HB3	50:2s:31:ILE:HD13	1.82	0.61
26:14:54:GLY:N	26:14:55:ARG:HA	2.14	0.61
1:1A:2849:U:OP2	15:1T:95:ARG:NH1	2.33	0.61
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.34	0.61
32:2a:673:G:H2'	32:2a:674:G:C8	2.35	0.61
37:2f:8:ILE:HD13	37:2f:26:ILE:HD13	1.83	0.61
50:2s:32:LYS:HA	50:2s:50:ALA:HB3	1.82	0.61
1:1A:11:G:H2'	1:1A:12:U:H5'	1.82	0.61
51:1t:43:LEU:HD13	51:1t:51:GLU:HG2	1.82	0.61
14:2S:3:ARG:NH2	14:2S:4:LEU:O	2.34	0.61
36:2e:31:LEU:HD22	36:2e:43:LEU:HD11	1.83	0.61
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.36	0.61
20:1Y:34:LYS:NZ	62:1Y:301:HOH:O	2.33	0.61
33:2b:126:GLU:CD	33:2b:126:GLU:H	2.08	0.61
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.32	0.61
27:25:40:LYS:NZ	27:25:44:THR:O	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:14:A:H61	54:2w:21:A:H2	1.49	0.61
1:2A:602:G:O2'	1:2A:655:A:N6	2.34	0.61
1:2A:2318:G:H21	14:2S:3:ARG:HD3	1.65	0.61
32:2a:1255:G:OP1	41:2j:45:ARG:NH2	2.34	0.61
32:2a:1263:C:N3	32:2a:1272:G:O6	2.34	0.61
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.00	0.61
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.82	0.61
32:2a:165:C:H2'	32:2a:166:G:C8	2.35	0.61
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.36	0.61
33:2b:185:ILE:HG22	33:2b:199:TYR:HB2	1.82	0.61
1:1A:1359:A:H61	1:1A:1372:U:H3	1.49	0.60
1:1A:2136:C:N4	1:1A:2155:G:C6	2.69	0.60
1:2A:397:G:N7	62:2A:4003:HOH:O	2.31	0.60
1:2A:855:G:O2'	22:20:27:GLU:OE2	2.18	0.60
12:1Q:10:ARG:HH11	12:1Q:11:LYS:HE2	1.66	0.60
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.15	0.60
1:2A:1639:U:H2'	1:2A:1640:C:H5"	1.82	0.60
11:2P:118:GLY:O	11:2P:137:LYS:NZ	2.34	0.60
38:2g:68:ASN:HD22	38:2g:128:ALA:HA	1.66	0.60
33:1b:78:GLN:NE2	33:1b:94:ASN:O	2.34	0.60
48:1q:67:LYS:HA	48:1q:70:ARG:HH12	1.67	0.60
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.32	0.60
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.34	0.60
32:2a:1492:A:H4'	43:2l:47:LYS:HD2	1.83	0.60
1:1A:2128:C:H42	1:1A:2160:G:H1	1.46	0.60
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.36	0.60
6:2G:41:GLN:HB3	6:2G:43:LEU:HD22	1.83	0.60
12:2Q:35:VAL:HG22	12:2Q:102:VAL:HG22	1.83	0.60
51:2t:60:GLU:HG3	51:2t:81:LYS:HD2	1.83	0.60
1:1A:2206:G:H3'	1:1A:2207:G:N7	2.16	0.60
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.36	0.60
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.34	0.60
36:1e:105:VAL:HG21	36:1e:128:PRO:HB3	1.84	0.60
1:2A:360:G:OP1	62:2A:3930:HOH:O	2.16	0.60
33:2b:87:ARG:NH2	33:2b:220:ASP:OD1	2.24	0.60
1:1A:1069:A:H2'	1:1A:1073:A:C8	2.37	0.60
1:2A:2171:A:N3	1:2A:2172:U:N3	2.50	0.60
41:2j:5:ARG:N	62:2j:301:HOH:O	2.35	0.60
1:1A:2102:U:H3	1:1A:2187:G:H1	1.50	0.60
8:1I:95:LYS:HE3	8:1I:99:GLU:HG3	1.83	0.60
1:2A:1754:C:OP1	15:2T:96:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:4:C:H42	2:2B:117:G:H1	1.50	0.60
6:2G:124:SER:O	6:2G:124:SER:OG	2.18	0.60
21:2Z:144:LEU:HD11	21:2Z:150:LEU:HD23	1.83	0.60
32:2a:1373:G:H5"	38:2g:36:LYS:HE2	1.83	0.60
1:1A:2124:G:H1	1:1A:2174:C:N4	1.99	0.60
44:2m:5:ALA:HB3	44:2m:22:ILE:HD12	1.84	0.60
21:1Z:155:LEU:HD12	21:1Z:156:LYS:H	1.65	0.60
54:1w:33:U:O4'	54:1w:37:MIA:H151	2.02	0.60
57:1y:55:PSU:C4	57:1y:57:G:H5'	2.37	0.60
1:2A:2759:G:OP2	62:2A:3931:HOH:O	2.17	0.60
62:2A:4322:HOH:O	5:2F:74:ARG:HD2	2.00	0.60
33:2b:91:PRO:HG2	33:2b:155:LEU:HD13	1.84	0.60
54:2w:51:U:H3	54:2w:63:G:H1	1.48	0.60
2:1B:75:G:H22	21:1Z:73:GLN:HE22	1.50	0.60
2:2B:66:A:H61	2:2B:109:C:H5'	1.67	0.60
12:2Q:57:HIS:HD2	12:2Q:117:ALA:HB2	1.66	0.60
32:2a:134:A:H61	47:2p:25:ARG:NH1	2.00	0.60
32:2a:1279:A:OP2	41:2j:9:ARG:NH2	2.29	0.60
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.83	0.60
1:1A:2690:C:OP2	13:1R:17:ARG:NH2	2.35	0.59
1:2A:307:G:H21	1:2A:330:A:H62	1.48	0.59
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.83	0.59
1:1A:1971:A:OP1	62:1A:4209:HOH:O	2.16	0.59
32:1a:877:C:OP1	39:1h:88:LYS:NZ	2.28	0.59
32:1a:1040:U:H2'	32:1a:1041:A:C8	2.37	0.59
21:2Z:153:SER:HB2	21:2Z:167:PRO:HB3	1.83	0.59
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.67	0.59
19:2X:94:GLY:H	19:2X:95:LEU:HB2	1.67	0.59
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.37	0.59
32:1a:501:C:H2'	32:1a:502:G:C8	2.38	0.59
33:1b:88:ALA:HB2	33:1b:219:VAL:HG13	1.83	0.59
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	1.84	0.59
57:2y:18:G:H22	57:2y:55:PSU:HN3	1.48	0.59
1:1A:1059:G:H1	1:1A:1079:C:N4	1.99	0.59
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.00	0.59
43:1l:88:GLY:O	43:1l:99:HIS:HD2	1.85	0.59
46:1o:26:GLU:HG3	46:1o:81:LEU:HD22	1.83	0.59
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.02	0.59
20:2Y:8:LYS:HD3	20:2Y:97:ARG:NH1	2.17	0.59
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.35	0.59
15:1T:117:ASP:OD2	15:1T:120:ARG:NE	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:173:TRP:CD2	35:1d:189:PRO:HG3	2.37	0.59
37:1f:2:ARG:HD2	37:1f:69:GLU:HB3	1.84	0.59
49:1r:56:THR:HG22	49:1r:58:LEU:HG	1.84	0.59
33:1b:19:HIS:HA	33:1b:39:ILE:HD13	1.83	0.59
48:1q:22:LEU:HD11	48:1q:39:SER:HB3	1.85	0.59
32:2a:148:G:H2'	32:2a:149:A:C8	2.35	0.59
32:2a:1518:MA6:H93	32:2a:1519:MA6:H92	1.85	0.59
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.83	0.59
41:1j:7:LYS:HE3	41:1j:9:ARG:HH12	1.67	0.59
1:2A:2136:C:N4	1:2A:2155:G:H1	2.00	0.59
20:2Y:28:LYS:NZ	20:2Y:64:GLU:OE1	2.27	0.59
32:2a:1271:G:C2	32:2a:1272:G:N7	2.71	0.59
47:2p:48:TRP:HH2	47:2p:76:GLN:HE22	1.50	0.59
32:1a:78:G:N2	32:1a:91:C:N3	2.50	0.59
32:1a:545:C:OP1	35:1d:61:LYS:NZ	2.36	0.59
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.03	0.59
57:1y:36:A:H2'	57:1y:37:MIA:O4'	2.03	0.59
1:1A:1071:G:H1'	1:1A:1089:G:H2'	1.84	0.59
1:1A:2128:C:N3	1:1A:2160:G:N2	2.48	0.59
1:1A:2165:G:H1	1:1A:2171:A:H2'	1.68	0.59
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	1.83	0.59
32:2a:976:G:H5'	32:2a:1358:U:O2'	2.03	0.59
54:2w:25:C:H2'	54:2w:26:A:H8	1.67	0.59
1:1A:2218:U:O4'	23:11:52:ARG:NH2	2.35	0.58
3:1D:147:LEU:HD13	3:1D:155:LEU:HD11	1.85	0.58
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.18	0.58
33:1b:162:ILE:O	33:1b:185:ILE:HG12	2.03	0.58
32:2a:1320:C:N3	50:2s:36:ARG:NH2	2.51	0.58
48:2q:81:ARG:HH21	48:2q:84:LEU:HD21	1.68	0.58
1:1A:1187:G:H5"	17:1V:81:TYR:CE1	2.38	0.58
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.38	0.58
1:1A:2790:A:H5'	1:1A:2893:G:H21	1.68	0.58
49:1r:56:THR:HG21	49:1r:63:GLN:HE22	1.68	0.58
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.03	0.58
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.52	0.58
32:2a:973:G:H3'	32:2a:974:A:H5"	1.85	0.58
33:2b:74:LYS:HD2	33:2b:166:ASP:HB2	1.85	0.58
32:1a:78:G:N1	32:1a:91:C:N4	2.51	0.58
34:1c:150:LYS:HD3	34:1c:152:ILE:HD11	1.85	0.58
39:1h:86:ILE:HD12	39:1h:133:LEU:HD22	1.85	0.58
44:1m:3:ARG:HG2	44:1m:8:GLU:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1s:80:TYR:CZ	50:1s:82:GLY:HA2	2.38	0.58
11:2P:91:PHE:O	11:2P:121:LYS:NZ	2.31	0.58
26:24:46:GLN:C	26:24:48:ARG:H	2.11	0.58
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.02	0.58
2:1B:96:U:OP1	21:1Z:14:LYS:NZ	2.36	0.58
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	1.85	0.58
41:1j:49:VAL:HG21	45:1n:44:LEU:HD11	1.85	0.58
1:2A:706:A:OP1	3:2D:7:LYS:NZ	2.36	0.58
1:2A:922:U:H2'	1:2A:923:C:C6	2.38	0.58
1:1A:870:A:OP1	12:1Q:6:ARG:NH1	2.35	0.58
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.03	0.58
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.38	0.58
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.21	0.58
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.04	0.58
41:2j:44:VAL:HG22	41:2j:66:ARG:HB3	1.85	0.58
1:2A:143(A):C:O2'	19:2X:2:LYS:NZ	2.33	0.58
1:2A:856:C:N4	62:2A:3915:HOH:O	2.33	0.58
32:2a:942:G:N2	40:2i:124:GLN:OE1	2.33	0.58
32:2a:977:A:O2'	32:2a:981:U:N3	2.37	0.58
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.84	0.58
32:1a:828:A:OP1	39:1h:21:LYS:NZ	2.36	0.58
1:2A:330:A:H2	1:2A:1210:A:HO2'	1.52	0.58
1:2A:668:G:H5'	1:2A:669:G:OP2	2.03	0.58
7:2H:9:ILE:N	7:2H:50:VAL:O	2.21	0.58
32:2a:692:U:O2'	32:2a:694:A:N7	2.27	0.58
1:1A:763:G:OP1	62:1A:4230:HOH:O	2.17	0.58
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.84	0.58
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.37	0.58
32:2a:376:G:H5"	47:2p:5:ARG:HB2	1.85	0.58
50:2s:53:ASN:HD21	50:2s:56:GLN:HB2	1.69	0.58
5:1F:185:ASP:OD1	5:1F:188:ARG:NH1	2.36	0.58
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.69	0.58
1:2A:2135:A:C8	1:2A:2136:C:H5	2.21	0.58
32:2a:393:A:OP1	62:2a:1907:HOH:O	2.17	0.58
32:2a:560:U:H5'	32:2a:566:G:N2	2.19	0.58
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.39	0.58
1:1A:1079:C:H2'	1:1A:1080:C:O4'	2.04	0.58
3:1D:2:ALA:N	3:1D:200:ASP:OD2	2.37	0.58
26:14:59:PHE:CD2	50:1s:64:GLU:HB3	2.39	0.58
32:1a:222:U:H2'	32:1a:223:U:C6	2.39	0.58
32:1a:266:G:H5"	32:1a:268:C:H41	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:157:LEU:HD22	35:1d:161:ASN:HD21	1.69	0.58
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.86	0.58
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.17	0.58
32:2a:179:A:N7	62:2a:1928:HOH:O	2.32	0.58
32:2a:651:C:N4	32:2a:753:A:OP2	2.36	0.58
34:2c:22:TRP:CH2	34:2c:32:LEU:HB3	2.39	0.58
37:2f:46:ARG:HH22	49:2r:37:VAL:HG11	1.69	0.58
38:2g:113:GLU:HG3	38:2g:119:ARG:HG2	1.86	0.58
54:2w:4:C:N4	54:2w:69:G:H1	2.01	0.58
54:2w:25:C:H2'	54:2w:26:A:C8	2.39	0.58
1:1A:2428:G:OP1	62:1A:4203:HOH:O	2.17	0.57
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.36	0.57
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.19	0.57
33:1b:91:PRO:HG2	33:1b:155:LEU:HD13	1.86	0.57
33:1b:208:ILE:H	33:1b:208:ILE:HD12	1.68	0.57
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.85	0.57
21:2Z:4:ARG:HG2	21:2Z:58:VAL:HB	1.86	0.57
43:2l:13:LYS:NZ	62:2l:301:HOH:O	2.36	0.57
15:1T:127:ALA:C	15:1T:129:ARG:H	2.10	0.57
32:1a:673:G:H2'	32:1a:674:G:C8	2.39	0.57
35:1d:15:GLU:OE2	35:1d:59:ARG:NH1	2.37	0.57
45:1n:24:CYS:HB3	45:1n:28:GLY:H	1.69	0.57
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.23	0.57
1:1A:741:G:OP2	62:1A:4231:HOH:O	2.17	0.57
13:1R:118:GLU:H	13:1R:118:GLU:CD	2.13	0.57
32:1a:749:C:H2'	32:1a:750:G:H8	1.70	0.57
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.40	0.57
33:2b:150:SER:OG	33:2b:151:GLY:N	2.38	0.57
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.38	0.57
32:1a:473:G:OP2	47:1p:75:ARG:NH1	2.36	0.57
32:1a:1036:G:H5"	32:1a:1037:C:C5	2.39	0.57
1:2A:947:G:OP2	62:2A:3934:HOH:O	2.18	0.57
1:2A:2506:U:O2'	54:2w:76:F3N:H4'	2.04	0.57
1:1A:2136:C:C2	1:1A:2155:G:N2	2.73	0.57
21:1Z:152:ALA:HB1	21:1Z:163:LEU:HD11	1.86	0.57
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.20	0.57
44:1m:2:ALA:N	44:1m:8:GLU:OE1	2.38	0.57
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.87	0.57
2:2B:7:G:N2	14:2S:38:GLN:HE22	2.01	0.57
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	1.87	0.57
32:2a:1004:A:C8	32:2a:1005:A:H4'	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1202:G:O4'	45:2n:29:ARG:NH1	2.38	0.57
1:1A:1062:G:H1	1:1A:1077:A:N6	1.98	0.57
1:1A:1506:C:H2'	1:1A:1507:A:C8	2.39	0.57
54:1w:29:G:H1	54:1w:41:C:H42	1.53	0.57
1:2A:1012:U:C5	9:2N:28:THR:HG21	2.40	0.57
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.51	0.57
32:2a:972:C:O2'	41:2j:55:LYS:O	2.21	0.57
40:2i:21:PRO:HA	40:2i:59:PHE:HA	1.86	0.57
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.85	0.57
44:2m:25:ILE:HD11	44:2m:60:VAL:HG11	1.86	0.57
48:2q:45:HIS:CD2	48:2q:47:PRO:HG3	2.40	0.57
13:2R:2:ARG:HG2	13:2R:5:LYS:HB2	1.87	0.57
32:2a:1329:A:OP2	52:2u:7:ARG:NH1	2.31	0.57
50:2s:80:TYR:O	50:2s:81:ARG:HG2	2.04	0.57
57:2y:8:4SU:H1'	57:2y:48:C:H1'	1.87	0.57
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.38	0.57
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.39	0.57
32:1a:548:G:OP1	62:1a:1923:HOH:O	2.16	0.57
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.87	0.57
48:1q:26:GLN:OE1	48:1q:37:LYS:NZ	2.38	0.57
34:2c:32:LEU:O	34:2c:36:ASP:HB2	2.04	0.57
1:1A:1762:A:H2'	62:1A:6137:HOH:O	2.04	0.57
11:1P:39:LYS:HB2	11:1P:45:LEU:HD13	1.87	0.57
32:1a:757:U:O4	62:1a:1922:HOH:O	2.16	0.57
1:2A:621:A:OP2	11:2P:108:LYS:NZ	2.29	0.57
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.38	0.57
40:2i:31:GLN:HE21	40:2i:36:TYR:HD1	1.53	0.57
1:1A:1068:G:C8	1:1A:1096:A:H1'	2.40	0.57
4:1E:127:ASP:OD2	62:1E:401:HOH:O	2.17	0.57
32:2a:1118:C:OP1	40:2i:104:ARG:NH1	2.35	0.57
33:2b:121:LEU:HD21	33:2b:130:ARG:HH12	1.69	0.57
42:2k:48:ILE:O	42:2k:50:TYR:N	2.34	0.57
8:1I:126:TYR:HB2	8:1I:142:VAL:HG23	1.85	0.56
57:1y:42:C:H2'	57:1y:43:C:C6	2.39	0.56
32:2a:838:G:H1	32:2a:848:C:H42	1.53	0.56
32:2a:1352:C:OP1	52:2u:3:LYS:NZ	2.27	0.56
57:2y:46:G7M:O2'	57:2y:48:C:OP2	2.20	0.56
1:1A:271(H):G:H1	1:1A:271(P):C:H42	1.53	0.56
1:1A:1053:C:H42	1:1A:1106:G:H1	1.51	0.56
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.05	0.56
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:370:G:OP2	62:2A:3932:HOH:O	2.17	0.56
1:2A:1365:A:O2'	23:21:11:ARG:NH1	2.38	0.56
32:1a:309:G:O2'	32:1a:607:A:N1	2.38	0.56
32:1a:1070:U:OP1	36:1e:18:ARG:NH2	2.36	0.56
33:1b:87:ARG:NH2	33:1b:220:ASP:OD1	2.36	0.56
1:2A:141:A:H8	1:2A:1408:C:HO2'	1.50	0.56
1:2A:1013:C:H42	1:2A:1149:G:H1	1.53	0.56
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.86	0.56
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.40	0.56
6:2G:114:ILE:HA	6:2G:140:ILE:HD11	1.87	0.56
18:2W:19:LEU:HB3	27:25:25:LEU:HG	1.86	0.56
32:2a:17:U:H2'	32:2a:18:C:C6	2.40	0.56
32:2a:1053:G:H4'	32:2a:1054:C:H3'	1.87	0.56
32:2a:1194:U:H4'	36:2e:22:GLY:HA2	1.87	0.56
35:2d:173:TRP:CD2	35:2d:189:PRO:HB3	2.41	0.56
36:2e:24:ARG:H	36:2e:24:ARG:HD2	1.69	0.56
54:2w:27:G:H1	54:2w:43:C:N4	2.00	0.56
1:1A:120:U:OP2	62:1A:4232:HOH:O	2.17	0.56
4:1E:29:GLY:HA3	62:1E:402:HOH:O	2.05	0.56
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	1.86	0.56
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.41	0.56
15:2T:24:PRO:HA	15:2T:49:VAL:HG12	1.88	0.56
32:2a:1029:C:N4	32:2a:1032:G:C6	2.73	0.56
40:2i:79:LEU:HG	40:2i:83:ARG:HD2	1.85	0.56
50:2s:12:ASP:OD1	50:2s:37:ARG:NH1	2.39	0.56
50:2s:30:LEU:HD11	50:2s:50:ALA:HB2	1.88	0.56
28:16:14:THR:HB	28:16:48:VAL:O	2.05	0.56
41:1j:8:LEU:HD22	41:1j:96:ILE:HG22	1.88	0.56
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.71	0.56
49:2r:52:PRO:HB2	49:2r:54:ARG:HG3	1.86	0.56
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.87	0.56
54:1w:26:A:H61	54:1w:44:G:H1	1.54	0.56
32:2a:773:G:N7	62:2a:1930:HOH:O	2.33	0.56
51:2t:57:ARG:HH12	51:2t:100:ILE:HD12	1.70	0.56
7:1H:41:MET:HE2	7:1H:65:HIS:HA	1.87	0.56
33:2b:178:ARG:HH22	39:2h:68:ARG:HH12	1.52	0.56
1:1A:1171:G:OP2	1:1A:1174:A:N6	2.39	0.56
1:1A:1671:U:O4	62:1A:4208:HOH:O	2.18	0.56
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.21	0.56
5:1F:31:HIS:NE2	5:1F:35:GLU:OE2	2.39	0.56
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:972:C:O2'	41:1j:55:LYS:O	2.23	0.56
32:1a:974:A:H8	32:1a:974:A:OP1	1.89	0.56
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.22	0.56
11:2P:121:LYS:O	11:2P:123:LEU:N	2.39	0.56
32:2a:56:U:H2'	32:2a:57:G:H8	1.71	0.56
32:2a:64:G:H4'	32:2a:65:U:H3'	1.88	0.56
32:2a:946:A:H2'	32:2a:947:G:C8	2.41	0.56
33:2b:214:ILE:HG22	33:2b:215:LEU:HD23	1.87	0.56
1:1A:271(O):C:H2'	1:1A:271(P):C:C6	2.41	0.56
33:1b:132:LYS:HA	33:1b:135:GLN:HB3	1.88	0.56
44:1m:3:ARG:HG3	44:1m:4:ILE:H	1.71	0.56
50:1s:63:THR:OG1	50:1s:65:ASN:OD1	2.21	0.56
1:2A:2163:C:H5'	1:2A:2172:U:OP2	2.06	0.56
1:2A:2889:C:H2'	1:2A:2891:G:O4'	2.06	0.56
62:2A:4025:HOH:O	27:25:2:ALA:N	2.39	0.56
3:2D:71:ASP:HB2	3:2D:103:ARG:HH12	1.71	0.56
12:2Q:77:LYS:NZ	12:2Q:86:GLY:O	2.39	0.56
32:2a:179:A:H2'	32:2a:180:U:C6	2.41	0.56
1:1A:2629:A:H1'	1:1A:2630:G:H5"	1.88	0.55
32:1a:731:G:H5'	32:1a:766:A:H4'	1.88	0.55
32:1a:1152:A:OP1	41:1j:68:HIS:ND1	2.39	0.55
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.38	0.55
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.40	0.55
1:1A:1092:C:C2'	1:1A:1093:G:H5'	2.36	0.55
1:1A:2685:G:H5'	10:1O:68:GLU:OE2	2.06	0.55
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.88	0.55
26:14:61:ARG:O	26:14:61:ARG:NE	2.30	0.55
33:1b:20:GLU:HG2	33:1b:23:ARG:NH1	2.22	0.55
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.32	0.55
57:1y:8:4SU:H4'	57:1y:48:C:H4'	1.89	0.55
32:2a:1103:C:P	33:2b:96:ARG:HH22	2.28	0.55
32:1a:953:G:H2'	32:1a:954:G:O4'	2.06	0.55
47:1p:59:TRP:HA	47:1p:62:VAL:HG12	1.86	0.55
13:2R:36:THR:HG22	13:2R:37:THR:H	1.71	0.55
24:22:31:GLU:HB3	24:22:53:LEU:HD11	1.88	0.55
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.89	0.55
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.41	0.55
34:2c:20:SER:HB3	34:2c:22:TRP:HE1	1.71	0.55
1:1A:247:G:H4'	1:1A:386:G:C5	2.41	0.55
1:1A:2226:C:OP2	62:1A:4233:HOH:O	2.18	0.55
23:11:72:GLU:OE2	23:11:76:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:43:ALA:HA	40:1i:74:ILE:HD13	1.87	0.55
1:2A:2058:A:N7	62:2A:4017:HOH:O	2.33	0.55
35:2d:140:VAL:HG11	35:2d:146:ILE:HD11	1.89	0.55
1:1A:2099:U:H3	1:1A:2190:G:H1	1.52	0.55
1:1A:2765:A:OP2	62:1A:4234:HOH:O	2.18	0.55
19:1X:60:ARG:HH22	29:17:47:ARG:HH22	1.55	0.55
21:1Z:103:ARG:O	21:1Z:139:VAL:N	2.39	0.55
54:1w:23:A:H3'	54:1w:24:G:H8	1.72	0.55
32:2a:419:C:OP1	32:2a:513:C:O2'	2.22	0.55
42:2k:87:THR:O	42:2k:87:THR:OG1	2.25	0.55
1:1A:528:A:O2'	1:1A:529:A:H5'	2.06	0.55
32:1a:1032:G:H2'	32:1a:1033:G:O4'	2.06	0.55
49:1r:52:PRO:O	49:1r:56:THR:OG1	2.14	0.55
1:2A:2136:C:HO2'	1:2A:2137:C:H6	1.53	0.55
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.24	0.55
5:2F:7:TYR:O	5:2F:22:ALA:N	2.37	0.55
26:24:10:VAL:HG22	26:24:11:PRO:HD2	1.88	0.55
32:2a:662:G:O2'	32:2a:836:G:OP1	2.24	0.55
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.20	0.55
33:2b:78:GLN:O	33:2b:94:ASN:ND2	2.40	0.55
1:1A:1039:G:H1	1:1A:1116:C:H42	1.55	0.55
1:1A:1057:A:N7	1:1A:1086:A:H2'	2.22	0.55
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	1.88	0.55
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.90	0.55
5:2F:180:GLY:O	5:2F:182:ASN:ND2	2.37	0.55
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.72	0.55
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.07	0.55
32:2a:1117:G:H5'	32:2a:1118:C:OP2	2.07	0.55
35:2d:22:LYS:O	35:2d:113:SER:HB3	2.06	0.55
46:2o:39:LEU:HD13	46:2o:56:LEU:HB2	1.87	0.55
1:1A:2153:G:H2'	1:1A:2154:G:C8	2.41	0.55
2:1B:23:G:O6	62:1B:301:HOH:O	2.18	0.55
32:1a:757:U:H2'	32:1a:758:G:O4'	2.06	0.55
35:1d:117:ALA:O	35:1d:121:VAL:HG23	2.07	0.55
57:1y:2:C:H42	57:1y:71:G:H1	1.54	0.55
1:2A:893:C:H5'	1:2A:894:C:C5	2.42	0.55
1:2A:1300:U:H4'	1:2A:1301:A:H5"	1.89	0.55
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.42	0.55
2:2B:103:G:H21	21:2Z:73:GLN:NE2	2.05	0.55
19:2X:60:ARG:HH22	29:27:47:ARG:NH2	2.04	0.55
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:620:C:C2	35:2d:135:LEU:HG	2.42	0.55
36:2e:81:GLU:HG2	36:2e:90:VAL:HG22	1.89	0.55
42:2k:27:ASN:OD1	42:2k:28:THR:N	2.39	0.55
45:2n:23:ARG:NH1	45:2n:28:GLY:O	2.40	0.55
1:1A:615:G:OP1	5:1F:40:GLN:NE2	2.35	0.55
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.36	0.55
1:1A:2518:A:OP1	62:1A:4235:HOH:O	2.18	0.55
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.89	0.55
33:1b:163:PHE:CD1	33:1b:185:ILE:HG13	2.42	0.55
45:1n:23:ARG:NH1	45:1n:30:ALA:HB2	2.21	0.55
1:2A:848:G:H2'	1:2A:849:A:C8	2.42	0.55
32:2a:1005:A:H3'	32:2a:1006:C:C6	2.42	0.55
32:2a:1051:C:H2'	32:2a:1052:U:C6	2.42	0.55
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.72	0.54
10:1O:35:VAL:HG21	10:1O:69:ILE:HD13	1.89	0.54
32:1a:1239:A:H62	32:1a:1299:A:N6	2.05	0.54
1:2A:531:C:OP1	1:2A:561:G:N1	2.39	0.54
33:2b:98:LEU:HB2	33:2b:101:MET:HE3	1.88	0.54
1:1A:1176:G:H21	1:1A:1178:C:P	2.29	0.54
1:1A:1800:C:OP1	3:1D:260:ARG:NH2	2.41	0.54
1:2A:987:G:O2'	1:2A:1000:A:N3	2.36	0.54
20:2Y:6:HIS:H	20:2Y:6:HIS:CD2	2.25	0.54
32:2a:275:G:H5'	48:2q:14:LYS:HB2	1.89	0.54
32:2a:876:G:O5'	39:2h:14:ARG:NH1	2.40	0.54
32:2a:1135:U:H4'	32:2a:1136:U:H5	1.73	0.54
32:2a:1176:A:H2'	32:2a:1177:G:C8	2.42	0.54
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.22	0.54
32:1a:1531:A:H8	32:1a:1531:A:O5'	1.90	0.54
45:1n:21:TYR:OH	45:1n:23:ARG:NH2	2.39	0.54
50:1s:22:LEU:HB3	50:1s:27:GLU:HB3	1.88	0.54
21:2Z:130:PRO:HA	21:2Z:133:ILE:HG13	1.89	0.54
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.88	0.54
33:2b:48:MET:HA	33:2b:51:LEU:HD12	1.90	0.54
39:2h:25:ASP:N	39:2h:25:ASP:OD1	2.38	0.54
8:1I:87:LYS:HZ3	8:1I:121:LYS:HE3	1.71	0.54
32:1a:1040:U:H2'	32:1a:1041:A:H8	1.70	0.54
1:2A:563:G:OP2	62:2A:3937:HOH:O	2.18	0.54
1:2A:2430:A:H2'	1:2A:2430:A:N3	2.21	0.54
1:2A:2805:G:H2'	1:2A:2807:G:H8	1.72	0.54
2:2B:9:G:H1	2:2B:112:U:H3	1.54	0.54
9:2N:15:LEU:HB2	9:2N:135:PRO:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:54:THR:HG21	33:2b:201:ILE:HD11	1.89	0.54
34:2c:40:ARG:HE	34:2c:55:VAL:HG13	1.72	0.54
40:2i:17:VAL:HG11	40:2i:81:ILE:HG12	1.89	0.54
1:1A:1041:C:H42	1:1A:1114:G:H1	1.55	0.54
1:2A:639:U:H2'	1:2A:640:C:C6	2.43	0.54
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.42	0.54
6:2G:41:GLN:O	6:2G:43:LEU:N	2.40	0.54
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.90	0.54
32:2a:148:G:H2'	32:2a:149:A:H8	1.73	0.54
1:1A:271(F):C:N4	62:1A:4228:HOH:O	2.41	0.54
1:1A:881:G:N2	1:1A:897:C:O2	2.41	0.54
1:1A:1048:A:N1	1:1A:1112:G:O2'	2.31	0.54
2:1B:8:U:O3'	14:1S:25:ARG:NH2	2.40	0.54
7:1H:113:VAL:HG11	7:1H:151:ILE:HD13	1.89	0.54
1:2A:884:C:H3'	1:2A:885:C:C6	2.41	0.54
1:2A:2100:G:H1	1:2A:2189:U:H3	1.56	0.54
32:2a:881:G:P	43:2l:12:ARG:HH22	2.29	0.54
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.08	0.54
32:1a:1035:A:N3	32:1a:1036:G:N2	2.56	0.54
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.89	0.54
33:1b:100:GLY:O	33:1b:104:ASN:N	2.34	0.54
35:1d:81:GLU:O	35:1d:85:LYS:HB2	2.08	0.54
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.23	0.54
12:2Q:135:ASP:OD2	21:2Z:81:ARG:NH1	2.40	0.54
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.89	0.54
19:2X:72:LYS:NZ	19:2X:75:ASP:OD1	2.36	0.54
32:2a:460:G:N2	32:2a:471:G:N7	2.55	0.54
32:1a:78:G:C6	32:1a:91:C:N4	2.75	0.54
32:1a:148:G:H2'	32:1a:149:A:H8	1.72	0.54
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.90	0.54
1:2A:2161:C:H2'	1:2A:2162:G:O4'	2.08	0.54
32:2a:7:G:O2'	36:2e:120:THR:O	2.24	0.54
51:2t:43:LEU:O	51:2t:47:GLY:N	2.35	0.54
21:1Z:163:LEU:HD23	21:1Z:167:PRO:HG3	1.89	0.54
26:14:13:ARG:HB3	26:14:30:GLU:HG2	1.89	0.54
39:1h:51:VAL:HG21	39:1h:60:ARG:HB2	1.88	0.54
14:2S:67:ARG:O	14:2S:71:ARG:HG3	2.08	0.54
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.23	0.54
32:2a:1030(A):G:N2	32:2a:1030(D):A:OP2	2.40	0.54
34:2c:125:GLU:HB2	34:2c:190:ARG:HH21	1.72	0.54
32:1a:501:C:H2'	32:1a:502:G:H8	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.08	0.54
11:2P:138:LEU:HD23	11:2P:145:PRO:HB3	1.89	0.54
32:2a:1147:C:O2	40:2i:16:ARG:NH1	2.41	0.54
32:2a:1330:U:H4'	44:2m:23:TYR:CE1	2.43	0.54
35:2d:98:GLU:OE1	35:2d:103:ASN:ND2	2.38	0.54
35:2d:165:MET:HE2	35:2d:168:ARG:CZ	2.38	0.54
1:1A:893:C:H2'	1:1A:894:C:C6	2.43	0.53
1:1A:2171:A:O2'	1:1A:2172:U:H5"	2.08	0.53
36:1e:69:VAL:HG11	36:1e:113:ALA:HB1	1.90	0.53
1:2A:2318:G:H21	14:2S:3:ARG:CD	2.21	0.53
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.89	0.53
32:2a:316:G:OP2	32:2a:351:G:O2'	2.26	0.53
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.43	0.53
1:1A:2448:A:OP1	62:1A:4214:HOH:O	2.19	0.53
11:1P:38:GLN:O	11:1P:40:SER:N	2.40	0.53
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.89	0.53
16:1U:81:HIS:CE1	16:1U:85:LYS:HD2	2.43	0.53
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.36	0.53
32:1a:347:G:H5'	62:1a:2131:HOH:O	2.09	0.53
33:1b:77:ALA:HB2	33:1b:211:ILE:HD13	1.89	0.53
38:1g:151:TYR:OH	42:1k:54:ARG:NH1	2.41	0.53
1:2A:2125:G:H1'	1:2A:2173:A:H61	1.73	0.53
6:2G:41:GLN:NE2	6:2G:153:ARG:HB3	2.24	0.53
7:2H:27:LYS:HG2	7:2H:32:GLU:HB3	1.91	0.53
19:2X:46:ALA:HB1	24:22:33:MET:HE1	1.89	0.53
32:2a:999:C:H42	32:2a:1042:G:H1	1.55	0.53
45:2n:24:CYS:HB2	45:2n:40:CYS:HB3	1.89	0.53
57:2y:55:PSU:HN1	57:2y:57:G:C5'	2.21	0.53
57:2y:66:U:H2'	57:2y:67:C:O4'	2.09	0.53
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.43	0.53
2:1B:75:G:H22	21:1Z:73:GLN:NE2	2.06	0.53
40:1i:3:GLN:HG2	40:1i:20:ARG:HE	1.73	0.53
40:1i:55:ALA:HB1	40:1i:58:HIS:HB2	1.90	0.53
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.07	0.53
15:2T:91:ARG:HB2	15:2T:121:ILE:HG13	1.91	0.53
1:1A:2096:U:H3	1:1A:2193:G:H1	1.56	0.53
1:1A:2336:A:H61	22:10:43:THR:HG22	1.73	0.53
35:1d:172:PRO:C	35:1d:174:LEU:H	2.16	0.53
25:23:39:ASP:OD1	25:23:44:ARG:NH1	2.41	0.53
32:2a:42:G:OP1	62:2a:1908:HOH:O	2.18	0.53
32:2a:1068:G:H8	32:2a:1068:G:OP2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1221:G:O3'	50:2s:77:THR:OG1	2.25	0.53
36:2e:105:VAL:HB	36:2e:106:PRO:HD3	1.90	0.53
37:2f:35:ALA:HA	37:2f:67:MET:HB3	1.90	0.53
16:1U:69:CYS:HB3	16:1U:74:LEU:HD13	1.90	0.53
1:2A:71:A:H5"	1:2A:73:A:C8	2.42	0.53
1:2A:247:G:H4'	1:2A:386:G:C5	2.43	0.53
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.09	0.53
1:2A:1287:A:C8	13:2R:104:ARG:HD3	2.44	0.53
17:2V:1:MET:HE2	17:2V:43:GLU:HB2	1.90	0.53
32:2a:1051:C:H2'	32:2a:1052:U:H6	1.73	0.53
33:2b:96:ARG:HG2	33:2b:98:LEU:HD12	1.91	0.53
40:1i:42:ARG:NH1	40:1i:71:SER:OG	2.42	0.53
43:1l:8:ASN:O	43:1l:11:VAL:HG12	2.08	0.53
32:2a:1280:A:O2'	32:2a:1281:U:H5'	2.09	0.53
36:2e:42:GLY:HA2	36:2e:65:ASN:O	2.07	0.53
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.90	0.53
41:2j:62:HIS:HB3	45:2n:59:ALA:HB3	1.91	0.53
1:1A:302:C:P	20:1Y:73:ARG:HH22	2.32	0.53
32:1a:17:U:H2'	32:1a:18:C:C6	2.43	0.53
32:1a:1183:A:O2'	32:1a:1184:G:OP1	2.22	0.53
33:1b:195:ASP:O	39:1h:68:ARG:NH2	2.42	0.53
41:1j:5:ARG:HG3	41:1j:71:LEU:HD11	1.91	0.53
1:2A:2102:U:H2'	1:2A:2103:C:C6	2.44	0.53
44:2m:33:ALA:HA	44:2m:59:TYR:HE2	1.73	0.53
25:13:7:LYS:HG3	25:13:34:GLU:HG3	1.91	0.53
32:1a:542:G:H5'	35:1d:41:GLY:HA3	1.91	0.53
32:2a:381:C:H2'	32:2a:382:A:O4'	2.08	0.53
32:2a:1104:G:O3'	33:2b:111:ARG:NH2	2.42	0.53
38:2g:79:ARG:HH21	38:2g:79:ARG:HB2	1.74	0.53
50:2s:53:ASN:OD1	50:2s:54:GLY:N	2.42	0.53
50:2s:66:MET:HB2	50:2s:74:PHE:CZ	2.44	0.53
57:2y:9:A:O2'	57:2y:11:C:N4	2.29	0.53
1:1A:674:G:O2'	5:1F:74:ARG:HD3	2.08	0.53
19:1X:72:LYS:HE2	19:1X:73:ARG:O	2.09	0.53
32:1a:1191:A:H5"	34:1c:4:LYS:HE3	1.90	0.53
39:1h:34:GLU:OE1	39:1h:37:ARG:NH1	2.42	0.53
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.74	0.53
5:2F:118:ALA:HB2	5:2F:123:LEU:HD23	1.91	0.53
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.44	0.53
17:2V:72:VAL:HB	17:2V:85:LYS:HB3	1.90	0.53
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:847:U:OP2	62:1A:4237:HOH:O	2.19	0.53
21:1Z:31:ARG:NE	21:1Z:94:GLU:OE2	2.39	0.53
32:1a:1284:C:H3'	32:1a:1285:A:H8	1.74	0.53
39:1h:98:LYS:NZ	39:1h:98:LYS:H	2.08	0.53
39:1h:121:ASP:OD2	39:1h:125:ARG:NH2	2.42	0.53
1:2A:657:U:H2'	1:2A:658:C:C6	2.44	0.53
1:2A:774:A:H2'	1:2A:774:A:N3	2.24	0.53
1:2A:884:C:H3'	1:2A:885:C:H6	1.74	0.53
1:2A:2552:2MU:OP2	62:2A:3938:HOH:O	2.18	0.53
1:2A:2820:A:OP2	13:2R:2:ARG:NH2	2.43	0.53
40:2i:55:ALA:HA	40:2i:58:HIS:CD2	2.44	0.53
57:2y:65:G:H2'	57:2y:66:U:C6	2.44	0.53
1:1A:1062:G:P	1:1A:1070:A:H1'	2.50	0.52
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.43	0.52
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.44	0.52
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.90	0.52
32:1a:1039:C:H2'	32:1a:1040:U:C6	2.44	0.52
1:2A:752:A:H3'	29:27:1:MET:HE1	1.91	0.52
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.24	0.52
32:2a:921:U:O2	36:2e:19:MET:HB2	2.09	0.52
32:2a:1202:G:N2	45:2n:46:GLU:OE2	2.36	0.52
54:2w:67:C:H2'	54:2w:68:C:C6	2.44	0.52
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.44	0.52
1:1A:2733:A:OP1	62:1A:4236:HOH:O	2.19	0.52
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.22	0.52
32:1a:1343:G:H1'	40:1i:121:ARG:NH1	2.25	0.52
44:1m:19:LEU:HD11	44:1m:56:LEU:HD21	1.91	0.52
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.44	0.52
1:2A:245:G:OP2	62:2A:3944:HOH:O	2.19	0.52
1:2A:818:G:OP2	62:2A:3943:HOH:O	2.19	0.52
32:2a:1144:G:N2	32:2a:1146:A:H62	2.07	0.52
32:2a:1228:C:OP1	44:2m:115:LYS:NZ	2.38	0.52
40:2i:99:LEU:HB3	40:2i:101:PHE:CE2	2.44	0.52
43:2l:56:ALA:HB2	43:2l:70:ILE:HD11	1.91	0.52
46:1o:16:ALA:HB1	46:1o:21:ASP:HB3	1.91	0.52
48:1q:45:HIS:NE2	48:1q:47:PRO:HG3	2.23	0.52
1:2A:2162:G:H2'	1:2A:2163:C:O4'	2.09	0.52
18:2W:34:ASN:OD1	18:2W:37:ARG:NH2	2.38	0.52
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.41	0.52
26:24:61:ARG:HA	26:24:61:ARG:HH11	1.73	0.52
32:2a:1129:C:H2'	32:2a:1139:G:N7	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:45:U:H2'	32:1a:46:G:C8	2.44	0.52
54:1w:43:C:H2'	54:1w:44:G:C8	2.45	0.52
1:2A:1973:G:OP1	62:2A:3940:HOH:O	2.18	0.52
5:2F:10:PRO:HB3	5:2F:17:ARG:NH1	2.24	0.52
6:2G:50:ALA:O	6:2G:52:ILE:N	2.42	0.52
36:2e:78:HIS:HE1	36:2e:143:ARG:H	1.58	0.52
40:2i:97:LYS:HA	40:2i:102:LEU:HG	1.92	0.52
57:2y:18:G:N2	57:2y:55:PSU:C4	2.75	0.52
21:1Z:23:LYS:NZ	21:1Z:40:ASP:OD1	2.42	0.52
1:2A:62:C:H42	1:2A:93:G:H1	1.58	0.52
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.45	0.52
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.25	0.52
6:2G:20:ILE:HA	6:2G:25:TYR:HD2	1.74	0.52
40:2i:33:PHE:HE2	40:2i:43:ALA:HB1	1.74	0.52
55:2x:50:U:H3	55:2x:64:G:H1	1.57	0.52
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.74	0.52
33:1b:201:ILE:HG21	33:1b:214:ILE:HG21	1.91	0.52
1:2A:534:U:H5'	16:2U:42:ALA:HB1	1.90	0.52
1:2A:851:U:H5'	25:23:49:LYS:HD2	1.90	0.52
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.44	0.52
1:2A:2609:U:H6	56:2z:2:THR:HG22	1.75	0.52
1:2A:2801(A):A:O2'	1:2A:2895:U:O4'	2.28	0.52
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.44	0.52
5:1F:132:VAL:HA	5:1F:138:GLU:HB3	1.91	0.52
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.09	0.52
32:1a:1239:A:H62	32:1a:1299:A:H62	1.57	0.52
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.43	0.52
1:2A:1580:A:H3'	1:2A:1581:G:H8	1.75	0.52
32:2a:1189:C:O2'	34:2c:176:HIS:ND1	2.38	0.52
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.77	0.52
51:2t:9:ASN:O	51:2t:10:LEU:HB2	2.10	0.52
1:1A:639:U:H2'	1:1A:640:C:C6	2.45	0.52
1:1A:1017:G:N7	62:1A:4295:HOH:O	2.34	0.52
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.44	0.52
15:1T:56:GLY:O	15:1T:59:THR:HG22	2.10	0.52
32:1a:333:G:H4'	51:1t:16:HIS:CE1	2.45	0.52
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.27	0.52
32:2a:1260:C:O5'	32:2a:1284:C:H4'	2.10	0.52
54:2w:51:U:H2'	54:2w:52:G:C8	2.45	0.52
57:2y:63:G:H2'	57:2y:64:A:C8	2.45	0.52
1:1A:828:U:P	62:1A:4251:HOH:O	2.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.74	0.52
1:1A:1359:A:N6	1:1A:1372:U:H3	2.07	0.52
6:1G:64:THR:HB	6:1G:94:LEU:HD21	1.92	0.52
32:1a:406:G:N2	35:1d:119:GLN:HE22	2.08	0.52
35:1d:178:VAL:C	35:1d:180:GLY:H	2.18	0.52
40:1i:32:ASP:OD1	40:1i:33:PHE:N	2.42	0.52
1:2A:620:G:O6	62:2A:3945:HOH:O	2.19	0.52
1:2A:2582:G:OP2	62:2A:3942:HOH:O	2.19	0.52
7:2H:124:GLU:HB2	7:2H:132:ARG:HB3	1.90	0.52
14:2S:67:ARG:HG2	14:2S:71:ARG:HD2	1.92	0.52
35:2d:82:ALA:HB1	35:2d:92:VAL:HG13	1.90	0.52
35:2d:104:VAL:HG21	35:2d:140:VAL:HG21	1.92	0.52
39:2h:86:ILE:HG21	39:2h:133:LEU:HD13	1.91	0.52
1:1A:530:G:N1	1:1A:2023:G:OP1	2.32	0.52
12:1Q:136:ALA:HB1	21:1Z:52:SER:HB2	1.91	0.52
32:1a:1353:G:OP1	52:1u:10:ARG:NH1	2.43	0.52
53:1v:14:A:H3'	53:1v:15:A:H8	1.75	0.52
1:2A:883:G:H22	1:2A:895:U:H1'	1.75	0.52
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.10	0.52
5:2F:192:LEU:HD21	5:2F:194:MET:HE2	1.92	0.52
9:2N:96:GLU:CD	9:2N:96:GLU:H	2.17	0.52
32:2a:1060:C:C5	34:2c:2:GLY:HA2	2.45	0.52
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.10	0.52
40:2i:26:VAL:HG22	40:2i:61:ALA:HB3	1.92	0.52
44:2m:23:TYR:HB3	44:2m:67:GLU:HA	1.92	0.52
44:2m:40:ASN:HD22	44:2m:43:THR:HG23	1.73	0.52
1:1A:2131:G:H5'	1:1A:2133:G:C8	2.45	0.51
32:1a:396:G:O2'	32:1a:398:C:OP1	2.23	0.51
1:2A:645:C:H5"	1:2A:646:A:OP2	2.09	0.51
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.10	0.51
1:2A:2612:C:OP2	27:25:2:ALA:N	2.43	0.51
13:2R:56:LYS:NZ	13:2R:90:ARG:O	2.43	0.51
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.25	0.51
32:2a:8:A:H5'	36:2e:101:ILE:HG22	1.92	0.51
1:1A:881:G:H3'	1:1A:882:G:H8	1.75	0.51
7:1H:41:MET:HE1	7:1H:54:ARG:HB3	1.92	0.51
8:1I:77:LEU:HG	8:1I:101:LEU:HD22	1.92	0.51
9:1N:46:VAL:HG23	9:1N:48:MET:HG2	1.92	0.51
37:1f:62:TRP:CH2	37:1f:64:GLN:HB2	2.44	0.51
1:2A:10:G:O2'	1:2A:2801(A):A:N7	2.43	0.51
1:2A:483:A:O2'	20:2Y:49:VAL:O	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2127:G:N2	1:2A:2161:C:C2	2.79	0.51
19:2X:11:PRO:HB3	19:2X:92:LEU:HD21	1.93	0.51
21:2Z:8:TYR:HB2	21:2Z:38:TYR:CE2	2.46	0.51
32:2a:779:C:H2'	32:2a:780:A:O4'	2.11	0.51
32:2a:838:G:H1	32:2a:848:C:N4	2.08	0.51
32:2a:1313:U:OP1	50:2s:5:LEU:HB2	2.10	0.51
44:2m:92:HIS:CE1	44:2m:98:VAL:HG21	2.45	0.51
1:1A:1365:A:O2'	23:11:11:ARG:NH1	2.44	0.51
5:1F:28:ILE:HD12	5:1F:119:ARG:HH21	1.76	0.51
6:1G:98:ARG:CZ	26:14:1:MET:HE3	2.40	0.51
32:1a:766:A:OP2	62:1a:1925:HOH:O	2.19	0.51
1:2A:2206:G:H5"	1:2A:2207:G:C5	2.45	0.51
7:2H:26:VAL:HG12	7:2H:79:VAL:HG21	1.91	0.51
21:2Z:31:ARG:HG3	21:2Z:32:HIS:CD2	2.44	0.51
32:2a:1238:A:OP2	62:2a:1910:HOH:O	2.19	0.51
33:2b:84:GLU:HB3	33:2b:219:VAL:HG21	1.93	0.51
40:2i:85:LEU:HB3	40:2i:92:TYR:HD2	1.74	0.51
44:2m:50:GLU:HA	44:2m:53:VAL:HG22	1.91	0.51
47:2p:28:ARG:HG2	47:2p:29:ASP:OD1	2.11	0.51
1:1A:566:U:H5"	11:1P:29:LYS:HE3	1.93	0.51
1:1A:897:C:N3	1:1A:898:C:N4	2.58	0.51
1:1A:2748:A:H5'	7:1H:4:ILE:HD13	1.92	0.51
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.75	0.51
34:1c:152:ILE:HG23	34:1c:167:TRP:HB3	1.91	0.51
1:2A:2059:A:O2'	5:2F:69:HIS:HD2	1.94	0.51
7:2H:80:SER:OG	7:2H:81:GLU:N	2.43	0.51
40:2i:9:ARG:HG2	40:2i:14:VAL:HG12	1.91	0.51
55:2x:55:PSU:O2'	55:2x:57:A:N7	2.40	0.51
1:1A:278:A:O2'	1:1A:279:C:OP1	2.27	0.51
1:1A:747:U:O2	1:1A:2014:A:H1'	2.10	0.51
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.25	0.51
32:1a:276:G:O3'	48:1q:68:ARG:NH1	2.43	0.51
32:1a:486:U:H2'	32:1a:487:A:H8	1.75	0.51
32:1a:1148:U:H2'	32:1a:1149:C:O4'	2.10	0.51
1:2A:217:G:OP2	62:2A:3936:HOH:O	2.18	0.51
1:2A:468:G:N7	29:27:39:ARG:NH2	2.53	0.51
1:2A:2117:A:H61	1:2A:2166:G:H22	1.58	0.51
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.74	0.51
21:2Z:159:PRO:HA	21:2Z:161:VAL:H	1.76	0.51
33:2b:68:ILE:O	33:2b:90:MET:HB3	2.11	0.51
33:2b:187:LEU:HD12	33:2b:214:ILE:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2y:63:G:H2'	57:2y:64:A:H8	1.76	0.51
32:1a:258:G:H2'	32:1a:259:G:H8	1.75	0.51
32:1a:353:A:H5'	32:1a:353:A:H8	1.76	0.51
32:1a:1292:U:H5'	40:1i:38:GLN:OE1	2.10	0.51
51:1t:47:GLY:N	51:1t:48:LYS:HB2	2.25	0.51
57:1y:5:G:H1'	57:1y:69:G:N2	2.25	0.51
1:2A:2125:G:H1'	1:2A:2173:A:N6	2.26	0.51
1:2A:2319:G:N2	14:2S:3:ARG:HD2	2.25	0.51
39:2h:64:LYS:HG2	39:2h:79:VAL:HG21	1.92	0.51
1:1A:817:C:H4'	1:1A:932:G:C5	2.46	0.51
32:1a:973:G:H3'	32:1a:974:A:H5"	1.92	0.51
32:1a:1456:G:O3'	51:1t:39:LYS:NZ	2.42	0.51
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.92	0.51
40:1i:4:TYR:CD1	40:1i:88:TYR:HB2	2.45	0.51
1:2A:2138:C:N4	1:2A:2153:G:H1	2.09	0.51
32:2a:1265:G:C2	32:2a:1271:G:C2	2.99	0.51
33:2b:158:LEU:HD23	33:2b:182:ILE:HD11	1.91	0.51
57:2y:15:G:H22	57:2y:48:C:N4	2.07	0.51
1:1A:1086:A:H3'	1:1A:1086:A:N3	2.26	0.51
21:1Z:132:ASN:N	21:1Z:132:ASN:OD1	2.42	0.51
32:1a:977:A:H1'	32:1a:982:U:O4	2.11	0.51
35:1d:172:PRO:O	35:1d:174:LEU:N	2.41	0.51
54:1w:1:G:H2'	54:1w:2:C:C6	2.46	0.51
11:2P:39:LYS:HB2	11:2P:45:LEU:HD13	1.91	0.51
32:2a:1006:C:H2'	32:2a:1007:C:O4'	2.11	0.51
1:1A:271(I):G:N7	1:1A:271(J):C:N4	2.58	0.51
1:1A:588:U:H2'	1:1A:589:C:C6	2.45	0.51
1:1A:1170:G:H1	1:1A:1179:C:H42	1.58	0.51
1:1A:2612:C:OP2	27:15:2:ALA:N	2.44	0.51
8:1I:77:LEU:HB3	8:1I:142:VAL:HG12	1.93	0.51
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.46	0.51
32:1a:662:G:H2'	32:1a:663:A:C8	2.45	0.51
43:1l:11:VAL:HG23	48:1q:29:HIS:CD2	2.45	0.51
1:2A:2096:U:H3	1:2A:2193:G:H1	1.58	0.51
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.25	0.51
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.43	0.51
15:2T:74:ARG:HG2	15:2T:76:PHE:CZ	2.46	0.51
19:2X:88:LYS:HE3	19:2X:93:GLU:HG3	1.93	0.51
32:2a:1149:C:H2'	32:2a:1150:U:C6	2.45	0.51
4:1E:50:GLY:HA3	4:1E:75:VAL:HG21	1.91	0.51
26:14:53:GLU:HB2	26:14:55:ARG:C	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:16:19:ARG:NH1	28:16:52:VAL:HG21	2.25	0.51
32:1a:1136:U:H5"	32:1a:1137:C:N3	2.26	0.51
1:2A:296:C:OP1	20:2Y:4:LYS:NZ	2.44	0.51
1:2A:646:A:H2'	1:2A:647:G:O4'	2.11	0.51
1:2A:910:A:N1	1:2A:2277:G:H1'	2.26	0.51
6:2G:28:VAL:O	6:2G:31:VAL:HG12	2.10	0.51
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	1.93	0.51
32:2a:920:U:H2'	32:2a:921:U:C6	2.46	0.51
32:2a:1029:C:C2	32:2a:1032:G:N2	2.77	0.51
40:2i:4:TYR:HB2	40:2i:19:LEU:HB2	1.91	0.51
54:2w:18:G:H4'	54:2w:60:U:C5	2.45	0.51
1:1A:2629:A:HO2'	1:1A:2630:G:P	2.33	0.50
1:1A:2774:C:H2'	1:1A:2775:A:O4'	2.11	0.50
10:1O:49:ARG:HH12	32:1a:1423:G:P	2.34	0.50
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.26	0.50
1:2A:2769:C:H2'	1:2A:2770:G:O4'	2.12	0.50
10:2O:63:VAL:HG23	10:2O:64:ARG:HG3	1.93	0.50
12:2Q:78:PRO:HD3	55:2x:1:C:N3	2.25	0.50
32:2a:662:G:H2'	32:2a:663:A:C8	2.46	0.50
32:2a:1003:G:H2'	32:2a:1004:A:O4'	2.09	0.50
44:2m:22:ILE:HG21	44:2m:66:LEU:HD13	1.92	0.50
36:1e:106:PRO:O	36:1e:110:LEU:HG	2.11	0.50
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.46	0.50
1:2A:2116:G:N1	1:2A:2162:G:OP1	2.44	0.50
12:2Q:137:TYR:CE1	21:2Z:83:PRO:HG3	2.47	0.50
21:2Z:73:GLN:O	21:2Z:87:ASP:N	2.44	0.50
46:2o:11:VAL:HG21	46:2o:34:LEU:HD22	1.93	0.50
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.92	0.50
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.47	0.50
1:2A:801:G:O6	5:2F:53:THR:OG1	2.29	0.50
42:2k:18:ARG:NH2	42:2k:35:PRO:O	2.43	0.50
1:1A:1794:U:H2'	1:1A:1795:C:H6	1.75	0.50
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.11	0.50
1:1A:2313:C:H4'	6:1G:91:ARG:HG3	1.91	0.50
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.80	0.50
35:1d:60:GLU:HG3	35:1d:202:LEU:HD12	1.94	0.50
1:2A:141:A:H8	1:2A:1408:C:O2'	1.94	0.50
1:2A:2875:C:OP1	15:2T:3:ARG:NH2	2.44	0.50
2:2B:14:U:H1'	2:2B:108:U:O2'	2.12	0.50
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.93	0.50
12:2Q:17:LEU:HB3	12:2Q:39:PRO:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:13:ARG:HA	26:24:22:ILE:O	2.11	0.50
1:1A:616:G:OP2	5:1F:106:ARG:NH2	2.45	0.50
32:1a:507:C:OP2	32:1a:508:C:O2'	2.22	0.50
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.59	0.50
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.94	0.50
57:1y:70:G:H3'	57:1y:71:G:H8	1.77	0.50
1:2A:2376:A:H2'	1:2A:2377:A:O4'	2.11	0.50
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.77	0.50
21:2Z:150:LEU:H	21:2Z:171:ILE:HD11	1.75	0.50
37:2f:95:GLU:O	49:2r:32:ARG:NH1	2.44	0.50
1:1A:2155:G:H2'	1:1A:2155:G:N3	2.26	0.50
1:1A:2790:A:H3'	1:1A:2790:A:N3	2.27	0.50
62:1A:5750:HOH:O	11:1P:44:GLY:HA2	2.10	0.50
40:1i:128:ARG:NH1	55:1x:35:A:OP2	2.45	0.50
57:1y:3:C:H42	57:1y:70:G:H1	1.57	0.50
1:2A:2507:C:H5"	1:2A:2573:C:N4	2.26	0.50
23:21:8:SER:HB3	23:21:66:HIS:CD2	2.46	0.50
37:2f:30:LEU:HD23	37:2f:75:LEU:HD11	1.92	0.50
1:1A:1054:A:N6	1:1A:1105:U:H3	2.05	0.50
54:1w:18:G:H4'	54:1w:60:U:C5	2.46	0.50
10:2O:73:ASP:OD2	15:2T:32:TYR:OH	2.26	0.50
21:2Z:99:TYR:HB3	21:2Z:123:ASP:OD2	2.12	0.50
32:2a:1003:G:N2	32:2a:1025:U:O4	2.43	0.50
32:2a:1313:U:OP2	50:2s:5:LEU:HD13	2.12	0.50
33:2b:47:THR:HA	33:2b:202:PRO:HG2	1.92	0.50
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.12	0.50
32:1a:1025:U:O2	32:1a:1036:G:O6	2.30	0.50
32:1a:1304:G:OP2	62:1a:1926:HOH:O	2.20	0.50
1:2A:2108:C:H42	1:2A:2181:G:H1	1.59	0.50
1:2A:2882:A:OP1	13:2R:96:ARG:NE	2.40	0.50
5:2F:28:ILE:HD11	5:2F:115:ALA:HB3	1.93	0.50
6:2G:126:ASP:OD2	6:2G:130:ASN:ND2	2.37	0.50
26:24:26:SER:OG	26:24:27:THR:N	2.45	0.50
34:2c:37:GLN:NE2	45:2n:52:GLN:OE1	2.41	0.50
38:2g:54:THR:O	38:2g:56:GLN:N	2.43	0.50
1:1A:752:A:H3'	29:17:1:MET:HE1	1.94	0.50
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.47	0.50
9:1N:13:TRP:CE2	9:1N:133:GLN:HG2	2.47	0.50
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.13	0.50
32:1a:562:C:H1'	43:1l:15:ARG:HB3	1.92	0.50
33:1b:93:VAL:HG11	33:1b:97:TRP:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:12:LEU:HD11	45:1n:51:GLY:HA2	1.94	0.50
37:1f:100:ASN:HB2	49:1r:28:GLU:HA	1.93	0.50
15:2T:26:ASP:OD1	15:2T:120:ARG:NH2	2.45	0.50
18:2W:65:LEU:HD12	18:2W:68:ARG:HD2	1.94	0.50
32:2a:45:U:H2'	32:2a:46:G:C8	2.47	0.50
32:2a:1016:A:H2'	32:2a:1017:G:O4'	2.11	0.50
33:2b:104:ASN:OD1	33:2b:107:THR:OG1	2.28	0.50
57:2y:18:G:H4'	57:2y:60:U:C5	2.46	0.50
1:1A:207:A:H2'	1:1A:208:C:O4'	2.10	0.49
8:1I:10:GLU:O	8:1I:12:LEU:N	2.45	0.49
8:1I:116:LEU:HD11	8:1I:120:ILE:HG13	1.94	0.49
19:1X:60:ARG:NH2	29:17:47:ARG:HH22	2.10	0.49
21:1Z:72:ARG:NH2	21:1Z:97:GLU:O	2.44	0.49
26:14:18:CYS:SG	26:14:20:ASN:HB2	2.52	0.49
32:1a:1048:G:OP1	62:1a:1924:HOH:O	2.18	0.49
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.47	0.49
1:2A:286:C:H2'	1:2A:287:C:C6	2.47	0.49
1:2A:804:A:OP1	62:2A:3947:HOH:O	2.19	0.49
1:2A:2727:G:O3'	10:2O:70:LYS:NZ	2.44	0.49
2:2B:106:G:H5'	21:2Z:31:ARG:HB3	1.94	0.49
5:2F:10:PRO:HB3	5:2F:17:ARG:HH11	1.77	0.49
12:2Q:15:GLY:O	12:2Q:16:ARG:HB2	2.12	0.49
26:24:16:CYS:SG	26:24:17:GLY:N	2.85	0.49
27:25:49:CYS:SG	27:25:51:TYR:HB2	2.52	0.49
32:2a:1225:A:OP1	44:2m:103:THR:OG1	2.30	0.49
43:2l:40:VAL:HG21	43:2l:78:GLN:HA	1.94	0.49
1:1A:579:G:H2'	1:1A:580:C:C6	2.47	0.49
1:1A:1113:U:H2'	1:1A:1114:G:H8	1.77	0.49
1:1A:1173:G:H22	1:1A:1177:A:P	2.36	0.49
6:1G:57:ALA:HA	6:1G:68:PRO:HG2	1.94	0.49
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.95	0.49
33:1b:98:LEU:HD12	33:1b:101:MET:HE3	1.92	0.49
33:1b:174:VAL:O	33:1b:178:ARG:HG2	2.13	0.49
41:1j:11:PHE:CE1	41:1j:67:THR:HG22	2.47	0.49
42:1k:85:ARG:NH2	42:1k:111:ASP:OD2	2.33	0.49
50:1s:27:GLU:HB2	50:1s:28:LYS:CA	2.41	0.49
1:2A:700:G:O2'	1:2A:1632:A:N3	2.42	0.49
1:2A:2166:G:N7	1:2A:2167:U:H2'	2.28	0.49
1:2A:2822:G:O2'	1:2A:2825:C:N4	2.44	0.49
21:2Z:102:LEU:HD23	21:2Z:139:VAL:HG21	1.95	0.49
26:24:68:ARG:HE	26:24:69:LYS:H	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:447:G:O6	32:2a:485:G:O2'	2.23	0.49
32:2a:448:A:P	32:2a:485:G:H22	2.35	0.49
33:2b:222:ILE:HG13	33:2b:223:ILE:N	2.25	0.49
38:2g:65:ALA:HB1	38:2g:127:ALA:HB3	1.94	0.49
1:1A:1628:G:H2'	1:1A:1629:U:C6	2.47	0.49
1:1A:1744:C:H2'	1:1A:1745:C:C6	2.47	0.49
1:1A:2585:U:H1'	56:1z:5:MET:HE3	1.94	0.49
3:1D:237:GLU:OE2	62:1D:401:HOH:O	2.19	0.49
32:1a:67:C:H2'	32:1a:68:G:C8	2.47	0.49
32:1a:1278:U:H5'	32:1a:1279:A:O4'	2.12	0.49
33:1b:105:PHE:C	33:1b:107:THR:H	2.20	0.49
41:1j:11:PHE:HE1	41:1j:67:THR:HG22	1.77	0.49
51:1t:36:LEU:HD12	51:1t:62:LEU:HD12	1.95	0.49
1:2A:191:A:H2'	1:2A:192:C:C6	2.46	0.49
1:2A:811:U:H2'	11:2P:21:ARG:HA	1.94	0.49
1:2A:2136:C:O2'	1:2A:2137:C:H6	1.95	0.49
33:2b:8:LYS:HB3	33:2b:217:ARG:HG3	1.94	0.49
47:2p:28:ARG:NH1	47:2p:29:ASP:OD1	2.45	0.49
1:1A:796:C:H2'	1:1A:797:C:C6	2.47	0.49
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.47	0.49
1:1A:1991:U:H2'	1:1A:1992:G:H5"	1.95	0.49
1:1A:2629:A:H1'	1:1A:2630:G:C5'	2.42	0.49
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.48	0.49
1:2A:2531:A:C8	7:2H:175:LYS:HD2	2.47	0.49
2:2B:75:G:N2	21:2Z:87:ASP:OD1	2.45	0.49
23:21:83:GLU:N	23:21:83:GLU:OE2	2.43	0.49
32:2a:975:A:N1	41:2j:48:THR:HB	2.27	0.49
44:2m:4:ILE:HG23	44:2m:5:ALA:H	1.76	0.49
2:1B:42:C:O2'	6:1G:66:GLN:HG2	2.13	0.49
20:1Y:92:ASN:HD22	20:1Y:92:ASN:C	2.16	0.49
32:1a:189(D):C:H2'	32:1a:189(E):U:O4'	2.13	0.49
34:1c:172:ARG:NH2	34:1c:206:GLU:OE2	2.46	0.49
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.46	0.49
1:2A:2849:U:O4	15:2T:23:ARG:NH1	2.39	0.49
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.13	0.49
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.12	0.49
32:2a:1427:U:H2'	32:2a:1428:A:C8	2.47	0.49
57:2y:62:C:H2'	57:2y:63:G:C8	2.48	0.49
32:1a:1073:U:O2'	33:1b:104:ASN:OD1	2.23	0.49
38:1g:74:GLU:HG2	38:1g:91:VAL:HG22	1.95	0.49
1:2A:184:C:H2'	1:2A:185:U:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:58:LEU:HD13	8:2I:59:ALA:N	2.28	0.49
8:2I:82:ARG:NH2	8:2I:90:GLY:N	2.60	0.49
8:2I:130:TYR:CE2	8:2I:132:PRO:HB3	2.48	0.49
19:2X:26:TYR:HB3	19:2X:92:LEU:HD12	1.95	0.49
32:2a:6:G:O6	36:2e:95:ALA:N	2.46	0.49
38:2g:16:LEU:HD22	40:2i:42:ARG:HA	1.94	0.49
1:1A:7:G:H2'	1:1A:8:A:O4'	2.12	0.49
1:1A:414:C:H2'	1:1A:415:A:C8	2.47	0.49
1:1A:880:G:H8	1:1A:880:G:OP2	1.95	0.49
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.28	0.49
1:1A:2439:A:N6	55:1x:76:8AN:O1P	2.45	0.49
5:1F:152:GLU:OE1	5:1F:191:ARG:HD2	2.13	0.49
9:1N:20:GLY:HA2	9:1N:61:ARG:HE	1.77	0.49
32:1a:382:A:H2'	32:1a:383:A:C8	2.47	0.49
33:1b:24:TRP:CD1	33:1b:24:TRP:H	2.31	0.49
36:1e:50:GLU:HB2	36:1e:53:LEU:HD13	1.93	0.49
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.17	0.49
1:2A:2572:A:C8	4:2E:144:ARG:HD3	2.47	0.49
15:2T:30:VAL:HG22	15:2T:86:ILE:HG12	1.94	0.49
33:2b:197:VAL:HB	33:2b:200:ILE:HG13	1.95	0.49
36:2e:57:LYS:HG2	36:2e:61:TYR:CE2	2.47	0.49
45:2n:21:TYR:HB3	62:2n:201:HOH:O	2.11	0.49
57:2y:8:4SU:H6	57:2y:8:4SU:O5'	2.12	0.49
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.12	0.49
21:1Z:52:SER:O	21:1Z:52:SER:OG	2.29	0.49
32:1a:1027:C:N4	32:1a:1034:G:H1	2.11	0.49
32:1a:1513:A:H2'	32:1a:1514:C:C6	2.48	0.49
39:1h:81:HIS:N	39:1h:138:TRP:O	2.45	0.49
42:1k:82:VAL:HB	42:1k:108:ILE:HG12	1.94	0.49
1:2A:299:A:N1	1:2A:322:A:O2'	2.37	0.49
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.13	0.49
23:21:44:PRO:HB2	23:21:46:LEU:HD13	1.94	0.49
32:2a:1243:C:H42	32:2a:1294:G:H1	1.60	0.49
1:1A:1876:A:H2'	1:1A:1877:A:C8	2.48	0.49
1:1A:1924:C:H4'	55:1x:13:C:O2'	2.12	0.49
3:1D:92:ILE:HD12	3:1D:104:TYR:CD1	2.48	0.49
32:1a:509:A:O2'	32:1a:510:A:OP1	2.26	0.49
32:1a:890:G:O2'	32:1a:906:G:O6	2.30	0.49
32:1a:1037:C:H2'	32:1a:1038:C:H6	1.77	0.49
1:2A:2112:G:C2	1:2A:2113:U:H1'	2.48	0.49
7:2H:45:VAL:HG13	7:2H:50:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2N:123:TYR:OH	9:2N:130:HIS:NE2	2.37	0.49
38:2g:15:ASP:OD1	38:2g:20:ASP:N	2.44	0.49
42:2k:73:MET:HG2	42:2k:103:LEU:HD21	1.93	0.49
55:2x:15:G:H2'	55:2x:59:A:N1	2.28	0.49
1:1A:1203:G:O6	62:1A:4229:HOH:O	2.17	0.49
1:1A:2319:G:H22	14:1S:3:ARG:CD	2.23	0.49
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	1.93	0.49
4:1E:52:LEU:O	4:1E:76:ARG:N	2.41	0.49
6:1G:122:PRO:HG3	6:1G:182:LYS:H	1.78	0.49
40:1i:89:ASN:O	40:1i:92:TYR:HB2	2.13	0.49
48:1q:3:LYS:HD3	48:1q:60:ILE:HD11	1.94	0.49
1:2A:652(B):A:N6	1:2A:655:A:O2'	2.44	0.49
1:2A:1354:A:H5"	3:2D:38:LYS:HD3	1.94	0.49
1:2A:2136:C:H42	1:2A:2155:G:H1	1.60	0.49
1:2A:2807:G:H22	1:2A:2892:A:N6	2.10	0.49
12:2Q:10:ARG:HH12	12:2Q:89:ASN:ND2	2.11	0.49
32:2a:1002:G:N3	32:2a:1003:G:H1'	2.27	0.49
1:1A:897:C:H5'	54:1w:56:C:OP1	2.13	0.48
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.28	0.48
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	1.95	0.48
32:1a:239:U:O4	62:1a:1921:HOH:O	2.16	0.48
32:1a:1381:U:H1'	38:1g:79:ARG:HG2	1.95	0.48
34:1c:111:LEU:HD11	34:1c:144:SER:O	2.13	0.48
37:1f:42:GLU:OE2	37:1f:59:TYR:OH	2.25	0.48
1:2A:1847:A:H3'	1:2A:1848:A:H5'	1.93	0.48
1:2A:2193:G:H2'	1:2A:2194:G:H8	1.77	0.48
9:2N:59:LYS:O	9:2N:61:ARG:NH2	2.46	0.48
32:2a:473:G:H2'	32:2a:474:G:H8	1.78	0.48
32:2a:1139:G:N2	32:2a:1142:G:O6	2.36	0.48
36:2e:63:ARG:C	36:2e:66:MET:HE1	2.38	0.48
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.95	0.48
32:1a:262:A:H2'	32:1a:263:A:C8	2.49	0.48
32:1a:1028:C:H2'	32:1a:1029:C:O4'	2.13	0.48
1:2A:796:C:H2'	1:2A:797:C:C6	2.48	0.48
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.48	0.48
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.94	0.48
8:2I:71:ILE:O	8:2I:75:LEU:HD13	2.14	0.48
12:2Q:32:TYR:OH	12:2Q:133:ARG:NH2	2.44	0.48
32:2a:278:G:OP2	48:2q:41:LYS:NZ	2.31	0.48
32:2a:1069:C:O2'	32:2a:1192:C:H1'	2.13	0.48
38:2g:78:ARG:HG3	38:2g:156:TRP:HZ3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:78:ASN:O	41:2j:80:LYS:N	2.46	0.48
45:2n:48:ALA:HB2	45:2n:53:LEU:HD12	1.95	0.48
1:1A:922:U:H2'	1:1A:923:C:C6	2.48	0.48
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	1.95	0.48
9:1N:109:LYS:HE2	62:1N:305:HOH:O	2.13	0.48
32:1a:1202:G:O4'	45:1n:29:ARG:NH1	2.46	0.48
1:2A:272:G:O2'	1:2A:421:U:OP2	2.21	0.48
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.49	0.48
34:2c:111:LEU:HD21	34:2c:146:ALA:HB2	1.94	0.48
38:2g:113:GLU:CG	38:2g:119:ARG:HG2	2.42	0.48
40:2i:31:GLN:HB3	40:2i:35:GLU:HG2	1.94	0.48
1:1A:593:G:H4'	30:18:4:MET:HE2	1.95	0.48
1:1A:1104:C:H2'	1:1A:1105:U:C6	2.49	0.48
1:1A:2723:C:OP1	13:1R:3:HIS:ND1	2.46	0.48
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.95	0.48
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.13	0.48
21:1Z:125:LEU:HB3	21:1Z:165:VAL:HG13	1.95	0.48
21:1Z:132:ASN:HD22	21:1Z:160:GLY:HA3	1.78	0.48
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.48	0.48
44:1m:96:LEU:C	44:1m:110:ARG:HG2	2.38	0.48
1:2A:338:G:OP2	62:2A:3949:HOH:O	2.20	0.48
1:2A:1011:G:OP1	16:2U:77:SER:OG	2.26	0.48
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.95	0.48
1:2A:1991:U:H2'	1:2A:1992:G:H5"	1.95	0.48
5:2F:20:LEU:HG	5:2F:21:ALA:H	1.79	0.48
21:2Z:17:ALA:HA	21:2Z:20:ARG:HB3	1.95	0.48
32:2a:23:C:H5	32:2a:561:U:O4	1.97	0.48
32:2a:73:G:H1	32:2a:96:U:H3	1.61	0.48
32:2a:1047:G:H5"	45:2n:4:LYS:HD3	1.95	0.48
41:2j:61:GLU:OE2	45:2n:58:LYS:NZ	2.34	0.48
1:1A:1139:G:OP2	9:1N:70:LYS:NZ	2.45	0.48
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.28	0.48
32:1a:750:G:N3	46:1o:23:GLY:HA3	2.28	0.48
32:1a:1060:C:C5	34:1c:2:GLY:HA3	2.47	0.48
32:1a:1244:C:N4	32:1a:1293:G:H1	2.11	0.48
41:1j:38:ILE:HD11	41:1j:40:LEU:HD23	1.96	0.48
54:1w:23:A:H3'	54:1w:24:G:C8	2.49	0.48
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.61	0.48
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.48	0.48
2:2B:103:G:N2	21:2Z:73:GLN:HE22	2.08	0.48
6:2G:50:ALA:C	6:2G:52:ILE:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:15:ARG:O	14:2S:19:LYS:HG2	2.13	0.48
33:2b:167:PRO:HD3	33:2b:187:LEU:O	2.14	0.48
35:2d:119:GLN:HG3	35:2d:123:HIS:CD2	2.48	0.48
41:2j:16:LEU:HD23	41:2j:94:VAL:HG22	1.96	0.48
1:1A:444:C:H5"	62:1A:5245:HOH:O	2.12	0.48
1:1A:2137:C:H2'	1:1A:2138:C:C6	2.48	0.48
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.13	0.48
7:1H:105:LEU:HD12	7:1H:151:ILE:HD12	1.95	0.48
12:1Q:78:PRO:HD3	55:1x:1:C:N3	2.29	0.48
25:13:11:SER:HA	25:13:31:LEU:HD11	1.94	0.48
1:2A:190:A:OP2	23:21:39:LYS:HE3	2.13	0.48
1:2A:883:G:N2	1:2A:895:U:H1'	2.28	0.48
1:2A:900:A:O2'	1:2A:901:A:OP1	2.30	0.48
1:2A:2131:G:C8	1:2A:2133:G:C2	3.02	0.48
10:2O:9:GLU:OE2	10:2O:18:LYS:NZ	2.46	0.48
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.95	0.48
21:2Z:40:ASP:OD2	21:2Z:43:GLU:N	2.43	0.48
34:2c:18:TRP:HE3	34:2c:18:TRP:H	1.60	0.48
42:2k:45:GLY:O	42:2k:50:TYR:HB2	2.14	0.48
44:2m:3:ARG:HH22	44:2m:11:ARG:HG3	1.78	0.48
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.11	0.48
1:1A:370:G:H8	1:1A:370:G:OP2	1.97	0.48
1:1A:1051:G:H2'	1:1A:1052:C:O4'	2.14	0.48
32:1a:269:C:H2'	32:1a:270:A:C8	2.48	0.48
42:1k:99:GLN:HG3	42:1k:105:VAL:HG21	1.94	0.48
57:1y:33:U:H2'	57:1y:34:G:H3'	1.95	0.48
2:2B:118:G:H2'	2:2B:119:G:O4'	2.14	0.48
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.94	0.48
28:26:38:LYS:HB2	28:26:49:HIS:CE1	2.48	0.48
32:2a:546:G:OP1	35:2d:73:ARG:HG2	2.14	0.48
33:2b:103:THR:HA	33:2b:180:LEU:HD11	1.94	0.48
37:2f:2:ARG:NE	37:2f:69:GLU:HG2	2.27	0.48
1:1A:518:G:H2'	1:1A:519:U:C6	2.49	0.48
1:1A:1090:U:C2	1:1A:1102:C:H1'	2.49	0.48
1:1A:1364:G:P	23:11:3:LYS:HG3	2.53	0.48
18:1W:68:ARG:NH1	18:1W:112:GLY:H	2.12	0.48
32:1a:156:G:H2'	32:1a:157:G:H8	1.78	0.48
32:1a:358:U:H2'	32:1a:359:U:C6	2.48	0.48
32:1a:1036:G:H3'	32:1a:1037:C:C6	2.49	0.48
43:1l:33:ARG:HA	43:1l:33:ARG:HD2	1.61	0.48
1:2A:2096:U:H2'	1:2A:2097:C:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2193:G:H2'	1:2A:2194:G:C8	2.49	0.48
3:2D:123:ALA:HB3	3:2D:131:LEU:HG	1.96	0.48
7:2H:143:GLN:NE2	7:2H:147:ASN:OD1	2.46	0.48
32:2a:735:C:H2'	32:2a:736:C:H6	1.78	0.48
33:2b:212:GLN:OE1	33:2b:216:SER:HB3	2.14	0.48
37:2f:76:ALA:HB1	37:2f:80:ARG:NH2	2.26	0.48
40:2i:37:PHE:HB3	40:2i:43:ALA:HB2	1.95	0.48
1:1A:2316:C:O2'	6:1G:128:ARG:NH2	2.47	0.48
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.95	0.48
21:1Z:48:PHE:CE1	21:1Z:52:SER:HA	2.49	0.48
32:1a:767:A:H2'	32:1a:768:A:O4'	2.14	0.48
32:1a:1525:G:OP1	42:1k:120:ARG:NH2	2.47	0.48
33:1b:222:ILE:O	33:1b:226:ARG:HG2	2.14	0.48
35:1d:111:ALA:HB2	35:1d:120:LEU:HD12	1.95	0.48
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.49	0.48
11:2P:38:GLN:O	11:2P:39:LYS:HB3	2.12	0.48
32:2a:624:C:H2'	32:2a:625:G:H8	1.78	0.48
32:2a:1478:C:H2'	32:2a:1479:C:H6	1.79	0.48
36:2e:27:ARG:NH1	62:2e:302:HOH:O	2.45	0.48
8:1I:6:LEU:O	8:1I:7:GLU:HG3	2.13	0.48
21:1Z:52:SER:C	21:1Z:54:HIS:N	2.71	0.48
24:12:51:ARG:O	24:12:55:ARG:HG2	2.13	0.48
32:1a:192:U:O2'	51:1t:60:GLU:OE1	2.24	0.48
32:1a:736:C:H2'	32:1a:737:A:C8	2.49	0.48
32:1a:865:A:H2	32:1a:918:A:H4'	1.78	0.48
32:1a:1456:G:N2	51:1t:51:GLU:OE2	2.40	0.48
40:1i:17:VAL:HG11	40:1i:80:GLY:C	2.39	0.48
1:2A:2552:2MU:H2'	1:2A:2554:U:OP2	2.14	0.48
1:2A:2602:A:N6	55:2x:76:8AN:H2'	2.29	0.48
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.49	0.48
2:2B:11:C:OP2	22:20:72:ARG:NH2	2.47	0.48
3:2D:146:GLU:HG2	3:2D:152:GLY:C	2.39	0.48
4:2E:143:ASN:HB2	4:2E:147:PRO:HD2	1.96	0.48
12:2Q:110:THR:HG22	12:2Q:112:GLU:H	1.79	0.48
32:2a:818:G:O2'	32:2a:819:A:H5'	2.13	0.48
32:2a:1299:A:H2'	32:2a:1299:A:N3	2.29	0.48
35:2d:18:LYS:HG3	35:2d:33:MET:HG2	1.95	0.48
41:2j:35:SER:HB3	41:2j:73:ASP:HB2	1.96	0.48
44:2m:33:ALA:HA	44:2m:59:TYR:CE2	2.49	0.48
49:2r:84:LYS:H	49:2r:84:LYS:HD2	1.79	0.48
8:1I:38:LEU:HG	8:1I:40:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:1y:42:C:H2'	57:1y:43:C:H6	1.77	0.47
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.14	0.47
5:2F:9:ILE:HD11	5:2F:22:ALA:HB3	1.95	0.47
8:2I:77:LEU:HD21	8:2I:100:ALA:HB3	1.96	0.47
32:2a:67:C:H2'	32:2a:68:G:C8	2.49	0.47
32:2a:435:C:H2'	32:2a:436:C:H6	1.78	0.47
40:2i:50:LEU:HA	40:2i:53:VAL:HG22	1.96	0.47
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.39	0.47
51:2t:86:ARG:O	51:2t:90:GLN:HB2	2.14	0.47
1:1A:1058:G:N2	1:1A:1080:C:N3	2.51	0.47
1:1A:1082:U:C4	1:1A:1086:A:N1	2.79	0.47
1:1A:1698:A:C8	1:1A:1700:A:O4'	2.67	0.47
7:1H:98:LEU:HG	7:1H:125:VAL:HG23	1.96	0.47
32:1a:103:C:O2'	32:1a:172:A:N1	2.45	0.47
32:1a:828:A:H2'	32:1a:829:G:O4'	2.14	0.47
32:1a:1525:G:P	42:1k:120:ARG:HH22	2.37	0.47
1:2A:747:U:O2	1:2A:2014:A:H1'	2.14	0.47
1:2A:878:A:H61	1:2A:899:A:H1'	1.80	0.47
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.49	0.47
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.14	0.47
1:2A:2561:A:H4'	10:2O:22:ILE:HD11	1.97	0.47
5:2F:33:LEU:HB3	11:2P:6:LEU:HD21	1.95	0.47
21:2Z:102:LEU:HD13	21:2Z:123:ASP:HA	1.96	0.47
32:2a:1320:C:H2'	32:2a:1321:C:O4'	2.13	0.47
41:2j:74:ILE:HG22	62:2j:301:HOH:O	2.13	0.47
1:1A:1075:C:H2'	1:1A:1076:C:H5'	1.95	0.47
11:1P:121:LYS:O	11:1P:123:LEU:N	2.47	0.47
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.79	0.47
23:11:82:LEU:HA	23:11:85:LEU:HD12	1.95	0.47
32:1a:1223:C:P	50:1s:78:ARG:HH21	2.37	0.47
33:1b:109:SER:O	33:1b:112:VAL:HG22	2.13	0.47
35:1d:13:ARG:HB3	35:1d:38:TYR:O	2.14	0.47
45:1n:33:VAL:HA	45:1n:40:CYS:HA	1.94	0.47
53:1v:14:A:H3'	53:1v:15:A:C8	2.49	0.47
1:2A:711:G:H1	1:2A:720:C:H42	1.62	0.47
1:2A:1889:A:N1	1:2A:2234:G:H1'	2.29	0.47
1:2A:2099:U:H3	1:2A:2190:G:H1	1.63	0.47
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.96	0.47
32:2a:1119:C:OP2	40:2i:9:ARG:NH2	2.48	0.47
32:2a:1251:A:H2'	32:2a:1252:A:C8	2.49	0.47
1:1A:2611:U:H5'	1:1A:2611:U:H6	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:33:LEU:HD21	7:1H:136:ILE:HG13	1.96	0.47
30:18:4:MET:HE3	30:18:63:PRO:HG3	1.95	0.47
32:1a:1002:G:H3'	32:1a:1003:G:C4'	2.44	0.47
32:1a:1298:C:H4'	32:1a:1299:A:C4	2.49	0.47
33:1b:97:TRP:HZ2	33:1b:102:LEU:HD13	1.80	0.47
42:1k:21:ILE:HG12	42:1k:30:VAL:HG22	1.96	0.47
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.40	0.47
6:2G:101:ILE:HD13	26:24:25:TYR:HB2	1.97	0.47
6:2G:151:ALA:HB3	6:2G:153:ARG:HH12	1.79	0.47
32:2a:707:C:H2'	32:2a:708:C:H6	1.78	0.47
32:2a:1014:A:H4'	50:2s:14:HIS:CD2	2.50	0.47
57:2y:61:C:H2'	57:2y:62:C:C6	2.49	0.47
1:1A:192:C:OP1	62:1A:4239:HOH:O	2.20	0.47
1:1A:2428:G:N7	62:1A:4302:HOH:O	2.36	0.47
32:1a:421:U:O4	34:1c:127:ARG:NH2	2.47	0.47
32:1a:435:C:H2'	32:1a:436:C:H6	1.80	0.47
32:1a:693:G:OP2	62:1a:1928:HOH:O	2.20	0.47
32:1a:1314:C:H2'	32:1a:1315:U:C6	2.50	0.47
32:1a:1458:G:OP1	51:1t:35:THR:OG1	2.28	0.47
46:1o:5:LYS:O	46:1o:9:GLN:HG2	2.14	0.47
48:1q:67:LYS:O	48:1q:68:ARG:HB2	2.15	0.47
57:1y:19:G:O4'	57:1y:57:G:N1	2.47	0.47
1:2A:839:U:H2'	1:2A:840:C:C6	2.49	0.47
1:2A:893:C:H2'	1:2A:894:C:C2	2.50	0.47
1:2A:1539:G:H2'	1:2A:1540:U:O4'	2.13	0.47
1:2A:2121:G:H1	1:2A:2177:C:H42	1.61	0.47
1:2A:2467:C:H4'	12:2Q:123:HIS:CD2	2.50	0.47
32:2a:112:G:HO2'	32:2a:354:G:HO2'	1.62	0.47
34:2c:35:GLU:O	34:2c:39:ILE:HG13	2.14	0.47
47:2p:53:VAL:HG13	47:2p:79:VAL:HG22	1.95	0.47
50:2s:33:THR:HG21	50:2s:49:ILE:HD11	1.97	0.47
1:1A:1429:G:H2'	1:1A:1430:C:H6	1.79	0.47
1:1A:1803:A:H4'	3:1D:259:THR:HG23	1.95	0.47
1:1A:1948:G:O6	62:1A:4238:HOH:O	2.19	0.47
62:1A:5864:HOH:O	56:1z:2:THR:HB	2.15	0.47
12:1Q:12:GLN:NE2	12:1Q:72:LYS:HG3	2.29	0.47
12:1Q:89:ASN:HB2	55:1x:1:C:N3	2.29	0.47
32:1a:38:G:N2	32:1a:397:A:H5"	2.26	0.47
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.50	0.47
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.48	0.47
33:1b:134:GLU:HA	33:1b:137:ARG:HE	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:108:ASN:HB3	34:1c:111:LEU:HD13	1.95	0.47
1:2A:579:G:H2'	1:2A:580:C:C6	2.49	0.47
2:2B:83:G:H5"	25:23:52:HIS:CD2	2.49	0.47
11:2P:39:LYS:HB2	11:2P:45:LEU:HD22	1.97	0.47
26:24:50:VAL:HG21	44:2m:64:TRP:C	2.40	0.47
32:2a:1128:C:O2'	32:2a:1129:C:OP1	2.31	0.47
32:2a:1174:G:N7	62:2a:1934:HOH:O	2.34	0.47
32:2a:1381:U:H1'	38:2g:79:ARG:HD2	1.96	0.47
35:2d:50:ARG:HH12	36:2e:10:MET:HG3	1.79	0.47
46:2o:82:ILE:HD12	46:2o:88:ARG:HB2	1.96	0.47
50:2s:16:LEU:HG	50:2s:20:LEU:HD12	1.96	0.47
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.49	0.47
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.79	0.47
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.49	0.47
1:1A:2156:G:H2'	1:1A:2157:G:C2	2.49	0.47
1:1A:2206:G:H8	1:1A:2207:G:N7	2.13	0.47
4:1E:77:ILE:HD12	4:1E:195:LEU:HD13	1.96	0.47
5:1F:14:PRO:HD2	5:1F:127:GLU:OE1	2.14	0.47
18:1W:67:ASP:N	18:1W:67:ASP:OD1	2.46	0.47
32:1a:149:A:N1	32:1a:172:A:N6	2.63	0.47
32:1a:219:C:H2'	32:1a:220:G:O4'	2.14	0.47
32:1a:571:U:OP1	62:1a:1930:HOH:O	2.21	0.47
39:1h:21:LYS:O	39:1h:65:TYR:OH	2.28	0.47
40:1i:70:LYS:O	40:1i:74:ILE:HG13	2.14	0.47
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.96	0.47
1:2A:981:A:N1	1:2A:2027:G:O2'	2.48	0.47
1:2A:1041:C:H6	1:2A:1041:C:O5'	1.97	0.47
1:2A:1778:U:OP1	62:2A:3951:HOH:O	2.20	0.47
1:2A:2152:G:N2	1:2A:2153:G:N3	2.63	0.47
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.50	0.47
3:2D:179:SER:O	3:2D:275:LYS:HG2	2.15	0.47
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.58	0.47
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.97	0.47
8:2I:134:PRO:C	8:2I:136:VAL:H	2.23	0.47
10:2O:85:VAL:HG11	10:2O:114:ILE:HG12	1.96	0.47
17:2V:1:MET:HE1	17:2V:44:LYS:H	1.80	0.47
21:2Z:53:ILE:HA	21:2Z:71:VAL:HG23	1.97	0.47
32:2a:1278:U:H5'	32:2a:1279:A:OP1	2.15	0.47
32:2a:1288:A:N1	32:2a:1371:G:H1'	2.29	0.47
32:2a:1368:G:OP1	40:2i:111:ARG:NH2	2.47	0.47
34:2c:39:ILE:HG22	34:2c:43:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:81:THR:C	41:2j:83:GLU:N	2.73	0.47
44:2m:49:THR:OG1	44:2m:52:GLU:HG3	2.14	0.47
57:2y:8:4SU:H2'	57:2y:46:G7M:H22	1.80	0.47
1:1A:242:G:C8	30:18:5:LYS:HG2	2.49	0.47
1:1A:2576:G:H1'	62:1A:5264:HOH:O	2.15	0.47
6:1G:18:GLU:O	6:1G:22:ARG:HB2	2.14	0.47
8:1I:60:GLU:HG3	8:1I:61:ARG:HD2	1.97	0.47
12:1Q:89:ASN:HB2	55:1x:1:C:C4	2.49	0.47
32:1a:1241:G:H2'	32:1a:1242:C:C6	2.50	0.47
33:1b:196:LEU:HD12	33:1b:196:LEU:HA	1.80	0.47
35:1d:23:GLY:HA3	35:1d:112:VAL:HG22	1.97	0.47
1:2A:686:G:N2	1:2A:788:A:H61	2.12	0.47
1:2A:2148:G:H2'	1:2A:2149:G:C8	2.50	0.47
1:2A:2892:A:H2'	1:2A:2893:G:H5'	1.97	0.47
6:2G:129:GLY:O	6:2G:161:THR:HB	2.15	0.47
9:2N:35:ARG:O	9:2N:42:TRP:NE1	2.48	0.47
17:2V:24:LYS:HB3	17:2V:24:LYS:HE2	1.70	0.47
21:2Z:98:MET:O	21:2Z:125:LEU:HD12	2.15	0.47
32:2a:157:G:H1	32:2a:164:U:H3	1.61	0.47
32:2a:222:U:H2'	32:2a:223:U:C6	2.49	0.47
32:2a:444:C:H2'	32:2a:445:G:H8	1.77	0.47
32:2a:620:C:H2'	32:2a:621:A:O4'	2.15	0.47
32:2a:1305:G:H5'	52:2u:4:GLY:HA3	1.97	0.47
32:2a:1309:G:N7	44:2m:99:ARG:NH2	2.62	0.47
35:2d:176:LEU:HD12	35:2d:182:LYS:O	2.15	0.47
57:2y:18:G:N2	57:2y:55:PSU:HN3	2.08	0.47
8:1I:87:LYS:NZ	8:1I:121:LYS:HE3	2.29	0.47
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.68	0.47
32:1a:96:U:H2'	32:1a:97:G:C8	2.50	0.47
33:1b:97:TRP:CZ2	33:1b:102:LEU:HD13	2.50	0.47
36:1e:75:THR:HG23	36:1e:76:ILE:O	2.15	0.47
42:1k:27:ASN:OD1	42:1k:28:THR:N	2.48	0.47
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.14	0.47
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.50	0.47
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.50	0.47
5:2F:40:GLN:NE2	5:2F:182:ASN:HB2	2.30	0.47
32:2a:297:G:N2	32:2a:300:A:OP2	2.45	0.47
32:2a:404:U:H2'	32:2a:405:U:C6	2.50	0.47
48:2q:45:HIS:NE2	48:2q:47:PRO:HG3	2.30	0.47
49:2r:73:ALA:HB3	49:2r:79:LEU:HD12	1.96	0.47
1:1A:2331:G:O2'	22:10:43:THR:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.15	0.47
3:1D:2:ALA:O	3:1D:20:ASP:HB3	2.15	0.47
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.97	0.47
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.78	0.47
1:2A:297:C:OP2	62:2A:3952:HOH:O	2.21	0.47
1:2A:1639:U:C2'	1:2A:1640:C:H5"	2.45	0.47
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.47	0.47
8:2I:48:GLU:HG3	8:2I:52:ARG:NH1	2.30	0.47
9:2N:73:THR:HB	9:2N:82:LEU:HD11	1.97	0.47
12:2Q:89:ASN:HB2	55:2x:1:C:C4	2.50	0.47
32:2a:266:G:H2'	32:2a:266:G:N3	2.30	0.47
32:2a:1010:G:C2	32:2a:1020:U:H1'	2.50	0.47
32:2a:1273:G:C6	32:2a:1274:G:C4	3.03	0.47
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.50	0.47
32:2a:1328:C:OP1	52:2u:21:TYR:OH	2.28	0.47
1:1A:857:C:N4	1:1A:858:U:O4	2.48	0.46
17:1V:1:MET:HG2	17:1V:43:GLU:OE1	2.15	0.46
26:14:56:VAL:HG13	26:14:60:GLN:HG3	1.97	0.46
32:1a:266:G:H2'	32:1a:266:G:N3	2.30	0.46
1:2A:7:G:H2'	1:2A:8:A:C8	2.49	0.46
1:2A:2886:G:H2'	1:2A:2887:U:C6	2.49	0.46
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.80	0.46
32:2a:826:C:O2	39:2h:15:ASN:ND2	2.48	0.46
32:2a:955:U:O2'	50:2s:83:HIS:HD2	1.98	0.46
32:2a:1142:G:H2'	32:2a:1143:G:O4'	2.15	0.46
32:2a:1152:A:H2'	32:2a:1153:C:C6	2.50	0.46
33:2b:54:THR:O	33:2b:58:ILE:HG13	2.16	0.46
1:1A:295:G:H4'	20:1Y:1:MET:HE3	1.96	0.46
4:1E:72:VAL:HG12	4:1E:73:GLU:O	2.15	0.46
32:1a:447:G:H2'	32:1a:485:G:N2	2.30	0.46
32:1a:619:U:C2	35:1d:135:LEU:HD22	2.50	0.46
32:1a:1125:U:H4'	41:1j:5:ARG:HH22	1.79	0.46
1:2A:271(A):A:N1	1:2A:272(D):G:O2'	2.45	0.46
1:2A:995:C:O2	9:2N:3:THR:OG1	2.29	0.46
1:2A:1026:U:OP1	62:2A:3916:HOH:O	2.20	0.46
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.15	0.46
3:2D:206:LEU:HD22	3:2D:211:ARG:HG2	1.96	0.46
5:2F:95:ARG:NH1	5:2F:97:TYR:OH	2.48	0.46
9:2N:12:ARG:NH2	9:2N:50:ASP:OD2	2.45	0.46
12:2Q:78:PRO:HD3	55:2x:1:C:C4	2.50	0.46
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:101:LEU:HD13	34:2c:102:ASN:H	1.80	0.46
39:2h:49:GLU:HG2	39:2h:62:TYR:HE2	1.79	0.46
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.48	0.46
55:2x:61:C:H2'	55:2x:62:C:C6	2.50	0.46
1:1A:1173:G:N2	1:1A:1177:A:OP2	2.40	0.46
1:1A:1176:G:N2	1:1A:1178:C:OP2	2.40	0.46
1:1A:1300:U:H4'	1:1A:1301:A:H5"	1.97	0.46
1:1A:1775:U:OP1	1:1A:1979:C:O2'	2.22	0.46
1:1A:1799:G:O2'	3:1D:181:GLU:OE2	2.30	0.46
1:1A:2864:G:OP1	15:1T:119:LYS:HD2	2.16	0.46
15:1T:98:LYS:NZ	62:1T:302:HOH:O	2.43	0.46
21:1Z:54:HIS:HD2	21:1Z:99:TYR:O	1.98	0.46
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.97	0.46
26:14:40:HIS:HB3	26:14:43:TYR:HD2	1.79	0.46
32:1a:1226:C:H4'	50:1s:80:TYR:OH	2.15	0.46
32:1a:1370:G:C2	32:1a:1371:G:C8	3.03	0.46
39:1h:81:HIS:ND1	39:1h:138:TRP:OXT	2.32	0.46
40:1i:48:GLU:HA	40:1i:51:ARG:HD3	1.96	0.46
1:2A:800:A:H8	1:2A:800:A:OP1	1.98	0.46
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.50	0.46
8:2I:75:LEU:HG	8:2I:105:HIS:CD2	2.51	0.46
21:2Z:4:ARG:NH2	21:2Z:66:SER:OG	2.47	0.46
26:24:34:GLU:HG2	26:24:35:VAL:HG23	1.97	0.46
35:2d:74:GLN:O	35:2d:78:LEU:HD13	2.15	0.46
48:2q:45:HIS:HB3	48:2q:72:ARG:HG2	1.98	0.46
51:2t:16:HIS:O	51:2t:19:SER:OG	2.23	0.46
1:1A:185:U:H4'	1:1A:218:A:H4'	1.97	0.46
1:1A:271(K):U:O2'	1:1A:271(M):G:N2	2.49	0.46
11:1P:46:LYS:HB3	11:1P:46:LYS:HE3	1.78	0.46
32:1a:1070:U:H2'	32:1a:1071:C:H6	1.81	0.46
32:1a:1137:C:H5'	32:1a:1138:G:C5	2.50	0.46
33:1b:19:HIS:NE2	33:1b:20:GLU:HG3	2.31	0.46
46:1o:74:ASP:HB3	46:1o:77:ARG:HB2	1.97	0.46
1:2A:570:G:H2'	1:2A:2030:A:C5	2.50	0.46
1:2A:1252:G:N3	16:2U:33:ARG:HG2	2.31	0.46
1:2A:1843:C:H5'	3:2D:253:GLN:OE1	2.16	0.46
8:2I:72:LEU:HA	8:2I:75:LEU:HD22	1.97	0.46
16:2U:69:CYS:HB3	16:2U:74:LEU:HD13	1.96	0.46
22:20:23:VAL:HG22	22:20:38:VAL:HG22	1.97	0.46
32:2a:328:C:H4'	32:2a:329:A:H5'	1.98	0.46
33:2b:142:LEU:HG	33:2b:146:GLN:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:111:LEU:HA	34:2c:111:LEU:HD23	1.78	0.46
40:2i:50:LEU:HD13	40:2i:56:LEU:HA	1.98	0.46
57:2y:52:G:H5'	57:2y:53:G:OP2	2.16	0.46
1:1A:1062:G:C8	1:1A:1070:A:H4'	2.50	0.46
1:1A:1074:G:N1	1:1A:1075:C:H1'	2.30	0.46
1:1A:2319:G:H1	14:1S:3:ARG:HA	1.81	0.46
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.26	0.46
4:1E:59:VAL:O	4:1E:64:LYS:HE2	2.16	0.46
33:1b:8:LYS:HE2	33:1b:8:LYS:HB2	1.76	0.46
39:1h:113:SER:HB2	39:1h:134:ILE:HD11	1.96	0.46
1:2A:784:A:C8	1:2A:792:G:C5	3.04	0.46
1:2A:2331:G:O2'	22:20:43:THR:HG22	2.16	0.46
1:2A:2888:C:H2'	1:2A:2889:C:C6	2.50	0.46
10:2O:36:GLY:HA2	10:2O:106:LEU:HD23	1.97	0.46
11:2P:29:LYS:HD3	11:2P:30:THR:HG23	1.97	0.46
13:2R:104:ARG:HD2	13:2R:107:ASP:OD1	2.16	0.46
14:2S:36:TYR:CD1	14:2S:52:SER:HB3	2.51	0.46
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.48	0.46
23:21:64:ALA:HA	23:21:67:ILE:HG13	1.98	0.46
26:24:61:ARG:HA	26:24:61:ARG:NH1	2.30	0.46
32:2a:93:G:H2'	32:2a:96:U:O4'	2.16	0.46
32:2a:203:U:H2'	32:2a:203:U:OP2	2.15	0.46
35:2d:60:GLU:HG3	35:2d:202:LEU:HD12	1.97	0.46
36:2e:32:VAL:HG21	36:2e:55:VAL:HG23	1.98	0.46
40:2i:42:ARG:NH2	40:2i:71:SER:HG	2.13	0.46
50:2s:38:SER:HB2	50:2s:71:LEU:HD12	1.97	0.46
57:2y:5:G:H2'	57:2y:6:G:O4'	2.15	0.46
1:1A:385:C:O2	11:1P:71:VAL:HG21	2.16	0.46
7:1H:6:ARG:HH12	7:1H:54:ARG:HH22	1.61	0.46
17:1V:55:ALA:CA	17:1V:101:GLY:HA2	2.44	0.46
32:1a:664:G:P	49:1r:64:ARG:HH21	2.38	0.46
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.49	0.46
1:2A:2150:U:H2'	1:2A:2151:G:C8	2.45	0.46
1:2A:2360:A:H2'	1:2A:2361:A:O4'	2.16	0.46
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.44	0.46
4:2E:4:ILE:HD11	4:2E:29:GLY:HA2	1.98	0.46
32:2a:189(F):U:O2	48:2q:63:ARG:NH2	2.49	0.46
32:2a:565:U:OP2	32:2a:566:G:O2'	2.31	0.46
34:2c:148:GLY:HA3	34:2c:172:ARG:O	2.15	0.46
36:2e:36:ASP:O	36:2e:38:GLN:N	2.43	0.46
50:2s:28:LYS:CB	50:2s:29:ARG:HA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:106:C:H1'	20:1Y:1:MET:HE2	1.97	0.46
1:1A:1006:C:C2	1:1A:1138:G:N2	2.83	0.46
1:1A:1055:G:H1	1:1A:1104:C:N4	2.12	0.46
1:1A:2139:C:H2'	1:1A:2140:C:O4'	2.16	0.46
2:1B:2:C:H2'	2:1B:3:C:C6	2.51	0.46
4:1E:56:PRO:C	4:1E:58:ARG:H	2.23	0.46
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.16	0.46
14:1S:61:ASN:HB3	14:1S:64:GLU:HG2	1.97	0.46
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.50	0.46
26:14:63:TYR:N	26:14:64:GLY:HA2	2.29	0.46
32:1a:68:G:H1	32:1a:101:A:H61	1.64	0.46
32:1a:666:G:H5'	32:1a:726:C:H1'	1.97	0.46
1:2A:623:G:H2'	1:2A:624:C:C6	2.51	0.46
1:2A:1309:G:O2'	1:2A:1611:C:O2'	2.29	0.46
1:2A:2166:G:H3'	1:2A:2167:U:H5"	1.98	0.46
1:2A:2552:2MU:H6	1:2A:2552:2MU:O5'	2.16	0.46
3:2D:168:ARG:HG2	3:2D:173:VAL:HG12	1.97	0.46
12:2Q:85:LYS:HE2	22:20:7:LEU:HD12	1.98	0.46
30:28:4:MET:HE3	30:28:63:PRO:HG3	1.98	0.46
33:2b:111:ARG:HA	33:2b:111:ARG:HD3	1.74	0.46
39:2h:73:ASP:OD2	39:2h:75:ARG:NH2	2.44	0.46
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.97	0.46
55:2x:5:G:H1	55:2x:68:C:H42	1.63	0.46
1:1A:184:C:H2'	1:1A:185:U:C6	2.51	0.46
1:1A:2609:U:H2'	56:1z:2:THR:HG22	1.98	0.46
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.97	0.46
6:1G:53:LEU:HD11	6:1G:87:PRO:HB2	1.97	0.46
7:1H:125:VAL:HG22	7:1H:131:VAL:HG22	1.97	0.46
26:14:16:CYS:HB3	26:14:20:ASN:HB3	1.97	0.46
32:1a:591:U:H2'	32:1a:592:G:C8	2.51	0.46
32:1a:946:A:H2'	32:1a:947:G:C8	2.51	0.46
32:1a:1148:U:O4'	40:1i:16:ARG:HD2	2.15	0.46
34:1c:95:THR:C	34:1c:97:LYS:H	2.24	0.46
38:1g:152:ALA:O	38:1g:155:ARG:HB3	2.15	0.46
42:1k:45:GLY:O	42:1k:50:TYR:HB2	2.16	0.46
1:2A:1790:C:H5"	1:2A:1791:A:OP1	2.14	0.46
1:2A:2163:C:OP1	1:2A:2165:G:N2	2.48	0.46
1:2A:2572:A:OP1	1:2A:2574:G:O2'	2.33	0.46
12:2Q:65:PHE:HB2	12:2Q:105:GLU:HB2	1.98	0.46
21:2Z:150:LEU:HD12	21:2Z:151:HIS:O	2.16	0.46
32:2a:444:C:H2'	32:2a:445:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2y:15:G:N2	57:2y:48:C:H42	2.12	0.46
1:1A:1693:U:H1'	3:1D:14:ARG:NH1	2.31	0.46
1:1A:2049:G:H5"	62:1A:4933:HOH:O	2.14	0.46
1:1A:2081:C:OP1	23:11:19:GLN:NE2	2.47	0.46
3:1D:146:GLU:HG2	3:1D:152:GLY:C	2.41	0.46
5:1F:101:LEU:HD12	5:1F:102:PRO:HD2	1.98	0.46
25:13:44:ARG:O	25:13:48:GLU:HG3	2.15	0.46
32:1a:1318:A:H5"	50:1s:3:ARG:NH1	2.24	0.46
1:2A:154(A):C:H42	1:2A:171:G:H1	1.63	0.46
32:2a:410:G:OP1	35:2d:30:LYS:NZ	2.31	0.46
32:2a:924:C:O2'	32:2a:1502:A:N1	2.45	0.46
35:2d:108:LEU:HD13	35:2d:183:GLY:HA3	1.97	0.46
35:2d:150:GLU:H	35:2d:150:GLU:CD	2.23	0.46
51:2t:22:ARG:NH2	62:2t:301:HOH:O	2.48	0.46
1:1A:800:A:H8	1:1A:800:A:OP1	1.99	0.46
1:1A:910:A:N1	1:1A:2277:G:H1'	2.31	0.46
1:1A:2098:U:H3	1:1A:2191:G:H1	1.63	0.46
9:1N:59:LYS:O	9:1N:61:ARG:NH2	2.49	0.46
32:1a:148:G:H2'	32:1a:149:A:C8	2.50	0.46
37:1f:35:ALA:HA	37:1f:67:MET:HB3	1.98	0.46
38:1g:78:ARG:NH1	38:1g:154:TYR:O	2.49	0.46
39:1h:73:ASP:OD1	39:1h:75:ARG:NE	2.48	0.46
1:2A:1012:U:H5	9:2N:28:THR:HG21	1.79	0.46
1:2A:1580:A:H8	1:2A:1580:A:OP2	1.99	0.46
1:2A:2886:G:H2'	1:2A:2887:U:H6	1.80	0.46
21:2Z:171:ILE:CD1	21:2Z:172:ALA:H	2.28	0.46
32:2a:1010:G:H2'	32:2a:1011:G:H8	1.81	0.46
32:2a:1316:G:N2	32:2a:1318:A:H3'	2.30	0.46
40:2i:105:ASP:HB2	40:2i:107:ARG:HG3	1.97	0.46
42:2k:82:VAL:HB	42:2k:108:ILE:HD13	1.97	0.46
57:2y:7:A:N6	57:2y:65:G:H1	2.14	0.46
1:1A:1055:G:H3'	1:1A:1056:G:H8	1.81	0.45
1:1A:1453:U:O2'	1:1A:1455:G:N7	2.49	0.45
7:1H:7:LEU:HD12	7:1H:8:PRO:HD2	1.97	0.45
13:1R:2:ARG:HA	13:1R:5:LYS:HD2	1.98	0.45
32:1a:861:G:OP2	62:1a:1927:HOH:O	2.20	0.45
34:1c:18:TRP:O	34:1c:54:ARG:NH2	2.49	0.45
34:1c:79:ARG:O	34:1c:82:GLU:HG2	2.16	0.45
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.98	0.45
1:2A:524:U:H2'	1:2A:525:U:C6	2.51	0.45
1:2A:2298:A:H62	1:2A:2318:G:H8	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2864:G:OP1	15:2T:119:LYS:HD3	2.16	0.45
14:2S:31:SER:HG	14:2S:34:HIS:H	1.64	0.45
21:2Z:5:LEU:HD11	21:2Z:44:PHE:HA	1.97	0.45
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.98	0.45
32:2a:337:C:H2'	32:2a:338:A:C8	2.51	0.45
32:2a:719:C:N4	49:2r:71:LYS:HE2	2.31	0.45
1:1A:821:A:H2'	1:1A:946:G:H5"	1.96	0.45
1:1A:1071:G:OP1	1:1A:1071:G:H3'	2.16	0.45
2:1B:88:C:H2'	2:1B:89:G:O4'	2.16	0.45
5:1F:28:ILE:O	5:1F:30:PRO:HD3	2.16	0.45
6:1G:60:LEU:HB3	6:1G:68:PRO:HG3	1.98	0.45
19:1X:94:GLY:H	19:1X:95:LEU:C	2.24	0.45
32:1a:486:U:H2'	32:1a:487:A:C8	2.51	0.45
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.51	0.45
33:1b:55:PHE:HD1	33:1b:221:LEU:HG	1.81	0.45
51:1t:22:ARG:O	51:1t:26:ASN:ND2	2.49	0.45
1:2A:131:G:OP1	62:2A:3954:HOH:O	2.21	0.45
1:2A:1359:A:H2	1:2A:1372:U:O4	1.99	0.45
1:2A:1359:A:C2	1:2A:1372:U:O4	2.70	0.45
1:2A:1657:C:H2'	1:2A:1658:C:H6	1.81	0.45
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.17	0.45
4:2E:181:LEU:HD11	15:2T:6:LEU:HD22	1.97	0.45
14:2S:103:GLU:O	14:2S:107:GLU:HG3	2.17	0.45
32:2a:438:G:H4'	35:2d:123:HIS:CE1	2.52	0.45
32:2a:730:G:C5	32:2a:731:G:H1'	2.51	0.45
32:2a:1087:G:N2	32:2a:1099:G:H1'	2.30	0.45
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.79	0.45
34:2c:152:ILE:HG13	34:2c:199:LYS:HB2	1.98	0.45
1:1A:2143:C:H2'	1:1A:2144:U:O4'	2.16	0.45
1:1A:2359:C:H2'	1:1A:2360:A:O4'	2.17	0.45
25:13:39:ASP:OD1	25:13:44:ARG:HD2	2.17	0.45
32:1a:626:U:C2	32:1a:627:G:C8	3.05	0.45
33:1b:185:ILE:HG22	33:1b:199:TYR:HD2	1.81	0.45
57:1y:19:G:H5"	57:1y:60:U:O4	2.17	0.45
57:1y:26:A:N6	57:1y:44:G:N1	2.62	0.45
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.31	0.45
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.16	0.45
1:2A:2142:C:H2'	1:2A:2143:C:O4'	2.16	0.45
1:2A:2555:U:O4	62:2A:3948:HOH:O	2.20	0.45
5:2F:165:ARG:HG2	5:2F:168:ARG:NH2	2.32	0.45
8:2I:26:ALA:O	8:2I:31:LEU:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:45:ASP:CG	21:2Z:49:ARG:HE	2.23	0.45
32:2a:21:G:H2'	32:2a:22:G:C8	2.52	0.45
42:2k:79:SER:HA	42:2k:104:GLN:HB3	1.99	0.45
44:2m:79:LYS:HG2	44:2m:83:ASP:OD2	2.15	0.45
44:2m:88:ARG:HG2	44:2m:98:VAL:HG12	1.98	0.45
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.16	0.45
1:1A:774:A:N3	1:1A:774:A:H2'	2.30	0.45
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.16	0.45
1:1A:2464:C:H1'	62:1A:5500:HOH:O	2.16	0.45
5:1F:150:GLY:HA2	5:1F:172:TRP:CD2	2.52	0.45
8:1I:84:GLY:O	8:1I:86:THR:N	2.43	0.45
21:1Z:136:PHE:O	21:1Z:137:ILE:HG13	2.17	0.45
32:1a:406:G:N3	35:1d:119:GLN:NE2	2.63	0.45
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.52	0.45
32:1a:1288:A:H2'	32:1a:1289:A:C8	2.51	0.45
32:1a:1503:A:N3	53:1v:13:A:N6	2.65	0.45
1:2A:910:A:C5	12:2Q:13:GLN:HG3	2.51	0.45
1:2A:1027:A:C2	1:2A:2488:A:H5'	2.52	0.45
1:2A:1721:G:H8	1:2A:1741:A:H62	1.63	0.45
1:2A:2131:G:H4'	1:2A:2132:U:H3'	1.97	0.45
1:2A:2637:U:OP1	4:2E:82:ARG:NH1	2.48	0.45
9:2N:99:LEU:O	9:2N:103:VAL:HG23	2.17	0.45
25:23:17:LYS:HA	25:23:20:LYS:HG3	1.97	0.45
30:28:50:LEU:HD23	30:28:50:LEU:HA	1.82	0.45
32:2a:109:A:C6	32:2a:326:G:C6	3.05	0.45
32:2a:114:U:H2'	32:2a:115:G:C8	2.52	0.45
32:2a:646:U:H2'	32:2a:647:C:C6	2.52	0.45
32:2a:736:C:H2'	32:2a:737:A:C8	2.51	0.45
32:2a:1194:U:H2'	32:2a:1195:C:C6	2.52	0.45
49:2r:33:ASP:OD2	49:2r:36:ASN:HB2	2.17	0.45
1:1A:271(T):C:H2'	1:1A:271(U):G:C8	2.51	0.45
1:1A:284:U:H2'	1:1A:285:C:C6	2.52	0.45
1:1A:1062:G:C4	1:1A:1088:A:H2'	2.51	0.45
1:1A:2512:C:H2'	1:1A:2513:G:O4'	2.17	0.45
1:1A:2820:A:O2'	1:1A:2821:A:OP1	2.32	0.45
5:1F:89:VAL:O	62:1F:401:HOH:O	2.21	0.45
10:1O:97:ARG:NH1	32:1a:339:C:OP2	2.41	0.45
32:1a:472:A:OP1	47:1p:75:ARG:NH2	2.41	0.45
32:1a:975:A:H5'	32:1a:975:A:C8	2.52	0.45
35:1d:209:ARG:OXT	62:1d:401:HOH:O	2.21	0.45
46:1o:3:ILE:HG21	46:1o:34:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2390:U:P	30:28:35:GLN:HE22	2.39	0.45
1:2A:2888:C:H2'	1:2A:2889:C:H6	1.81	0.45
6:2G:45:GLU:H	6:2G:45:GLU:HG2	1.39	0.45
7:2H:121:ILE:HD11	7:2H:140:LYS:HG2	1.98	0.45
8:2I:6:LEU:O	8:2I:7:GLU:HG3	2.17	0.45
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.17	0.45
42:2k:84:VAL:HG21	42:2k:95:ILE:HD11	1.99	0.45
47:2p:8:ARG:HB3	47:2p:28:ARG:NH1	2.32	0.45
51:2t:67:ALA:HA	51:2t:72:LEU:O	2.17	0.45
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.98	0.45
11:1P:89:ALA:HA	11:1P:121:LYS:HD3	1.98	0.45
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.58	0.45
32:1a:903:G:OP1	62:1a:1931:HOH:O	2.21	0.45
33:1b:69:LEU:HD13	33:1b:91:PRO:HB2	1.98	0.45
54:1w:48:C:C2	54:1w:59:U:H1'	2.52	0.45
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.52	0.45
1:2A:2531:A:N7	7:2H:175:LYS:HD2	2.31	0.45
1:2A:2819:G:H2'	1:2A:2821:A:N7	2.32	0.45
6:2G:16:ARG:HB2	6:2G:17:PRO:HD3	1.97	0.45
6:2G:114:ILE:HB	6:2G:117:PHE:HD1	1.82	0.45
7:2H:127:GLU:HG3	7:2H:130:ARG:HB3	1.98	0.45
31:29:10:ILE:HD12	31:29:32:HIS:HA	1.99	0.45
32:2a:130:A:O2'	32:2a:131:C:O5'	2.31	0.45
32:2a:984:C:H2'	32:2a:985:C:C6	2.52	0.45
32:2a:1076:C:OP1	33:2b:179:LYS:NZ	2.50	0.45
1:1A:603:A:O4'	1:1A:655:A:N6	2.49	0.45
1:1A:637:A:H4'	1:1A:638:G:O5'	2.17	0.45
1:1A:1173:G:OP2	1:1A:1173:G:H2'	2.17	0.45
1:1A:2273:A:H2'	1:1A:2274:A:C8	2.51	0.45
35:1d:119:GLN:HG2	35:1d:123:HIS:CD2	2.51	0.45
57:1y:51:U:H3	57:1y:63:G:H1	1.65	0.45
1:2A:839:U:H1'	1:2A:1191:G:H1'	1.97	0.45
1:2A:2632:A:O2'	1:2A:2811:G:O2'	2.25	0.45
15:2T:27:THR:HG22	15:2T:89:VAL:HB	1.98	0.45
32:2a:160:A:H1'	32:2a:344:A:C5	2.52	0.45
44:2m:91:ARG:NH1	44:2m:96:LEU:HD13	2.32	0.45
54:2w:21:A:O2'	54:2w:22:G:OP1	2.35	0.45
54:2w:43:C:H2'	54:2w:44:G:C8	2.51	0.45
1:1A:2461:C:H2'	1:1A:2462:U:C6	2.52	0.45
8:1I:39:ALA:HB1	8:1I:44:LEU:HD13	1.97	0.45
32:1a:975:A:H5'	32:1a:975:A:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1016:A:H2'	32:1a:1017:G:O4'	2.17	0.45
33:1b:61:LEU:HG	33:1b:66:GLY:HA3	1.99	0.45
38:1g:78:ARG:HA	38:1g:78:ARG:HD2	1.54	0.45
38:1g:89:MET:SD	38:1g:155:ARG:HB2	2.56	0.45
44:1m:15:VAL:HG13	44:1m:43:THR:O	2.17	0.45
1:2A:176:G:O2'	1:2A:177:G:H5'	2.17	0.45
1:2A:271(S):G:C6	1:2A:271(T):C:C4	3.05	0.45
1:2A:307:G:N1	1:2A:310:A:OP2	2.48	0.45
1:2A:2019:A:N7	27:25:9:LYS:HE2	2.31	0.45
8:2I:57:ARG:CG	8:2I:61:ARG:HH21	2.29	0.45
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.51	0.45
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.16	0.45
38:2g:50:ILE:HD11	38:2g:58:PRO:HB3	1.98	0.45
49:2r:30:ASP:C	49:2r:32:ARG:H	2.25	0.45
55:2x:53:G:H2'	55:2x:54:5MU:C6	2.52	0.45
1:1A:996:A:H4'	16:1U:91:ASP:OD2	2.17	0.45
1:1A:1045:A:H1'	1:1A:1047:G:N3	2.31	0.45
1:1A:1183:G:O2'	25:13:29:ARG:NH2	2.50	0.45
1:1A:2023:G:H4'	1:1A:2617:C:O3'	2.17	0.45
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.99	0.45
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.52	0.45
32:1a:1004:A:H5"	32:1a:1025:U:C5	2.51	0.45
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.80	0.45
35:1d:107:ARG:NH2	35:1d:194:LEU:HD11	2.31	0.45
38:1g:126:ASP:HB3	38:1g:131:LYS:HB2	1.98	0.45
1:2A:27:G:N2	1:2A:512:G:H1'	2.32	0.45
1:2A:764:A:H5"	3:2D:210:GLY:CA	2.47	0.45
1:2A:1589:C:H2'	1:2A:1590:U:H6	1.81	0.45
1:2A:2334:G:H5'	14:2S:9:ARG:HG2	1.98	0.45
1:2A:2507:C:H2'	1:2A:2508:G:O4'	2.17	0.45
5:2F:157:VAL:HG12	5:2F:178:PRO:HA	1.98	0.45
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.99	0.45
6:2G:122:PRO:HB3	6:2G:170:ARG:HH21	1.82	0.45
15:2T:127:ALA:C	15:2T:129:ARG:H	2.25	0.45
28:26:50:ARG:HG3	28:26:51:GLU:H	1.82	0.45
32:2a:108:G:C6	51:2t:15:ARG:HG2	2.51	0.45
32:2a:755:G:OP2	46:2o:65:ARG:HD2	2.17	0.45
33:2b:187:LEU:HA	33:2b:201:ILE:HB	1.98	0.45
45:2n:59:ALA:HB1	45:2n:61:TRP:HZ3	1.82	0.45
51:2t:43:LEU:HD13	51:2t:51:GLU:HG3	1.99	0.45
52:2u:6:ARG:HD3	52:2u:15:ARG:HE	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:479:A:N3	1:1A:481:G:H5”	2.32	0.45
1:1A:668:G:H5’	1:1A:669:G:OP2	2.17	0.45
1:1A:829:A:N7	1:1A:2248:C:H5’	2.32	0.45
1:1A:2160:G:C6	1:1A:2161:C:N4	2.84	0.45
12:1Q:51:ARG:HD3	12:1Q:66:ILE:HD11	1.97	0.45
32:1a:200:G:H1	32:1a:217:C:N4	2.15	0.45
32:1a:406:G:H21	35:1d:119:GLN:HE22	1.65	0.45
32:1a:963:G:H5’	62:1a:2046:HOH:O	2.17	0.45
33:1b:66:GLY:O	33:1b:90:MET:HE1	2.17	0.45
33:1b:78:GLN:HA	33:1b:78:GLN:HE21	1.82	0.45
35:1d:155:LEU:HD23	35:1d:155:LEU:HA	1.77	0.45
44:1m:49:THR:HB	44:1m:52:GLU:HG3	1.99	0.45
57:1y:24:G:H2’	57:1y:25:C:O4’	2.17	0.45
1:2A:2811:G:N2	1:2A:2891:G:H1’	2.32	0.45
5:2F:143:ALA:HB1	5:2F:148:LEU:HB2	1.99	0.45
21:2Z:45:ASP:OD1	21:2Z:49:ARG:NE	2.40	0.45
22:20:32:ARG:H	22:20:35:ASN:ND2	2.14	0.45
27:25:45:VAL:HG11	27:25:58:LEU:HD22	1.97	0.45
32:2a:991:U:C5	32:2a:1212:U:H1’	2.51	0.45
32:2a:1346:A:N6	38:2g:10:ARG:HH12	2.14	0.45
33:2b:8:LYS:O	33:2b:8:LYS:HG2	2.17	0.45
33:2b:10:LEU:HD12	33:2b:10:LEU:HA	1.73	0.45
33:2b:185:ILE:HG22	33:2b:199:TYR:HD2	1.81	0.45
34:2c:43:LEU:HD13	34:2c:55:VAL:HG21	1.99	0.45
54:2w:14:A:N6	54:2w:21:A:H2	2.14	0.45
1:1A:213:A:H2’	1:1A:214:G:O4’	2.17	0.44
1:1A:271(C):C:H42	1:1A:271(U):G:H1	1.65	0.44
1:1A:272(G):C:H42	1:1A:363(C):G:H1	1.63	0.44
1:1A:1059:G:H2’	1:1A:1060:U:C5	2.52	0.44
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.18	0.44
35:1d:63:LYS:HD2	35:1d:198:VAL:HG22	1.99	0.44
37:1f:76:ALA:O	37:1f:80:ARG:HG3	2.17	0.44
54:1w:4:C:H42	54:1w:69:G:H1	1.65	0.44
1:2A:1003:G:O2’	1:2A:1010:A:N1	2.42	0.44
1:2A:1019:U:O2’	1:2A:1021:A:H2	1.98	0.44
1:2A:2098:U:H3	1:2A:2191:G:H1	1.64	0.44
1:2A:2651:C:H42	1:2A:2669:G:H1	1.65	0.44
5:2F:12:LEU:HG	5:2F:124:LEU:HD11	1.99	0.44
5:2F:20:LEU:HD12	5:2F:20:LEU:HA	1.81	0.44
5:2F:108:LYS:O	5:2F:112:MET:HG3	2.17	0.44
8:2I:129:THR:HA	8:2I:138:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1346:A:N1	32:2a:1374:A:H5"	2.32	0.44
39:2h:110:ALA:HB3	39:2h:121:ASP:HB3	1.99	0.44
40:2i:31:GLN:NE2	40:2i:36:TYR:HD1	2.15	0.44
44:2m:108:ARG:HD3	44:2m:108:ARG:HA	1.73	0.44
1:1A:484:C:H2'	1:1A:485:C:C6	2.53	0.44
1:1A:1345:C:OP2	62:1A:4241:HOH:O	2.21	0.44
3:1D:72:LYS:NZ	3:1D:99:ASP:OD2	2.43	0.44
33:1b:9:GLU:O	33:1b:10:LEU:HD23	2.18	0.44
33:1b:84:GLU:HB3	33:1b:219:VAL:HG21	1.99	0.44
37:1f:89:MET:HE3	37:1f:91:VAL:HG21	1.99	0.44
1:2A:263:C:H2'	1:2A:264:C:O4'	2.17	0.44
1:2A:2839:G:H5'	13:2R:46:GLY:CA	2.47	0.44
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.49	0.44
32:2a:737:A:H2'	32:2a:738:C:C6	2.53	0.44
32:2a:974:A:P	45:2n:29:ARG:HH21	2.40	0.44
32:2a:1040:U:H2'	32:2a:1041:A:C8	2.52	0.44
34:2c:57:ILE:HG12	34:2c:66:VAL:HG22	1.98	0.44
50:2s:81:ARG:HE	50:2s:81:ARG:HB3	1.50	0.44
62:1A:5997:HOH:O	27:15:3:LYS:HE2	2.16	0.44
5:1F:39:TRP:CZ2	5:1F:43:LYS:HE2	2.52	0.44
32:1a:358:U:H2'	32:1a:359:U:H6	1.82	0.44
32:1a:971:G:N2	32:1a:1363(A):A:OP2	2.45	0.44
32:1a:1345:U:H3'	62:1a:1972:HOH:O	2.17	0.44
37:1f:33:TYR:CD2	37:1f:75:LEU:HD23	2.52	0.44
50:1s:19:VAL:HG23	50:1s:47:HIS:CE1	2.53	0.44
57:1y:59:U:H3'	57:1y:60:U:H6	1.81	0.44
1:2A:1448:G:H2'	1:2A:1449:A:C8	2.52	0.44
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.52	0.44
2:2B:7:G:H21	14:2S:38:GLN:NE2	2.03	0.44
8:2I:48:GLU:HG3	8:2I:52:ARG:HH11	1.82	0.44
17:2V:58:VAL:HB	17:2V:98:GLU:HG3	2.00	0.44
32:2a:157:G:H2'	32:2a:158:G:H8	1.82	0.44
32:2a:624:C:H2'	32:2a:625:G:C8	2.52	0.44
32:2a:642:A:N3	39:2h:113:SER:OG	2.44	0.44
32:2a:811:C:O2'	32:2a:901:A:N1	2.48	0.44
32:2a:1145:C:H4'	32:2a:1146:A:H8	1.81	0.44
54:2w:37:MIA:H8	54:2w:37:MIA:O5'	2.18	0.44
1:1A:2051:A:H5'	1:1A:2578:G:O4'	2.18	0.44
23:11:81:LYS:HE3	23:11:81:LYS:HB2	1.70	0.44
32:1a:193:C:H2'	32:1a:194:C:C6	2.52	0.44
32:1a:198:G:H2'	32:1a:199:G:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:406:G:H5'	35:1d:5:ILE:HD12	1.99	0.44
32:1a:591:U:H2'	32:1a:592:G:H8	1.81	0.44
33:1b:37:ASN:C	33:1b:39:ILE:H	2.26	0.44
33:1b:59:GLU:HG2	33:1b:225:ALA:HB2	1.99	0.44
34:1c:8:ILE:HG13	34:1c:9:GLY:N	2.31	0.44
34:1c:28:GLN:HA	34:1c:31:HIS:ND1	2.32	0.44
35:1d:162:LEU:HD13	35:1d:181:MET:HG2	2.00	0.44
41:1j:46:ARG:NH2	41:1j:64:GLU:OE1	2.50	0.44
1:2A:580:C:H2'	1:2A:581:C:C6	2.52	0.44
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.33	0.44
6:2G:50:ALA:C	6:2G:52:ILE:N	2.76	0.44
21:2Z:100:VAL:HA	21:2Z:101:PRO:HD3	1.87	0.44
32:2a:201:C:H5'	32:2a:202:U:OP2	2.18	0.44
32:2a:390:C:O3'	47:2p:28:ARG:NH2	2.51	0.44
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.51	0.44
32:2a:1236:A:O2'	32:2a:1304:G:H4'	2.17	0.44
35:2d:88:VAL:O	35:2d:92:VAL:HG12	2.18	0.44
40:2i:4:TYR:CE1	40:2i:88:TYR:HA	2.52	0.44
40:2i:88:TYR:HD2	40:2i:89:ASN:HB2	1.82	0.44
1:1A:1268:A:C2	1:1A:2013:A:C4	3.06	0.44
1:1A:1541:G:OP2	62:1A:4243:HOH:O	2.21	0.44
7:1H:88:LEU:HD23	7:1H:130:ARG:HG3	2.00	0.44
32:1a:300:A:H1'	32:1a:565:U:O2	2.17	0.44
32:1a:450:G:OP1	47:1p:43:LYS:NZ	2.51	0.44
34:1c:18:TRP:H	34:1c:18:TRP:HE3	1.66	0.44
57:1y:5:G:C2	57:1y:69:G:C5	3.06	0.44
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.51	0.44
1:2A:2466:C:H5"	31:29:6:SER:HB2	1.99	0.44
4:2E:178:GLU:OE1	4:2E:178:GLU:N	2.35	0.44
8:2I:81:VAL:O	8:2I:146:ALA:HA	2.18	0.44
32:2a:540:G:H2'	32:2a:541:G:O4'	2.18	0.44
1:1A:467:G:OP1	29:17:33:ARG:NH1	2.50	0.44
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.18	0.44
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	2.00	0.44
10:1O:120:GLU:OE2	10:1O:122:LEU:HD21	2.18	0.44
32:1a:7:G:H5'	32:1a:298:A:O4'	2.17	0.44
32:1a:109:A:H2'	32:1a:326:G:N2	2.33	0.44
1:2A:271(N):U:OP1	1:2A:271(N):U:H2'	2.17	0.44
1:2A:300:A:P	20:2Y:86:ARG:HH12	2.41	0.44
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.53	0.44
1:2A:1721:G:H3'	1:2A:1722:A:H2'	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1866:C:H2'	1:2A:1876:A:O4'	2.17	0.44
5:2F:32:LEU:O	5:2F:36:VAL:HG23	2.18	0.44
6:2G:97:ASP:O	6:2G:101:ILE:HG13	2.18	0.44
7:2H:8:PRO:O	7:2H:10:PRO:HD3	2.17	0.44
7:2H:26:VAL:O	7:2H:79:VAL:HG11	2.18	0.44
22:20:52:GLY:O	22:20:59:LEU:HA	2.18	0.44
32:2a:441:A:OP2	32:2a:441:A:H8	2.00	0.44
32:2a:512:U:H2'	32:2a:513:C:H6	1.82	0.44
32:2a:986:A:H2'	32:2a:987:G:O4'	2.16	0.44
32:2a:1224:G:H1	32:2a:1363:C:H42	1.65	0.44
32:2a:1321:C:O2'	50:2s:77:THR:HG21	2.18	0.44
36:2e:41:VAL:O	36:2e:66:MET:HA	2.17	0.44
47:2p:6:LEU:HD23	47:2p:17:TYR:CG	2.53	0.44
1:1A:1584:C:O2'	1:1A:1586:A:H5'	2.18	0.44
6:1G:70:VAL:HG11	6:1G:87:PRO:HB3	2.00	0.44
24:12:70:GLN:H	24:12:70:GLN:HG3	1.48	0.44
32:1a:141:A:H1'	32:1a:182:U:O2	2.18	0.44
33:1b:24:TRP:H	33:1b:24:TRP:HD1	1.65	0.44
35:1d:88:VAL:O	35:1d:92:VAL:HG23	2.17	0.44
36:1e:34:VAL:HG12	36:1e:62:ALA:HB1	1.99	0.44
39:1h:87:SER:HB2	39:1h:93:VAL:H	1.81	0.44
43:1l:53:ARG:HB3	43:1l:69:TYR:HE1	1.82	0.44
44:1m:15:VAL:HG11	44:1m:48:LEU:HD21	1.98	0.44
1:2A:403:U:H4'	1:2A:404:C:H5'	1.99	0.44
1:2A:580:C:H2'	1:2A:581:C:H6	1.83	0.44
1:2A:2155:G:N7	1:2A:2156:G:H1'	2.33	0.44
2:2B:31:C:H4'	6:2G:29:TRP:CZ2	2.53	0.44
6:2G:137:GLU:CD	6:2G:140:ILE:HD13	2.43	0.44
9:2N:56:ASN:N	9:2N:125:GLY:O	2.43	0.44
10:2O:76:ALA:HB3	15:2T:75:ILE:HB	2.00	0.44
11:2P:85:LEU:HD23	11:2P:88:LEU:HD12	2.00	0.44
32:2a:745:C:OP1	32:2a:851:G:O2'	2.31	0.44
32:2a:748:C:H4'	32:2a:749:C:O5'	2.18	0.44
32:2a:1263:C:C4	32:2a:1272:G:O6	2.71	0.44
36:2e:19:MET:SD	36:2e:24:ARG:HG3	2.58	0.44
1:1A:2097:C:H2'	1:1A:2098:U:C6	2.53	0.44
1:1A:2747:G:O6	1:1A:2755:C:H5"	2.17	0.44
26:14:50:VAL:HG11	44:1m:64:TRP:C	2.43	0.44
29:17:11:LYS:HE3	29:17:15:THR:OG1	2.18	0.44
32:1a:56:U:H2'	32:1a:57:G:C8	2.53	0.44
32:1a:57:G:H2'	32:1a:58:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:277:C:P	48:1q:68:ARG:HH12	2.41	0.44
32:1a:377:G:OP1	47:1p:3:LYS:HD3	2.18	0.44
32:1a:1023:G:H3'	32:1a:1024:G:C8	2.53	0.44
34:1c:62:ASP:O	34:1c:97:LYS:HB3	2.18	0.44
35:1d:101:LEU:HB2	35:1d:138:TYR:HB3	2.00	0.44
35:1d:107:ARG:NH2	35:1d:194:LEU:HD21	2.32	0.44
36:1e:48:ALA:HB3	36:1e:54:ALA:HB2	2.00	0.44
40:1i:100:GLY:O	40:1i:103:THR:HG23	2.18	0.44
48:1q:87:LYS:HD2	48:1q:87:LYS:HA	1.81	0.44
50:1s:31:ILE:O	50:1s:50:ALA:N	2.40	0.44
56:1z:6:ARG:NH1	62:1z:102:HOH:O	2.40	0.44
1:2A:236:C:H2'	1:2A:237:C:C6	2.52	0.44
1:2A:443:A:N7	5:2F:45:ARG:HG2	2.33	0.44
1:2A:764:A:H5"	3:2D:210:GLY:HA2	1.98	0.44
1:2A:862:G:H2'	1:2A:863:A:O4'	2.18	0.44
33:2b:170:GLU:HB3	33:2b:173:ALA:HB3	2.00	0.44
36:2e:99:GLY:O	36:2e:117:ASP:HA	2.17	0.44
40:2i:17:VAL:HG21	40:2i:81:ILE:HG13	1.99	0.44
57:2y:62:C:H2'	57:2y:63:G:H8	1.82	0.44
1:1A:1670:C:OP1	62:1A:4242:HOH:O	2.21	0.44
4:1E:168:MET:HE2	4:1E:168:MET:HB3	1.90	0.44
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.53	0.44
26:14:62:ARG:C	26:14:63:TYR:CG	2.96	0.44
30:18:61:LEU:C	30:18:63:PRO:HD3	2.42	0.44
32:1a:1269:A:H2	32:1a:1312:G:N3	2.16	0.44
35:1d:112:VAL:HG12	35:1d:116:GLN:NE2	2.33	0.44
39:1h:110:ALA:HB3	39:1h:121:ASP:HB3	1.98	0.44
44:1m:60:VAL:HG22	44:1m:64:TRP:HZ3	1.82	0.44
1:2A:11:G:C2'	1:2A:12:U:H5'	2.48	0.44
1:2A:1006:C:C2	1:2A:1138:G:N2	2.86	0.44
1:2A:2124:G:O6	1:2A:2125:G:N2	2.51	0.44
1:2A:2359:C:H2'	1:2A:2360:A:O4'	2.18	0.44
1:2A:2684:U:H1'	10:2O:70:LYS:HD2	2.00	0.44
2:2B:75:G:H22	21:2Z:73:GLN:HE21	1.65	0.44
2:2B:94:C:H2'	2:2B:95:C:H6	1.83	0.44
9:2N:1:MET:HE1	16:2U:94:ASN:ND2	2.33	0.44
10:2O:112:MET:HA	10:2O:115:VAL:HB	1.99	0.44
34:2c:134:ILE:HD11	34:2c:153:VAL:HG22	2.00	0.44
35:2d:8:VAL:HG22	35:2d:21:LEU:HD13	2.00	0.44
35:2d:200:GLU:OE1	35:2d:200:GLU:N	2.48	0.44
57:2y:9:A:H5'	57:2y:46:G7M:N3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:234:C:H2'	1:1A:235:U:H6	1.82	0.43
1:1A:1047:G:H2'	1:1A:1110:G:N2	2.32	0.43
1:1A:1053:C:N4	1:1A:1106:G:H1	2.16	0.43
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.52	0.43
1:1A:1508:A:H4'	1:1A:1509(A):A:C4	2.52	0.43
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.53	0.43
3:1D:221:VAL:HG22	3:1D:226:MET:HE2	2.00	0.43
35:1d:74:GLN:O	35:1d:78:LEU:HD13	2.18	0.43
51:1t:44:ALA:HB2	51:1t:88:VAL:HG22	2.00	0.43
1:2A:212:G:H2'	1:2A:213:A:O4'	2.18	0.43
1:2A:600:G:O3'	5:2F:108:LYS:HE3	2.18	0.43
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.18	0.43
1:2A:2030:A:H4'	1:2A:2031:A:C8	2.53	0.43
1:2A:2319:G:H22	14:2S:3:ARG:HD2	1.83	0.43
17:2V:29:PRO:HA	17:2V:61:VAL:HG12	2.00	0.43
19:2X:5:TYR:HD1	24:22:33:MET:HE2	1.83	0.43
22:20:70:GLN:OE1	22:20:80:HIS:NE2	2.38	0.43
32:2a:1478:C:H2'	32:2a:1479:C:C6	2.53	0.43
32:2a:1525:G:OP1	42:2k:120:ARG:NH2	2.51	0.43
33:2b:185:ILE:HG22	33:2b:199:TYR:CD2	2.53	0.43
48:2q:14:LYS:HE3	48:2q:14:LYS:HB3	1.71	0.43
1:1A:438:G:H2'	1:1A:440:G:C8	2.53	0.43
1:1A:636:G:OP1	11:1P:132:LYS:NZ	2.50	0.43
1:1A:875:G:H1	1:1A:902:C:H42	1.66	0.43
1:1A:2136:C:C4	1:1A:2155:G:N1	2.86	0.43
32:1a:399:G:H2'	32:1a:400:C:C6	2.53	0.43
32:1a:444:C:H2'	32:1a:445:G:H8	1.83	0.43
32:1a:1044:A:C5	32:1a:1045:C:H1'	2.53	0.43
33:1b:63:MET:HE2	33:1b:63:MET:HB3	1.77	0.43
34:1c:22:TRP:CZ2	45:1n:54:PRO:HG3	2.52	0.43
35:1d:173:TRP:CE2	35:1d:189:PRO:HG3	2.52	0.43
40:1i:53:VAL:O	40:1i:55:ALA:N	2.51	0.43
1:2A:340:A:H2'	1:2A:341:G:O4'	2.18	0.43
1:2A:973:A:H8	1:2A:973:A:OP1	2.01	0.43
1:2A:1697:G:OP2	1:2A:1698:A:O2'	2.31	0.43
1:2A:1782:C:H1'	1:2A:2609:U:H5'	1.99	0.43
1:2A:2303:G:O2'	6:2G:132:ASN:HB2	2.18	0.43
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.30	0.43
2:2B:17:C:H2'	2:2B:18:G:O4'	2.17	0.43
4:2E:1:MET:HB3	4:2E:83:ASP:O	2.18	0.43
8:2I:82:ARG:H	8:2I:82:ARG:HD3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:74:VAL:HB	21:2Z:86:VAL:HG23	2.00	0.43
27:25:41:PRO:O	27:25:44:THR:OG1	2.31	0.43
32:2a:772:U:H2'	32:2a:773:G:O4'	2.19	0.43
32:2a:1259:C:O2'	32:2a:1283:G:N2	2.47	0.43
32:2a:1469:G:H2'	32:2a:1470:G:H8	1.83	0.43
39:2h:82:HIS:CE1	39:2h:84:ARG:HD2	2.53	0.43
46:2o:39:LEU:HB3	46:2o:56:LEU:HD12	2.00	0.43
51:2t:10:LEU:HB3	51:2t:12:ALA:H	1.83	0.43
57:2y:67:C:H2'	57:2y:68:C:C6	2.53	0.43
1:1A:625:G:O6	11:1P:107:LYS:NZ	2.51	0.43
1:1A:768:G:O2'	1:1A:1379:A:N1	2.46	0.43
1:1A:1056:G:H4'	1:1A:1086:A:H8	1.83	0.43
1:1A:1153:C:H2'	1:1A:1154:G:O4'	2.18	0.43
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.53	0.43
2:1B:48:A:H2'	2:1B:49:C:C6	2.53	0.43
30:18:42:ARG:HD2	62:18:202:HOH:O	2.18	0.43
32:1a:1157:A:H5'	32:1a:1158:C:C6	2.54	0.43
32:1a:1504:G:OP1	32:1a:1507:A:H4'	2.18	0.43
38:1g:90:GLU:CD	38:1g:90:GLU:H	2.26	0.43
1:2A:1354:A:H2'	1:2A:1355:G:O4'	2.17	0.43
1:2A:1512:U:H2'	1:2A:1513:C:C6	2.53	0.43
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.53	0.43
1:2A:2114:A:H2'	1:2A:2114:A:N3	2.34	0.43
1:2A:2801(A):A:HO2'	1:2A:2895:U:C1'	2.30	0.43
3:2D:71:ASP:CB	3:2D:103:ARG:HH12	2.31	0.43
18:2W:14:PRO:O	18:2W:18:ARG:HG3	2.18	0.43
22:20:6:GLY:O	22:20:7:LEU:HD23	2.18	0.43
19:1X:44:GLU:HG2	19:1X:49:VAL:O	2.19	0.43
31:19:25:VAL:HB	31:19:34:GLN:HB2	2.00	0.43
32:1a:299:G:O5'	32:1a:299:G:H8	2.01	0.43
32:1a:1124:G:OP1	41:1j:36:GLY:N	2.42	0.43
32:1a:1140:C:H2'	32:1a:1141:C:C6	2.53	0.43
1:2A:1417:C:H2'	1:2A:1418:G:O4'	2.17	0.43
7:2H:149:ARG:HD3	7:2H:164:TYR:CE2	2.53	0.43
22:20:48:GLY:HA3	22:20:80:HIS:ND1	2.34	0.43
32:2a:141:A:H1'	32:2a:182:U:O2	2.18	0.43
33:2b:192:SER:O	33:2b:194:PRO:HD3	2.18	0.43
34:2c:23:TYR:CG	34:2c:24:ALA:N	2.86	0.43
38:2g:38:LEU:O	38:2g:42:ILE:HG13	2.17	0.43
55:2x:21:A:N6	55:2x:46:G:H2'	2.34	0.43
55:2x:61:C:H2'	55:2x:62:C:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2y:5:G:H1	57:2y:68:C:H42	1.64	0.43
1:1A:862:G:H2'	1:1A:863:A:O4'	2.18	0.43
1:1A:2291:U:OP1	1:1A:2380:C:O2'	2.30	0.43
1:1A:2439:A:H5'	1:1A:2439:A:C8	2.53	0.43
27:15:40:LYS:NZ	27:15:44:THR:O	2.47	0.43
32:1a:1066:C:O2'	32:1a:1067:A:H5'	2.18	0.43
32:1a:1126:U:O2	32:1a:1280:A:H2'	2.18	0.43
32:1a:1320:C:OP1	50:1s:70:LYS:NZ	2.46	0.43
33:1b:36:ARG:C	33:1b:38:GLY:H	2.26	0.43
35:1d:65:ARG:HG3	35:1d:75:PHE:CD1	2.52	0.43
40:1i:127:LYS:O	40:1i:128:ARG:HB3	2.18	0.43
44:1m:22:ILE:HB	44:1m:25:ILE:HD12	1.99	0.43
44:1m:67:GLU:HB3	44:1m:68:GLY:H	1.66	0.43
1:2A:647:G:H2'	1:2A:648:G:O4'	2.18	0.43
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.84	0.43
1:2A:1016:G:O6	62:2A:3946:HOH:O	2.19	0.43
1:2A:2512:C:H2'	1:2A:2513:G:O4'	2.18	0.43
1:2A:2893:G:H5"	1:2A:2894:G:O4'	2.19	0.43
2:2B:8:U:H3	2:2B:113:G:H1	1.66	0.43
8:2I:68:LEU:HG	8:2I:72:LEU:HD13	2.00	0.43
28:26:23:THR:OG1	28:26:24:GLU:N	2.51	0.43
32:2a:1030(A):G:O2'	32:2a:1030(C):G:N7	2.46	0.43
32:2a:1226:C:P	44:2m:91:ARG:HH12	2.41	0.43
1:1A:784:A:OP1	1:1A:2588:G:H5"	2.19	0.43
1:1A:1052:C:H2'	1:1A:1053:C:H6	1.84	0.43
1:1A:1170:G:H2'	1:1A:1171:G:O4'	2.18	0.43
1:1A:1509(A):A:H2'	1:1A:1509(B):A:O4'	2.19	0.43
1:1A:2304:G:H22	1:1A:2312:U:H3	1.67	0.43
4:1E:36:ARG:NH1	4:1E:85:ASN:OD1	2.51	0.43
9:1N:73:THR:HB	9:1N:82:LEU:HD11	1.99	0.43
12:1Q:78:PRO:HD3	55:1x:1:C:C4	2.54	0.43
13:1R:9:LYS:O	13:1R:17:ARG:HD3	2.18	0.43
22:10:43:THR:O	22:10:43:THR:HG23	2.19	0.43
32:1a:341:C:H2'	32:1a:342:C:C6	2.54	0.43
32:1a:875:C:O2'	39:1h:14:ARG:HD2	2.18	0.43
32:1a:966:M2G:HM13	32:1a:967:5MC:H1'	2.01	0.43
32:1a:1070:U:H2'	32:1a:1071:C:C6	2.53	0.43
33:1b:30:ARG:HH21	33:1b:194:PRO:HB2	1.84	0.43
41:1j:78:ASN:O	41:1j:80:LYS:N	2.52	0.43
49:1r:47:THR:O	49:1r:83:GLU:N	2.50	0.43
1:2A:411:G:C5	11:2P:72:PRO:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1589:C:H2'	1:2A:1590:U:C6	2.54	0.43
1:2A:1815:A:H8	1:2A:1815:A:OP1	2.02	0.43
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.18	0.43
3:2D:16:MET:HE3	3:2D:16:MET:HB2	1.92	0.43
9:2N:67:LEU:HB3	9:2N:88:GLU:HG3	2.01	0.43
33:2b:188:ALA:HB1	33:2b:192:SER:HB2	2.00	0.43
38:2g:101:LEU:O	38:2g:105:VAL:HG23	2.19	0.43
42:2k:18:ARG:O	42:2k:32:ILE:HA	2.18	0.43
57:2y:9:A:H4'	57:2y:46:G7M:H5'	2.00	0.43
1:1A:1041:C:N4	1:1A:1114:G:H1	2.16	0.43
1:1A:1697:G:OP2	1:1A:1698:A:O2'	2.31	0.43
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.53	0.43
8:1I:93:THR:O	8:1I:97:ILE:HG13	2.19	0.43
16:1U:34:LYS:HA	16:1U:34:LYS:HD2	1.84	0.43
32:1a:769:G:H4'	32:1a:1513:A:H4'	2.01	0.43
33:1b:83:MET:SD	33:1b:234:PRO:HG3	2.58	0.43
35:1d:100:ARG:HH12	35:1d:137:SER:HB3	1.84	0.43
1:2A:118:A:N3	1:2A:178:G:H1'	2.34	0.43
1:2A:887:A:H4'	1:2A:888:C:C5	2.54	0.43
1:2A:1364:G:P	23:21:3:LYS:HG3	2.59	0.43
1:2A:2387:U:H1'	22:20:41:ARG:HE	1.83	0.43
1:2A:2564:A:C2	1:2A:2647:U:H4'	2.54	0.43
5:2F:13:SER:OG	5:2F:16:GLY:O	2.29	0.43
6:2G:105:LYS:NZ	6:2G:143:GLU:OE2	2.45	0.43
8:2I:82:ARG:HH22	8:2I:90:GLY:HA3	1.84	0.43
17:2V:56:SER:HB3	17:2V:100:ARG:HB2	2.01	0.43
32:2a:707:C:H2'	32:2a:708:C:C6	2.54	0.43
34:2c:69:HIS:CD2	34:2c:104:GLN:HG2	2.54	0.43
40:2i:8:GLY:O	40:2i:15:ALA:N	2.41	0.43
44:2m:60:VAL:HG12	44:2m:66:LEU:HD11	2.00	0.43
1:1A:84:A:H5'	20:1Y:8:LYS:HG2	2.01	0.43
1:1A:1025:G:O2'	62:1A:4210:HOH:O	2.11	0.43
1:1A:1354:A:H5"	3:1D:38:LYS:HD3	2.00	0.43
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.54	0.43
8:1I:77:LEU:HD23	8:1I:77:LEU:HA	1.89	0.43
8:1I:109:ILE:HG23	8:1I:130:TYR:CZ	2.54	0.43
13:1R:2:ARG:HG2	13:1R:5:LYS:HB2	1.99	0.43
26:14:62:ARG:HB2	26:14:63:TYR:CE1	2.53	0.43
30:18:4:MET:HE3	30:18:63:PRO:CG	2.49	0.43
32:1a:192:U:H2'	32:1a:193:C:C6	2.54	0.43
32:1a:302:G:O2'	32:1a:556:C:H5"	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:620:C:H2'	32:1a:621:A:O4'	2.18	0.43
32:1a:1202:G:O3'	45:1n:3:ARG:NH1	2.48	0.43
35:1d:122:ARG:HA	35:1d:122:ARG:HD2	1.70	0.43
1:2A:222:A:H5"	1:2A:421:U:OP1	2.19	0.43
1:2A:748:G:C8	18:2W:89:ALA:HB1	2.53	0.43
1:2A:900:A:H2'	1:2A:901:A:H8	1.83	0.43
1:2A:1038:C:H42	1:2A:1117:G:H1	1.67	0.43
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.53	0.43
1:2A:2206:G:H8	1:2A:2207:G:N7	2.17	0.43
10:2O:49:ARG:HH12	32:2a:1423:G:P	2.42	0.43
12:2Q:26:TYR:CD1	12:2Q:28:ALA:HB2	2.54	0.43
14:2S:48:LEU:HD23	14:2S:82:ILE:HD11	2.01	0.43
32:2a:108:G:N1	51:2t:15:ARG:HG2	2.34	0.43
32:2a:1291:G:C6	32:2a:1292:U:C4	3.06	0.43
46:2o:5:LYS:H	46:2o:5:LYS:HG3	1.64	0.43
1:1A:271(J):C:H6	1:1A:271(J):C:H2'	1.66	0.43
1:1A:1075:C:C2'	1:1A:1076:C:H5'	2.49	0.43
1:1A:1076:C:H4'	1:1A:1077:A:OP1	2.19	0.43
1:1A:2147:G:H3'	1:1A:2147:G:N3	2.34	0.43
12:1Q:7:MET:HE2	12:1Q:7:MET:HB3	1.87	0.43
21:1Z:1:MET:HA	21:1Z:2:GLU:HA	1.70	0.43
32:1a:159:G:N2	32:1a:162:A:OP2	2.52	0.43
32:1a:1291:G:O2'	40:1i:38:GLN:OE1	2.29	0.43
32:1a:1320:C:O2	50:1s:36:ARG:NH2	2.52	0.43
35:1d:107:ARG:HD2	35:1d:107:ARG:HA	1.66	0.43
36:1e:91:LEU:HB3	36:1e:118:ILE:HD11	2.01	0.43
57:1y:69:G:H5'	57:1y:70:G:OP2	2.19	0.43
1:2A:125:G:O2'	29:27:48:LYS:HD3	2.18	0.43
1:2A:322:A:OP1	5:2F:168:ARG:HD2	2.19	0.43
1:2A:652(A):A:H3'	1:2A:652(B):A:H5"	2.01	0.43
1:2A:1269:A:N7	62:2A:4048:HOH:O	2.37	0.43
1:2A:2172:U:H5'	1:2A:2173:A:H8	1.83	0.43
4:2E:112:GLY:O	4:2E:159:HIS:HA	2.18	0.43
11:2P:59:LEU:HD11	30:28:10:ALA:HA	2.01	0.43
18:2W:68:ARG:NH1	18:2W:111:HIS:HA	2.34	0.43
32:2a:54:C:H2'	32:2a:352:C:H41	1.84	0.43
48:2q:81:ARG:NH2	48:2q:84:LEU:HD21	2.32	0.43
51:2t:50:GLU:HA	51:2t:100:ILE:HG12	2.00	0.43
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.18	0.43
1:1A:1649:G:O2'	13:1R:107:ASP:OD2	2.27	0.43
1:1A:2406:U:H2'	1:1A:2406:U:OP2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:71:ASP:HB3	3:1D:103:ARG:HH12	1.83	0.43
3:1D:145:VAL:HG12	3:1D:146:GLU:O	2.18	0.43
32:1a:426:G:H4'	35:1d:41:GLY:O	2.19	0.43
32:1a:964:A:N3	32:1a:969:A:O2'	2.46	0.43
32:1a:1002:G:C2	32:1a:1004:A:H1'	2.54	0.43
32:1a:1054:C:C5	54:1w:34:G:H1'	2.53	0.43
32:1a:1149:C:P	40:1i:9:ARG:HH21	2.42	0.43
32:1a:1310:G:OP2	44:1m:88:ARG:NH2	2.52	0.43
33:1b:92:TYR:OH	33:1b:150:SER:OG	2.29	0.43
57:1y:40:C:H2'	57:1y:41:C:C6	2.54	0.43
1:2A:236:C:H2'	1:2A:237:C:H6	1.84	0.43
1:2A:731:C:H5"	62:2A:3964:HOH:O	2.18	0.43
1:2A:985:C:H2'	1:2A:986:C:H6	1.84	0.43
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.19	0.43
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.37	0.43
1:2A:2010:G:H5"	18:2W:42:ARG:HB2	2.00	0.43
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.54	0.43
1:2A:2252:G:H2'	1:2A:2253:G:O4'	2.18	0.43
6:2G:125:PHE:CE2	6:2G:170:ARG:HD3	2.54	0.43
8:2I:78:THR:HA	8:2I:143:SER:HB3	2.01	0.43
17:2V:89:GLN:HA	17:2V:90:PRO:HD3	1.91	0.43
32:2a:15:G:H21	36:2e:18:ARG:HA	1.84	0.43
32:2a:1271:G:N2	32:2a:1272:G:C8	2.87	0.43
35:2d:65:ARG:NH1	35:2d:70:ILE:O	2.52	0.43
36:2e:146:ALA:O	36:2e:150:ARG:HG2	2.19	0.43
47:2p:3:LYS:O	47:2p:21:VAL:HA	2.19	0.43
54:2w:72:C:H2'	54:2w:73:A:C8	2.54	0.43
57:2y:74:C:H2'	57:2y:75:C:C6	2.53	0.43
1:1A:271(T):C:H2'	1:1A:271(U):G:H8	1.83	0.42
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.54	0.42
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.19	0.42
22:10:7:LEU:O	55:1x:2:G:H4'	2.19	0.42
32:1a:146:G:C2	32:1a:147:G:C4	3.07	0.42
32:1a:737:A:H2'	32:1a:738:C:C6	2.53	0.42
32:1a:857:C:H2'	32:1a:858:G:O4'	2.19	0.42
32:1a:1072:G:H2'	32:1a:1073:U:C6	2.53	0.42
32:1a:1486:G:H2'	32:1a:1487:G:O4'	2.19	0.42
40:1i:45:ALA:O	40:1i:78:LYS:HD3	2.18	0.42
41:1j:81:THR:HA	41:1j:84:GLN:HB3	2.00	0.42
47:1p:50:LYS:HD2	47:1p:50:LYS:HA	1.85	0.42
57:1y:47:U:H2'	57:1y:50:U:OP1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:37:C:H4'	1:2A:451:C:OP1	2.19	0.42
1:2A:880:G:C2	1:2A:881:G:C8	3.07	0.42
2:2B:105:A:H5'	2:2B:106:G:OP2	2.19	0.42
3:2D:232:PRO:HB3	3:2D:244:ARG:CZ	2.48	0.42
5:2F:178:PRO:HG2	5:2F:179:GLU:OE2	2.18	0.42
10:2O:49:ARG:NH1	32:2a:1422:G:O3'	2.52	0.42
14:2S:15:ARG:HE	14:2S:88:ASP:CG	2.26	0.42
32:2a:512:U:H2'	32:2a:513:C:C6	2.54	0.42
32:2a:1305:G:O2'	32:2a:1331:G:N2	2.52	0.42
34:2c:91:LEU:O	34:2c:94:LEU:N	2.50	0.42
34:2c:121:ALA:HB1	34:2c:188:LEU:O	2.19	0.42
35:2d:125:HIS:HD2	35:2d:152:SER:OG	2.02	0.42
36:2e:78:HIS:CE1	36:2e:143:ARG:H	2.37	0.42
40:2i:99:LEU:HB3	40:2i:101:PHE:HE2	1.81	0.42
1:1A:305:U:H2'	1:1A:306:U:C6	2.55	0.42
1:1A:1164:G:H2'	1:1A:1165:U:C6	2.54	0.42
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.54	0.42
6:1G:116:ASP:OD2	44:1m:68:GLY:HA3	2.19	0.42
16:1U:107:ALA:O	16:1U:110:VAL:HG22	2.19	0.42
32:1a:110:C:H2'	32:1a:111:G:O4'	2.20	0.42
32:1a:582:U:H2'	32:1a:583:A:C8	2.54	0.42
32:1a:691:G:H2'	32:1a:692:U:C6	2.54	0.42
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.53	0.42
32:1a:1111:A:N1	34:1c:177:THR:OG1	2.50	0.42
32:1a:1333:A:H2'	32:1a:1334:G:O4'	2.20	0.42
32:1a:1376:U:H2'	32:1a:1377:A:H8	1.83	0.42
43:1l:70:ILE:HD13	43:1l:77:LEU:HD12	2.01	0.42
54:1w:26:A:N6	54:1w:44:G:H1	2.16	0.42
1:2A:2363:C:O2	22:20:39:ARG:NH2	2.49	0.42
2:2B:2:C:H2'	2:2B:3:C:H6	1.83	0.42
2:2B:105:A:P	21:2Z:72:ARG:HE	2.42	0.42
6:2G:43:LEU:HD12	6:2G:45:GLU:HG3	2.01	0.42
7:2H:75:ALA:O	7:2H:79:VAL:HG13	2.19	0.42
16:2U:109:LEU:HD23	16:2U:109:LEU:HA	1.93	0.42
24:22:3:LEU:O	24:22:7:ARG:HG3	2.19	0.42
32:2a:10:A:OP2	36:2e:126:ARG:HD2	2.19	0.42
33:2b:9:GLU:C	33:2b:11:LEU:H	2.25	0.42
34:2c:20:SER:HB3	34:2c:22:TRP:NE1	2.34	0.42
35:2d:134:ASP:OD1	35:2d:134:ASP:N	2.49	0.42
37:2f:50:TYR:CE2	49:2r:77:GLY:HA2	2.54	0.42
45:2n:53:LEU:HD23	45:2n:53:LEU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:66:GLN:HB3	6:1G:92:VAL:HG21	2.00	0.42
32:1a:114:U:O2'	32:1a:115:G:H5'	2.20	0.42
32:1a:123:C:OP1	32:1a:311:C:O2'	2.34	0.42
32:1a:418:C:H1'	32:1a:540:G:O2'	2.18	0.42
32:1a:603:U:H2'	32:1a:604:G:H8	1.84	0.42
32:1a:618:C:H5"	32:1a:619:U:H5"	2.01	0.42
41:1j:47:PHE:N	41:1j:63:PHE:O	2.44	0.42
41:1j:64:GLU:HB3	45:1n:59:ALA:HB2	2.01	0.42
5:2F:28:ILE:HG13	5:2F:112:MET:HB3	2.01	0.42
10:2O:112:MET:O	10:2O:116:SER:OG	2.34	0.42
14:2S:87:PHE:CE1	14:2S:102:ALA:HB2	2.54	0.42
20:2Y:5:MET:HE2	20:2Y:5:MET:HB2	1.78	0.42
21:2Z:67:LEU:HD12	21:2Z:67:LEU:HA	1.83	0.42
26:24:68:ARG:HH21	26:24:69:LYS:H	1.67	0.42
32:2a:1067:A:N3	32:2a:1068:G:H1'	2.34	0.42
32:2a:1125:U:OP1	41:2j:35:SER:OG	2.28	0.42
37:2f:99:ALA:HB1	49:2r:23:LYS:NZ	2.34	0.42
38:2g:102:ARG:O	38:2g:106:GLN:HG3	2.20	0.42
38:2g:103:TRP:CH2	38:2g:141:VAL:HG21	2.55	0.42
40:2i:23:ASN:HD21	40:2i:25:LYS:HE2	1.84	0.42
42:2k:106:LYS:HB2	42:2k:106:LYS:HE2	1.90	0.42
54:2w:9:A:H5'	54:2w:46:G7M:H22	1.84	0.42
57:2y:64:A:C2'	57:2y:65:G:H5'	2.49	0.42
1:1A:191:A:H2'	1:1A:192:C:C6	2.54	0.42
1:1A:264:C:O2'	1:1A:265:A:H2'	2.19	0.42
1:1A:1478:G:O2'	1:1A:1558:A:N7	2.52	0.42
2:1B:75:G:O2'	21:1Z:85:HIS:NE2	2.46	0.42
3:1D:70:TRP:HB3	3:1D:190:TYR:CE2	2.55	0.42
5:1F:89:VAL:HG12	5:1F:90:PHE:CD2	2.55	0.42
7:1H:109:PHE:C	7:1H:111:HIS:H	2.26	0.42
20:1Y:14:LEU:HB2	20:1Y:75:ILE:HD11	2.01	0.42
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.54	0.42
24:12:65:ASN:O	24:12:69:ARG:HB2	2.19	0.42
32:1a:160:A:H2'	32:1a:161:A:O4'	2.19	0.42
32:1a:161:A:H2'	32:1a:162:A:C8	2.54	0.42
32:1a:236:G:H5"	48:1q:42:TYR:OH	2.19	0.42
32:1a:922:G:C6	32:1a:923:A:C6	3.08	0.42
34:1c:123:GLN:HB3	34:1c:128:PHE:HD2	1.84	0.42
36:1e:18:ARG:HD3	36:1e:27:ARG:NH1	2.26	0.42
38:1g:65:ALA:HB1	38:1g:127:ALA:HB3	2.00	0.42
49:1r:73:ALA:HB3	49:1r:79:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:1y:18:G:O2'	57:1y:57:G:O6	2.24	0.42
1:2A:84:A:H5"	20:2Y:8:LYS:HE3	2.01	0.42
1:2A:813:U:H2'	1:2A:814:C:C6	2.55	0.42
1:2A:829:A:N7	1:2A:2248:C:H5'	2.34	0.42
1:2A:892:G:H3'	1:2A:893:C:C5'	2.49	0.42
1:2A:945:A:C4	1:2A:2448:A:C2	3.07	0.42
1:2A:1204:A:H2	1:2A:1241:A:N6	2.09	0.42
1:2A:1270:C:H5"	1:2A:1271:G:O5'	2.19	0.42
1:2A:2439:A:H5'	1:2A:2439:A:C8	2.55	0.42
1:2A:2619:C:OP1	4:2E:152:LYS:NZ	2.44	0.42
1:2A:2741:A:H2'	1:2A:2742:C:O4'	2.18	0.42
32:2a:473:G:H2'	32:2a:474:G:C8	2.54	0.42
32:2a:652:U:O4	32:2a:752:G:O2'	2.27	0.42
32:2a:841:U:C5	32:2a:848:C:H1'	2.54	0.42
32:2a:1095:U:H5"	32:2a:1109:C:O2	2.18	0.42
33:2b:92:TYR:CE2	33:2b:151:GLY:HA3	2.55	0.42
38:2g:108:ALA:O	38:2g:119:ARG:HD2	2.19	0.42
1:1A:1069:A:O4'	1:1A:1096:A:O2'	2.38	0.42
4:1E:4:ILE:HD11	4:1E:29:GLY:HA2	2.02	0.42
26:14:24:THR:OG1	26:14:25:TYR:N	2.52	0.42
32:1a:189:G:C2	32:1a:189(L):G:C2	3.07	0.42
32:1a:316:G:OP2	32:1a:351:G:O2'	2.34	0.42
32:1a:1194:U:H4'	36:1e:22:GLY:HA2	2.01	0.42
46:1o:87:ILE:HG22	46:1o:88:ARG:N	2.28	0.42
54:1w:8:4SU:O5'	54:1w:8:4SU:H6	2.20	0.42
54:1w:11:C:H2'	54:1w:12:U:C6	2.55	0.42
55:1x:4:G:H2'	55:1x:5:G:C8	2.54	0.42
1:2A:324:A:N6	1:2A:338:G:O2'	2.47	0.42
1:2A:455:C:N3	1:2A:472:A:H2'	2.35	0.42
1:2A:482:A:H1'	1:2A:498:G:N2	2.34	0.42
1:2A:492:A:H2'	1:2A:493:G:O4'	2.20	0.42
1:2A:530:G:C5	1:2A:2022:U:H5"	2.54	0.42
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.55	0.42
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.55	0.42
1:2A:1814:G:H4'	3:2D:51:VAL:HG21	2.01	0.42
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.85	0.42
26:24:19:GLY:O	26:24:21:VAL:HG23	2.19	0.42
32:2a:157:G:H2'	32:2a:158:G:C8	2.55	0.42
32:2a:261:U:OP2	51:2t:79:ARG:NH2	2.52	0.42
32:2a:1148:U:H2'	32:2a:1149:C:O4'	2.18	0.42
32:2a:1265:G:C4	32:2a:1271:G:N2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1289:A:OP1	52:2u:10:ARG:NH2	2.52	0.42
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.54	0.42
41:2j:8:LEU:HB3	41:2j:96:ILE:HG23	2.02	0.42
41:2j:33:GLN:HG2	41:2j:34:VAL:H	1.84	0.42
46:2o:55:GLY:HA2	46:2o:58:MET:HE3	2.02	0.42
57:2y:71:G:H2'	57:2y:72:C:C6	2.55	0.42
1:1A:271(V):G:O6	62:1A:4240:HOH:O	2.21	0.42
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.53	0.42
1:1A:1009:A:OP2	9:1N:37:LYS:NZ	2.47	0.42
1:1A:1372:U:H2'	1:1A:1373:A:O4'	2.19	0.42
2:1B:55:U:H2'	2:1B:56:G:O4'	2.20	0.42
2:1B:78:A:C2	2:1B:100:A:C4	3.07	0.42
15:1T:20:PRO:HD2	15:1T:86:ILE:HB	2.02	0.42
21:1Z:63:ASP:OD2	21:1Z:65:GLN:NE2	2.47	0.42
24:12:51:ARG:HE	24:12:51:ARG:HB2	1.63	0.42
28:16:47:THR:HG22	28:16:49:HIS:CE1	2.54	0.42
32:1a:7:G:O2'	36:1e:120:THR:O	2.38	0.42
32:1a:258:G:H2'	32:1a:259:G:C8	2.54	0.42
1:2A:222:A:H3'	1:2A:421:U:H5'	2.02	0.42
1:2A:330:A:H2	1:2A:1210:A:H2'	1.84	0.42
1:2A:1178:C:H2'	1:2A:1179:C:C6	2.55	0.42
1:2A:1263:U:C4	1:2A:1264:G:C6	3.07	0.42
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.45	0.42
1:2A:1924:C:H4'	55:2x:13:C:O2'	2.19	0.42
1:2A:2064:C:H2'	1:2A:2065:C:C6	2.55	0.42
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.19	0.42
7:2H:7:LEU:HD23	7:2H:69:ARG:NH2	2.34	0.42
8:2I:51:ILE:HD12	8:2I:51:ILE:HA	1.81	0.42
13:2R:78:LYS:HE2	13:2R:83:ILE:HD11	2.01	0.42
14:2S:41:ASP:OD1	14:2S:44:LYS:N	2.50	0.42
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	2.00	0.42
19:2X:44:GLU:HG2	19:2X:49:VAL:O	2.19	0.42
32:2a:1072:G:H2'	32:2a:1073:U:C6	2.55	0.42
33:2b:8:LYS:HD3	33:2b:8:LYS:N	2.34	0.42
57:2y:8:4SU:H5"	57:2y:49:C:H5'	2.02	0.42
1:1A:196:A:O2'	1:1A:805:G:O6	2.29	0.42
1:1A:1314:C:OP1	62:1A:4219:HOH:O	2.22	0.42
5:1F:129:PHE:CD2	5:1F:163:VAL:HG21	2.55	0.42
10:1O:98:VAL:HG21	10:1O:114:ILE:HG23	2.01	0.42
21:1Z:9:TYR:CZ	21:1Z:61:LEU:HD22	2.55	0.42
32:1a:92:C:H2'	32:1a:93:G:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:487:A:H2'	32:1a:488:C:O4'	2.20	0.42
37:1f:48:LEU:HD23	37:1f:48:LEU:HA	1.82	0.42
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.19	0.42
51:1t:62:LEU:HD23	51:1t:62:LEU:HA	1.86	0.42
1:2A:2784:C:H1'	4:2E:37:ARG:NH1	2.34	0.42
5:2F:9:ILE:HG22	5:2F:10:PRO:HD2	2.02	0.42
6:2G:33:ARG:O	6:2G:161:THR:HG23	2.20	0.42
7:2H:8:PRO:HA	7:2H:51:ARG:HB3	2.02	0.42
33:2b:124:SER:HB3	33:2b:125:PRO:HD3	2.02	0.42
44:2m:13:LYS:HA	44:2m:44:ARG:NH1	2.29	0.42
48:2q:24:GLU:OE2	48:2q:37:LYS:HE3	2.20	0.42
55:2x:23:C:H2'	55:2x:24:U:C6	2.55	0.42
1:1A:1170:G:H1	1:1A:1179:C:N4	2.18	0.42
1:1A:1448:G:H4'	1:1A:1542:A:OP1	2.19	0.42
1:1A:2180:U:H2'	1:1A:2181:G:O4'	2.20	0.42
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	2.01	0.42
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.34	0.42
32:1a:96:U:H2'	32:1a:97:G:H8	1.84	0.42
32:1a:390:C:H2'	32:1a:391:G:C8	2.54	0.42
32:1a:1146:A:H2'	32:1a:1147:C:O4'	2.18	0.42
32:1a:1284:C:H3'	32:1a:1285:A:C8	2.53	0.42
33:1b:15:VAL:HG21	33:1b:213:LEU:HD22	2.01	0.42
33:1b:80:ILE:H	33:1b:80:ILE:HD12	1.85	0.42
38:1g:50:ILE:HG22	38:1g:58:PRO:HG3	2.02	0.42
41:1j:81:THR:C	41:1j:83:GLU:N	2.78	0.42
51:1t:59:ALA:O	51:1t:63:ILE:HG13	2.20	0.42
1:2A:890:A:H2'	1:2A:892:G:H8	1.81	0.42
1:2A:1750:G:N3	1:2A:2860:A:H2	2.17	0.42
1:2A:2125:G:N1	1:2A:2172:U:OP1	2.52	0.42
1:2A:2773:C:OP1	4:2E:166:THR:OG1	2.34	0.42
3:2D:8:PRO:HB3	3:2D:14:ARG:HG3	2.02	0.42
6:2G:11:TYR:HB2	6:2G:176:LEU:HD21	2.01	0.42
9:2N:30:ILE:O	9:2N:34:LEU:HG	2.20	0.42
32:2a:971:G:H1'	32:2a:1365:G:O2'	2.19	0.42
32:2a:983:A:H3'	32:2a:983:A:N3	2.35	0.42
40:2i:63:ILE:HG21	40:2i:77:ILE:HG12	2.00	0.42
48:2q:41:LYS:NZ	48:2q:92:ARG:HH21	2.18	0.42
57:2y:8:4SU:H2'	57:2y:46:G7M:N2	2.33	0.42
1:1A:39:C:H2'	1:1A:40:C:C6	2.54	0.42
1:1A:125:G:O2'	29:17:48:LYS:HD3	2.19	0.42
1:1A:1021:A:H3'	1:1A:1021:A:N3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2556:C:H2'	1:1A:2557:G:O4'	2.20	0.42
1:1A:2732:G:H3'	1:1A:2733:A:O4'	2.19	0.42
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	2.02	0.42
4:1E:168:MET:HE2	4:1E:203:LYS:HG2	2.01	0.42
5:1F:136:THR:HA	5:1F:166:ALA:O	2.20	0.42
24:12:62:THR:O	24:12:66:GLU:HG3	2.20	0.42
32:1a:62:U:OP1	32:1a:385:C:O2'	2.36	0.42
32:1a:865:A:C2	32:1a:918:A:H4'	2.55	0.42
32:1a:1229:A:OP2	44:1m:114:ARG:HD3	2.20	0.42
54:1w:18:G:H4'	54:1w:60:U:C6	2.55	0.42
1:2A:567:A:H4'	1:2A:808:G:OP1	2.19	0.42
1:2A:656:G:H2'	1:2A:657:U:O4'	2.20	0.42
1:2A:1669:A:H5"	1:2A:2550:G:OP1	2.20	0.42
1:2A:2331:G:C6	1:2A:2332:U:C4	3.08	0.42
11:2P:28:GLY:O	11:2P:30:THR:N	2.44	0.42
16:2U:50:ARG:NH2	17:2V:72:VAL:HG22	2.32	0.42
32:2a:33:A:N3	43:2l:32:PHE:HE2	2.18	0.42
32:2a:625:G:H2'	32:2a:626:U:C6	2.55	0.42
32:2a:1012:U:H2'	32:2a:1013:G:C8	2.54	0.42
32:2a:1112:C:N3	34:2c:178:LEU:HD12	2.35	0.42
36:2e:31:LEU:HD11	36:2e:129:ILE:HA	2.01	0.42
39:2h:23:SER:OG	39:2h:24:THR:N	2.53	0.42
48:2q:10:VAL:HA	48:2q:20:THR:O	2.20	0.42
48:2q:40:LYS:HD3	48:2q:42:TYR:CZ	2.55	0.42
56:2z:5:MET:HE3	56:2z:5:MET:HB2	1.84	0.42
1:1A:1790:C:H2'	1:1A:1791:A:C5	2.55	0.42
1:1A:2110:G:C2	1:1A:2120:G:H1'	2.55	0.42
14:1S:3:ARG:HD3	14:1S:3:ARG:HA	1.86	0.42
21:1Z:42:VAL:O	21:1Z:46:LYS:HG3	2.20	0.42
32:1a:742:G:OP2	46:1o:35:ARG:NH2	2.45	0.42
32:1a:1316:G:N2	32:1a:1318:A:H3'	2.35	0.42
33:1b:21:ARG:O	33:1b:23:ARG:N	2.52	0.42
33:1b:140:HIS:CE1	33:1b:144:ARG:HD2	2.55	0.42
34:1c:85:ARG:O	34:1c:89:GLU:HG3	2.20	0.42
35:1d:173:TRP:CE3	35:1d:174:LEU:HG	2.54	0.42
39:1h:83:ILE:HG13	39:1h:137:VAL:HG22	2.02	0.42
51:1t:48:LYS:HA	51:1t:48:LYS:HD3	1.89	0.42
54:1w:33:U:H5'	54:1w:37:MIA:H161	2.02	0.42
1:2A:1408:C:H2'	1:2A:1409:C:C6	2.55	0.42
1:2A:2130:U:C2'	1:2A:2158:A:H61	2.28	0.42
3:2D:132:PRO:HG3	3:2D:190:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:73:GLU:HG3	8:2I:138:ILE:HG23	2.01	0.42
15:2T:82:LEU:H	15:2T:82:LEU:HD12	1.84	0.42
29:27:24:THR:HG22	29:27:26:GLY:N	2.35	0.42
32:2a:273:A:N6	32:2a:274:A:C6	2.88	0.42
32:2a:685:G:O2'	32:2a:686:U:H5'	2.20	0.42
33:2b:7:VAL:N	33:2b:221:LEU:HD11	2.34	0.42
33:2b:169:LYS:O	33:2b:169:LYS:HD3	2.20	0.42
34:2c:6:HIS:HD2	34:2c:7:PRO:HD2	1.85	0.42
34:2c:77:ILE:H	34:2c:77:ILE:HG12	1.69	0.42
36:2e:31:LEU:HD23	36:2e:31:LEU:HA	1.87	0.42
40:2i:106:ALA:O	40:2i:108:VAL:HG22	2.20	0.42
48:2q:22:LEU:HD13	48:2q:41:LYS:HG2	2.01	0.42
50:2s:80:TYR:O	50:2s:82:GLY:N	2.47	0.42
3:1D:206:LEU:HA	3:1D:211:ARG:NH1	2.35	0.41
6:1G:25:TYR:CZ	6:1G:32:PRO:HD3	2.55	0.41
10:1O:9:GLU:OE2	10:1O:18:LYS:NZ	2.53	0.41
32:1a:8:A:N7	35:1d:208:SER:OG	2.52	0.41
32:1a:179:A:H2'	32:1a:180:U:C6	2.54	0.41
33:1b:111:ARG:HB3	33:1b:149:LEU:HD11	2.01	0.41
38:1g:144:MET:HE2	38:1g:144:MET:HB3	1.92	0.41
40:1i:6:GLY:O	40:1i:17:VAL:HG12	2.20	0.41
41:1j:46:ARG:HH11	41:1j:46:ARG:HB2	1.85	0.41
44:1m:108:ARG:HD3	44:1m:108:ARG:HA	1.52	0.41
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.45	0.41
1:2A:699:A:H2'	1:2A:700:G:O4'	2.20	0.41
1:2A:1301:A:O2'	1:2A:1302:A:H3'	2.20	0.41
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.35	0.41
1:2A:2336:A:H61	22:20:43:THR:HG22	1.84	0.41
1:2A:2577:A:H5"	1:2A:2578:G:H5'	2.02	0.41
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	2.02	0.41
8:2I:90:GLY:O	8:2I:121:LYS:HE3	2.20	0.41
25:23:4:LEU:O	25:23:36:VAL:HA	2.19	0.41
32:2a:984:C:H2'	32:2a:985:C:H6	1.85	0.41
32:2a:1366:C:O2'	41:2j:60:ARG:NH2	2.53	0.41
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.55	0.41
33:2b:76:GLN:HB2	33:2b:208:ILE:HG12	2.00	0.41
36:2e:33:VAL:HG13	36:2e:112:LEU:HD12	2.01	0.41
41:2j:54:PHE:CD2	41:2j:55:LYS:HB3	2.55	0.41
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	2.02	0.41
1:1A:743:G:N7	62:1A:4314:HOH:O	2.37	0.41
1:1A:1274:A:N3	1:1A:1297:C:H1'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2522:U:OP1	62:1A:4245:HOH:O	2.22	0.41
12:1Q:89:ASN:HD22	12:1Q:89:ASN:HA	1.66	0.41
18:1W:68:ARG:HH12	18:1W:112:GLY:H	1.67	0.41
26:14:60:GLN:O	26:14:62:ARG:N	2.45	0.41
32:1a:156:G:H2'	32:1a:157:G:C8	2.55	0.41
32:1a:524:G:H2'	32:1a:525:C:C6	2.55	0.41
32:1a:881:G:P	43:1l:12:ARG:HH22	2.43	0.41
32:1a:1260:C:O5'	32:1a:1284:C:H4'	2.20	0.41
34:1c:79:ARG:C	34:1c:81:GLY:H	2.29	0.41
42:1k:34:ASP:HB2	42:1k:35:PRO:HD2	2.02	0.41
46:1o:64:ARG:HH11	46:1o:68:ARG:HH21	1.67	0.41
51:1t:18:GLN:O	51:1t:22:ARG:HG3	2.19	0.41
57:1y:18:G:H4'	57:1y:19:G:OP1	2.20	0.41
1:2A:893:C:H2'	1:2A:894:C:N3	2.35	0.41
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.20	0.41
1:2A:1882:C:H2'	1:2A:1883:G:O4'	2.20	0.41
1:2A:2469:A:H5"	1:2A:2470:G:OP2	2.20	0.41
1:2A:2539:C:H4'	31:29:3:VAL:HG21	2.02	0.41
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.20	0.41
2:2B:61:G:C6	2:2B:62:C:C4	3.09	0.41
7:2H:70:THR:HG22	7:2H:74:ASN:OD1	2.21	0.41
9:2N:120:LEU:HG	9:2N:122:VAL:HG23	2.02	0.41
14:2S:37:ALA:HB1	14:2S:73:LEU:HD22	2.00	0.41
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.21	0.41
26:24:46:GLN:C	26:24:48:ARG:N	2.78	0.41
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.85	0.41
32:2a:1452:C:H4'	32:2a:1457:G:C8	2.55	0.41
37:2f:28:ARG:O	37:2f:31:GLU:HG3	2.20	0.41
38:2g:77:SER:HA	38:2g:85:TYR:O	2.20	0.41
42:2k:44:SER:OG	42:2k:47:VAL:HG23	2.20	0.41
1:1A:2642:G:OP2	9:1N:83:LYS:NZ	2.53	0.41
1:1A:2648:C:H2'	1:1A:2649:U:C6	2.55	0.41
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	2.02	0.41
15:1T:51:ARG:HG3	15:1T:98:LYS:HE3	2.02	0.41
28:16:8:LYS:HB2	28:16:54:ILE:HD13	2.02	0.41
32:1a:250:A:H4'	32:1a:251:G:O5'	2.20	0.41
32:1a:690:G:C6	32:1a:691:G:C6	3.08	0.41
32:1a:1002:G:C8	32:1a:1003:G:H1'	2.55	0.41
32:1a:1225:A:H2'	32:1a:1226:C:C5	2.55	0.41
33:1b:12:GLU:HB2	33:1b:213:LEU:HD21	2.01	0.41
33:1b:167:PRO:HG2	33:1b:192:SER:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:16:ARG:HH11	40:1i:64:THR:HG21	1.84	0.41
57:1y:41:C:H2'	57:1y:42:C:C6	2.54	0.41
1:2A:921:G:H2'	1:2A:922:U:C6	2.55	0.41
1:2A:1363:C:O2'	1:2A:1809:A:N3	2.52	0.41
1:2A:1526:G:C6	1:2A:1527:G:C2	3.09	0.41
1:2A:1955:U:N3	62:2A:4000:HOH:O	2.31	0.41
1:2A:2106:G:H2'	1:2A:2107:C:O4'	2.20	0.41
1:2A:2802:G:H8	1:2A:2802:G:O5'	2.02	0.41
1:2A:2807:G:H22	1:2A:2892:A:H62	1.69	0.41
16:2U:16:LYS:HE2	16:2U:16:LYS:HB3	1.78	0.41
16:2U:74:LEU:H	16:2U:74:LEU:HD12	1.85	0.41
20:2Y:7:VAL:CG1	20:2Y:27:VAL:HG21	2.51	0.41
32:2a:833:U:H3	32:2a:853:G:H1	1.68	0.41
35:2d:79:PHE:HE1	35:2d:204:ILE:HD13	1.85	0.41
36:2e:20:GLN:HG2	36:2e:25:ARG:HD2	2.02	0.41
36:2e:100:VAL:O	36:2e:107:ARG:NH1	2.45	0.41
38:2g:70:LYS:O	38:2g:138:LYS:HD2	2.20	0.41
46:2o:9:GLN:O	46:2o:13:GLN:HB2	2.20	0.41
1:1A:118:A:C8	1:1A:119:A:C8	3.08	0.41
1:1A:288:C:H2'	1:1A:289:A:H8	1.85	0.41
1:1A:908:C:OP1	12:1Q:22:LYS:HB3	2.19	0.41
1:1A:1063:G:C2	1:1A:1064:C:N4	2.89	0.41
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.86	0.41
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.35	0.41
9:1N:1:MET:O	9:1N:2:LYS:HB2	2.21	0.41
15:1T:127:ALA:C	15:1T:129:ARG:N	2.74	0.41
21:1Z:105:VAL:O	21:1Z:141:VAL:HG23	2.19	0.41
21:1Z:125:LEU:HG	21:1Z:164:ALA:HB3	2.02	0.41
32:1a:1023:G:H3'	32:1a:1024:G:H8	1.85	0.41
33:1b:189:ASP:HB3	33:1b:204:ASN:HA	2.02	0.41
40:1i:4:TYR:CG	40:1i:88:TYR:HB2	2.56	0.41
57:1y:2:C:N4	57:1y:71:G:H1	2.18	0.41
1:2A:1810:A:H2'	1:2A:1811:G:O4'	2.19	0.41
2:2B:2:C:H2'	2:2B:3:C:C6	2.55	0.41
7:2H:41:MET:HE2	7:2H:64:LEU:HB2	2.02	0.41
11:2P:81:GLN:NE2	11:2P:106:LEU:HA	2.35	0.41
11:2P:135:LEU:HD23	11:2P:135:LEU:HA	1.76	0.41
16:2U:81:HIS:O	16:2U:84:LYS:HB3	2.21	0.41
32:2a:828:A:H2'	32:2a:829:G:O4'	2.21	0.41
32:2a:1326:C:H2'	32:2a:1327:C:C6	2.55	0.41
32:2a:1355:G:H2'	32:2a:1356:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:69:LEU:HD13	33:2b:91:PRO:HB2	2.03	0.41
57:2y:68:C:C4	57:2y:69:G:C8	3.08	0.41
1:1A:363(C):G:H2'	1:1A:363(D):G:H8	1.85	0.41
8:1I:125:GLU:OE2	8:1I:143:SER:HB2	2.21	0.41
15:1T:20:PRO:HG3	15:1T:86:ILE:O	2.20	0.41
32:1a:629:G:H2'	32:1a:630:G:H8	1.85	0.41
33:1b:21:ARG:H	33:1b:21:ARG:HD3	1.86	0.41
38:1g:31:MET:HG3	38:1g:36:LYS:HA	2.03	0.41
47:1p:57:ARG:HG3	47:1p:79:VAL:HG12	2.02	0.41
48:1q:53:LEU:HD23	48:1q:82:MET:HE1	2.03	0.41
51:1t:50:GLU:HB2	51:1t:99:LEU:O	2.21	0.41
1:2A:74:A:H4'	1:2A:75:G:O5'	2.20	0.41
1:2A:284:U:H2'	1:2A:285:C:C6	2.56	0.41
1:2A:608:A:H2'	1:2A:609:A:C8	2.55	0.41
1:2A:881:G:C2	1:2A:882:G:H1'	2.56	0.41
1:2A:1837:C:OP1	32:2a:784:C:H4'	2.20	0.41
1:2A:1969:A:O2'	1:2A:1972:A:N3	2.49	0.41
1:2A:2118:U:OP1	1:2A:2148:G:H4'	2.21	0.41
4:2E:32:PRO:HA	4:2E:90:THR:HG22	2.00	0.41
4:2E:50:GLY:HA3	4:2E:75:VAL:HG21	2.02	0.41
5:2F:196:LEU:HD23	5:2F:196:LEU:HA	1.79	0.41
6:2G:109:VAL:HG11	26:24:14:ILE:HG21	2.03	0.41
21:2Z:158:PRO:O	21:2Z:161:VAL:HG12	2.20	0.41
32:2a:54:C:N4	32:2a:353:A:OP2	2.39	0.41
32:2a:542:G:P	35:2d:10:ARG:HH22	2.42	0.41
32:2a:741:G:H2'	32:2a:742:G:O4'	2.21	0.41
32:2a:868:C:H2'	32:2a:869:G:O4'	2.21	0.41
32:2a:1157:A:C6	32:2a:1180:A:C5	3.08	0.41
32:2a:1469:G:H2'	32:2a:1470:G:C8	2.56	0.41
41:2j:38:ILE:HG13	41:2j:71:LEU:HB3	2.02	0.41
46:2o:26:GLU:HG3	46:2o:81:LEU:HD13	2.02	0.41
1:1A:185:U:H2'	1:1A:186:G:C8	2.56	0.41
1:1A:218:A:C2	1:1A:235:U:H4'	2.55	0.41
1:1A:224:G:H2'	1:1A:225:A:O4'	2.20	0.41
1:1A:271(D):G:H2'	1:1A:271(E):U:O4'	2.21	0.41
2:1B:24:G:N7	2:1B:56:G:H2'	2.35	0.41
5:1F:116:ASP:OD2	11:1P:1:MET:HB3	2.21	0.41
10:1O:16:ALA:HB2	10:1O:52:VAL:CG2	2.50	0.41
14:1S:71:ARG:NH1	14:1S:107:GLU:OE1	2.40	0.41
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.56	0.41
19:1X:92:LEU:O	19:1X:94:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:161:A:H2'	32:1a:162:A:O4'	2.21	0.41
32:1a:189(B):C:C2	32:1a:189(J):G:C2	3.09	0.41
32:1a:198:G:H2'	32:1a:199:G:C8	2.56	0.41
32:1a:224:C:OP1	51:1t:74:LYS:NZ	2.40	0.41
32:1a:582:U:H2'	32:1a:583:A:H8	1.85	0.41
33:1b:17:PHE:HB3	33:1b:44:LEU:HD11	2.03	0.41
36:1e:152:ARG:HA	39:1h:64:LYS:NZ	2.35	0.41
38:1g:58:PRO:O	38:1g:61:VAL:HG12	2.20	0.41
44:1m:11:ARG:HA	44:1m:45:VAL:HB	2.01	0.41
1:2A:795:C:H2'	1:2A:796:C:C6	2.56	0.41
1:2A:2316:C:O2'	6:2G:128:ARG:NH2	2.53	0.41
1:2A:2364:C:OP1	22:20:55:ARG:HD3	2.21	0.41
7:2H:101:ARG:NH2	7:2H:121:ILE:O	2.50	0.41
11:2P:81:GLN:NE2	11:2P:105:LEU:O	2.47	0.41
14:2S:51:ALA:HB3	14:2S:73:LEU:HB2	2.03	0.41
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.56	0.41
22:20:27:GLU:HG3	22:20:68:GLU:HA	2.01	0.41
32:2a:7:G:H5'	32:2a:298:A:O4'	2.21	0.41
32:2a:142:G:H2'	32:2a:143:A:C8	2.55	0.41
32:2a:195:A:OP2	62:2a:1912:HOH:O	2.22	0.41
33:2b:16:HIS:CB	33:2b:210:SER:HB2	2.48	0.41
34:2c:162:GLN:NE2	53:2v:24:A:O3'	2.53	0.41
36:2e:28:PHE:O	36:2e:47:LYS:HA	2.21	0.41
37:2f:91:VAL:HG11	49:2r:72:ARG:NH1	2.35	0.41
39:2h:39:LEU:HD12	39:2h:39:LEU:HA	1.87	0.41
39:2h:119:LEU:HB3	39:2h:123:GLU:HB2	2.03	0.41
1:1A:957:A:N1	1:1A:2458:G:H4'	2.35	0.41
1:1A:1155:A:OP1	16:1U:55:ARG:HG2	2.21	0.41
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.20	0.41
1:1A:2563:U:O2'	10:1O:28:SER:HB2	2.20	0.41
1:1A:2693:A:H2'	1:1A:2694:G:C8	2.55	0.41
2:1B:92:C:OP1	21:1Z:79:ARG:NH1	2.49	0.41
30:18:23:VAL:CG1	30:18:47:LYS:HD3	2.50	0.41
32:1a:235:C:H2'	32:1a:236:G:H8	1.85	0.41
32:1a:731:G:OP1	32:1a:766:A:H1'	2.21	0.41
32:1a:1402:4OC:O5'	32:1a:1402:4OC:H6	2.20	0.41
34:1c:29:TYR:CD2	34:1c:29:TYR:C	2.99	0.41
57:1y:66:U:C4	57:1y:67:C:C4	3.09	0.41
1:2A:588:U:H2'	1:2A:589:C:C6	2.56	0.41
1:2A:1031:G:N3	31:29:36:GLN:NE2	2.65	0.41
1:2A:1423:G:OP1	1:2A:1492:G:O2'	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1580:A:H3'	1:2A:1581:G:C8	2.53	0.41
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.55	0.41
1:2A:2186:G:H2'	1:2A:2187:G:C8	2.56	0.41
1:2A:2506:U:C2	1:2A:2585:U:O4	2.73	0.41
32:2a:353:A:H5'	32:2a:353:A:H8	1.85	0.41
32:2a:742:G:P	46:2o:35:ARG:HH22	2.41	0.41
32:2a:976:G:C8	32:2a:1358:U:C2	3.08	0.41
39:2h:31:PHE:O	39:2h:35:ILE:HG13	2.21	0.41
40:2i:85:LEU:HB3	40:2i:92:TYR:CD2	2.55	0.41
44:2m:10:PRO:HB2	44:2m:13:LYS:HD2	2.03	0.41
1:1A:234:C:H2'	1:1A:235:U:C6	2.56	0.41
1:1A:782:A:H5'	1:1A:783:A:N7	2.36	0.41
1:1A:899:A:N3	1:1A:899:A:H2'	2.34	0.41
1:1A:1108:U:H2'	1:1A:1109:C:O4'	2.21	0.41
1:1A:1851:U:H2'	1:1A:1852:C:O4'	2.21	0.41
10:1O:24:VAL:HG13	10:1O:33:ALA:HB2	2.01	0.41
12:1Q:17:LEU:HD23	12:1Q:17:LEU:HA	1.76	0.41
13:1R:55:ALA:HA	13:1R:80:PHE:CZ	2.56	0.41
32:1a:453:A:C5	32:1a:454:C:C4	3.09	0.41
32:1a:1315:U:H2'	32:1a:1316:G:O4'	2.20	0.41
32:1a:1342:C:O2'	40:1i:124:GLN:HG3	2.21	0.41
32:1a:1346:A:O2'	38:1g:10:ARG:NH2	2.51	0.41
32:1a:1367:C:H5'	41:1j:60:ARG:NH1	2.35	0.41
33:1b:84:GLU:OE1	33:1b:216:SER:HA	2.21	0.41
45:1n:29:ARG:HG2	45:1n:31:ARG:H	1.85	0.41
1:2A:2396:G:H1'	23:21:30:VAL:HG12	2.02	0.41
13:2R:117:VAL:HG12	13:2R:118:GLU:H	1.84	0.41
21:2Z:92:SER:O	21:2Z:130:PRO:HG3	2.21	0.41
32:2a:430:A:H4'	35:2d:7:PRO:HG3	2.02	0.41
32:2a:922:G:N3	32:2a:1398:A:H2	2.19	0.41
32:2a:947:G:H1	32:2a:1234:C:H42	1.68	0.41
32:2a:952:U:H2'	32:2a:953:G:H8	1.85	0.41
32:2a:967:5MC:H2'	32:2a:968:A:N7	2.36	0.41
32:2a:1004:A:N6	32:2a:1037:C:H1'	2.36	0.41
32:2a:1216:G:OP1	45:2n:2:ALA:HA	2.19	0.41
1:1A:272(B):G:H2'	1:1A:272(C):G:C8	2.56	0.41
1:1A:329:G:OP2	20:1Y:71:LYS:HD2	2.21	0.41
1:1A:489:G:N7	18:1W:49:LYS:NZ	2.69	0.41
1:1A:813:U:H2'	1:1A:814:C:C6	2.56	0.41
1:1A:858:U:O2	1:1A:2268:A:H2'	2.20	0.41
1:1A:1056:G:O2'	1:1A:1086:A:H1'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.56	0.41
1:1A:1494:A:OP1	62:1A:4246:HOH:O	2.22	0.41
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.56	0.41
1:1A:2698:U:H2'	1:1A:2699:C:C6	2.56	0.41
1:1A:2705:A:H2'	1:1A:2706:G:O4'	2.21	0.41
7:1H:97:ARG:NE	7:1H:104:GLU:OE1	2.50	0.41
21:1Z:158:PRO:O	21:1Z:161:VAL:HG22	2.21	0.41
28:16:12:GLU:OE1	28:16:52:VAL:HG11	2.21	0.41
32:1a:18:C:H2'	32:1a:19:C:O4'	2.20	0.41
32:1a:36:C:OP1	43:1l:123:LYS:NZ	2.52	0.41
32:1a:204:U:H4'	32:1a:216:G:H5"	2.03	0.41
40:1i:11:LYS:C	40:1i:13:ALA:H	2.29	0.41
44:1m:121:LYS:H	44:1m:121:LYS:HD2	1.85	0.41
46:1o:24:SER:O	46:1o:28:GLN:HG3	2.21	0.41
50:1s:69:HIS:HB3	50:1s:73:GLU:CD	2.46	0.41
57:1y:11:C:H2'	57:1y:12:U:O4'	2.21	0.41
1:2A:6:A:N3	9:2N:133:GLN:NE2	2.69	0.41
1:2A:27:G:C2	1:2A:512:G:N3	2.88	0.41
1:2A:252:G:P	11:2P:50:ARG:HH12	2.43	0.41
1:2A:271(K):U:H4'	1:2A:271(L):U:OP1	2.18	0.41
1:2A:582:G:H2'	1:2A:583:G:C8	2.56	0.41
1:2A:956:G:N2	1:2A:959:A:H3'	2.36	0.41
1:2A:1040:C:H2'	1:2A:1041:C:C6	2.56	0.41
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.21	0.41
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.56	0.41
1:2A:1885:A:H2'	1:2A:1886:C:O4'	2.21	0.41
2:2B:119:G:H5'	2:2B:120:A:OP2	2.20	0.41
8:2I:4:ILE:HD11	8:2I:44:LEU:HD23	2.03	0.41
9:2N:73:THR:HG22	9:2N:84:LYS:HG2	2.03	0.41
10:2O:120:GLU:HG2	10:2O:122:LEU:HG	2.03	0.41
11:2P:121:LYS:HE2	11:2P:123:LEU:HD11	2.02	0.41
13:2R:117:VAL:HG12	13:2R:118:GLU:N	2.36	0.41
26:24:15:ILE:HG23	26:24:21:VAL:HG22	2.01	0.41
26:24:68:ARG:HH21	26:24:69:LYS:HB3	1.86	0.41
32:2a:502:G:H2'	32:2a:503:C:O4'	2.21	0.41
32:2a:683:G:H2'	32:2a:684:A:C8	2.55	0.41
32:2a:828:A:H5"	32:2a:859:A:C2	2.56	0.41
32:2a:950:U:H2'	32:2a:951:G:C8	2.56	0.41
32:2a:1240:U:H3	38:2g:30:ILE:HG23	1.86	0.41
32:2a:1326:C:H2'	32:2a:1327:C:H6	1.86	0.41
33:2b:9:GLU:C	33:2b:11:LEU:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:67:THR:HA	34:2c:102:ASN:HB2	2.02	0.41
34:2c:179:ARG:NH1	34:2c:206:GLU:HB2	2.36	0.41
35:2d:112:VAL:H	35:2d:116:GLN:NE2	2.19	0.41
37:2f:67:MET:HE1	37:2f:75:LEU:HD22	2.02	0.41
41:2j:81:THR:C	41:2j:83:GLU:H	2.28	0.41
42:2k:121:PRO:HG2	42:2k:126:ARG:HG2	2.02	0.41
44:2m:40:ASN:ND2	44:2m:43:THR:HG23	2.34	0.41
48:2q:41:LYS:HZ2	48:2q:92:ARG:HH21	1.69	0.41
54:2w:10:G:H8	54:2w:10:G:OP1	2.03	0.41
1:1A:892:G:C2'	1:1A:893:C:H5'	2.50	0.41
1:1A:1805:U:O2	3:1D:50:THR:HB	2.20	0.41
1:1A:1999:C:H4'	1:1A:2723:C:O2	2.21	0.41
5:1F:9:ILE:HD13	5:1F:22:ALA:HB3	2.03	0.41
7:1H:11:VAL:HA	7:1H:12:PRO:HD3	1.95	0.41
8:1I:66:GLU:HA	8:1I:69:LYS:HB3	2.03	0.41
12:1Q:10:ARG:NH1	12:1Q:11:LYS:HE2	2.34	0.41
14:1S:55:ALA:O	14:1S:57:LYS:HG3	2.21	0.41
21:1Z:93:ASP:HA	21:1Z:131:ARG:HH12	1.86	0.41
32:1a:815:A:N7	32:1a:1509:C:O2'	2.47	0.41
32:1a:953:G:H5'	32:1a:965:A:N6	2.30	0.41
32:1a:986:A:H1'	50:1s:54:GLY:O	2.20	0.41
33:1b:164:VAL:HG22	33:1b:186:ALA:HB2	2.03	0.41
33:1b:219:VAL:O	33:1b:223:ILE:HG13	2.21	0.41
34:1c:29:TYR:C	34:1c:29:TYR:HD2	2.29	0.41
35:1d:85:LYS:HD3	35:1d:92:VAL:HG11	2.03	0.41
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	2.03	0.41
39:1h:98:LYS:HE2	39:1h:98:LYS:HB2	1.80	0.41
42:1k:44:SER:OG	42:1k:47:VAL:HG23	2.20	0.41
54:1w:66:U:C4	54:1w:67:C:C4	3.08	0.41
57:1y:3:C:N4	57:1y:70:G:H1	2.19	0.41
57:1y:66:U:H2'	57:1y:67:C:C6	2.56	0.41
57:1y:67:C:H2'	57:1y:68:C:C6	2.56	0.41
1:2A:900:A:HO2'	1:2A:901:A:P	2.42	0.41
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.35	0.41
1:2A:1598:C:H2'	1:2A:1599:C:H6	1.86	0.41
2:2B:94:C:H2'	2:2B:95:C:C6	2.55	0.41
10:2O:48:PRO:CB	32:2a:1422:G:H5"	2.44	0.41
19:2X:92:LEU:O	19:2X:94:GLY:N	2.54	0.41
32:2a:21:G:OP1	62:2a:1913:HOH:O	2.22	0.41
32:2a:361:G:H2'	32:2a:362:G:O4'	2.21	0.41
32:2a:952:U:H2'	32:2a:953:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1135:U:H2'	32:2a:1137:C:C4	2.55	0.41
32:2a:1264:C:C4	32:2a:1272:G:O6	2.74	0.41
32:2a:1279:A:O2'	32:2a:1281:U:OP2	2.28	0.41
48:2q:67:LYS:O	48:2q:68:ARG:HB2	2.21	0.41
54:2w:76:F3N:HE2	56:2z:6:ARG:HG2	2.03	0.41
1:1A:969:U:H2'	1:1A:970:C:C6	2.56	0.40
1:1A:2001:A:H2'	1:1A:2002:G:C8	2.56	0.40
1:1A:2298:A:H2'	1:1A:2299:G:O4'	2.21	0.40
1:1A:2649:U:H2'	1:1A:2650:U:C6	2.56	0.40
5:1F:110:LEU:HD11	5:1F:181:LEU:HG	2.03	0.40
6:1G:41:GLN:O	6:1G:43:LEU:HD22	2.21	0.40
7:1H:104:GLU:HG3	7:1H:114:VAL:HG12	2.04	0.40
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.56	0.40
18:1W:1:MET:HE2	18:1W:62:HIS:ND1	2.37	0.40
25:13:59:VAL:O	25:13:60:GLU:HG2	2.21	0.40
26:14:53:GLU:HB2	26:14:55:ARG:O	2.21	0.40
32:1a:165:C:H2'	32:1a:166:G:C8	2.48	0.40
32:1a:174:C:H2'	32:1a:175:C:C6	2.56	0.40
40:1i:40:LEU:HD11	40:1i:70:LYS:HD2	2.02	0.40
44:1m:70:LEU:HD23	44:1m:70:LEU:HA	1.88	0.40
1:2A:1006:C:O2'	9:2N:106:MET:HB3	2.21	0.40
1:2A:1341:U:OP2	1:2A:1394:U:O2'	2.25	0.40
1:2A:1652:A:OP1	13:2R:8:ARG:HD3	2.20	0.40
1:2A:2474:C:H5"	1:2A:2475:C:OP2	2.21	0.40
1:2A:2516:G:C6	1:2A:2517:C:C4	3.09	0.40
1:2A:2583:G:H4'	62:2A:4532:HOH:O	2.21	0.40
1:2A:2809:A:OP2	1:2A:2891:G:N1	2.40	0.40
20:2Y:6:HIS:H	20:2Y:6:HIS:HD2	1.67	0.40
32:2a:811:C:N4	62:2a:1971:HOH:O	2.54	0.40
32:2a:1239:A:H62	32:2a:1299:A:H62	1.68	0.40
32:2a:1358:U:H5"	45:2n:33:VAL:O	2.22	0.40
32:2a:1440:C:H2'	32:2a:1441:G:O4'	2.21	0.40
46:2o:15:PHE:CZ	46:2o:84:LYS:HD2	2.56	0.40
1:1A:195:A:OP1	11:1P:46:LYS:NZ	2.49	0.40
1:1A:1063:G:H2'	1:1A:1064:C:C5	2.50	0.40
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.22	0.40
1:1A:1669:A:H5"	1:1A:2550:G:OP1	2.21	0.40
1:1A:2250:G:OP1	12:1Q:85:LYS:NZ	2.43	0.40
1:1A:2820:A:P	13:1R:2:ARG:HH22	2.44	0.40
17:1V:1:MET:HE1	17:1V:44:LYS:O	2.21	0.40
17:1V:81:TYR:C	17:1V:82:ARG:HD2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:93:ASP:HB3	21:1Z:131:ARG:HH22	1.86	0.40
37:1f:61:LEU:HB3	37:1f:63:TYR:HE2	1.86	0.40
45:1n:24:CYS:SG	45:1n:39:LEU:HA	2.61	0.40
50:1s:32:LYS:HA	50:1s:50:ALA:HB3	2.03	0.40
57:1y:34:G:H2'	57:1y:35:A:C8	2.56	0.40
1:2A:870:A:OP1	12:2Q:6:ARG:NH1	2.53	0.40
1:2A:1364:G:C8	23:21:3:LYS:HD2	2.56	0.40
1:2A:2528:U:H2'	1:2A:2530:A:H5"	2.03	0.40
2:2B:28:C:OP1	14:2S:36:TYR:OH	2.36	0.40
8:2I:27:ARG:HD3	23:21:71:TYR:CE2	2.57	0.40
11:2P:3:LEU:HD23	11:2P:6:LEU:HD12	2.03	0.40
24:22:35:LEU:HD23	24:22:35:LEU:HA	1.91	0.40
32:2a:435:C:H2'	32:2a:436:C:C6	2.56	0.40
32:2a:637:G:H2'	32:2a:638:G:H8	1.86	0.40
32:2a:993:G:H2'	32:2a:993:G:N3	2.37	0.40
33:2b:51:LEU:HD23	33:2b:201:ILE:HD12	2.03	0.40
33:2b:74:LYS:HB3	33:2b:74:LYS:HE2	1.82	0.40
33:2b:108:ILE:HD13	33:2b:108:ILE:HA	1.88	0.40
35:2d:196:LEU:O	35:2d:198:VAL:N	2.47	0.40
36:2e:47:LYS:HB2	36:2e:47:LYS:HE2	1.87	0.40
39:2h:6:ILE:HD12	39:2h:35:ILE:HD12	2.01	0.40
39:2h:6:ILE:O	39:2h:10:LEU:HG	2.21	0.40
43:2l:117:ARG:NH2	43:2l:124:LYS:HB2	2.37	0.40
44:2m:4:ILE:HG23	44:2m:22:ILE:HD11	2.03	0.40
50:2s:15:LEU:HD21	50:2s:49:ILE:HD11	2.03	0.40
1:1A:55:G:O2'	1:1A:127:A:N1	2.51	0.40
1:1A:271(F):C:H2'	1:1A:271(G):C:C6	2.57	0.40
1:1A:839:U:H1'	1:1A:1191:G:H1'	2.03	0.40
1:1A:2334:G:O6	22:10:74:ARG:NH2	2.46	0.40
6:1G:146:TYR:O	6:1G:149:VAL:HG12	2.21	0.40
26:14:44:THR:O	26:14:44:THR:OG1	2.39	0.40
32:1a:1243:C:H2'	32:1a:1244:C:C6	2.55	0.40
35:1d:81:GLU:OE1	35:1d:139:ARG:NH2	2.42	0.40
38:1g:27:ILE:HD12	38:1g:40:ALA:HA	2.02	0.40
38:1g:50:ILE:HD11	38:1g:125:MET:HG2	2.03	0.40
43:1l:113:ARG:HA	43:1l:113:ARG:HD2	1.92	0.40
48:1q:78:GLU:HG2	48:1q:79:SER:N	2.36	0.40
1:2A:271(X):G:C2	1:2A:271(Y):U:O4	2.74	0.40
1:2A:392:C:H5"	1:2A:409:C:H5"	2.03	0.40
1:2A:515:A:H1'	1:2A:581:C:H1'	2.04	0.40
1:2A:2142:C:C4	1:2A:2143:C:C4	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.21	0.40
1:2A:2818:G:OP1	1:2A:2837:G:O2'	2.26	0.40
2:2B:90:A:C5	2:2B:91:C:H1'	2.56	0.40
3:2D:177:LEU:HD12	3:2D:181:GLU:HG2	2.02	0.40
15:2T:26:ASP:CG	15:2T:120:ARG:HH22	2.29	0.40
15:2T:118:ARG:HG2	32:2a:1442(A):G:C8	2.56	0.40
20:2Y:55:TYR:N	20:2Y:56:PRO:HD3	2.36	0.40
32:2a:114:U:O2'	32:2a:115:G:H5'	2.22	0.40
32:2a:582:U:C2	32:2a:760:G:C6	3.10	0.40
32:2a:1151:A:O2'	32:2a:1152:A:H8	2.02	0.40
62:2a:1933:HOH:O	45:2n:4:LYS:HG3	2.20	0.40
1:1A:363(C):G:H2'	1:1A:363(D):G:C8	2.55	0.40
1:1A:710:G:H2'	1:1A:711:G:C8	2.57	0.40
1:1A:811:U:H2'	11:1P:21:ARG:HA	2.04	0.40
1:1A:1865:G:N2	1:1A:1877:A:OP2	2.47	0.40
1:1A:2506:U:C2	1:1A:2585:U:O4	2.74	0.40
1:1A:2801(A):A:H1'	1:1A:2895:U:H1'	2.04	0.40
1:1A:2854:G:H2'	1:1A:2855:C:C6	2.57	0.40
2:1B:29:A:H2'	2:1B:30:C:O4'	2.22	0.40
9:1N:137:LYS:NZ	9:1N:139:GLU:OE2	2.50	0.40
20:1Y:6:HIS:H	20:1Y:6:HIS:CD2	2.39	0.40
32:1a:970:C:H42	40:1i:128:ARG:C	2.29	0.40
32:1a:1323:G:H2'	32:1a:1324:A:C8	2.56	0.40
39:1h:49:GLU:HG2	39:1h:62:TYR:HE2	1.86	0.40
43:1l:56:ALA:HB2	43:1l:70:ILE:HD11	2.04	0.40
49:1r:43:PHE:HD1	49:1r:56:THR:HG23	1.86	0.40
57:1y:9:A:H4'	57:1y:46:G7M:OP2	2.22	0.40
1:2A:709:U:H2'	1:2A:710:G:C8	2.57	0.40
1:2A:2469:A:O3'	12:2Q:56:ARG:NH1	2.55	0.40
1:2A:2611:U:H6	1:2A:2611:U:H5'	1.86	0.40
4:2E:183:LEU:HD21	15:2T:10:VAL:HG11	2.03	0.40
23:21:73:LEU:HA	23:21:73:LEU:HD23	1.82	0.40
24:22:11:GLU:O	24:22:15:LYS:HG3	2.21	0.40
32:2a:377:G:OP1	47:2p:3:LYS:HE2	2.21	0.40
32:2a:983:A:N1	32:2a:1222:G:N2	2.68	0.40
32:2a:1206:G:H2'	32:2a:1207:2MG:C8	2.57	0.40
32:2a:1221:G:OP1	32:2a:1320:C:N4	2.49	0.40
32:2a:1359:C:H5"	62:2a:2142:HOH:O	2.21	0.40
33:2b:77:ALA:HA	33:2b:80:ILE:HG22	2.03	0.40
43:2l:39:VAL:HG11	43:2l:41:ARG:NH1	2.37	0.40
54:2w:76:F3N:CE2	56:2z:6:ARG:HG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:536:A:H2'	1:1A:537:C:C6	2.57	0.40
1:1A:1448:G:O2'	1:1A:1528(A):A:N1	2.54	0.40
1:1A:1845:G:OP1	3:1D:258:LYS:NZ	2.52	0.40
1:1A:2848:G:H3'	15:1T:95:ARG:O	2.22	0.40
3:1D:38:LYS:HE2	3:1D:39:LYS:O	2.21	0.40
8:1I:72:LEU:HD11	8:1I:107:VAL:HG11	2.03	0.40
10:1O:91:LEU:HB3	10:1O:111:PHE:CE1	2.57	0.40
17:1V:1:MET:HE2	17:1V:43:GLU:H	1.87	0.40
18:1W:2:GLU:OE2	18:1W:72:LYS:NZ	2.44	0.40
19:1X:88:LYS:HB2	19:1X:88:LYS:HE3	1.87	0.40
32:1a:445:G:H2'	32:1a:446:G:O4'	2.22	0.40
32:1a:692:U:H5'	32:1a:797:C:H5'	2.02	0.40
32:1a:941:G:O6	62:1a:1932:HOH:O	2.21	0.40
32:1a:1092:A:H5"	38:1g:4:ARG:NH1	2.36	0.40
32:1a:1261:A:H3'	32:1a:1262:C:H6	1.85	0.40
33:1b:24:TRP:CZ3	33:1b:26:PRO:HA	2.57	0.40
33:1b:50:GLU:HB3	33:1b:200:ILE:O	2.22	0.40
33:1b:216:SER:C	33:1b:218:ALA:H	2.29	0.40
34:1c:73:PRO:HB3	34:1c:103:VAL:HG11	2.03	0.40
36:1e:10:MET:HE3	36:1e:10:MET:HB3	1.91	0.40
57:1y:6:G:C6	57:1y:7:A:C6	3.09	0.40
1:2A:514:A:N3	1:2A:581:C:O2'	2.51	0.40
1:2A:1171:G:O5'	1:2A:1171:G:H8	2.05	0.40
3:2D:72:LYS:HE3	3:2D:72:LYS:HB3	1.94	0.40
10:2O:77:ILE:HB	15:2T:74:ARG:HD2	2.03	0.40
18:2W:88:ARG:HB2	18:2W:92:ARG:HB3	2.02	0.40
32:2a:580:U:H2'	32:2a:581:G:O4'	2.22	0.40
32:2a:920:U:H2'	32:2a:921:U:H6	1.86	0.40
41:2j:8:LEU:HD11	41:2j:20:ALA:HB2	2.03	0.40
44:2m:48:LEU:HD23	44:2m:48:LEU:HA	1.82	0.40
50:2s:36:ARG:NH1	50:2s:75:ALA:HB3	2.37	0.40
54:2w:10:G:H2'	54:2w:11:C:H6	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	25	32
4	2E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	25	32
5	1F	200/210 (95%)	196 (98%)	3 (2%)	1 (0%)	25	32
5	2F	200/210 (95%)	190 (95%)	9 (4%)	1 (0%)	25	32
6	1G	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	22	28
6	2G	179/182 (98%)	159 (89%)	15 (8%)	5 (3%)	4	2
7	1H	172/180 (96%)	162 (94%)	10 (6%)	0	100	100
7	2H	172/180 (96%)	159 (92%)	12 (7%)	1 (1%)	22	28
8	1I	144/148 (97%)	123 (85%)	20 (14%)	1 (1%)	19	24
8	2I	144/148 (97%)	125 (87%)	18 (12%)	1 (1%)	19	24
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	130 (94%)	6 (4%)	2 (1%)	9	9
10	1O	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	133 (90%)	11 (8%)	3 (2%)	6	5
11	2P	147/150 (98%)	133 (90%)	10 (7%)	4 (3%)	4	2
12	1Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
12	2Q	139/141 (99%)	127 (91%)	11 (8%)	1 (1%)	19	24
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	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%)	14	18
15	1T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	16	21
15	2T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	13	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	2V	99/101 (98%)	92 (93%)	7 (7%)	0	100 100
18	1W	110/113 (97%)	110 (100%)	0	0	100 100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
19	1X	93/96 (97%)	88 (95%)	3 (3%)	2 (2%)	5 4
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	12 13
20	1Y	105/110 (96%)	99 (94%)	6 (6%)	0	100 100
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100 100
21	1Z	148/206 (72%)	130 (88%)	17 (12%)	1 (1%)	19 24
21	2Z	156/206 (76%)	131 (84%)	21 (14%)	4 (3%)	4 2
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100 100
22	20	81/85 (95%)	78 (96%)	3 (4%)	0	100 100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	12 13
23	21	95/98 (97%)	94 (99%)	1 (1%)	0	100 100
24	12	68/72 (94%)	65 (96%)	3 (4%)	0	100 100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
26	14	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1 0
26	24	67/71 (94%)	57 (85%)	7 (10%)	3 (4%)	2 0
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%)	50 (98%)	1 (2%)	0	100 100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
29	17	46/49 (94%)	46 (100%)	0	0	100 100
29	27	46/49 (94%)	46 (100%)	0	0	100 100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100 100
30	28	62/65 (95%)	62 (100%)	0	0	100 100
31	19	35/37 (95%)	35 (100%)	0	0	100 100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
33	1b	229/256 (90%)	194 (85%)	26 (11%)	9 (4%)	2 1
33	2b	229/256 (90%)	197 (86%)	28 (12%)	4 (2%)	7 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
34	1c	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	25 32
34	2c	204/239 (85%)	176 (86%)	21 (10%)	7 (3%)	3 1
35	1d	206/209 (99%)	194 (94%)	9 (4%)	3 (2%)	8 8
35	2d	206/209 (99%)	191 (93%)	15 (7%)	0	100 100
36	1e	146/162 (90%)	130 (89%)	13 (9%)	3 (2%)	5 4
36	2e	146/162 (90%)	133 (91%)	10 (7%)	3 (2%)	5 4
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%)	143 (94%)	9 (6%)	1 (1%)	19 24
38	2g	153/156 (98%)	139 (91%)	11 (7%)	3 (2%)	6 5
39	1h	135/138 (98%)	123 (91%)	12 (9%)	0	100 100
39	2h	135/138 (98%)	126 (93%)	8 (6%)	1 (1%)	19 24
40	1i	125/128 (98%)	106 (85%)	18 (14%)	1 (1%)	16 21
40	2i	125/128 (98%)	115 (92%)	9 (7%)	1 (1%)	16 21
41	1j	95/105 (90%)	83 (87%)	9 (10%)	3 (3%)	3 1
41	2j	94/105 (90%)	78 (83%)	13 (14%)	3 (3%)	3 1
42	1k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	14 18
42	2k	112/129 (87%)	102 (91%)	7 (6%)	3 (3%)	4 2
43	1l	119/132 (90%)	113 (95%)	4 (3%)	2 (2%)	7 6
43	2l	119/132 (90%)	113 (95%)	6 (5%)	0	100 100
44	1m	121/126 (96%)	109 (90%)	10 (8%)	2 (2%)	7 6
44	2m	120/126 (95%)	110 (92%)	9 (8%)	1 (1%)	16 21
45	1n	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7 6
45	2n	58/61 (95%)	52 (90%)	6 (10%)	0	100 100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100 100
46	2o	86/89 (97%)	80 (93%)	6 (7%)	0	100 100
47	1p	80/88 (91%)	66 (82%)	13 (16%)	1 (1%)	10 10
47	2p	80/88 (91%)	72 (90%)	8 (10%)	0	100 100
48	1q	97/105 (92%)	91 (94%)	5 (5%)	1 (1%)	13 14
48	2q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	13 14
49	1r	66/88 (75%)	63 (96%)	3 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100 100
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100 100
50	2s	81/93 (87%)	69 (85%)	10 (12%)	2 (2%)	4 3
51	1t	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	3 1
51	2t	94/106 (89%)	85 (90%)	7 (7%)	2 (2%)	5 4
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
56	1z	5/7 (71%)	5 (100%)	0	0	100 100
56	2z	5/7 (71%)	5 (100%)	0	0	100 100
All	All	11378/12142 (94%)	10554 (93%)	718 (6%)	106 (1%)	14 18

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	1Z	53	ILE
33	1b	17	PHE
33	1b	126	GLU
35	1d	173	TRP
40	1i	54	ASP
42	1k	49	GLY
44	1m	67	GLU
5	2F	130	ALA
12	2Q	16	ARG
26	24	45	GLY
33	2b	17	PHE
38	2g	4	ARG
38	2g	55	GLY
44	2m	106	ASN
5	1F	130	ALA
8	1I	11	ASN
11	1P	44	GLY
17	1V	43	GLU
19	1X	93	GLU
23	11	3	LYS
26	14	61	ARG
36	1e	21	ALA
36	1e	85	GLY
45	1n	12	ARG
48	1q	68	ARG

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Mol	Chain	Res	Type
6	2G	42	GLY
6	2G	43	LEU
6	2G	50	ALA
6	2G	51	ARG
11	2P	36	LYS
21	2Z	52	SER
33	2b	126	GLU
34	2c	107	GLN
40	2i	56	LEU
48	2q	68	ARG
50	2s	81	ARG
11	1P	38	GLN
26	14	49	PHE
26	14	62	ARG
33	1b	228	GLY
34	1c	107	GLN
38	1g	79	ARG
41	1j	79	ARG
47	1p	75	ARG
9	2N	2	LYS
9	2N	23	LEU
11	2P	38	GLN
19	2X	93	GLU
21	2Z	144	LEU
26	24	47	GLN
26	24	49	PHE
34	2c	43	LEU
36	2e	69	VAL
41	2j	78	ASN
41	2j	79	ARG
42	2k	49	GLY
4	1E	52	LEU
6	1G	43	LEU
33	1b	8	LYS
33	1b	22	LYS
33	1b	106	LYS
35	1d	88	VAL
41	1j	78	ASN
43	1l	91	LYS
43	1l	105	TYR
44	1m	106	ASN
4	2E	52	LEU

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Mol	Chain	Res	Type
14	2S	84	GLN
34	2c	91	LEU
34	2c	95	THR
38	2g	80	VAL
42	2k	117	ASN
51	2t	10	LEU
15	1T	55	ASN
19	1X	2	LYS
26	14	51	ASP
51	1t	47	GLY
6	2G	181	ARG
7	2H	126	PRO
11	2P	122	PRO
21	2Z	146	ILE
33	2b	123	ALA
34	2c	53	ALA
33	1b	20	GLU
51	1t	100	ILE
8	2I	10	GLU
11	2P	45	LEU
34	2c	179	ARG
51	2t	95	ALA
35	1d	172	PRO
33	2b	231	GLU
34	2c	51	GLY
41	2j	75	ILE
42	2k	105	VAL
41	1j	39	PRO
50	2s	9	VAL
11	1P	122	PRO
36	2e	11	ILE
39	2h	73	ASP
33	1b	231	GLU
36	1e	69	VAL
51	1t	96	GLY
21	2Z	171	ILE
26	14	50	VAL
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%)	203 (94%)	12 (6%)	17 24
3	2D	215/218 (99%)	205 (95%)	10 (5%)	22 32
4	1E	164/166 (99%)	160 (98%)	4 (2%)	44 60
4	2E	164/166 (99%)	159 (97%)	5 (3%)	36 51
5	1F	160/166 (96%)	144 (90%)	16 (10%)	6 6
5	2F	159/166 (96%)	152 (96%)	7 (4%)	24 36
6	1G	143/156 (92%)	133 (93%)	10 (7%)	12 15
6	2G	143/156 (92%)	129 (90%)	14 (10%)	6 6
7	1H	144/148 (97%)	139 (96%)	5 (4%)	31 45
7	2H	144/148 (97%)	138 (96%)	6 (4%)	25 38
8	1I	113/124 (91%)	97 (86%)	16 (14%)	2 2
8	2I	105/124 (85%)	89 (85%)	16 (15%)	2 1
9	1N	118/119 (99%)	110 (93%)	8 (7%)	13 16
9	2N	118/119 (99%)	109 (92%)	9 (8%)	11 13
10	1O	100/100 (100%)	98 (98%)	2 (2%)	50 65
10	2O	100/100 (100%)	94 (94%)	6 (6%)	16 22
11	1P	115/116 (99%)	107 (93%)	8 (7%)	12 15
11	2P	115/116 (99%)	107 (93%)	8 (7%)	12 15
12	1Q	111/111 (100%)	109 (98%)	2 (2%)	54 68
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	15 20
13	1R	101/101 (100%)	99 (98%)	2 (2%)	50 65
13	2R	101/101 (100%)	99 (98%)	2 (2%)	50 65
14	1S	86/88 (98%)	81 (94%)	5 (6%)	17 23
14	2S	85/88 (97%)	78 (92%)	7 (8%)	9 10
15	1T	115/127 (91%)	108 (94%)	7 (6%)	15 21
15	2T	113/127 (89%)	107 (95%)	6 (5%)	19 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	1U	93/94 (99%)	90 (97%)	3 (3%)	34 48
16	2U	93/94 (99%)	87 (94%)	6 (6%)	14 18
17	1V	80/82 (98%)	78 (98%)	2 (2%)	42 58
17	2V	80/82 (98%)	75 (94%)	5 (6%)	15 20
18	1W	90/92 (98%)	87 (97%)	3 (3%)	33 47
18	2W	90/92 (98%)	88 (98%)	2 (2%)	47 62
19	1X	77/78 (99%)	74 (96%)	3 (4%)	27 41
19	2X	77/78 (99%)	76 (99%)	1 (1%)	65 78
20	1Y	85/91 (93%)	78 (92%)	7 (8%)	9 10
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	12 15
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	9 11
21	2Z	137/179 (76%)	122 (89%)	15 (11%)	5 4
22	10	65/67 (97%)	65 (100%)	0	100 100
22	20	65/67 (97%)	64 (98%)	1 (2%)	60 74
23	11	80/83 (96%)	79 (99%)	1 (1%)	65 78
23	21	80/83 (96%)	76 (95%)	4 (5%)	20 29
24	12	65/67 (97%)	62 (95%)	3 (5%)	23 33
24	22	65/67 (97%)	63 (97%)	2 (3%)	35 50
25	13	51/52 (98%)	48 (94%)	3 (6%)	16 23
25	23	50/52 (96%)	45 (90%)	5 (10%)	6 6
26	14	59/63 (94%)	52 (88%)	7 (12%)	4 3
26	24	53/63 (84%)	44 (83%)	9 (17%)	1 1
27	15	50/52 (96%)	47 (94%)	3 (6%)	16 22
27	25	50/52 (96%)	46 (92%)	4 (8%)	10 11
28	16	51/52 (98%)	46 (90%)	5 (10%)	6 6
28	26	50/52 (96%)	45 (90%)	5 (10%)	6 6
29	17	41/42 (98%)	38 (93%)	3 (7%)	11 14
29	27	41/42 (98%)	36 (88%)	5 (12%)	4 3
30	18	54/55 (98%)	51 (94%)	3 (6%)	17 24
30	28	54/55 (98%)	51 (94%)	3 (6%)	17 24
31	19	34/34 (100%)	34 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
31	29	34/34 (100%)	33 (97%)	1 (3%)	37 52
33	1b	192/220 (87%)	167 (87%)	25 (13%)	3 2
33	2b	187/220 (85%)	158 (84%)	29 (16%)	2 1
34	1c	142/188 (76%)	128 (90%)	14 (10%)	6 6
34	2c	140/188 (74%)	122 (87%)	18 (13%)	3 2
35	1d	169/181 (93%)	150 (89%)	19 (11%)	5 4
35	2d	173/181 (96%)	157 (91%)	16 (9%)	7 7
36	1e	113/123 (92%)	104 (92%)	9 (8%)	10 11
36	2e	114/123 (93%)	100 (88%)	14 (12%)	4 3
37	1f	84/90 (93%)	77 (92%)	7 (8%)	9 10
37	2f	85/90 (94%)	75 (88%)	10 (12%)	4 3
38	1g	119/127 (94%)	105 (88%)	14 (12%)	4 3
38	2g	120/127 (94%)	105 (88%)	15 (12%)	3 3
39	1h	114/119 (96%)	106 (93%)	8 (7%)	12 15
39	2h	114/119 (96%)	107 (94%)	7 (6%)	15 21
40	1i	90/99 (91%)	78 (87%)	12 (13%)	3 2
40	2i	89/99 (90%)	78 (88%)	11 (12%)	4 3
41	1j	66/92 (72%)	57 (86%)	9 (14%)	3 2
41	2j	69/92 (75%)	60 (87%)	9 (13%)	3 2
42	1k	82/99 (83%)	78 (95%)	4 (5%)	21 30
42	2k	83/99 (84%)	75 (90%)	8 (10%)	7 6
43	1l	96/108 (89%)	92 (96%)	4 (4%)	25 38
43	2l	96/108 (89%)	87 (91%)	9 (9%)	7 7
44	1m	93/101 (92%)	84 (90%)	9 (10%)	6 6
44	2m	92/101 (91%)	84 (91%)	8 (9%)	8 8
45	1n	49/50 (98%)	40 (82%)	9 (18%)	1 0
45	2n	49/50 (98%)	47 (96%)	2 (4%)	26 39
46	1o	78/80 (98%)	75 (96%)	3 (4%)	28 41
46	2o	78/80 (98%)	73 (94%)	5 (6%)	14 19
47	1p	69/74 (93%)	64 (93%)	5 (7%)	12 14
47	2p	68/74 (92%)	60 (88%)	8 (12%)	4 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
48	1q	94/97 (97%)	90 (96%)	4 (4%)	25 37
48	2q	94/97 (97%)	88 (94%)	6 (6%)	14 19
49	1r	59/77 (77%)	56 (95%)	3 (5%)	20 28
49	2r	59/77 (77%)	54 (92%)	5 (8%)	8 9
50	1s	69/80 (86%)	65 (94%)	4 (6%)	17 23
50	2s	67/80 (84%)	59 (88%)	8 (12%)	4 3
51	1t	70/82 (85%)	63 (90%)	7 (10%)	6 6
51	2t	70/82 (85%)	69 (99%)	1 (1%)	62 76
52	1u	18/22 (82%)	17 (94%)	1 (6%)	17 24
52	2u	18/22 (82%)	17 (94%)	1 (6%)	17 24
56	1z	6/6 (100%)	5 (83%)	1 (17%)	2 1
56	2z	6/6 (100%)	4 (67%)	2 (33%)	0 0
All	All	9315/10076 (92%)	8621 (92%)	694 (8%)	11 13

All (694) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	37	LEU
3	1D	71	ASP
3	1D	111	LEU
3	1D	142	VAL
3	1D	173	VAL
3	1D	174	ILE
3	1D	204	ILE
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
4	1E	47	VAL
4	1E	116	VAL
4	1E	184	VAL
4	1E	188	VAL
5	1F	13	SER
5	1F	24	LEU
5	1F	27	GLU
5	1F	53	THR
5	1F	57	VAL

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Mol	Chain	Res	Type
5	1F	60	SER
5	1F	70	THR
5	1F	88	VAL
5	1F	106	ARG
5	1F	132	VAL
5	1F	144	LYS
5	1F	168	ARG
5	1F	175	THR
5	1F	183	VAL
5	1F	192	LEU
5	1F	195	ASP
6	1G	3	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	22	ARG
6	1G	31	VAL
6	1G	43	LEU
6	1G	91	ARG
6	1G	139	LEU
6	1G	145	THR
6	1G	159	VAL
7	1H	95	ARG
7	1H	127	GLU
7	1H	134	SER
7	1H	149	ARG
7	1H	160	LYS
8	1I	12	LEU
8	1I	20	ASP
8	1I	38	LEU
8	1I	47	LEU
8	1I	69	LYS
8	1I	76	THR
8	1I	77	LEU
8	1I	85	GLU
8	1I	86	THR
8	1I	92	VAL
8	1I	101	LEU
8	1I	116	LEU
8	1I	133	HIS
8	1I	140	LEU
8	1I	143	SER
8	1I	144	VAL

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Mol	Chain	Res	Type
9	1N	1	MET
9	1N	8	GLN
9	1N	9	VAL
9	1N	28	THR
9	1N	48	MET
9	1N	61	ARG
9	1N	62	VAL
9	1N	83	LYS
10	1O	28	SER
10	1O	66	LYS
11	1P	7	ARG
11	1P	15	ARG
11	1P	45	LEU
11	1P	75	ILE
11	1P	98	GLU
11	1P	125	VAL
11	1P	133	SER
11	1P	147	LEU
12	1Q	75	THR
12	1Q	109	VAL
13	1R	36	THR
13	1R	114	VAL
14	1S	14	VAL
14	1S	46	VAL
14	1S	69	VAL
14	1S	73	LEU
14	1S	110	LEU
15	1T	28	VAL
15	1T	34	VAL
15	1T	36	GLU
15	1T	96	ARG
15	1T	108	ARG
15	1T	115	ARG
15	1T	128	GLU
16	1U	31	SER
16	1U	74	LEU
16	1U	95	LEU
17	1V	56	SER
17	1V	73	SER
18	1W	11	ARG
18	1W	17	VAL
18	1W	67	ASP

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Mol	Chain	Res	Type
19	1X	38	GLU
19	1X	72	LYS
19	1X	92	LEU
20	1Y	1	MET
20	1Y	7	VAL
20	1Y	31	LEU
20	1Y	64	GLU
20	1Y	67	LEU
20	1Y	91	GLU
20	1Y	99	CYS
21	1Z	1	MET
21	1Z	33	LEU
21	1Z	42	VAL
21	1Z	72	ARG
21	1Z	80	ARG
21	1Z	129	SER
21	1Z	132	ASN
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	170	THR
21	1Z	171	ILE
23	11	46	LEU
24	12	40	SER
24	12	55	ARG
24	12	70	GLN
25	13	23	LEU
25	13	37	LEU
25	13	54	VAL
26	14	1	MET
26	14	49	PHE
26	14	50	VAL
26	14	61	ARG
26	14	63	TYR
26	14	66	SER
26	14	69	LYS
27	15	6	VAL
27	15	40	LYS
27	15	58	LEU
28	16	6	ARG
28	16	7	ILE
28	16	14	THR
28	16	17	LYS

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Mol	Chain	Res	Type
28	16	47	THR
29	17	24	THR
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	23	VAL
30	18	29	LYS
33	1b	7	VAL
33	1b	12	GLU
33	1b	44	LEU
33	1b	45	GLN
33	1b	59	GLU
33	1b	74	LYS
33	1b	78	GLN
33	1b	81	VAL
33	1b	83	MET
33	1b	93	VAL
33	1b	108	ILE
33	1b	112	VAL
33	1b	156	LYS
33	1b	164	VAL
33	1b	170	GLU
33	1b	185	ILE
33	1b	196	LEU
33	1b	197	VAL
33	1b	212	GLN
33	1b	215	LEU
33	1b	220	ASP
33	1b	221	LEU
33	1b	229	VAL
33	1b	233	SER
33	1b	236	TYR
34	1c	3	ASN
34	1c	8	ILE
34	1c	17	ASP
34	1c	29	TYR
34	1c	32	LEU
34	1c	49	SER
34	1c	70	VAL
34	1c	89	GLU
34	1c	91	LEU
34	1c	165	THR

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Mol	Chain	Res	Type
34	1c	178	LEU
34	1c	195	VAL
34	1c	198	VAL
34	1c	207	VAL
35	1d	3	ARG
35	1d	10	ARG
35	1d	17	VAL
35	1d	19	LEU
35	1d	28	SER
35	1d	31	CYS
35	1d	59	ARG
35	1d	83	SER
35	1d	89	THR
35	1d	91	SER
35	1d	107	ARG
35	1d	135	LEU
35	1d	137	SER
35	1d	140	VAL
35	1d	157	LEU
35	1d	158	ILE
35	1d	175	SER
35	1d	188	LEU
35	1d	194	LEU
36	1e	10	MET
36	1e	18	ARG
36	1e	31	LEU
36	1e	41	VAL
36	1e	64	ARG
36	1e	75	THR
36	1e	79	GLU
36	1e	120	THR
36	1e	126	ARG
37	1f	45	LEU
37	1f	57	GLN
37	1f	65	VAL
37	1f	72	VAL
37	1f	73	ASN
37	1f	75	LEU
37	1f	92	LYS
38	1g	9	VAL
38	1g	12	LEU
38	1g	21	VAL

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Mol	Chain	Res	Type
38	1g	31	MET
38	1g	50	ILE
38	1g	59	LEU
38	1g	78	ARG
38	1g	80	VAL
38	1g	85	TYR
38	1g	87	VAL
38	1g	90	GLU
38	1g	104	LEU
38	1g	110	GLN
38	1g	114	ARG
39	1h	25	ASP
39	1h	26	VAL
39	1h	38	ILE
39	1h	51	VAL
39	1h	52	ASP
39	1h	54	ASP
39	1h	98	LYS
39	1h	133	LEU
40	1i	23	ASN
40	1i	25	LYS
40	1i	27	THR
40	1i	29	ASN
40	1i	53	VAL
40	1i	60	ASP
40	1i	64	THR
40	1i	88	TYR
40	1i	92	TYR
40	1i	103	THR
40	1i	109	VAL
40	1i	128	ARG
41	1j	5	ARG
41	1j	38	ILE
41	1j	43	ARG
41	1j	44	VAL
41	1j	46	ARG
41	1j	51	ARG
41	1j	81	THR
41	1j	92	THR
41	1j	98	ILE
42	1k	18	ARG
42	1k	31	THR

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Mol	Chain	Res	Type
42	1k	48	ILE
42	1k	114	VAL
43	1l	18	VAL
43	1l	33	ARG
43	1l	36	VAL
43	1l	62	SER
44	1m	4	ILE
44	1m	11	ARG
44	1m	12	ASN
44	1m	17	VAL
44	1m	43	THR
44	1m	70	LEU
44	1m	106	ASN
44	1m	109	THR
44	1m	121	LYS
45	1n	13	THR
45	1n	15	LYS
45	1n	17	LYS
45	1n	18	VAL
45	1n	24	CYS
45	1n	35	ARG
45	1n	44	LEU
45	1n	53	LEU
45	1n	60	SER
46	1o	3	ILE
46	1o	76	GLU
46	1o	84	LYS
47	1p	19	ILE
47	1p	29	ASP
47	1p	67	THR
47	1p	75	ARG
47	1p	79	VAL
48	1q	9	VAL
48	1q	34	LYS
48	1q	60	ILE
48	1q	99	SER
49	1r	35	ARG
49	1r	37	VAL
49	1r	63	GLN
50	1s	5	LEU
50	1s	6	LYS
50	1s	12	ASP

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Mol	Chain	Res	Type
50	1s	15	LEU
51	1t	10	LEU
51	1t	13	LEU
51	1t	24	LEU
51	1t	37	SER
51	1t	88	VAL
51	1t	90	GLN
51	1t	100	ILE
52	1u	15	ARG
56	1z	2	THR
3	2D	37	LEU
3	2D	38	LYS
3	2D	64	ILE
3	2D	127	VAL
3	2D	142	VAL
3	2D	181	GLU
3	2D	183	ARG
3	2D	221	VAL
3	2D	242	ARG
3	2D	259	THR
4	2E	38	THR
4	2E	73	GLU
4	2E	77	ILE
4	2E	87	GLU
4	2E	116	VAL
5	2F	9	ILE
5	2F	33	LEU
5	2F	74	ARG
5	2F	145	GLU
5	2F	157	VAL
5	2F	161	GLU
5	2F	183	VAL
6	2G	4	ASP
6	2G	5	VAL
6	2G	18	GLU
6	2G	28	VAL
6	2G	43	LEU
6	2G	45	GLU
6	2G	79	ASN
6	2G	115	ARG
6	2G	124	SER
6	2G	130	ASN

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Mol	Chain	Res	Type
6	2G	140	ILE
6	2G	150	ASP
6	2G	152	LEU
6	2G	165	THR
7	2H	17	VAL
7	2H	88	LEU
7	2H	90	LYS
7	2H	127	GLU
7	2H	129	THR
7	2H	136	ILE
8	2I	2	LYS
8	2I	19	VAL
8	2I	38	LEU
8	2I	51	ILE
8	2I	58	LEU
8	2I	68	LEU
8	2I	75	LEU
8	2I	85	GLU
8	2I	87	LYS
8	2I	101	LEU
8	2I	102	SER
8	2I	117	GLU
8	2I	123	LEU
8	2I	127	VAL
8	2I	129	THR
8	2I	142	VAL
9	2N	1	MET
9	2N	8	GLN
9	2N	9	VAL
9	2N	22	THR
9	2N	28	THR
9	2N	61	ARG
9	2N	62	VAL
9	2N	68	GLU
9	2N	83	LYS
10	2O	1	MET
10	2O	22	ILE
10	2O	66	LYS
10	2O	78	ARG
10	2O	112	MET
10	2O	116	SER
11	2P	45	LEU

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Mol	Chain	Res	Type
11	2P	95	VAL
11	2P	119	GLU
11	2P	125	VAL
11	2P	133	SER
11	2P	135	LEU
11	2P	148	LEU
11	2P	149	GLU
12	2Q	1	MET
12	2Q	6	ARG
12	2Q	22	LYS
12	2Q	38	GLU
12	2Q	56	ARG
12	2Q	75	THR
12	2Q	127	ILE
13	2R	36	THR
13	2R	114	VAL
14	2S	3	ARG
14	2S	21	THR
14	2S	26	LEU
14	2S	43	GLU
14	2S	52	SER
14	2S	84	GLN
14	2S	110	LEU
15	2T	40	THR
15	2T	63	VAL
15	2T	66	VAL
15	2T	67	SER
15	2T	72	VAL
15	2T	87	ASP
16	2U	5	LYS
16	2U	9	VAL
16	2U	31	SER
16	2U	74	LEU
16	2U	77	SER
16	2U	95	LEU
17	2V	15	GLU
17	2V	46	VAL
17	2V	53	GLU
17	2V	79	VAL
17	2V	98	GLU
18	2W	11	ARG
18	2W	17	VAL

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Mol	Chain	Res	Type
19	2X	38	GLU
20	2Y	3	VAL
20	2Y	5	MET
20	2Y	7	VAL
20	2Y	14	LEU
20	2Y	26	LYS
20	2Y	99	CYS
21	2Z	6	LYS
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	67	LEU
21	2Z	71	VAL
21	2Z	74	VAL
21	2Z	100	VAL
21	2Z	121	HIS
21	2Z	129	SER
21	2Z	131	ARG
21	2Z	137	ILE
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	161	VAL
21	2Z	171	ILE
22	20	63	VAL
23	21	40	ARG
23	21	46	LEU
23	21	72	GLU
23	21	85	LEU
24	22	53	LEU
24	22	70	GLN
25	23	18	ASP
25	23	31	LEU
25	23	34	GLU
25	23	37	LEU
25	23	58	VAL
26	24	5	ILE
26	24	10	VAL
26	24	37	SER
26	24	48	ARG
26	24	50	VAL
26	24	61	ARG
26	24	63	TYR
26	24	67	TYR

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Mol	Chain	Res	Type
26	24	68	ARG
27	25	6	VAL
27	25	55	ARG
27	25	58	LEU
27	25	59	GLU
28	26	19	ARG
28	26	20	ASN
28	26	34	LEU
28	26	40	CYS
28	26	48	VAL
29	27	1	MET
29	27	23	ARG
29	27	24	THR
29	27	43	THR
29	27	46	VAL
30	28	14	VAL
30	28	23	VAL
30	28	37	SER
31	29	33	LYS
33	2b	7	VAL
33	2b	8	LYS
33	2b	9	GLU
33	2b	11	LEU
33	2b	16	HIS
33	2b	35	GLU
33	2b	44	LEU
33	2b	71	VAL
33	2b	76	GLN
33	2b	82	ARG
33	2b	83	MET
33	2b	93	VAL
33	2b	107	THR
33	2b	110	GLN
33	2b	112	VAL
33	2b	117	GLU
33	2b	127	ILE
33	2b	138	LEU
33	2b	142	LEU
33	2b	150	SER
33	2b	164	VAL
33	2b	185	ILE
33	2b	189	ASP

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Mol	Chain	Res	Type
33	2b	196	LEU
33	2b	197	VAL
33	2b	208	ILE
33	2b	224	GLN
33	2b	230	VAL
33	2b	236	TYR
34	2c	4	LYS
34	2c	5	ILE
34	2c	15	THR
34	2c	16	ARG
34	2c	26	LYS
34	2c	34	LEU
34	2c	35	GLU
34	2c	55	VAL
34	2c	91	LEU
34	2c	101	LEU
34	2c	116	VAL
34	2c	132	ARG
34	2c	152	ILE
34	2c	153	VAL
34	2c	161	GLU
34	2c	190	ARG
34	2c	196	LEU
34	2c	202	ILE
35	2d	5	ILE
35	2d	8	VAL
35	2d	47	ARG
35	2d	53	ASP
35	2d	58	LEU
35	2d	59	ARG
35	2d	86	LYS
35	2d	107	ARG
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	155	LEU
35	2d	156	GLU
35	2d	175	SER
35	2d	178	VAL
35	2d	196	LEU
36	2e	11	ILE
36	2e	13	ILE

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Mol	Chain	Res	Type
36	2e	20	GLN
36	2e	38	GLN
36	2e	41	VAL
36	2e	51	VAL
36	2e	53	LEU
36	2e	55	VAL
36	2e	68	GLU
36	2e	91	LEU
36	2e	120	THR
36	2e	148	VAL
36	2e	149	GLU
36	2e	151	LEU
37	2f	10	LEU
37	2f	17	SER
37	2f	21	LEU
37	2f	37	VAL
37	2f	45	LEU
37	2f	63	TYR
37	2f	69	GLU
37	2f	81	ILE
37	2f	92	LYS
37	2f	95	GLU
38	2g	6	ARG
38	2g	9	VAL
38	2g	13	GLN
38	2g	24	THR
38	2g	30	ILE
38	2g	32	ARG
38	2g	63	LYS
38	2g	78	ARG
38	2g	79	ARG
38	2g	85	TYR
38	2g	94	ARG
38	2g	113	GLU
38	2g	135	VAL
38	2g	144	MET
38	2g	154	TYR
39	2h	18	ARG
39	2h	25	ASP
39	2h	29	SER
39	2h	51	VAL
39	2h	99	GLU

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Mol	Chain	Res	Type
39	2h	112	LEU
39	2h	133	LEU
40	2i	12	GLU
40	2i	27	THR
40	2i	35	GLU
40	2i	38	GLN
40	2i	41	VAL
40	2i	47	LEU
40	2i	54	ASP
40	2i	65	VAL
40	2i	66	ARG
40	2i	89	ASN
40	2i	102	LEU
41	2j	8	LEU
41	2j	16	LEU
41	2j	23	ILE
41	2j	38	ILE
41	2j	66	ARG
41	2j	81	THR
41	2j	89	ASP
41	2j	94	VAL
41	2j	97	GLU
42	2k	14	VAL
42	2k	28	THR
42	2k	48	ILE
42	2k	62	GLN
42	2k	84	VAL
42	2k	87	THR
42	2k	103	LEU
42	2k	114	VAL
43	2l	18	VAL
43	2l	36	VAL
43	2l	40	VAL
43	2l	46	LYS
43	2l	47	LYS
43	2l	62	SER
43	2l	65	GLU
43	2l	83	VAL
43	2l	89	ARG
44	2m	17	VAL
44	2m	32	GLU
44	2m	90	LEU

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Mol	Chain	Res	Type
44	2m	93	ARG
44	2m	98	VAL
44	2m	103	THR
44	2m	106	ASN
44	2m	122	LYS
45	2n	3	ARG
45	2n	33	VAL
46	2o	3	ILE
46	2o	13	GLN
46	2o	24	SER
46	2o	26	GLU
46	2o	39	LEU
47	2p	2	VAL
47	2p	8	ARG
47	2p	11	SER
47	2p	20	VAL
47	2p	21	VAL
47	2p	60	LEU
47	2p	73	LEU
47	2p	74	LEU
48	2q	14	LYS
48	2q	41	LYS
48	2q	60	ILE
48	2q	63	ARG
48	2q	77	VAL
48	2q	84	LEU
49	2r	31	LEU
49	2r	35	ARG
49	2r	41	LYS
49	2r	56	THR
49	2r	86	VAL
50	2s	21	GLU
50	2s	37	ARG
50	2s	43	GLU
50	2s	45	VAL
50	2s	47	HIS
50	2s	48	THR
50	2s	56	GLN
50	2s	81	ARG
51	2t	93	GLU
52	2u	7	ARG
56	2z	2	THR

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Mol	Chain	Res	Type
56	2z	5	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (137) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	126	GLN
4	1E	121	ASN
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
7	1H	74	ASN
8	1I	104	GLN
8	1I	133	HIS
9	1N	8	GLN
12	1Q	12	GLN
12	1Q	57	HIS
12	1Q	89	ASN
12	1Q	123	HIS
12	1Q	141	GLN
13	1R	31	HIS
13	1R	50	HIS
15	1T	58	ASN
15	1T	90	GLN
16	1U	81	HIS
16	1U	94	ASN
18	1W	60	ASN
19	1X	31	HIS
21	1Z	34	ASN
21	1Z	54	HIS
21	1Z	151	HIS
24	12	9	GLN
33	1b	16	HIS
33	1b	78	GLN
33	1b	94	ASN
33	1b	140	HIS
33	1b	212	GLN
34	1c	6	HIS
34	1c	102	ASN
34	1c	162	GLN
34	1c	170	GLN
35	1d	45	GLN

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Mol	Chain	Res	Type
35	1d	116	GLN
35	1d	125	HIS
35	1d	160	GLN
35	1d	161	ASN
36	1e	38	GLN
36	1e	65	ASN
37	1f	13	ASN
37	1f	57	GLN
37	1f	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	56	GLN
38	1g	86	GLN
38	1g	106	GLN
39	1h	15	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	58	HIS
40	1i	124	GLN
41	1j	56	HIS
41	1j	62	HIS
42	1k	104	GLN
43	1l	99	HIS
44	1m	92	HIS
47	1p	13	HIS
49	1r	63	GLN
50	1s	47	HIS
50	1s	83	HIS
51	1t	16	HIS
51	1t	75	ASN
51	1t	90	GLN
56	1z	3	HIS
4	2E	48	GLN
4	2E	143	ASN
5	2F	69	HIS
5	2F	75	HIS
6	2G	41	GLN
6	2G	132	ASN
8	2I	11	ASN
8	2I	43	ASN

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Mol	Chain	Res	Type
9	2N	8	GLN
9	2N	69	GLN
11	2P	128	HIS
12	2Q	12	GLN
12	2Q	89	ASN
12	2Q	123	HIS
13	2R	71	GLN
14	2S	38	GLN
14	2S	95	HIS
15	2T	58	ASN
15	2T	84	GLN
16	2U	94	ASN
19	2X	31	HIS
19	2X	82	GLN
20	2Y	6	HIS
21	2Z	55	HIS
21	2Z	73	GLN
22	20	50	ASN
25	23	32	GLN
26	24	40	HIS
26	24	46	GLN
30	28	35	GLN
33	2b	76	GLN
33	2b	94	ASN
33	2b	110	GLN
33	2b	135	GLN
33	2b	146	GLN
34	2c	162	GLN
34	2c	170	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
36	2e	78	HIS
36	2e	130	ASN
36	2e	141	GLN
37	2f	73	ASN
37	2f	100	ASN
38	2g	13	GLN
38	2g	28	ASN
38	2g	68	ASN

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Mol	Chain	Res	Type
40	2i	3	GLN
40	2i	31	GLN
41	2j	33	GLN
41	2j	62	HIS
42	2k	104	GLN
43	2l	99	HIS
44	2m	92	HIS
46	2o	9	GLN
47	2p	16	HIS
47	2p	76	GLN
48	2q	93	GLN
49	2r	63	GLN
50	2s	83	HIS
51	2t	45	GLN
51	2t	75	ASN
51	2t	90	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	408 (14%)	29 (1%)
1	2A	2791/2915 (95%)	432 (15%)	23 (0%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	118/121 (97%)	24 (20%)	0
32	1a	1497/1521 (98%)	228 (15%)	0
32	2a	1501/1521 (98%)	256 (17%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	71/76 (93%)	18 (25%)	0
54	2w	68/76 (89%)	18 (26%)	0
55	1x	75/77 (97%)	7 (9%)	0
55	2x	75/77 (97%)	6 (8%)	0
57	1y	72/76 (94%)	29 (40%)	0
57	2y	70/76 (92%)	24 (34%)	0
All	All	9345/9620 (97%)	1464 (15%)	52 (0%)

All (1464) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C

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Mol	Chain	Res	Type
1	1A	36	G
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	119	A
1	1A	120	U
1	1A	139(A)	G
1	1A	196	A
1	1A	197	A
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	265	A
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	272(B)	G
1	1A	272(G)	C
1	1A	272(I)	U
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	353	G
1	1A	357	A
1	1A	363	G

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Mol	Chain	Res	Type
1	1A	370	G
1	1A	386	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	455	C
1	1A	456	C
1	1A	457	A
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	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	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	651	G
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	669	G

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Mol	Chain	Res	Type
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	746	A
1	1A	747	U
1	1A	764	A
1	1A	765	G
1	1A	774	A
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	792	G
1	1A	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	884	C
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	894	C
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	899	A
1	1A	910	A
1	1A	932	G

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Mol	Chain	Res	Type
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	963	U
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	1038	C
1	1A	1040	C
1	1A	1044	G
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1060	U
1	1A	1063	G
1	1A	1068	G
1	1A	1069	A
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1081	U
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U

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Mol	Chain	Res	Type
1	1A	1097	U
1	1A	1098	A
1	1A	1099	G
1	1A	1106	G
1	1A	1110	G
1	1A	1112	G
1	1A	1116	C
1	1A	1117	G
1	1A	1135	C
1	1A	1136	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	1220	A
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1319	G
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	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G

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Mol	Chain	Res	Type
1	1A	1459	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1543	C
1	1A	1558	A
1	1A	1569	A
1	1A	1578	U
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1647	G
1	1A	1648	C
1	1A	1674	G
1	1A	1700	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1756	G
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1828	G
1	1A	1829	A
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

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Mol	Chain	Res	Type
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
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	2110	G
1	1A	2113	U
1	1A	2116	G
1	1A	2121	G
1	1A	2127	G
1	1A	2130	U
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	2137	C
1	1A	2140	C
1	1A	2142	C
1	1A	2143	C

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Mol	Chain	Res	Type
1	1A	2144	U
1	1A	2146	C
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	2160	G
1	1A	2161	C
1	1A	2163	C
1	1A	2165	G
1	1A	2166	G
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2180	U
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2189	U
1	1A	2190	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2267	A
1	1A	2268	A
1	1A	2280	G
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G

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Mol	Chain	Res	Type
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
1	1A	2372	G
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2407	G
1	1A	2422	A
1	1A	2424	C
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2474	C
1	1A	2476	A
1	1A	2478	A
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2549	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2602	A
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2641	G
1	1A	2654	A

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Mol	Chain	Res	Type
1	1A	2669	G
1	1A	2689	U
1	1A	2691	C
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2757	A
1	1A	2765	A
1	1A	2778	A
1	1A	2790	A
1	1A	2791	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	2825	C
1	1A	2835	A
1	1A	2839	G
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	13	A
2	1B	32	C
2	1B	35	U
2	1B	45	A
2	1B	50	G
2	1B	56	G
2	1B	73	A
2	1B	84	C
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	39	G

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Mol	Chain	Res	Type
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	52	G
32	1a	61	G
32	1a	68	G
32	1a	77	G
32	1a	78	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	115	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	139	G
32	1a	144	G
32	1a	154	C
32	1a	164	U
32	1a	174	C
32	1a	182	U
32	1a	189(G)	G
32	1a	189(H)	G
32	1a	195	A
32	1a	197	A
32	1a	203	U
32	1a	204	U
32	1a	218	C
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	262	A
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	306	G
32	1a	321	A
32	1a	328	C
32	1a	330	C
32	1a	332	G
32	1a	342	C

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Mol	Chain	Res	Type
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	355	C
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	388	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	452	A
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G

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Mol	Chain	Res	Type
32	1a	577	G
32	1a	607	A
32	1a	630	G
32	1a	653	A
32	1a	657	G
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	703	G
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	749	C
32	1a	753	A
32	1a	755	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	857	C
32	1a	870	U
32	1a	902	G
32	1a	913	A
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A

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Mol	Chain	Res	Type
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	996	A
32	1a	1000	U
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1013	G
32	1a	1017	G
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	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1030(D)	A
32	1a	1031	G
32	1a	1033	G
32	1a	1039	C
32	1a	1044	A
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1111	A
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1134	G
32	1a	1135	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G

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Mol	Chain	Res	Type
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1174	G
32	1a	1176	A
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	1214	C
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1250	A
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1370	G
32	1a	1419	G
32	1a	1442	G

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Mol	Chain	Res	Type
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1456	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	7	A
54	1w	8	4SU
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	62	C
54	1w	68	C
54	1w	70	G
54	1w	73	A
54	1w	74	C
55	1x	9	G
55	1x	13	C
55	1x	19	G
55	1x	20	U
55	1x	21	A
55	1x	47	U
55	1x	61	C
57	1y	5	G
57	1y	7	A

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Mol	Chain	Res	Type
57	1y	9	A
57	1y	12	U
57	1y	13	C
57	1y	14	A
57	1y	19	G
57	1y	20	U
57	1y	21	A
57	1y	22	G
57	1y	27	G
57	1y	28	G
57	1y	35	A
57	1y	44	G
57	1y	45	U
57	1y	46	G7M
57	1y	47	U
57	1y	48	C
57	1y	53	G
57	1y	54	5MU
57	1y	56	C
57	1y	57	G
57	1y	58	A
57	1y	59	U
57	1y	61	C
57	1y	66	U
57	1y	70	G
57	1y	71	G
57	1y	72	C
1	2A	12	U
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	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

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Mol	Chain	Res	Type
1	2A	141	A
1	2A	157	U
1	2A	173	G
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	230	U
1	2A	232	G
1	2A	233	A
1	2A	248	G
1	2A	271(I)	G
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(B)	G
1	2A	272(J)	C
1	2A	274	G
1	2A	277	C
1	2A	278	A
1	2A	294	A
1	2A	311	A
1	2A	312	G
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	405	U
1	2A	411	G

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Mol	Chain	Res	Type
1	2A	412	A
1	2A	421	U
1	2A	435	C
1	2A	440	G
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	504	U
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	573	G
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	615	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	701	G
1	2A	717	G
1	2A	730	C

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Mol	Chain	Res	Type
1	2A	739	G
1	2A	752	A
1	2A	753	C
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	783	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	878	A
1	2A	879	G
1	2A	880	G
1	2A	882	G
1	2A	884	C
1	2A	886	C
1	2A	888	C
1	2A	889	C
1	2A	892	G
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	903	C
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	936	C
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G

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Mol	Chain	Res	Type
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
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	1114	G
1	2A	1116	C
1	2A	1117	G
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1171	G
1	2A	1195	G
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1236	G
1	2A	1244	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1314	C
1	2A	1352	U

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Mol	Chain	Res	Type
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1370	C
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1496	A
1	2A	1497	U
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	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1608	A
1	2A	1609	A

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Mol	Chain	Res	Type
1	2A	1610	A
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1741	A
1	2A	1746	G
1	2A	1756	G
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1828	G
1	2A	1829	A
1	2A	1835	G
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
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	1955	U
1	2A	1963	U
1	2A	1967	C

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Mol	Chain	Res	Type
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2099	U
1	2A	2110	G
1	2A	2111	C
1	2A	2113	U
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2145	C
1	2A	2149	G
1	2A	2150	U

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Mol	Chain	Res	Type
1	2A	2151	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2176	A
1	2A	2178	C
1	2A	2184	G
1	2A	2185	C
1	2A	2186	G
1	2A	2187	G
1	2A	2189	U
1	2A	2193	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2268	A
1	2A	2275	C
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	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C

Continued on next page...

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Mol	Chain	Res	Type
1	2A	2350	C
1	2A	2354	G
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2403	C
1	2A	2406	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2431	U
1	2A	2434	A
1	2A	2435	A
1	2A	2439	A
1	2A	2440	C
1	2A	2441	C
1	2A	2448	A
1	2A	2459	A
1	2A	2468	G
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A
1	2A	2478	A
1	2A	2487	G
1	2A	2490	G
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2530	A
1	2A	2549	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2582	G
1	2A	2602	A
1	2A	2609	U

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Mol	Chain	Res	Type
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2656	U
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2757	A
1	2A	2758	A
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	2803	C
1	2A	2810	A
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G
1	2A	2873	A
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	9	G

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Mol	Chain	Res	Type
2	2B	13	A
2	2B	17	C
2	2B	20	C
2	2B	33	G
2	2B	34	U
2	2B	40	U
2	2B	41	U
2	2B	45	A
2	2B	51	G
2	2B	53	A
2	2B	56	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	105	A
2	2B	106	G
2	2B	109	C
2	2B	110	G
2	2B	111	G
2	2B	119	G
2	2B	120	A
32	2a	9	G
32	2a	22	G
32	2a	31	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	52	G
32	2a	65	U
32	2a	66	G
32	2a	76	C
32	2a	79	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	115	G
32	2a	116	A
32	2a	121	C

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Mol	Chain	Res	Type
32	2a	131	C
32	2a	156	G
32	2a	161	A
32	2a	163	C
32	2a	182	U
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	217	C
32	2a	231	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	345	C
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	400	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	429	U

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Mol	Chain	Res	Type
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	470	C
32	2a	471	G
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	524	G
32	2a	527	G7M
32	2a	528	C
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	545	C
32	2a	547	A
32	2a	559	A
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	653	A
32	2a	661	G
32	2a	665	A
32	2a	666	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	723	U
32	2a	731	G

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Mol	Chain	Res	Type
32	2a	733	A
32	2a	749	C
32	2a	755	G
32	2a	774	G
32	2a	777	A
32	2a	793	U
32	2a	794	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	874	G
32	2a	884	U
32	2a	887	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	958	A
32	2a	960	U
32	2a	961	U
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	984	C
32	2a	991	U
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	997	U
32	2a	998	G
32	2a	999	C
32	2a	1002	G

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Mol	Chain	Res	Type
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1008	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1019	C
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1037	C
32	2a	1039	C
32	2a	1040	U
32	2a	1044	A
32	2a	1050	G
32	2a	1051	C
32	2a	1053	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1086	U
32	2a	1092	A
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1104	G
32	2a	1108	G
32	2a	1117	G
32	2a	1122	U

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Mol	Chain	Res	Type
32	2a	1125	U
32	2a	1128	C
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1141	C
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1160	G
32	2a	1182	G
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1211	U
32	2a	1213	A
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1270	C
32	2a	1272	G
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1286	A
32	2a	1287	A
32	2a	1299	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G

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Mol	Chain	Res	Type
32	2a	1312	G
32	2a	1320	C
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	1370	G
32	2a	1379	G
32	2a	1394	A
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
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	9	A
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	29	G
54	2w	46	G7M
54	2w	48	C
54	2w	50	U
54	2w	65	G
54	2w	66	U
54	2w	68	C

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Mol	Chain	Res	Type
54	2w	69	G
54	2w	70	G
54	2w	72	C
54	2w	74	C
55	2x	9	G
55	2x	21	A
55	2x	47	U
55	2x	52	G
55	2x	53	G
55	2x	61	C
57	2y	12	U
57	2y	14	A
57	2y	15	G
57	2y	19	G
57	2y	24	G
57	2y	27	G
57	2y	28	G
57	2y	43	C
57	2y	45	U
57	2y	48	C
57	2y	49	C
57	2y	52	G
57	2y	53	G
57	2y	54	5MU
57	2y	56	C
57	2y	57	G
57	2y	58	A
57	2y	59	U
57	2y	61	C
57	2y	63	G
57	2y	65	G
57	2y	69	G
57	2y	70	G
57	2y	71	G

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	195	A
1	1A	196	A
1	1A	266	G
1	1A	271(J)	C

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Mol	Chain	Res	Type
1	1A	278	A
1	1A	548	A
1	1A	573	G
1	1A	685	A
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	974	G
1	1A	1067	A
1	1A	1174	A
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	2170	A
1	1A	2183	C
1	1A	2406	U
1	1A	2430	A
1	1A	2439	A
1	1A	2629	A
1	1A	2756	U
1	2A	196	A
1	2A	228	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	900	A
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1992	G

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Mol	Chain	Res	Type
1	2A	2119	A
1	2A	2126	A
1	2A	2430	A
1	2A	2439	A
1	2A	2689	U
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	MA6	2a	1518	32	19,26,27	1.01	2 (10%)	18,38,41	1.96	3 (16%)
54	F3N	1w	76	1,54	29,36,37	1.41	4 (13%)	28,51,54	1.46	2 (7%)
32	5MC	2a	1404	32	19,22,23	1.79	3 (15%)	26,32,35	1.18	2 (7%)
1	PSU	2A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	2.12	4 (19%)
57	G7M	1y	46	57	20,26,27	1.30	1 (5%)	16,39,42	0.54	0
32	5MC	1a	1404	32	19,22,23	1.63	3 (15%)	26,32,35	1.12	2 (7%)
55	PSU	2x	55	55	18,21,22	1.38	3 (16%)	21,30,33	1.95	4 (19%)
1	OMG	1A	2251	55,1,58	19,26,27	0.90	1 (5%)	21,38,41	1.01	1 (4%)
57	MIA	2y	37	57	17,24,32	0.98	1 (5%)	16,35,47	1.23	2 (12%)
32	5MC	2a	967	32	19,22,23	1.61	3 (15%)	26,32,35	1.13	4 (15%)
57	PSU	2y	39	57	18,21,22	1.36	2 (11%)	21,30,33	1.93	3 (14%)
1	5MU	2A	1915	1	19,22,23	1.42	6 (31%)	27,32,35	2.30	6 (22%)
32	MA6	2a	1519	32	19,26,27	1.04	2 (10%)	18,38,41	2.01	3 (16%)
32	PSU	2a	516	32,58	18,21,22	1.32	2 (11%)	21,30,33	2.10	4 (19%)
54	PSU	1w	55	54	18,21,22	1.31	2 (11%)	21,30,33	2.12	4 (19%)
32	G7M	2a	527	32,58	20,26,27	1.22	2 (10%)	16,39,42	0.50	0
57	PSU	1y	55	57	18,21,22	1.42	2 (11%)	21,30,33	2.06	3 (14%)
1	PSU	1A	2605	1,58	18,21,22	1.49	3 (16%)	21,30,33	1.94	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
57	4SU	2y	8	57	18,21,22	1.80	4 (22%)	25,30,33	1.70	4 (16%)
32	UR3	2a	1498	32	19,22,23	1.07	1 (5%)	26,32,35	1.73	3 (11%)
54	PSU	2w	55	54	18,21,22	1.36	2 (11%)	21,30,33	1.97	3 (14%)
1	PSU	2A	2605	1	18,21,22	1.27	2 (11%)	21,30,33	2.28	4 (19%)
54	F3N	2w	76	1,54	29,36,37	1.40	5 (17%)	28,51,54	1.48	2 (7%)
32	5MC	1a	1400	32	19,22,23	1.64	3 (15%)	26,32,35	1.11	2 (7%)
32	2MG	2a	1207	32,58	18,26,27	0.93	1 (5%)	16,38,41	1.41	3 (18%)
57	PSU	1y	32	57	18,21,22	1.35	2 (11%)	21,30,33	1.95	3 (14%)
54	G7M	2w	46	54	20,26,27	1.24	1 (5%)	16,39,42	0.57	0
1	5MU	1A	1915	1	19,22,23	1.36	4 (21%)	27,32,35	2.13	7 (25%)
32	2MG	1a	1207	32	18,26,27	0.93	1 (5%)	16,38,41	1.33	3 (18%)
55	5MU	1x	54	55	19,22,23	1.46	4 (21%)	27,32,35	1.90	6 (22%)
1	PSU	2A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	1.96	4 (19%)
54	PSU	1w	32	58,54	18,21,22	1.35	2 (11%)	21,30,33	2.04	5 (23%)
32	PSU	1a	516	32,58	18,21,22	1.39	2 (11%)	21,30,33	2.08	6 (28%)
57	5MU	1y	54	57	19,22,23	1.49	4 (21%)	27,32,35	2.09	6 (22%)
1	5MC	1A	1962	1,58	19,22,23	1.68	3 (15%)	26,32,35	1.20	3 (11%)
32	5MC	2a	1407	32,58	19,22,23	1.61	3 (15%)	26,32,35	1.22	3 (11%)
56	FME	1z	1	56	8,9,10	1.00	0	8,9,11	1.58	1 (12%)
55	5MC	2x	32	55	19,22,23	1.56	3 (15%)	26,32,35	1.25	3 (11%)
32	4OC	1a	1402	32	20,23,24	0.74	0	25,32,35	0.96	1 (4%)
1	5MC	1A	1942	1	19,22,23	1.76	3 (15%)	26,32,35	1.22	3 (11%)
32	MA6	1a	1518	32	19,26,27	1.02	2 (10%)	18,38,41	1.90	3 (16%)
56	FME	2z	1	56	8,9,10	0.97	0	8,9,11	1.32	2 (25%)
55	4SU	2x	8	55	18,21,22	2.13	6 (33%)	25,30,33	1.34	5 (20%)
32	5MC	1a	967	32	19,22,23	1.71	2 (10%)	26,32,35	1.09	2 (7%)
1	2MU	2A	2552	1,58	19,22,24	1.24	3 (15%)	25,31,36	1.83	6 (24%)
1	5MU	2A	1939	1,58	19,22,23	1.48	6 (31%)	27,32,35	2.23	6 (22%)
32	MA6	1a	1519	32	19,26,27	1.04	2 (10%)	18,38,41	1.98	3 (16%)
57	PSU	2y	55	57	18,21,22	1.39	3 (16%)	21,30,33	1.95	5 (23%)
54	4SU	1w	8	54	18,21,22	1.76	4 (22%)	25,30,33	2.14	4 (16%)
55	5MU	2x	54	55	19,22,23	1.38	5 (26%)	27,32,35	2.17	6 (22%)
43	0TD	1l	92	43	8,9,10	4.48	1 (12%)	6,11,13	2.11	3 (50%)
1	OMC	2A	1920	1	19,22,23	0.81	0	25,31,34	0.92	1 (4%)
54	PSU	2w	32	54	18,21,22	1.36	2 (11%)	21,30,33	1.99	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	1A	1917	1	18,21,22	1.33	2 (11%)	21,30,33	2.07	3 (14%)
43	0TD	2l	92	43	8,9,10	4.55	2 (25%)	6,11,13	5.17	3 (50%)
1	8AH	2A	2503	1,58	18,26,27	0.62	0	22,39,42	1.89	4 (18%)
55	8AN	2x	76	55,56,58	17,24,25	1.13	2 (11%)	13,35,38	3.32	4 (30%)
54	5MU	1w	54	54	19,22,23	1.42	5 (26%)	27,32,35	1.99	6 (22%)
55	PSU	1x	55	55	18,21,22	1.35	2 (11%)	21,30,33	1.99	4 (19%)
54	4SU	2w	8	54	18,21,22	1.66	3 (16%)	25,30,33	2.37	5 (20%)
54	MIA	2w	37	54	19,27,32	1.91	3 (15%)	18,39,47	1.50	5 (27%)
1	2MU	1A	2552	1,58	19,22,24	1.20	2 (10%)	25,31,36	1.83	6 (24%)
1	8AH	1A	2503	1,58	18,26,27	0.58	0	22,39,42	1.88	3 (13%)
57	4SU	1y	8	57	18,21,22	1.73	5 (27%)	25,30,33	1.81	4 (16%)
54	5MU	2w	54	54	19,22,23	1.30	4 (21%)	27,32,35	1.91	7 (25%)
57	MIA	1y	37	57	17,24,32	1.03	1 (5%)	16,35,47	1.30	2 (12%)
57	PSU	1y	39	57	18,21,22	1.41	2 (11%)	21,30,33	1.82	4 (19%)
32	G7M	1a	527	32,58	20,26,27	1.16	2 (10%)	16,39,42	0.64	0
55	4SU	1x	8	55	18,21,22	2.34	6 (33%)	25,30,33	1.77	6 (24%)
54	MIA	1w	37	54	24,31,32	2.07	3 (12%)	22,44,47	2.70	7 (31%)
1	OMC	1A	1920	1	19,22,23	0.76	0	25,31,34	0.87	0
54	PSU	1w	39	54	18,21,22	1.38	2 (11%)	21,30,33	1.80	3 (14%)
1	OMG	2A	2251	55,1,58	19,26,27	0.91	1 (5%)	21,38,41	1.15	2 (9%)
55	5MC	1x	32	55	19,22,23	1.65	3 (15%)	26,32,35	1.22	3 (11%)
1	5MC	2A	1962	1,58	19,22,23	1.57	3 (15%)	26,32,35	1.25	3 (11%)
1	5MC	2A	1942	1	19,22,23	1.63	3 (15%)	26,32,35	1.09	2 (7%)
32	5MC	2a	1400	32	19,22,23	1.71	3 (15%)	26,32,35	1.25	4 (15%)
57	G7M	2y	46	57	20,26,27	1.37	2 (10%)	16,39,42	0.64	0
1	5MU	1A	1939	1,58	19,22,23	1.60	6 (31%)	27,32,35	2.12	7 (25%)
57	PSU	2y	32	57	18,21,22	1.36	2 (11%)	21,30,33	2.03	3 (14%)
32	UR3	1a	1498	32	19,22,23	0.98	2 (10%)	26,32,35	1.77	4 (15%)
1	PSU	1A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	2.10	6 (28%)
57	5MU	2y	54	57	19,22,23	1.46	5 (26%)	27,32,35	1.93	6 (22%)
55	8AN	1x	76	55,56,58	17,24,25	1.18	1 (5%)	13,35,38	3.68	3 (23%)
54	G7M	1w	46	54	20,26,27	1.26	2 (10%)	16,39,42	0.60	0
32	M2G	2a	966	32	20,27,28	1.29	2 (10%)	19,40,43	1.06	1 (5%)
54	PSU	2w	39	54	18,21,22	1.49	2 (11%)	21,30,33	1.54	4 (19%)
32	5MC	1a	1407	32	19,22,23	1.63	3 (15%)	26,32,35	1.17	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	M2G	1a	966	32	20,27,28	1.38	3 (15%)	19,40,43	1.09	2 (10%)
32	4OC	2a	1402	32	20,23,24	0.80	0	25,32,35	0.97	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
54	F3N	1w	76	1,54	-	0/15/37/38	0/4/4/4
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
57	G7M	1y	46	57	-	2/3/25/26	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	55,1,58	-	0/5/27/28	0/3/3/3
57	MIA	2y	37	57	-	1/3/25/34	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
57	PSU	2y	39	57	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
32	PSU	2a	516	32,58	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32,58	-	3/3/25/26	0/3/3/3
57	PSU	1y	55	57	-	2/7/25/26	0/2/2/2
1	PSU	1A	2605	1,58	-	0/7/25/26	0/2/2/2
57	4SU	2y	8	57	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	F3N	2w	76	1,54	-	0/15/37/38	0/4/4/4
32	5MC	1a	1400	32	-	1/7/25/26	0/2/2/2
32	2MG	2a	1207	32,58	-	0/5/27/28	0/3/3/3
57	PSU	1y	32	57	-	2/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	1/3/25/26	0/3/3/3
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	2/5/27/28	0/3/3/3
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	58,54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PSU	1a	516	32,58	-	0/7/25/26	0/2/2/2
57	5MU	1y	54	57	-	2/7/25/26	0/2/2/2
1	5MC	1A	1962	1,58	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32,58	-	0/7/25/26	0/2/2/2
56	FME	1z	1	56	-	3/7/9/11	-
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
56	FME	2z	1	56	-	4/7/9/11	-
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
1	2MU	2A	2552	1,58	-	0/9/27/28	0/2/2/2
1	5MU	2A	1939	1,58	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
57	PSU	2y	55	57	-	2/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
1	8AH	2A	2503	1,58	-	0/3/25/26	0/3/3/3
55	8AN	2x	76	55,56,58	-	3/3/25/26	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/7/29/34	0/3/3/3
1	2MU	1A	2552	1,58	-	0/9/27/28	0/2/2/2
1	8AH	1A	2503	1,58	-	1/3/25/26	0/3/3/3
57	4SU	1y	8	57	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
57	MIA	1y	37	57	-	0/3/25/34	0/3/3/3
57	PSU	1y	39	57	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,58	-	3/3/25/26	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	3/11/33/34	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	2A	2251	55,1,58	-	0/5/27/28	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,58	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
57	G7M	2y	46	57	-	1/3/25/26	0/3/3/3
1	5MU	1A	1939	1,58	-	0/7/25/26	0/2/2/2
57	PSU	2y	32	57	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
57	5MU	2y	54	57	-	2/7/25/26	0/2/2/2
55	8AN	1x	76	55,56,58	-	3/3/25/26	0/3/3/3
54	G7M	1w	46	54	-	1/3/25/26	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2

All (223) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.33	1.69	1.82
43	1l	92	0TD	CB-SB	-12.22	1.70	1.82
54	2w	37	MIA	C2-S10	-7.11	1.69	1.75
54	1w	37	MIA	C13-C14	6.75	1.52	1.32
1	1A	1942	5MC	C5-C4	6.54	1.49	1.44
32	2a	1404	5MC	C5-C4	6.47	1.49	1.44
54	1w	37	MIA	C2-S10	-6.32	1.70	1.75
32	1a	967	5MC	C5-C4	6.29	1.48	1.44
32	2a	1400	5MC	C5-C4	6.29	1.48	1.44
1	1A	1962	5MC	C5-C4	6.14	1.48	1.44
55	1x	8	4SU	C4-N3	-6.06	1.31	1.37
55	1x	32	5MC	C5-C4	5.91	1.48	1.44
32	1a	1400	5MC	C5-C4	5.84	1.48	1.44
32	2a	967	5MC	C5-C4	5.83	1.48	1.44
1	2A	1942	5MC	C5-C4	5.80	1.48	1.44
32	1a	1404	5MC	C5-C4	5.79	1.48	1.44
32	1a	1407	5MC	C5-C4	5.77	1.48	1.44
32	2a	1407	5MC	C5-C4	5.73	1.48	1.44
55	2x	32	5MC	C5-C4	5.46	1.48	1.44
1	2A	1962	5MC	C5-C4	5.46	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	8	4SU	C4-N3	-5.09	1.32	1.37
54	1w	8	4SU	C4-S4	-4.89	1.60	1.68
57	2y	8	4SU	C4-S4	-4.68	1.60	1.68
54	2w	76	F3N	CB-CG	-4.63	1.40	1.51
54	2w	8	4SU	C4-S4	-4.62	1.60	1.68
57	1y	8	4SU	C4-S4	-4.51	1.60	1.68
55	2x	8	4SU	C4-S4	-4.49	1.60	1.68
54	1w	76	F3N	CB-CG	-4.44	1.40	1.51
55	1x	8	4SU	C4-S4	-4.38	1.60	1.68
57	2y	46	G7M	C5-C4	4.21	1.47	1.39
54	2w	39	PSU	C6-C5	4.20	1.39	1.35
55	1x	8	4SU	C2-N3	-4.17	1.30	1.38
57	1y	55	PSU	C6-C5	4.14	1.39	1.35
32	1a	966	M2G	C2-N3	4.11	1.36	1.30
54	1w	76	F3N	O4'-C1'	4.10	1.46	1.40
57	1y	39	PSU	C6-C5	4.07	1.39	1.35
57	1y	46	G7M	C5-C4	4.03	1.47	1.39
57	1y	32	PSU	C6-C5	3.96	1.39	1.35
57	2y	39	PSU	C6-C5	3.92	1.39	1.35
57	2y	32	PSU	C6-C5	3.89	1.39	1.35
1	1A	2605	PSU	C6-C5	3.85	1.39	1.35
32	2a	966	M2G	C2-N3	3.84	1.36	1.30
32	1a	516	PSU	C6-C5	3.82	1.39	1.35
54	2w	55	PSU	C6-C5	3.82	1.39	1.35
54	2w	46	G7M	C5-C4	3.81	1.46	1.39
1	1A	1911	PSU	C6-C5	3.78	1.39	1.35
54	1w	46	G7M	C5-C4	3.77	1.46	1.39
32	2a	516	PSU	C6-C5	3.75	1.39	1.35
32	2a	527	G7M	C5-C4	3.70	1.46	1.39
55	2x	55	PSU	C6-C5	3.69	1.39	1.35
54	1w	32	PSU	C6-C5	3.65	1.39	1.35
1	2A	1911	PSU	C6-C5	3.62	1.39	1.35
32	1a	527	G7M	C5-C4	3.57	1.46	1.39
54	2w	32	PSU	C6-C5	3.55	1.39	1.35
55	1x	55	PSU	C6-C5	3.54	1.39	1.35
54	1w	55	PSU	C6-C5	3.46	1.39	1.35
55	2x	8	4SU	C2-N3	-3.45	1.32	1.38
1	2A	1917	PSU	C6-C5	3.37	1.39	1.35
54	2w	76	F3N	O4'-C1'	3.37	1.45	1.40
57	1y	8	4SU	C4-N3	-3.31	1.34	1.37
32	2a	1404	5MC	C6-C5	3.27	1.39	1.34
57	2y	55	PSU	C6-C5	3.25	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	39	PSU	C6-C5	3.24	1.38	1.35
1	1A	1917	PSU	C6-C5	3.23	1.38	1.35
57	2y	8	4SU	C4-N3	-3.20	1.34	1.37
1	1A	1939	5MU	C4-N3	-3.16	1.32	1.38
1	1A	1939	5MU	C2-N3	-3.14	1.32	1.38
55	1x	8	4SU	C5-C4	-3.12	1.38	1.42
32	1a	967	5MC	C6-C5	3.07	1.39	1.34
55	2x	8	4SU	C5-C4	-3.07	1.38	1.42
57	1y	54	5MU	C6-C5	3.04	1.39	1.34
55	1x	54	5MU	C6-C5	3.02	1.39	1.34
54	1w	8	4SU	C4-N3	-3.01	1.34	1.37
57	1y	37	MIA	C2-N3	2.98	1.36	1.32
1	1A	2605	PSU	C4-N3	-2.97	1.33	1.38
32	1a	966	M2G	C2-N2	2.94	1.40	1.35
32	1a	1407	5MC	C6-C5	2.94	1.39	1.34
1	2A	2605	PSU	C6-C5	2.94	1.38	1.35
1	2A	1915	5MU	C6-C5	2.93	1.39	1.34
1	2A	1939	5MU	C6-C5	2.92	1.39	1.34
1	2A	1942	5MC	C6-C5	2.90	1.39	1.34
54	2w	8	4SU	C4-N3	-2.87	1.34	1.37
54	2w	39	PSU	C4-N3	-2.87	1.33	1.38
54	1w	39	PSU	C4-N3	-2.86	1.33	1.38
57	1y	54	5MU	C4-C5	2.82	1.49	1.44
55	1x	54	5MU	C4-N3	-2.81	1.33	1.38
57	2y	8	4SU	C5-C4	-2.81	1.39	1.42
32	2a	1407	5MC	C6-C5	2.80	1.39	1.34
57	2y	54	5MU	C6-C5	2.79	1.39	1.34
55	2x	54	5MU	C6-C5	2.79	1.39	1.34
32	1a	1404	5MC	C6-C5	2.78	1.39	1.34
54	1w	54	5MU	C6-C5	2.78	1.39	1.34
1	1A	1915	5MU	C6-C5	2.78	1.39	1.34
57	2y	37	MIA	C2-N3	2.77	1.36	1.32
57	1y	54	5MU	C2-N1	2.76	1.42	1.38
1	2A	1939	5MU	C4-N3	-2.76	1.33	1.38
32	1a	1400	5MC	C6-C5	2.74	1.39	1.34
1	1A	1939	5MU	C6-C5	2.74	1.39	1.34
55	2x	32	5MC	C6-C5	2.72	1.39	1.34
32	2a	966	M2G	C2-N2	2.70	1.40	1.35
1	2A	1917	PSU	C4-N3	-2.69	1.33	1.38
57	2y	54	5MU	C4-C5	2.68	1.49	1.44
55	1x	32	5MC	C6-C5	2.68	1.39	1.34
32	2a	1400	5MC	C6-C5	2.68	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2552	2MU	C4-N3	-2.67	1.34	1.38
1	1A	1939	5MU	C4-C5	2.67	1.49	1.44
54	1w	54	5MU	C4-C5	2.67	1.49	1.44
1	1A	1917	PSU	C4-N3	-2.64	1.33	1.38
1	1A	1915	5MU	C2-N1	2.63	1.42	1.38
1	1A	1942	5MC	C6-C5	2.62	1.38	1.34
54	1w	32	PSU	C4-N3	-2.61	1.34	1.38
54	1w	55	PSU	C4-N3	-2.61	1.34	1.38
55	2x	76	8AN	C6-C5	-2.61	1.33	1.43
1	1A	1962	5MC	C6-C5	2.61	1.38	1.34
54	1w	54	5MU	C4-N3	-2.60	1.34	1.38
55	1x	8	4SU	O2-C2	2.60	1.27	1.23
55	1x	54	5MU	C4-C5	2.59	1.49	1.44
1	2A	1962	5MC	C6-C5	2.58	1.38	1.34
32	1a	516	PSU	C4-N3	-2.57	1.34	1.38
1	1A	1939	5MU	C2-N1	2.56	1.42	1.38
1	2A	1911	PSU	C4-N3	-2.56	1.34	1.38
1	1A	1911	PSU	C4-N3	-2.56	1.34	1.38
54	2w	54	5MU	C4-N3	-2.55	1.34	1.38
54	2w	37	MIA	C6-C5	2.55	1.48	1.44
1	1A	1962	5MC	C6-N1	-2.55	1.33	1.38
57	2y	55	PSU	C4-N3	-2.54	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.53	1.34	1.38
57	2y	54	5MU	C4-N3	-2.53	1.34	1.38
1	2A	1939	5MU	C2-N1	2.52	1.42	1.38
1	1A	1942	5MC	C6-N1	-2.51	1.33	1.38
1	1A	2251	OMG	C6-N1	-2.51	1.34	1.37
54	2w	76	F3N	C6-C5	-2.50	1.34	1.43
57	1y	39	PSU	C4-N3	-2.50	1.34	1.38
55	2x	54	5MU	C4-C5	2.50	1.48	1.44
57	2y	54	5MU	C2-N1	2.48	1.42	1.38
55	1x	76	8AN	C6-C5	-2.48	1.34	1.43
54	2w	55	PSU	C4-N3	-2.48	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.47	1.33	1.38
55	2x	55	PSU	C4-N3	-2.47	1.34	1.38
54	1w	37	MIA	C6-C5	2.46	1.48	1.44
32	2a	967	5MC	C6-C5	2.46	1.38	1.34
54	1w	8	4SU	C5-C4	-2.46	1.39	1.42
1	2A	2251	OMG	C6-N1	-2.45	1.34	1.37
55	1x	55	PSU	C4-N3	-2.45	1.34	1.38
1	2A	2552	2MU	C5-C4	2.44	1.49	1.43
57	1y	54	5MU	C4-N3	-2.44	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	54	5MU	C4-N3	-2.44	1.34	1.38
1	2A	2552	2MU	C4-N3	-2.43	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.43	1.34	1.37
55	1x	32	5MC	C6-N1	-2.42	1.33	1.38
32	1a	1518	MA6	C6-C5	-2.42	1.41	1.44
54	1w	76	F3N	C6-C5	-2.42	1.34	1.43
1	2A	1915	5MU	C4-C5	2.42	1.48	1.44
55	2x	32	5MC	C6-N1	-2.41	1.33	1.38
1	2A	1915	5MU	C2-N1	2.40	1.42	1.38
32	1a	1519	MA6	C6-C5	-2.39	1.41	1.44
1	2A	1962	5MC	C6-N1	-2.39	1.33	1.38
1	1A	1915	5MU	C4-N3	-2.38	1.34	1.38
57	1y	55	PSU	C4-N3	-2.36	1.34	1.38
57	2y	39	PSU	C4-N3	-2.36	1.34	1.38
32	2a	1518	MA6	C6-C5	-2.36	1.41	1.44
54	1w	46	G7M	C6-N1	-2.36	1.34	1.37
1	1A	1939	5MU	C6-N1	-2.36	1.34	1.38
32	2a	967	5MC	C6-N1	-2.35	1.34	1.38
1	2A	1939	5MU	C4-C5	2.34	1.48	1.44
54	2w	54	5MU	C6-C5	2.34	1.38	1.34
54	2w	32	PSU	C4-N3	-2.33	1.34	1.38
57	2y	46	G7M	C6-N1	-2.33	1.34	1.37
1	2A	2605	PSU	C4-N3	-2.33	1.34	1.38
57	1y	32	PSU	C4-N3	-2.33	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.32	1.34	1.37
32	1a	966	M2G	C6-N1	-2.31	1.34	1.37
54	1w	54	5MU	C2-N1	2.30	1.42	1.38
57	2y	32	PSU	C4-N3	-2.30	1.34	1.38
54	2w	8	4SU	C5-C4	-2.29	1.39	1.42
32	2a	1498	UR3	C2-N1	2.29	1.41	1.38
57	1y	8	4SU	C5-C4	-2.29	1.39	1.42
1	2A	1939	5MU	C6-N1	-2.28	1.34	1.38
55	2x	54	5MU	C2-N1	2.28	1.42	1.38
32	2a	1519	MA6	C6-C5	-2.28	1.41	1.44
32	2a	516	PSU	C4-N3	-2.28	1.34	1.38
32	1a	1498	UR3	C2-N1	2.27	1.41	1.38
32	1a	1404	5MC	C6-N1	-2.27	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.26	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.25	1.34	1.38
32	2a	527	G7M	C6-N1	-2.24	1.34	1.37
1	1A	1915	5MU	C4-C5	2.24	1.48	1.44
43	2l	92	0TD	CB-CA	2.23	1.55	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	54	5MU	C2-N3	-2.23	1.34	1.38
57	2y	8	4SU	C2-N3	-2.20	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.19	1.34	1.38
55	2x	8	4SU	O2-C2	2.18	1.26	1.23
32	2a	1400	5MC	C6-N1	-2.17	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.15	1.34	1.38
32	2a	1518	MA6	C6-N1	2.13	1.35	1.32
57	1y	8	4SU	C2-N3	-2.13	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.12	1.34	1.38
54	2w	37	MIA	C2-N3	2.12	1.37	1.34
55	1x	8	4SU	C6-C5	2.12	1.40	1.35
55	2x	8	4SU	C6-C5	2.11	1.40	1.35
55	2x	76	8AN	C5-N7	-2.10	1.32	1.39
54	1w	76	F3N	C5-N7	-2.09	1.32	1.39
32	1a	1407	5MC	C6-N1	-2.09	1.34	1.38
54	1w	8	4SU	C2-N3	-2.09	1.34	1.38
54	2w	54	5MU	C6-N1	-2.08	1.34	1.38
32	1a	1498	UR3	C6-C5	2.07	1.39	1.35
1	2A	2552	2MU	C2-N3	-2.07	1.34	1.38
32	2a	1519	MA6	C6-N1	2.06	1.35	1.32
32	1a	1519	MA6	C6-N1	2.06	1.35	1.32
54	2w	76	F3N	C5-N7	-2.06	1.32	1.39
1	1A	2552	2MU	C2-N3	-2.06	1.34	1.38
55	2x	54	5MU	C6-N1	-2.05	1.34	1.38
55	2x	55	PSU	C4-C5	2.04	1.50	1.44
57	2y	55	PSU	C2-N3	-2.04	1.34	1.37
1	1A	2605	PSU	C2-N3	-2.04	1.34	1.37
57	2y	54	5MU	C2-N3	-2.03	1.34	1.38
32	1a	1518	MA6	C6-N1	2.03	1.35	1.32
32	1a	527	G7M	C6-N1	-2.03	1.34	1.37
54	1w	54	5MU	C2-N3	-2.03	1.34	1.38
54	2w	54	5MU	C4-C5	2.02	1.48	1.44
57	1y	8	4SU	C6-C5	2.01	1.39	1.35
1	2A	1915	5MU	C2-N3	-2.01	1.34	1.38
54	2w	76	F3N	C2'-C3'	-2.00	1.50	1.53

All (307) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-11.86	81.05	102.36
54	1w	37	MIA	C12-C13-C14	-9.58	109.82	127.01
55	2x	76	8AN	C4'-O4'-C1'	-8.39	102.24	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	76	8AN	O4'-C1'-N9	8.10	119.49	108.75
54	2w	8	4SU	C4-N3-C2	-7.38	120.24	127.31
55	1x	76	8AN	C4'-O4'-C1'	-7.17	103.36	109.92
1	2A	2503	8AH	C2-N3-C4	6.91	121.04	115.46
55	1x	76	8AN	N3-C2-N1	-6.87	119.34	128.67
32	1a	1498	UR3	C4-N3-C2	-6.84	119.08	124.58
32	2a	1498	UR3	C4-N3-C2	-6.79	119.11	124.58
54	1w	76	F3N	N3-C2-N1	-6.77	119.48	128.67
1	2A	2605	PSU	N1-C2-N3	6.76	122.30	115.17
1	1A	2503	8AH	C2-N3-C4	6.75	120.91	115.46
54	2w	76	F3N	N3-C2-N1	-6.66	119.63	128.67
55	2x	76	8AN	N3-C2-N1	-6.64	119.66	128.67
1	1A	1911	PSU	N1-C2-N3	6.57	122.10	115.17
1	2A	1911	PSU	N1-C2-N3	6.56	122.08	115.17
32	1a	516	PSU	N1-C2-N3	6.48	122.00	115.17
57	1y	55	PSU	N1-C2-N3	6.45	121.97	115.17
54	1w	8	4SU	C4-N3-C2	-6.37	121.21	127.31
54	2w	32	PSU	N1-C2-N3	6.33	121.84	115.17
1	1A	1917	PSU	N1-C2-N3	6.33	121.84	115.17
57	2y	32	PSU	N1-C2-N3	6.30	121.82	115.17
54	1w	32	PSU	N1-C2-N3	6.29	121.80	115.17
32	2a	516	PSU	N1-C2-N3	6.27	121.79	115.17
55	1x	55	PSU	N1-C2-N3	6.21	121.72	115.17
54	1w	55	PSU	N1-C2-N3	6.20	121.71	115.17
55	2x	55	PSU	N1-C2-N3	6.18	121.68	115.17
54	2w	55	PSU	N1-C2-N3	6.04	121.54	115.17
57	2y	39	PSU	N1-C2-N3	5.93	121.42	115.17
1	2A	1917	PSU	N1-C2-N3	5.92	121.42	115.17
1	1A	2605	PSU	N1-C2-N3	5.87	121.36	115.17
57	1y	32	PSU	N1-C2-N3	5.83	121.32	115.17
57	2y	55	PSU	N1-C2-N3	5.78	121.27	115.17
54	1w	8	4SU	C5-C4-N3	5.78	120.13	114.75
54	1w	39	PSU	N1-C2-N3	5.77	121.25	115.17
57	1y	39	PSU	N1-C2-N3	5.75	121.23	115.17
54	2w	8	4SU	C5-C4-N3	5.72	120.07	114.75
1	2A	1915	5MU	C4-N3-C2	-5.63	119.96	127.34
32	2a	1519	MA6	N3-C2-N1	-5.58	121.10	128.67
1	2A	1939	5MU	C4-N3-C2	-5.57	120.04	127.34
32	1a	1519	MA6	N3-C2-N1	-5.49	121.22	128.67
32	2a	1518	MA6	N3-C2-N1	-5.45	121.27	128.67
57	1y	54	5MU	N3-C2-N1	5.35	121.85	114.89
55	2x	54	5MU	C4-N3-C2	-5.33	120.35	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1518	MA6	N3-C2-N1	-5.29	121.48	128.67
1	2A	1939	5MU	N3-C2-N1	5.29	121.77	114.89
1	2A	1915	5MU	N3-C2-N1	5.21	121.68	114.89
1	2A	1915	5MU	C5-C4-N3	5.20	119.84	115.32
55	2x	54	5MU	N3-C2-N1	5.20	121.66	114.89
57	1y	54	5MU	C4-N3-C2	-5.19	120.53	127.34
57	1y	8	4SU	C4-N3-C2	-5.18	122.35	127.31
54	1w	54	5MU	N3-C2-N1	5.15	121.60	114.89
1	1A	1915	5MU	N3-C2-N1	5.13	121.57	114.89
1	1A	1939	5MU	C4-N3-C2	-5.09	120.67	127.34
1	1A	1939	5MU	C5-C4-N3	5.06	119.72	115.32
32	2a	1518	MA6	C2-N1-C6	5.06	121.80	116.84
1	2A	2605	PSU	C4-N3-C2	-5.05	119.42	126.37
1	1A	1915	5MU	C4-N3-C2	-5.04	120.73	127.34
1	2A	1939	5MU	C5-C4-N3	5.03	119.69	115.32
57	2y	8	4SU	C5-C4-N3	5.00	119.40	114.75
32	1a	1519	MA6	C2-N1-C6	4.97	121.71	116.84
32	2a	1519	MA6	C2-N1-C6	4.93	121.67	116.84
1	2A	2552	2MU	N3-C2-N1	4.90	121.27	114.89
32	1a	1518	MA6	C2-N1-C6	4.88	121.62	116.84
55	1x	54	5MU	N3-C2-N1	4.85	121.21	114.89
1	1A	2552	2MU	N3-C2-N1	4.84	121.19	114.89
54	1w	54	5MU	C4-N3-C2	-4.83	121.01	127.34
1	1A	1939	5MU	N3-C2-N1	4.80	121.13	114.89
54	2w	39	PSU	N1-C2-N3	4.77	120.20	115.17
1	1A	1915	5MU	O4-C4-C5	-4.73	119.51	124.92
1	2A	1915	5MU	O4-C4-C5	-4.70	119.54	124.92
54	2w	8	4SU	N3-C2-N1	4.66	120.95	114.89
54	1w	55	PSU	C4-N3-C2	-4.64	119.98	126.37
57	1y	8	4SU	C5-C4-N3	4.63	119.06	114.75
1	1A	1939	5MU	C5-C6-N1	-4.54	118.38	123.31
57	2y	54	5MU	C4-N3-C2	-4.53	121.40	127.34
55	2x	76	8AN	O4'-C1'-N9	4.52	114.74	108.75
1	2A	2552	2MU	C4-N3-C2	-4.51	121.02	126.61
57	2y	54	5MU	N3-C2-N1	4.50	120.75	114.89
1	1A	2552	2MU	C4-N3-C2	-4.47	121.06	126.61
54	1w	32	PSU	C4-N3-C2	-4.47	120.21	126.37
32	1a	516	PSU	C4-N3-C2	-4.46	120.22	126.37
1	1A	1911	PSU	C4-N3-C2	-4.44	120.25	126.37
55	1x	54	5MU	C4-N3-C2	-4.44	121.52	127.34
55	2x	54	5MU	C5-C4-N3	4.38	119.13	115.32
1	2A	1939	5MU	O4-C4-C5	-4.34	119.95	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2w	54	5MU	C4-N3-C2	-4.34	121.65	127.34
54	1w	37	MIA	C15-C14-C13	-4.32	109.68	122.66
32	2a	516	PSU	C4-N3-C2	-4.31	120.43	126.37
1	2A	1911	PSU	O2-C2-N1	-4.26	118.39	122.79
1	1A	1915	5MU	C5-C4-N3	4.25	119.02	115.32
54	2w	54	5MU	O4-C4-C5	-4.21	120.10	124.92
1	1A	1917	PSU	C4-N3-C2	-4.20	120.59	126.37
55	2x	54	5MU	O4-C4-C5	-4.19	120.12	124.92
57	1y	54	5MU	C5-C4-N3	4.19	118.97	115.32
55	1x	55	PSU	C4-N3-C2	-4.16	120.64	126.37
54	2w	54	5MU	N3-C2-N1	4.15	120.29	114.89
32	2a	516	PSU	O2-C2-N1	-4.12	118.54	122.79
1	2A	1917	PSU	C4-N3-C2	-4.11	120.71	126.37
1	2A	1911	PSU	C4-N3-C2	-4.09	120.74	126.37
1	2A	2605	PSU	O2-C2-N1	-4.09	118.58	122.79
57	2y	54	5MU	C5-C4-N3	4.07	118.86	115.32
54	2w	54	5MU	C5-C4-N3	4.06	118.86	115.32
57	2y	55	PSU	C4-N3-C2	-4.05	120.79	126.37
55	1x	8	4SU	C6-C5-C4	-4.05	116.45	119.95
55	2x	55	PSU	C4-N3-C2	-3.99	120.88	126.37
55	1x	8	4SU	S4-C4-N3	-3.98	116.04	120.20
57	2y	8	4SU	C4-N3-C2	-3.97	123.51	127.31
57	2y	32	PSU	O2-C2-N1	-3.97	118.69	122.79
54	2w	32	PSU	C4-N3-C2	-3.96	120.91	126.37
57	1y	32	PSU	C4-N3-C2	-3.96	120.91	126.37
1	2A	1939	5MU	C5-C6-N1	-3.95	119.02	123.31
1	1A	2605	PSU	C4-N3-C2	-3.95	120.93	126.37
54	1w	54	5MU	C5-C4-N3	3.94	118.75	115.32
54	2w	55	PSU	C4-N3-C2	-3.91	120.98	126.37
57	1y	55	PSU	O2-C2-N1	-3.89	118.78	122.79
1	1A	1917	PSU	O2-C2-N1	-3.88	118.78	122.79
57	1y	55	PSU	C4-N3-C2	-3.87	121.04	126.37
57	2y	32	PSU	C4-N3-C2	-3.87	121.04	126.37
54	1w	8	4SU	C5-C4-S4	-3.85	119.91	124.31
57	1y	37	MIA	N3-C2-N1	-3.84	123.46	128.67
57	2y	39	PSU	C4-N3-C2	-3.82	121.11	126.37
55	1x	54	5MU	C5-C6-N1	-3.81	119.17	123.31
54	2w	8	4SU	C5-C4-S4	-3.77	120.00	124.31
1	1A	1942	5MC	C5-C6-N1	-3.76	119.23	123.31
54	1w	8	4SU	N3-C2-N1	3.76	119.79	114.89
32	1a	967	5MC	C5-C6-N1	-3.75	119.24	123.31
56	1z	1	FME	CA-N-CN	3.75	128.59	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	8	4SU	O2-C2-N1	3.74	127.67	122.80
57	1y	8	4SU	N3-C2-N1	3.72	119.73	114.89
1	2A	1915	5MU	C5-C6-N1	-3.70	119.30	123.31
57	2y	37	MIA	N3-C2-N1	-3.69	123.66	128.67
55	2x	54	5MU	C5-C6-N1	-3.68	119.31	123.31
32	2a	1404	5MC	C5-C6-N1	-3.64	119.36	123.31
32	2a	1400	5MC	C5-C6-N1	-3.64	119.36	123.31
54	1w	37	MIA	C16-C14-C13	-3.63	111.77	122.66
55	1x	54	5MU	C5-C4-N3	3.60	118.45	115.32
57	1y	54	5MU	C5-C6-N1	-3.60	119.41	123.31
57	1y	39	PSU	C4-N3-C2	-3.59	121.43	126.37
55	1x	32	5MC	C5-C6-N1	-3.59	119.42	123.31
54	1w	54	5MU	O4-C4-C5	-3.58	120.83	124.92
54	2w	32	PSU	O2-C2-N1	-3.57	119.11	122.79
57	1y	54	5MU	O4-C4-C5	-3.51	120.90	124.92
55	2x	32	5MC	C5-C6-N1	-3.51	119.50	123.31
57	1y	32	PSU	O2-C2-N1	-3.48	119.20	122.79
32	1a	1404	5MC	C5-C6-N1	-3.45	119.57	123.31
32	2a	1407	5MC	C5-C6-N1	-3.44	119.57	123.31
57	2y	54	5MU	O4-C4-C5	-3.37	121.06	124.92
43	2l	92	0TD	OD2-CG-CB	3.36	120.41	113.15
55	1x	32	5MC	C5-C4-N3	-3.36	118.31	121.75
54	2w	55	PSU	O2-C2-N1	-3.36	119.33	122.79
57	2y	54	5MU	C5-C6-N1	-3.36	119.67	123.31
54	1w	55	PSU	O2-C2-N1	-3.36	119.33	122.79
1	2A	1917	PSU	O2-C2-N1	-3.35	119.33	122.79
54	1w	54	5MU	C5-C6-N1	-3.33	119.69	123.31
1	2A	1942	5MC	C5-C6-N1	-3.33	119.70	123.31
54	2w	37	MIA	C11-S10-C2	-3.32	99.76	102.25
54	1w	39	PSU	C4-N3-C2	-3.31	121.81	126.37
57	2y	55	PSU	O2-C2-N1	-3.31	119.38	122.79
57	2y	39	PSU	O2-C2-N1	-3.23	119.46	122.79
32	1a	1400	5MC	C5-C6-N1	-3.19	119.84	123.31
32	2a	1498	UR3	C5-C4-N3	3.19	119.23	115.04
43	1l	92	0TD	CSB-SB-CB	-3.18	96.65	102.36
1	2A	1962	5MC	C5-C4-N3	-3.17	118.50	121.75
32	1a	1207	2MG	C8-N7-C5	3.17	107.95	102.55
1	1A	2552	2MU	O4-C4-C5	-3.17	119.69	125.16
32	1a	1404	5MC	C5-C4-N3	-3.15	118.53	121.75
57	2y	8	4SU	C5-C4-S4	-3.15	120.71	124.31
1	1A	1962	5MC	C5-C6-N1	-3.14	119.91	123.31
32	1a	1407	5MC	C5-C6-N1	-3.14	119.91	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1498	UR3	C5-C4-N3	3.10	119.13	115.04
32	2a	1519	MA6	C4-C5-N7	-3.08	106.08	109.34
54	1w	37	MIA	C2-N1-C6	3.07	122.88	117.42
55	1x	55	PSU	O2-C2-N1	-3.06	119.63	122.79
43	1l	92	0TD	OD2-CG-CB	3.06	119.76	113.15
55	2x	8	4SU	C5-C4-N3	3.05	117.58	114.75
1	2A	2552	2MU	C5-C4-N3	3.04	119.06	114.80
55	1x	54	5MU	O4-C4-C5	-3.04	121.44	124.92
32	2a	1207	2MG	N1-C2-N2	3.03	119.65	116.56
55	2x	8	4SU	C6-C5-C4	-3.02	117.33	119.95
1	2A	2251	OMG	C8-N7-C5	3.01	107.67	102.55
32	2a	1404	5MC	C5-C4-N3	-3.00	118.68	121.75
1	2A	2552	2MU	O2-C2-N1	-2.98	118.91	122.80
1	1A	1911	PSU	O2-C2-N1	-2.97	119.72	122.79
1	1A	1942	5MC	C5-C4-N3	-2.97	118.72	121.75
32	2a	1407	5MC	C5-C4-N3	-2.96	118.72	121.75
55	1x	8	4SU	C4-N3-C2	2.95	130.14	127.31
54	1w	39	PSU	O2-C2-N1	-2.95	119.75	122.79
55	2x	55	PSU	O2-C2-N1	-2.93	119.77	122.79
54	2w	8	4SU	O2-C2-N1	-2.93	118.99	122.80
1	1A	2552	2MU	C5-C4-N3	2.92	118.89	114.80
32	1a	1519	MA6	C4-C5-N7	-2.91	106.26	109.34
55	2x	54	5MU	O2-C2-N1	-2.91	119.01	122.80
56	2z	1	FME	CA-N-CN	2.91	127.29	122.82
32	2a	967	5MC	C5-C6-N1	-2.89	120.17	123.31
32	2a	966	M2G	C8-N7-C5	2.89	107.47	102.55
32	1a	516	PSU	O2-C2-N1	-2.89	119.81	122.79
1	1A	2251	OMG	C8-N7-C5	2.87	107.44	102.55
54	2w	54	5MU	C5-C6-N1	-2.87	120.20	123.31
55	2x	32	5MC	C5-C4-N3	-2.84	118.85	121.75
32	1a	1407	5MC	C5-C4-N3	-2.82	118.86	121.75
1	2A	1962	5MC	C5-C6-N1	-2.82	120.25	123.31
32	2a	1207	2MG	C8-N7-C5	2.82	107.34	102.55
1	1A	1962	5MC	C5-C4-N3	-2.81	118.88	121.75
32	2a	1518	MA6	C4-C5-N7	-2.80	106.38	109.34
1	1A	1915	5MU	C5-C6-N1	-2.79	120.28	123.31
32	1a	966	M2G	C8-N7-C5	2.76	107.26	102.55
1	2A	1942	5MC	C5-C4-N3	-2.75	118.93	121.75
54	1w	32	PSU	O2-C2-N1	-2.75	119.96	122.79
55	1x	54	5MU	O2-C2-N1	-2.74	119.23	122.80
1	2A	1915	5MU	O2-C2-N1	-2.72	119.26	122.80
1	1A	2552	2MU	O2-C2-N1	-2.70	119.28	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	1y	8	4SU	C5-C4-S4	-2.67	121.25	124.31
32	1a	1400	5MC	C5-C4-N3	-2.67	119.02	121.75
54	1w	54	5MU	O2-C2-N1	-2.65	119.34	122.80
1	2A	2552	2MU	O4-C4-C5	-2.62	120.65	125.16
32	1a	1402	4OC	C6-C5-C4	2.60	120.13	117.00
32	2a	1400	5MC	O2-C2-N3	-2.59	118.25	122.33
54	1w	37	MIA	N3-C2-N1	-2.56	122.34	127.03
1	1A	1939	5MU	O4-C4-C5	-2.55	122.00	124.92
1	1A	2503	8AH	C2-N1-C6	2.55	122.02	118.10
54	1w	37	MIA	C11-S10-C2	-2.55	100.34	102.25
55	2x	8	4SU	S4-C4-N3	-2.54	117.54	120.20
32	1a	1498	UR3	C3U-N3-C4	2.54	121.39	117.87
1	2A	2503	8AH	C2-N1-C6	2.49	121.93	118.10
55	2x	8	4SU	O2-C2-N1	2.49	126.04	122.80
54	1w	37	MIA	C4-C5-N7	-2.49	106.71	109.34
1	1A	1911	PSU	C5-C6-N1	-2.48	118.69	122.14
55	1x	8	4SU	C5-C4-N3	2.48	117.06	114.75
54	2w	37	MIA	C2-N1-C6	2.47	121.82	117.42
32	1a	516	PSU	C5-C6-N1	-2.47	118.71	122.14
54	2w	37	MIA	C12-N6-C6	-2.46	120.57	122.85
1	2A	1939	5MU	O2-C2-N1	-2.46	119.59	122.80
1	2A	2503	8AH	C4-C5-N7	-2.46	106.86	109.40
54	2w	39	PSU	C4-N3-C2	-2.46	122.99	126.37
32	1a	1407	5MC	O2-C2-N3	-2.45	118.46	122.33
57	2y	8	4SU	N3-C2-N1	2.45	118.08	114.89
32	2a	1207	2MG	N2-C2-N3	-2.45	117.39	120.51
32	1a	967	5MC	C5-C4-N3	-2.45	119.25	121.75
1	2A	2605	PSU	C5-C6-N1	-2.45	118.74	122.14
1	1A	2503	8AH	C4-C5-N7	-2.44	106.87	109.40
1	1A	1962	5MC	O2-C2-N3	-2.44	118.49	122.33
54	2w	54	5MU	O2-C2-N1	-2.43	119.63	122.80
32	1a	1518	MA6	C4-C5-N7	-2.43	106.77	109.34
57	2y	37	MIA	C4-C5-N7	-2.43	106.77	109.34
54	1w	55	PSU	C5-C6-N1	-2.42	118.78	122.14
32	1a	1498	UR3	C6-N1-C2	-2.41	119.83	121.80
32	2a	967	5MC	C5-C4-N3	-2.40	119.30	121.75
1	1A	1939	5MU	O2-C2-N3	-2.38	117.10	121.49
43	2l	92	0TD	OD1-CG-CB	-2.37	117.49	122.44
57	1y	54	5MU	O2-C2-N1	-2.36	119.72	122.80
57	1y	37	MIA	C4-C5-N7	-2.35	106.85	109.34
1	2A	2251	OMG	C5-C6-N1	2.33	118.51	114.07
32	2a	1407	5MC	O2-C2-N3	-2.32	118.67	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1920	OMC	O2-C2-N3	-2.32	118.67	122.33
1	2A	1917	PSU	C5-C6-N1	-2.32	118.93	122.14
55	2x	32	5MC	O2-C2-N3	-2.31	118.69	122.33
1	1A	1915	5MU	O2-C2-N1	-2.28	119.82	122.80
54	1w	32	PSU	C5-C6-N1	-2.28	118.97	122.14
32	2a	1402	4OC	C6-C5-C4	2.27	119.74	117.00
55	1x	8	4SU	C5-C4-S4	2.27	126.90	124.31
32	2a	1400	5MC	C5-C4-N3	-2.27	119.43	121.75
1	1A	2605	PSU	O2-C2-N1	-2.27	120.45	122.79
57	2y	54	5MU	C5M-C5-C4	2.26	121.20	118.78
57	2y	55	PSU	C5-C6-N1	-2.25	119.02	122.14
57	1y	39	PSU	O2-C2-N1	-2.23	120.48	122.79
54	2w	37	MIA	C4-C5-N7	-2.22	106.99	109.34
55	1x	55	PSU	C5-C6-N1	-2.21	119.07	122.14
1	2A	2552	2MU	C2'-C1'-N1	-2.20	110.06	114.24
54	2w	39	PSU	C6-C5-C4	-2.20	116.69	118.17
32	2a	967	5MC	C1'-N1-C6	-2.18	117.57	121.15
32	2a	1498	UR3	C6-N1-C2	-2.17	120.02	121.80
1	2A	1962	5MC	N4-C4-N3	2.17	122.43	118.51
54	2w	54	5MU	C5M-C5-C4	2.13	121.06	118.78
57	2y	55	PSU	O4'-C1'-C2'	2.13	108.09	105.15
1	1A	1911	PSU	O4'-C1'-C2'	2.12	108.08	105.15
32	1a	1207	2MG	N1-C2-N2	2.12	118.72	116.56
32	2a	967	5MC	CM5-C5-C6	-2.11	119.99	122.85
43	1l	92	0TD	OD1-CG-CB	-2.11	118.03	122.44
1	1A	1942	5MC	CM5-C5-C6	-2.10	120.01	122.85
1	1A	2552	2MU	C2'-C1'-N1	-2.09	110.27	114.24
54	2w	39	PSU	O2-C2-N3	-2.09	118.15	121.86
54	1w	76	F3N	C4'-O4'-C1'	-2.08	108.02	109.92
1	1A	1911	PSU	O2-C2-N3	-2.08	118.17	121.86
54	2w	76	F3N	C4'-O4'-C1'	-2.07	108.03	109.92
32	1a	516	PSU	O4'-C1'-C2'	2.07	108.02	105.15
54	2w	37	MIA	C1'-N9-C4	2.07	130.28	126.64
32	1a	516	PSU	O2-C2-N3	-2.07	118.19	121.86
1	1A	2605	PSU	O2-C2-N3	-2.07	118.19	121.86
1	1A	2605	PSU	C6-C5-C4	-2.07	116.78	118.17
32	2a	516	PSU	O4'-C1'-C2'	2.06	108.01	105.15
55	2x	55	PSU	C5-C6-N1	-2.06	119.28	122.14
32	1a	966	M2G	O6-C6-C5	-2.06	120.23	124.32
1	1A	1939	5MU	C5M-C5-C4	2.05	120.97	118.78
56	2z	1	FME	CB-CA-N	2.04	114.24	110.52
54	1w	32	PSU	O2-C2-N3	-2.04	118.24	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1207	2MG	C5-C6-N1	2.04	117.95	114.07
54	2w	32	PSU	C5-C6-N1	-2.03	119.32	122.14
1	2A	2503	8AH	O4'-C1'-N9	-2.03	106.06	108.75
1	1A	1915	5MU	C1'-N1-C2	2.02	121.23	117.59
55	2x	8	4SU	C1'-N1-C2	2.02	121.23	117.59
57	1y	39	PSU	O2-C2-N3	-2.01	118.29	121.86
32	2a	1400	5MC	C1'-N1-C6	-2.01	117.84	121.15
55	2x	76	8AN	O2'-C2'-C3'	2.01	116.91	111.61
55	1x	32	5MC	O2-C2-N3	-2.01	119.17	122.33
1	2A	1911	PSU	C5-C6-N1	-2.00	119.36	122.14

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
43	1l	92	0TD	SB-CB-CG-OD2
43	1l	92	0TD	SB-CB-CG-OD1
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16
55	1x	76	8AN	O4'-C4'-C5'-O5'
55	1x	76	8AN	C3'-C4'-C5'-O5'
57	1y	46	G7M	C4'-C5'-O5'-P
57	1y	54	5MU	O4'-C4'-C5'-O5'
43	2l	92	0TD	O-C-CA-CB
43	2l	92	0TD	CG-CB-SB-CSB
54	2w	37	MIA	C5-C6-N6-C12
54	2w	37	MIA	N1-C6-N6-C12
55	2x	76	8AN	C3'-C4'-C5'-O5'
57	2y	54	5MU	O4'-C4'-C5'-O5'
56	1z	1	FME	N-CA-CB-CG
56	1z	1	FME	C-CA-CB-CG
56	2z	1	FME	O-C-CA-CB
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
55	2x	76	8AN	O4'-C4'-C5'-O5'
54	1w	46	G7M	C4'-C5'-O5'-P
32	2a	527	G7M	C3'-C4'-C5'-O5'
57	1y	54	5MU	C3'-C4'-C5'-O5'
57	2y	54	5MU	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
56	2z	1	FME	CB-CG-SD-CE
32	2a	527	G7M	O4'-C4'-C5'-O5'
56	2z	1	FME	N-CA-CB-CG
55	1x	76	8AN	C4'-C5'-O5'-P
54	2w	46	G7M	C4'-C5'-O5'-P
56	2z	1	FME	CA-CB-CG-SD
57	1y	32	PSU	O4'-C1'-C5-C4
57	1y	55	PSU	O4'-C1'-C5-C4
57	1y	46	G7M	C3'-C4'-C5'-O5'
56	1z	1	FME	CA-CB-CG-SD
54	1w	37	MIA	N6-C12-C13-C14
32	2a	527	G7M	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
57	2y	46	G7M	O4'-C4'-C5'-O5'
55	2x	76	8AN	C4'-C5'-O5'-P
32	1a	1400	5MC	O4'-C4'-C5'-O5'
43	2l	92	0TD	CA-CB-SB-CSB
32	1a	527	G7M	C4'-C5'-O5'-P
57	1y	32	PSU	O4'-C1'-C5-C6
57	1y	55	PSU	O4'-C1'-C5-C6
57	2y	55	PSU	O4'-C1'-C5-C6
32	1a	1519	MA6	C4'-C5'-O5'-P
57	2y	37	MIA	C3'-C4'-C5'-O5'
1	1A	2503	8AH	C4'-C5'-O5'-P
43	1l	92	0TD	CG-CB-SB-CSB
57	2y	55	PSU	C2'-C1'-C5-C6
32	1a	527	G7M	O4'-C4'-C5'-O5'
1	1A	1920	OMC	C2'-C1'-N1-C2
32	1a	967	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

28 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1518	MA6	1	0
57	1y	46	G7M	1	0
55	2x	55	PSU	1	0
32	2a	967	5MC	1	0
1	2A	1915	5MU	1	0
32	2a	1519	MA6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	1y	55	PSU	1	0
57	2y	8	4SU	5	0
54	2w	76	F3N	4	0
32	2a	1207	2MG	1	0
54	2w	46	G7M	1	0
32	1a	1402	4OC	1	0
32	1a	1518	MA6	1	0
32	1a	967	5MC	1	0
1	2A	2552	2MU	3	0
32	1a	1519	MA6	1	0
57	2y	55	PSU	6	0
54	1w	8	4SU	1	0
55	2x	54	5MU	1	0
55	2x	76	8AN	1	0
54	2w	37	MIA	1	0
57	1y	8	4SU	2	0
57	1y	37	MIA	2	0
55	1x	8	4SU	1	0
54	1w	37	MIA	2	0
57	2y	46	G7M	5	0
55	1x	76	8AN	1	0
32	1a	966	M2G	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2765 ligands modelled in this entry, 2763 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	$\#\|Z\| > 2$
61	SF4	2d	303	35	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
61	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
61	SF4	2d	303	35	-	-	0/6/5/5
61	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%)	-0.41	180 (6%) 27 28	24, 43, 98, 108	0
1	2A	2789/2915 (95%)	0.06	148 (5%) 33 33	39, 61, 97, 107	0
2	1B	120/121 (99%)	-0.25	0 100 100	39, 58, 72, 91	0
2	2B	120/121 (99%)	0.44	1 (0%) 82 83	68, 77, 86, 93	0
3	1D	275/276 (99%)	-0.16	4 (1%) 71 73	26, 44, 57, 86	0
3	2D	275/276 (99%)	0.16	5 (1%) 67 69	36, 54, 65, 84	0
4	1E	204/206 (99%)	-0.23	1 (0%) 87 88	26, 45, 64, 75	0
4	2E	204/206 (99%)	0.70	5 (2%) 58 61	42, 64, 76, 81	0
5	1F	202/210 (96%)	0.01	4 (1%) 64 67	24, 48, 70, 87	0
5	2F	202/210 (96%)	0.39	5 (2%) 58 61	41, 67, 80, 85	0
6	1G	181/182 (99%)	0.51	9 (4%) 35 35	48, 64, 75, 89	0
6	2G	181/182 (99%)	1.03	16 (8%) 17 17	66, 78, 85, 91	0
7	1H	174/180 (96%)	0.33	5 (2%) 54 56	44, 58, 71, 78	0
7	2H	174/180 (96%)	1.50	44 (25%) 2 2	72, 85, 93, 97	0
8	1I	146/148 (98%)	1.01	13 (8%) 17 17	51, 75, 82, 85	0
8	2I	146/148 (98%)	1.05	17 (11%) 11 10	55, 75, 83, 87	0
9	1N	140/140 (100%)	-0.12	1 (0%) 84 85	32, 43, 63, 75	0
9	2N	140/140 (100%)	0.77	6 (4%) 40 41	52, 69, 81, 88	0
10	1O	122/122 (100%)	-0.19	0 100 100	32, 46, 62, 66	0
10	2O	122/122 (100%)	0.67	3 (2%) 58 61	52, 64, 74, 80	0
11	1P	149/150 (99%)	0.01	2 (1%) 74 76	25, 54, 71, 77	0
11	2P	149/150 (99%)	0.63	6 (4%) 43 44	45, 69, 83, 89	0
12	1Q	141/141 (100%)	0.03	2 (1%) 73 75	31, 47, 62, 74	0
12	2Q	141/141 (100%)	0.96	11 (7%) 20 20	54, 70, 80, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.24	0 100 100	32, 41, 53, 62	0
13	2R	118/118 (100%)	0.24	0 100 100	47, 58, 68, 75	0
14	1S	110/112 (98%)	0.31	2 (1%) 67 69	45, 58, 69, 73	0
14	2S	110/112 (98%)	0.93	6 (5%) 32 32	62, 74, 80, 83	0
15	1T	131/146 (89%)	0.15	4 (3%) 51 54	40, 50, 74, 83	0
15	2T	131/146 (89%)	0.80	9 (6%) 24 25	56, 66, 78, 83	0
16	1U	116/118 (98%)	-0.48	1 (0%) 81 81	27, 35, 50, 69	0
16	2U	116/118 (98%)	0.60	3 (2%) 57 60	47, 67, 76, 81	0
17	1V	101/101 (100%)	-0.34	0 100 100	28, 44, 59, 70	0
17	2V	101/101 (100%)	0.57	4 (3%) 43 44	46, 74, 80, 85	0
18	1W	112/113 (99%)	-0.34	0 100 100	28, 36, 54, 82	0
18	2W	112/113 (99%)	0.25	2 (1%) 67 69	46, 54, 69, 95	0
19	1X	95/96 (98%)	-0.02	3 (3%) 50 53	33, 44, 68, 80	0
19	2X	95/96 (98%)	0.66	4 (4%) 41 42	50, 63, 75, 84	0
20	1Y	107/110 (97%)	0.27	3 (2%) 55 57	38, 56, 73, 82	0
20	2Y	107/110 (97%)	1.26	13 (12%) 10 10	62, 73, 83, 88	0
21	1Z	154/206 (74%)	0.79	16 (10%) 13 13	43, 69, 87, 91	0
21	2Z	160/206 (77%)	1.60	47 (29%) 1 1	71, 83, 90, 92	0
22	10	83/85 (97%)	-0.03	0 100 100	33, 44, 58, 67	0
22	20	83/85 (97%)	0.74	3 (3%) 46 48	47, 66, 75, 82	0
23	11	97/98 (98%)	0.31	2 (2%) 63 65	35, 52, 76, 82	0
23	21	97/98 (98%)	0.49	3 (3%) 51 54	43, 59, 76, 83	0
24	12	70/72 (97%)	0.14	0 100 100	39, 54, 64, 76	0
24	22	70/72 (97%)	0.66	3 (4%) 40 41	60, 71, 77, 85	0
25	13	59/60 (98%)	-0.11	2 (3%) 48 50	32, 41, 67, 82	0
25	23	59/60 (98%)	0.48	3 (5%) 34 35	60, 68, 77, 85	0
26	14	69/71 (97%)	1.10	14 (20%) 3 3	61, 80, 89, 91	0
26	24	69/71 (97%)	1.41	18 (26%) 2 2	76, 86, 91, 93	0
27	15	59/60 (98%)	-0.37	0 100 100	26, 38, 57, 61	0
27	25	59/60 (98%)	0.24	2 (3%) 48 50	42, 56, 72, 80	0
28	16	53/54 (98%)	0.09	0 100 100	41, 50, 65, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.38	0 100 100	49, 62, 71, 75	0
29	17	48/49 (97%)	0.04	4 (8%) 19 18	27, 34, 60, 70	0
29	27	48/49 (97%)	0.53	6 (12%) 9 9	40, 46, 70, 75	0
30	18	64/65 (98%)	-0.32	0 100 100	35, 41, 47, 62	0
30	28	64/65 (98%)	0.39	0 100 100	50, 58, 65, 66	0
31	19	37/37 (100%)	-0.09	0 100 100	36, 44, 59, 62	0
31	29	37/37 (100%)	1.26	4 (10%) 12 12	67, 74, 81, 83	0
32	1a	1488/1521 (97%)	0.33	62 (4%) 41 42	40, 71, 94, 108	0
32	2a	1491/1521 (98%)	0.52	82 (5%) 32 32	49, 76, 95, 108	0
33	1b	231/256 (90%)	1.15	38 (16%) 5 5	66, 80, 90, 94	0
33	2b	231/256 (90%)	1.69	83 (35%) 1 1	72, 86, 91, 94	0
34	1c	206/239 (86%)	0.94	12 (5%) 30 30	65, 76, 86, 89	0
34	2c	206/239 (86%)	1.49	48 (23%) 2 2	74, 83, 88, 94	0
35	1d	208/209 (99%)	0.84	13 (6%) 27 28	61, 72, 81, 88	0
35	2d	208/209 (99%)	0.88	12 (5%) 30 30	60, 70, 79, 87	0
36	1e	148/162 (91%)	0.70	8 (5%) 32 32	51, 67, 77, 82	0
36	2e	148/162 (91%)	0.97	8 (5%) 32 32	60, 74, 82, 91	0
37	1f	100/101 (99%)	0.74	3 (3%) 52 55	60, 71, 78, 81	0
37	2f	100/101 (99%)	0.63	1 (1%) 79 80	58, 69, 77, 87	0
38	1g	155/156 (99%)	0.94	18 (11%) 11 10	67, 75, 86, 90	0
38	2g	155/156 (99%)	1.05	18 (11%) 11 10	71, 80, 88, 94	0
39	1h	137/138 (99%)	0.71	5 (3%) 46 48	58, 69, 76, 82	0
39	2h	137/138 (99%)	0.79	6 (4%) 39 40	67, 76, 80, 84	0
40	1i	127/128 (99%)	1.57	31 (24%) 2 2	58, 80, 85, 89	0
40	2i	127/128 (99%)	1.90	52 (40%) 1 0	71, 85, 90, 93	0
41	1j	97/105 (92%)	1.42	19 (19%) 4 3	62, 80, 89, 91	0
41	2j	96/105 (91%)	2.40	60 (62%) 0 0	74, 88, 93, 96	0
42	1k	114/129 (88%)	0.46	6 (5%) 33 33	48, 69, 79, 81	0
42	2k	114/129 (88%)	0.96	12 (10%) 13 13	58, 74, 84, 88	0
43	1l	121/132 (91%)	0.34	3 (2%) 58 61	51, 57, 69, 76	0
43	2l	121/132 (91%)	0.90	8 (6%) 26 26	60, 68, 76, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	1.08	12 (9%) 14 15	59, 74, 82, 90	0
44	2m	122/126 (96%)	1.47	24 (19%) 3 3	73, 82, 87, 91	0
45	1n	60/61 (98%)	1.40	7 (11%) 10 10	67, 74, 82, 86	0
45	2n	60/61 (98%)	2.27	33 (55%) 0 0	77, 84, 89, 90	0
46	1o	88/89 (98%)	0.62	4 (4%) 39 39	50, 69, 76, 80	0
46	2o	88/89 (98%)	0.82	4 (4%) 39 39	59, 72, 82, 85	0
47	1p	82/88 (93%)	1.03	8 (9%) 14 15	64, 73, 80, 88	0
47	2p	82/88 (93%)	0.92	4 (4%) 36 36	63, 71, 78, 81	0
48	1q	99/105 (94%)	0.80	5 (5%) 34 35	57, 69, 77, 79	0
48	2q	99/105 (94%)	0.75	8 (8%) 19 19	62, 74, 82, 84	0
49	1r	68/88 (77%)	0.58	1 (1%) 71 73	58, 68, 78, 82	0
49	2r	68/88 (77%)	0.75	5 (7%) 22 23	63, 71, 80, 84	0
50	1s	83/93 (89%)	1.07	11 (13%) 8 8	67, 77, 85, 89	0
50	2s	83/93 (89%)	1.84	28 (33%) 1 1	78, 86, 91, 96	0
51	1t	96/106 (90%)	1.19	16 (16%) 5 5	63, 74, 82, 84	0
51	2t	96/106 (90%)	1.15	15 (15%) 6 6	63, 73, 84, 86	0
52	1u	23/27 (85%)	1.37	4 (17%) 5 4	67, 71, 76, 79	0
52	2u	23/27 (85%)	1.84	10 (43%) 1 0	70, 79, 83, 88	0
53	1v	13/24 (54%)	0.90	2 (15%) 6 6	52, 59, 93, 103	0
53	2v	13/24 (54%)	1.48	4 (30%) 1 1	65, 73, 97, 102	0
54	1w	66/76 (86%)	1.37	16 (24%) 2 2	34, 88, 99, 103	0
54	2w	64/76 (84%)	1.33	13 (20%) 3 3	50, 95, 100, 103	0
55	1x	72/77 (93%)	0.26	4 (5%) 31 31	31, 65, 83, 90	0
55	2x	72/77 (93%)	0.44	1 (1%) 73 75	48, 77, 88, 98	0
56	1z	6/7 (85%)	1.30	2 (33%) 1 1	33, 41, 67, 73	0
56	2z	6/7 (85%)	1.75	2 (33%) 1 1	52, 58, 77, 78	0
57	1y	67/76 (88%)	2.04	29 (43%) 1 0	62, 99, 103, 104	0
57	2y	66/76 (86%)	2.18	35 (53%) 0 0	70, 102, 104, 106	0
All	All	20883/21762 (95%)	0.42	1584 (7%) 21 21	24, 67, 90, 108	0

All (1584) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	9.8
1	2A	652(U)	G	9.8
1	1A	653	A	8.6
1	1A	652(V)	C	8.6
1	2A	653	A	8.4
1	2A	652(V)	C	8.4
1	1A	654	A	7.8
44	2m	124	PRO	7.8
1	1A	652(U)	G	7.7
44	1m	123	ALA	7.4
45	2n	2	ALA	7.3
21	1Z	141	VAL	7.1
45	1n	2	ALA	7.1
1	2A	652(C)	G	6.8
21	1Z	146	ILE	6.7
1	2A	652(T)	C	6.5
1	1A	652(C)	G	6.4
1	1A	2115	G	6.4
1	2A	883	G	6.3
33	2b	237	ALA	6.2
1	2A	654	A	6.0
50	2s	2	PRO	5.9
23	21	2	SER	5.9
1	1A	652(S)	C	5.7
56	1z	2	THR	5.7
32	2a	1032	G	5.6
1	1A	652(T)	C	5.6
51	2t	103	GLY	5.6
1	2A	2147	G	5.5
32	2a	1001(A)	G	5.5
1	1A	2114	A	5.5
32	1a	1035	A	5.5
15	1T	131	ALA	5.4
1	2A	884	C	5.4
44	1m	124	PRO	5.3
7	1H	2	SER	5.3
23	11	2	SER	5.3
1	2A	2111	C	5.3
1	2A	2802	G	5.3
1	2A	2803	C	5.2
56	2z	2	THR	5.2
3	1D	276	LYS	5.2
1	2A	652(B)	A	5.2

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Mol	Chain	Res	Type	RSRZ
29	17	48	LYS	5.2
45	1n	25	VAL	5.2
38	2g	83	ALA	5.1
38	2g	82	GLY	5.1
44	2m	102	ARG	5.1
1	2A	885	C	5.0
29	27	48	LYS	5.0
33	2b	236	TYR	5.0
41	2j	32	ALA	5.0
1	2A	2146	C	4.9
34	2c	2	GLY	4.9
43	2l	18	VAL	4.9
1	2A	2112	G	4.9
3	2D	276	LYS	4.9
44	1m	2	ALA	4.9
1	1A	2117	A	4.9
54	2w	71	G	4.8
1	1A	1096	A	4.8
1	1A	2119	A	4.8
1	1A	652(D)	C	4.8
41	2j	65	LEU	4.8
32	2a	1002	G	4.7
11	2P	15	ARG	4.7
20	2Y	1	MET	4.7
18	2W	112	GLY	4.7
32	1a	1027	C	4.7
32	2a	1033	G	4.7
32	2a	1030(B)	C	4.7
44	1m	122	LYS	4.7
1	1A	2166	G	4.7
40	1i	56	LEU	4.6
51	2t	98	PRO	4.6
1	1A	2135	A	4.6
1	2A	882	G	4.6
45	2n	38	GLY	4.6
54	1w	73	A	4.6
1	1A	2159	G	4.6
1	2A	2115	G	4.6
32	1a	1034	G	4.6
5	2F	207	GLY	4.5
33	1b	237	ALA	4.5
1	1A	1095	A	4.5

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Mol	Chain	Res	Type	RSRZ
44	2m	121	LYS	4.5
1	2A	2893	G	4.5
40	1i	2	GLU	4.5
54	1w	72	C	4.5
1	1A	2116	G	4.5
1	2A	652(D)	C	4.5
1	1A	1094	U	4.4
57	2y	19	G	4.4
1	1A	1057	A	4.4
41	2j	91	PRO	4.4
32	1a	1036	G	4.4
38	2g	16	LEU	4.4
40	2i	102	LEU	4.4
45	2n	34	TYR	4.4
1	1A	1078	U	4.3
32	2a	1001	A	4.3
50	1s	13	ASP	4.3
1	1A	652(E)	G	4.3
34	2c	4	LYS	4.3
1	2A	2145	C	4.3
34	2c	207	VAL	4.3
1	1A	2112	G	4.2
21	2Z	164	ALA	4.2
51	2t	99	LEU	4.2
1	2A	2805	G	4.2
32	1a	1003	G	4.2
21	2Z	144	LEU	4.2
26	24	63	TYR	4.2
26	24	56	VAL	4.2
33	2b	136	VAL	4.2
57	1y	35	A	4.2
54	1w	1	G	4.2
26	14	51	ASP	4.2
34	2c	62	ASP	4.2
1	1A	897	C	4.2
44	2m	122	LYS	4.2
32	1a	1531	A	4.2
1	1A	2110	G	4.1
40	2i	14	VAL	4.1
53	2v	13	A	4.1
26	14	55	ARG	4.1
34	1c	39	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
41	2j	75	ILE	4.1
27	25	29	THR	4.1
38	2g	80	VAL	4.1
32	2a	1030(A)	G	4.1
38	2g	154	TYR	4.1
1	1A	888	C	4.1
1	1A	2111	C	4.1
41	2j	74	ILE	4.1
1	1A	1068	G	4.1
38	2g	84	ASN	4.1
51	1t	103	GLY	4.1
54	1w	70	G	4.1
57	2y	15	G	4.1
19	1X	95	LEU	4.1
1	1A	896	A	4.1
32	2a	1030	C	4.1
32	2a	1038	C	4.1
8	2I	146	ALA	4.1
38	2g	85	TYR	4.0
38	1g	80	VAL	4.0
1	2A	2113	U	4.0
1	1A	1176	G	4.0
1	2A	2125	G	4.0
21	2Z	105	VAL	4.0
26	14	56	VAL	4.0
1	1A	655	A	4.0
32	2a	1039	C	4.0
20	2Y	54	LYS	4.0
1	1A	1063	G	4.0
57	1y	15	G	4.0
21	2Z	172	ALA	4.0
1	1A	652(A)	A	4.0
1	1A	885	C	4.0
1	1A	1509	C	4.0
32	2a	1030(D)	A	4.0
7	2H	45	VAL	4.0
33	2b	7	VAL	4.0
34	2c	190	ARG	3.9
52	1u	24	ARG	3.9
1	1A	1058	G	3.9
38	1g	81	GLY	3.9
1	1A	884	C	3.9

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Mol	Chain	Res	Type	RSRZ
53	1v	12	A	3.9
1	2A	2159	G	3.9
32	2a	1031	G	3.9
1	1A	2136	C	3.9
1	1A	2164	C	3.9
57	2y	36	A	3.9
26	14	58	ARG	3.9
1	1A	1081	U	3.9
1	1A	2113	U	3.9
32	1a	1025	U	3.9
1	2A	2793	G	3.9
32	2a	1286	A	3.9
1	2A	2896	C	3.8
40	1i	67	GLY	3.8
21	1Z	1	MET	3.8
40	1i	19	LEU	3.8
1	1A	652(F)	G	3.8
1	1A	1069	A	3.8
33	2b	77	ALA	3.8
1	2A	2804	C	3.8
54	2w	72	C	3.8
41	2j	59	SER	3.8
5	1F	207	GLY	3.8
6	1G	50	ALA	3.8
1	1A	2145	C	3.8
1	2A	2137	C	3.8
1	2A	2148	G	3.8
1	2A	2154	G	3.8
32	1a	630	G	3.8
41	2j	96	ILE	3.8
7	2H	2	SER	3.8
33	1b	236	TYR	3.8
33	2b	121	LEU	3.8
7	2H	43	VAL	3.8
40	2i	91	ASP	3.8
57	2y	14	A	3.8
50	1s	9	VAL	3.7
29	27	45	ALA	3.7
32	1a	1023	G	3.7
43	2l	64	TYR	3.7
45	2n	13	THR	3.7
44	2m	104	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	2A	896	A	3.7
32	1a	1001	A	3.7
57	2y	7	A	3.7
35	1d	194	LEU	3.7
45	2n	39	LEU	3.7
50	2s	15	LEU	3.7
1	2A	2139	C	3.7
7	2H	15	VAL	3.7
7	2H	17	VAL	3.7
29	27	46	VAL	3.7
41	2j	100	THR	3.7
1	1A	2160	G	3.7
45	2n	11	LYS	3.7
53	2v	12	A	3.7
38	2g	156	TRP	3.7
12	2Q	121	ALA	3.7
51	2t	97	ALA	3.7
1	1A	2141	G	3.7
41	2j	78	ASN	3.6
22	20	84	LEU	3.6
33	1b	232	PRO	3.6
33	2b	17	PHE	3.6
1	1A	2109	U	3.6
6	1G	48	GLU	3.6
32	1a	1447	A	3.6
54	1w	71	G	3.6
33	1b	19	HIS	3.6
38	1g	84	ASN	3.6
3	2D	38	LYS	3.6
40	2i	21	PRO	3.6
36	2e	114	GLY	3.6
29	17	47	ARG	3.6
40	1i	64	THR	3.6
45	2n	12	ARG	3.6
1	2A	2128	C	3.6
40	2i	99	LEU	3.6
1	1A	1059	G	3.6
1	2A	2165	G	3.6
21	1Z	170	THR	3.6
42	2k	14	VAL	3.6
1	1A	1082	U	3.6
1	1A	1098	A	3.6

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Mol	Chain	Res	Type	RSRZ
1	2A	2126	A	3.6
41	2j	14	LYS	3.6
21	2Z	136	PHE	3.6
38	2g	5	ARG	3.6
21	2Z	146	ILE	3.6
40	2i	36	TYR	3.6
1	1A	2170	A	3.5
1	2A	887	A	3.5
21	2Z	157	LEU	3.5
1	1A	898	C	3.5
1	2A	2138	C	3.5
52	2u	24	ARG	3.5
40	1i	8	GLY	3.5
50	2s	9	VAL	3.5
50	2s	71	LEU	3.5
12	2Q	10	ARG	3.5
32	1a	1286	A	3.5
25	23	60	GLU	3.5
1	1A	2138	C	3.5
1	1A	1060	U	3.5
1	2A	2156	G	3.5
32	2a	1034	G	3.5
21	1Z	136	PHE	3.5
1	1A	2169	A	3.5
53	1v	13	A	3.5
1	1A	2140	C	3.5
1	2A	2136	C	3.5
7	2H	136	ILE	3.5
15	1T	130	ALA	3.5
15	2T	130	ALA	3.5
1	1A	1065	U	3.5
1	1A	1066	U	3.5
33	2b	234	PRO	3.5
1	1A	2793	G	3.5
41	2j	31	GLY	3.5
41	2j	34	VAL	3.5
41	2j	49	VAL	3.5
47	1p	82	GLN	3.5
1	2A	2117	A	3.5
1	2A	2135	A	3.5
1	2A	2169	A	3.5
41	1j	98	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
51	1t	10	LEU	3.4
32	2a	1150	U	3.4
44	2m	12	ASN	3.4
32	1a	1026	G	3.4
32	1a	1030(A)	G	3.4
44	2m	100	GLY	3.4
33	1b	229	VAL	3.4
6	2G	50	ALA	3.4
49	1r	20	ALA	3.4
1	2A	2134	A	3.4
32	2a	1005	A	3.4
40	2i	56	LEU	3.4
1	2A	2794	C	3.4
33	2b	33	TYR	3.4
38	1g	156	TRP	3.4
55	2x	47	U	3.4
6	2G	182	LYS	3.4
33	2b	132	LYS	3.4
36	1e	85	GLY	3.4
41	2j	10	GLY	3.4
45	1n	55	GLY	3.4
1	1A	2165	G	3.4
15	2T	131	ALA	3.4
32	1a	1033	G	3.4
40	2i	82	ALA	3.4
57	1y	27	G	3.4
54	2w	73	A	3.4
21	2Z	159	PRO	3.4
1	1A	2803	C	3.4
1	2A	886	C	3.4
40	2i	4	TYR	3.4
32	2a	1040	U	3.4
33	1b	17	PHE	3.4
44	2m	6	GLY	3.4
21	2Z	166	SER	3.4
41	2j	46	ARG	3.4
1	2A	2318	G	3.4
32	1a	1021	G	3.4
57	2y	34	G	3.4
1	1A	2790	A	3.4
32	1a	1028	C	3.4
32	2a	1149	C	3.4

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Mol	Chain	Res	Type	RSRZ
32	1a	1257	U	3.4
33	2b	11	LEU	3.3
40	2i	19	LEU	3.3
52	2u	23	PRO	3.3
21	1Z	148	ASP	3.3
26	24	65	ASP	3.3
46	2o	89	GLY	3.3
1	2A	2174	C	3.3
32	2a	1043	C	3.3
1	1A	2172	U	3.3
34	2c	182	ILE	3.3
38	1g	79	ARG	3.3
8	1I	10	GLU	3.3
1	1A	879	G	3.3
1	2A	2160	G	3.3
32	2a	1036	G	3.3
57	1y	19	G	3.3
57	1y	34	G	3.3
1	1A	1054	A	3.3
1	2A	2158	A	3.3
32	2a	1035	A	3.3
33	1b	127	ILE	3.3
33	2b	165	VAL	3.3
41	2j	50	ILE	3.3
38	2g	76	ARG	3.3
41	2j	9	ARG	3.3
50	2s	81	ARG	3.3
1	1A	2137	C	3.3
32	2a	1018	C	3.3
11	2P	109	GLY	3.3
1	1A	899	A	3.3
1	2A	2119	A	3.3
1	2A	2801(A)	A	3.3
7	2H	19	VAL	3.3
21	2Z	174	VAL	3.3
51	2t	8	ARG	3.3
1	1A	1087	G	3.3
1	1A	2151	G	3.3
20	2Y	90	LEU	3.3
32	1a	1001(A)	G	3.3
32	2a	1004	A	3.3
33	1b	11	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	2A	2109	U	3.3
31	29	20	HIS	3.3
26	24	49	PHE	3.3
34	2c	8	ILE	3.2
33	2b	93	VAL	3.2
8	1I	146	ALA	3.2
1	1A	2150	U	3.2
1	1A	2162	G	3.2
1	2A	2127	G	3.2
1	2A	2792	G	3.2
21	2Z	167	PRO	3.2
32	1a	1024	G	3.2
1	2A	2142	C	3.2
1	2A	2143	C	3.2
56	2z	3	HIS	3.2
41	1j	66	ARG	3.2
42	2k	25	TYR	3.2
42	2k	75	TYR	3.2
44	1m	121	LYS	3.2
5	2F	6	VAL	3.2
1	1A	2130	U	3.2
1	1A	2173	A	3.2
32	1a	1532	U	3.2
54	1w	20	U	3.2
57	2y	35	A	3.2
1	1A	2168	G	3.2
32	2a	1003	G	3.2
1	1A	2804	C	3.2
32	1a	1008	C	3.2
26	14	69	LYS	3.2
51	1t	74	LYS	3.2
21	2Z	171	ILE	3.2
6	1G	146	TYR	3.2
50	2s	45	VAL	3.2
25	13	2	PRO	3.2
1	1A	2167	U	3.2
1	2A	2130	U	3.2
57	1y	20	U	3.2
32	1a	1005	A	3.2
57	1y	36	A	3.2
1	2A	881	G	3.2
1	2A	2149	G	3.2

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Mol	Chain	Res	Type	RSRZ
32	1a	1032	G	3.2
54	2w	70	G	3.2
1	1A	1064	C	3.2
1	2A	2164	C	3.2
32	1a	1038	C	3.2
41	2j	36	GLY	3.2
57	2y	68	C	3.2
41	2j	71	LEU	3.2
20	2Y	55	TYR	3.2
21	2Z	149	SER	3.2
32	2a	1278	U	3.2
1	1A	2158	A	3.2
4	2E	29	GLY	3.1
33	1b	10	LEU	3.1
1	2A	888	C	3.1
1	2A	1536	C	3.1
1	2A	2133	G	3.1
32	2a	1027	C	3.1
41	2j	77	PRO	3.1
43	1l	64	TYR	3.1
26	24	57	GLU	3.1
5	1F	15	SER	3.1
6	1G	182	LYS	3.1
7	2H	175	LYS	3.1
21	2Z	103	ARG	3.1
41	2j	5	ARG	3.1
45	2n	35	ARG	3.1
20	1Y	1	MET	3.1
42	2k	49	GLY	3.1
1	2A	2114	A	3.1
7	2H	7	LEU	3.1
19	2X	95	LEU	3.1
41	2j	88	LEU	3.1
33	1b	230	VAL	3.1
33	1b	125	PRO	3.1
41	1j	77	PRO	3.1
1	1A	2207	G	3.1
1	2A	2110	G	3.1
57	2y	18	G	3.1
3	2D	275	LYS	3.1
33	2b	39	ILE	3.1
50	2s	13	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
32	1a	1030(D)	A	3.1
34	1c	207	VAL	3.1
45	2n	18	VAL	3.1
40	2i	114	TYR	3.1
50	2s	80	TYR	3.1
1	1A	2128	C	3.1
32	2a	1037	C	3.1
54	2w	2	C	3.1
1	2A	2751	G	3.1
40	2i	126	SER	3.1
57	2y	6	G	3.1
7	2H	174	GLY	3.1
35	2d	2	GLY	3.1
38	2g	81	GLY	3.1
32	2a	1257	U	3.1
32	2a	1532	U	3.1
6	2G	2	PRO	3.1
7	2H	26	VAL	3.1
38	1g	83	ALA	3.1
1	1A	1070	A	3.1
1	1A	1508	A	3.1
32	2a	1531	A	3.1
40	2i	9	ARG	3.1
50	2s	29	ARG	3.1
50	2s	4	SER	3.1
1	2A	2140	C	3.1
32	2a	1006	C	3.1
1	1A	1071	G	3.0
1	2A	11	G	3.0
32	1a	346	G	3.0
32	1a	1009	G	3.0
41	2j	63	PHE	3.0
45	1n	44	LEU	3.0
42	2k	48	ILE	3.0
33	1b	131	PRO	3.0
41	2j	37	PRO	3.0
15	2T	28	VAL	3.0
33	2b	34	ALA	3.0
40	2i	106	ALA	3.0
51	1t	97	ALA	3.0
41	2j	13	HIS	3.0
42	2k	126	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
36	2e	20	GLN	3.0
1	1A	2171	A	3.0
57	1y	21	A	3.0
45	2n	61	TRP	3.0
26	14	59	PHE	3.0
36	2e	45	PHE	3.0
1	1A	2792	G	3.0
1	2A	2155	G	3.0
26	24	50	VAL	3.0
34	2c	195	VAL	3.0
38	1g	9	VAL	3.0
57	2y	12	U	3.0
4	1E	204	ALA	3.0
40	2i	20	ARG	3.0
41	2j	42	THR	3.0
34	2c	201	TYR	3.0
12	2Q	104	PHE	3.0
33	2b	41	ILE	3.0
44	1m	4	ILE	3.0
1	2A	2129	C	3.0
21	2Z	158	PRO	3.0
32	1a	1037	C	3.0
32	2a	999	C	3.0
33	2b	22	LYS	3.0
21	2Z	74	VAL	3.0
4	2E	204	ALA	3.0
45	2n	5	ALA	3.0
54	1w	5	G	3.0
1	2A	1026	U	3.0
32	1a	204	U	3.0
39	2h	70	GLN	3.0
42	2k	13	GLN	3.0
26	24	67	TYR	3.0
40	1i	79	LEU	3.0
41	2j	8	LEU	3.0
48	1q	98	LEU	3.0
1	2A	2173	A	3.0
4	2E	115	GLY	3.0
6	2G	52	ILE	3.0
19	1X	94	GLY	3.0
35	1d	167	GLY	3.0
40	1i	18	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
45	2n	7	ILE	3.0
44	2m	120	LYS	3.0
26	24	51	ASP	3.0
50	1s	12	ASP	3.0
45	2n	57	ARG	3.0
1	1A	2108	C	3.0
1	1A	2146	C	3.0
1	2A	1509	C	3.0
54	1w	2	C	3.0
33	2b	207	ALA	3.0
38	1g	7	ALA	3.0
41	1j	32	ALA	3.0
41	2j	76	ASN	3.0
7	2H	33	LEU	2.9
26	24	32	TYR	2.9
50	2s	16	LEU	2.9
3	1D	275	LYS	2.9
34	1c	2	GLY	2.9
1	1A	548	A	2.9
1	1A	2134	A	2.9
57	2y	21	A	2.9
29	27	47	ARG	2.9
41	2j	61	GLU	2.9
20	2Y	107	ASP	2.9
21	1Z	105	VAL	2.9
33	2b	189	ASP	2.9
34	2c	95	THR	2.9
1	1A	895	U	2.9
1	1A	2189	U	2.9
1	2A	2118	U	2.9
1	1A	2133	G	2.9
1	2A	1171	G	2.9
1	2A	2166	G	2.9
32	2a	1026	G	2.9
40	2i	90	PRO	2.9
40	2i	17	VAL	2.9
46	2o	60	VAL	2.9
34	2c	189	ALA	2.9
54	1w	4	C	2.9
32	2a	1126	U	2.9
35	2d	5	ILE	2.9
7	1H	174	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
21	2Z	147	GLY	2.9
19	2X	68	ARG	2.9
1	1A	883	G	2.9
1	2A	2116	G	2.9
1	2A	2168	G	2.9
33	2b	134	GLU	2.9
57	2y	57	G	2.9
40	1i	13	ALA	2.9
49	2r	20	ALA	2.9
53	2v	14	A	2.9
40	2i	27	THR	2.9
41	2j	16	LEU	2.9
1	1A	2142	C	2.9
1	2A	2144	U	2.9
6	1G	51	ARG	2.9
7	2H	60	ARG	2.9
51	2t	101	GLY	2.9
26	14	49	PHE	2.9
20	2Y	5	MET	2.9
33	1b	9	GLU	2.9
33	1b	134	GLU	2.9
40	2i	2	GLU	2.9
9	2N	9	VAL	2.9
21	2Z	165	VAL	2.9
32	2a	1117	G	2.9
33	2b	123	ALA	2.9
45	2n	22	THR	2.9
1	1A	1067	A	2.8
33	2b	44	LEU	2.8
51	2t	10	LEU	2.8
8	2I	82	ARG	2.8
38	1g	4	ARG	2.8
50	2s	68	GLY	2.8
7	2H	123	PHE	2.8
25	23	2	PRO	2.8
41	2j	47	PHE	2.8
1	1A	2161	C	2.8
21	2Z	2	GLU	2.8
32	1a	1029	C	2.8
48	2q	99	SER	2.8
33	2b	31	TYR	2.8
38	1g	85	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
40	2i	65	VAL	2.8
33	2b	75	LYS	2.8
1	2A	652(E)	G	2.8
32	2a	1021	G	2.8
42	2k	117	ASN	2.8
33	2b	175	ARG	2.8
33	2b	201	ILE	2.8
41	2j	38	ILE	2.8
51	2t	100	ILE	2.8
50	1s	8	GLY	2.8
41	2j	35	SER	2.8
1	1A	2129	C	2.8
21	2Z	128	VAL	2.8
45	1n	56	VAL	2.8
4	2E	195	LEU	2.8
40	2i	10	ARG	2.8
1	1A	2802	G	2.8
1	2A	1170	G	2.8
1	2A	2131	G	2.8
1	2A	2157	G	2.8
26	14	54	GLY	2.8
44	1m	6	GLY	2.8
1	2A	2170	A	2.8
26	24	59	PHE	2.8
33	2b	122	PHE	2.8
45	2n	36	PHE	2.8
21	1Z	52	SER	2.8
1	2A	895	U	2.8
26	14	63	TYR	2.8
55	1x	47	U	2.8
33	1b	133	LYS	2.8
1	1A	2143	C	2.8
1	2A	645	C	2.8
21	2Z	173	ALA	2.8
32	1a	1030	C	2.8
33	2b	120	ALA	2.8
34	2c	188	LEU	2.8
50	2s	30	LEU	2.8
33	2b	97	TRP	2.8
35	1d	154	ASN	2.8
41	2j	6	ILE	2.8
51	1t	100	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
51	2t	41	ILE	2.8
40	1i	39	GLY	2.8
43	2l	63	GLY	2.8
1	2A	2141	G	2.8
1	1A	1088	A	2.8
47	2p	82	GLN	2.8
40	1i	4	TYR	2.8
7	2H	113	VAL	2.8
33	1b	7	VAL	2.8
35	1d	198	VAL	2.8
1	1A	2174	C	2.7
1	2A	2179	C	2.7
32	1a	1030(B)	C	2.7
32	2a	470	C	2.7
40	2i	128	ARG	2.7
6	2G	20	ILE	2.7
9	2N	44	PRO	2.7
50	2s	14	HIS	2.7
7	2H	14	GLY	2.7
12	2Q	15	GLY	2.7
46	1o	89	GLY	2.7
1	1A	2131	G	2.7
1	1A	2801(A)	A	2.7
1	2A	2100	G	2.7
32	2a	1280	A	2.7
1	2A	2167	U	2.7
33	1b	165	VAL	2.7
33	2b	71	VAL	2.7
54	2w	45	U	2.7
33	1b	34	ALA	2.7
41	2j	90	LEU	2.7
9	2N	1	MET	2.7
41	2j	87	THR	2.7
1	1A	2139	C	2.7
32	1a	163	C	2.7
32	1a	1007	C	2.7
32	2a	1007	C	2.7
57	2y	13	C	2.7
41	1j	33	GLN	2.7
7	2H	52	VAL	2.7
33	1b	15	VAL	2.7
1	2A	271(K)	U	2.7

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Mol	Chain	Res	Type	RSRZ
32	2a	1000	U	2.7
38	2g	32	ARG	2.7
57	1y	12	U	2.7
57	2y	33	U	2.7
1	1A	880	G	2.7
1	2A	1112	G	2.7
1	2A	2124	G	2.7
1	2A	2182	G	2.7
32	2a	1023	G	2.7
32	2a	1024	G	2.7
57	2y	5	G	2.7
7	2H	128	PRO	2.7
21	2Z	137	ILE	2.7
41	1j	4	ILE	2.7
35	1d	173	TRP	2.7
38	1g	82	GLY	2.7
1	1A	889	C	2.7
57	2y	49	C	2.7
57	2y	67	C	2.7
37	1f	60	PHE	2.7
40	2i	101	PHE	2.7
41	2j	44	VAL	2.7
12	1Q	32	TYR	2.7
14	2S	3	ARG	2.7
38	1g	154	TYR	2.7
45	2n	10	ALA	2.7
1	1A	1175	U	2.7
1	1A	2122	U	2.7
1	2A	9	U	2.7
1	2A	2150	U	2.7
57	1y	59	U	2.7
1	1A	1509(A)	A	2.7
1	2A	1509(A)	A	2.7
21	2Z	121	HIS	2.7
41	2j	62	HIS	2.7
11	2P	76	LYS	2.7
1	1A	1093	G	2.7
1	1A	2120	G	2.7
32	2a	1030(C)	G	2.7
54	2w	5	G	2.7
45	2n	8	GLU	2.7
51	2t	96	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
52	2u	16	GLY	2.7
21	2Z	104	PHE	2.7
33	2b	70	PHE	2.7
1	2A	894	C	2.7
21	2Z	141	VAL	2.6
41	2j	85	LEU	2.6
45	2n	25	VAL	2.6
36	1e	21	ALA	2.6
42	1k	25	TYR	2.6
8	2I	109	ILE	2.6
21	2Z	95	PRO	2.6
34	2c	57	ILE	2.6
1	1A	1084	A	2.6
26	14	64	GLY	2.6
1	1A	11	G	2.6
1	1A	2121	G	2.6
32	2a	485	G	2.6
11	2P	79	ARG	2.6
41	1j	46	ARG	2.6
52	2u	22	ARG	2.6
1	1A	886	C	2.6
1	2A	897	C	2.6
40	1i	126	SER	2.6
7	2H	11	VAL	2.6
38	2g	2	ALA	2.6
40	2i	94	ALA	2.6
44	2m	42	ALA	2.6
33	2b	19	HIS	2.6
45	2n	4	LYS	2.6
26	14	67	TYR	2.6
7	2H	12	PRO	2.6
35	1d	29	PRO	2.6
41	1j	87	THR	2.6
45	2n	14	PRO	2.6
11	1P	149	GLU	2.6
21	2Z	168	GLU	2.6
19	2X	94	GLY	2.6
1	1A	1073	A	2.6
1	2A	652(A)	A	2.6
34	2c	186	PHE	2.6
33	2b	21	ARG	2.6
36	2e	27	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	1A	10	G	2.6
1	1A	2805	G	2.6
41	1j	86	MET	2.6
21	2Z	125	LEU	2.6
57	1y	22	G	2.6
35	2d	112	VAL	2.6
44	2m	27	LYS	2.6
1	1A	1053	C	2.6
1	2A	2175	C	2.6
33	2b	113	HIS	2.6
56	1z	3	HIS	2.6
29	27	24	THR	2.6
3	1D	28	GLU	2.6
23	11	93	GLU	2.6
35	2d	156	GLU	2.6
9	2N	45	ASN	2.6
1	1A	1097	U	2.6
1	1A	2118	U	2.6
35	1d	87	GLY	2.6
50	1s	84	GLY	2.6
57	1y	47	U	2.6
14	1S	3	ARG	2.6
35	2d	73	ARG	2.6
40	2i	66	ARG	2.6
45	1n	57	ARG	2.6
52	1u	9	ARG	2.6
52	2u	6	ARG	2.6
1	1A	1046	A	2.6
32	1a	162	A	2.6
32	1a	344	A	2.6
48	1q	100	LYS	2.6
21	2Z	126	VAL	2.6
33	1b	40	HIS	2.6
1	1A	1056	G	2.6
1	1A	2152	G	2.6
32	1a	79	G	2.6
32	1a	1002	G	2.6
33	2b	29	ALA	2.6
34	2c	24	ALA	2.6
35	1d	195	ALA	2.6
54	2w	15	G	2.6
57	1y	24	G	2.6

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Mol	Chain	Res	Type	RSRZ
57	2y	1	G	2.6
1	1A	2794	C	2.6
26	14	57	GLU	2.6
26	24	52	THR	2.6
40	1i	103	THR	2.6
48	2q	96	GLU	2.6
32	1a	223	U	2.6
33	2b	105	PHE	2.6
34	1c	79	ARG	2.6
7	2H	64	LEU	2.5
17	2V	94	LEU	2.5
34	2c	87	LEU	2.5
40	1i	102	LEU	2.5
41	2j	7	LYS	2.5
45	2n	6	LEU	2.5
1	1A	278	A	2.5
1	1A	1077	A	2.5
33	2b	173	ALA	2.5
34	2c	200	ALA	2.5
49	2r	24	ALA	2.5
41	2j	39	PRO	2.5
26	24	31	ILE	2.5
33	1b	129	GLU	2.5
33	2b	222	ILE	2.5
34	2c	14	ILE	2.5
1	2A	2151	G	2.5
1	2A	2153	G	2.5
8	1I	40	THR	2.5
57	1y	53	G	2.5
57	2y	69	G	2.5
1	1A	34	C	2.5
23	21	28	GLY	2.5
54	1w	67	C	2.5
3	1D	38	LYS	2.5
32	1a	1000	U	2.5
40	2i	95	LYS	2.5
41	2j	99	LYS	2.5
50	2s	7	LYS	2.5
40	2i	79	LEU	2.5
50	2s	20	LEU	2.5
51	1t	13	LEU	2.5
52	2u	14	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
50	2s	19	VAL	2.5
41	2j	26	ALA	2.5
6	2G	17	PRO	2.5
8	2I	7	GLU	2.5
33	2b	80	ILE	2.5
44	2m	4	ILE	2.5
33	2b	168	THR	2.5
47	2p	45	THR	2.5
33	2b	166	ASP	2.5
33	1b	33	TYR	2.5
51	1t	102	GLY	2.5
20	1Y	92	ASN	2.5
1	1A	271(M)	G	2.5
1	1A	1062	G	2.5
1	2A	171	G	2.5
1	1A	1075	C	2.5
8	1I	131	LYS	2.5
33	1b	22	LYS	2.5
50	2s	10	PHE	2.5
32	2a	1119	C	2.5
19	2X	92	LEU	2.5
39	1h	112	LEU	2.5
1	1A	271(K)	U	2.5
1	1A	2897	U	2.5
1	2A	2897	U	2.5
7	2H	79	VAL	2.5
40	1i	14	VAL	2.5
43	1l	18	VAL	2.5
21	1Z	167	PRO	2.5
40	2i	49	PRO	2.5
8	1I	109	ILE	2.5
33	1b	39	ILE	2.5
34	2c	5	ILE	2.5
35	2d	192	GLU	2.5
44	2m	9	ILE	2.5
1	2A	2629	A	2.5
53	2v	15	A	2.5
48	1q	7	THR	2.5
40	2i	39	GLY	2.5
33	2b	147	LYS	2.5
33	2b	169	LYS	2.5
50	2s	32	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
40	1i	47	LEU	2.5
40	1i	99	LEU	2.5
49	2r	66	LEU	2.5
1	1A	271(I)	G	2.5
1	2A	2107	C	2.5
1	2A	2120	G	2.5
32	1a	1031	G	2.5
41	2j	68	HIS	2.5
57	1y	18	G	2.5
12	2Q	106	VAL	2.5
40	1i	106	ALA	2.5
40	2i	84	ALA	2.5
45	2n	30	ALA	2.5
6	2G	48	GLU	2.5
8	2I	64	GLU	2.5
16	2U	62	ILE	2.5
21	2Z	127	LYS	2.5
41	1j	100	THR	2.5
43	2l	126	LYS	2.5
48	2q	100	LYS	2.5
1	1A	887	A	2.5
1	1A	1177	A	2.5
21	2Z	70	LEU	2.4
41	2j	40	LEU	2.4
50	1s	16	LEU	2.4
1	1A	2149	G	2.4
32	2a	1020	U	2.4
33	1b	136	VAL	2.4
36	1e	69	VAL	2.4
40	1i	17	VAL	2.4
40	1i	108	VAL	2.4
43	2l	39	VAL	2.4
45	2n	33	VAL	2.4
57	1y	67	C	2.4
40	1i	21	PRO	2.4
55	1x	46	G	2.4
33	2b	170	GLU	2.4
47	2p	59	TRP	2.4
48	1q	97	SER	2.4
34	2c	79	ARG	2.4
46	1o	88	ARG	2.4
52	2u	17	THR	2.4

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Mol	Chain	Res	Type	RSRZ
8	2I	20	ASP	2.4
1	1A	890	A	2.4
8	2I	38	LEU	2.4
34	2c	34	LEU	2.4
33	2b	16	HIS	2.4
33	2b	40	HIS	2.4
33	1b	234	PRO	2.4
33	2b	232	PRO	2.4
1	2A	2189	U	2.4
33	1b	120	ALA	2.4
33	2b	12	GLU	2.4
40	1i	15	ALA	2.4
41	2j	64	GLU	2.4
51	1t	59	ALA	2.4
1	1A	1072	C	2.4
6	1G	52	ILE	2.4
3	2D	262	ARG	2.4
7	1H	6	ARG	2.4
9	2N	83	LYS	2.4
32	1a	221	C	2.4
32	2a	1019	C	2.4
33	2b	133	LYS	2.4
46	1o	3	ILE	2.4
35	2d	132	ARG	2.4
44	1m	102	ARG	2.4
52	2u	15	ARG	2.4
1	1A	2123	G	2.4
1	1A	2125	G	2.4
1	2A	1533	G	2.4
1	2A	2123	G	2.4
32	1a	181	G	2.4
32	1a	1030(C)	G	2.4
57	2y	44	G	2.4
34	2c	9	GLY	2.4
40	2i	8	GLY	2.4
42	2k	17	GLY	2.4
21	2Z	148	ASP	2.4
6	2G	3	LEU	2.4
21	1Z	150	LEU	2.4
38	1g	16	LEU	2.4
26	14	32	TYR	2.4
7	2H	36	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
21	2Z	162	GLU	2.4
33	2b	101	MET	2.4
40	2i	11	LYS	2.4
7	2H	6	ARG	2.4
41	2j	33	GLN	2.4
41	2j	70	ARG	2.4
51	1t	95	ALA	2.4
41	2j	98	ILE	2.4
42	1k	13	GLN	2.4
57	2y	59	U	2.4
1	1A	645	C	2.4
1	1A	1052	C	2.4
1	1A	1076	C	2.4
1	1A	2107	C	2.4
1	1A	2163	C	2.4
33	2b	38	GLY	2.4
34	2c	25	GLY	2.4
35	2d	124	GLY	2.4
36	1e	97	GLY	2.4
1	2A	10	G	2.4
1	2A	614(B)	G	2.4
1	2A	2319	G	2.4
14	2S	32	LEU	2.4
32	2a	1124	G	2.4
36	2e	5	ASP	2.4
37	1f	83	ASP	2.4
41	1j	88	LEU	2.4
42	1k	36	ASP	2.4
54	1w	69	G	2.4
57	1y	44	G	2.4
57	1y	57	G	2.4
6	2G	132	ASN	2.4
39	1h	62	TYR	2.4
1	1A	1460	A	2.4
7	1H	175	LYS	2.4
32	2a	1041	A	2.4
33	2b	83	MET	2.4
39	1h	98	LYS	2.4
40	1i	127	LYS	2.4
57	2y	23	A	2.4
44	2m	7	VAL	2.4
48	2q	77	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
12	1Q	6	ARG	2.4
15	1T	129	ARG	2.4
26	24	68	ARG	2.4
33	2b	129	GLU	2.4
7	2H	145	ALA	2.4
10	2O	69	ILE	2.4
34	2c	61	ALA	2.4
34	2c	149	ALA	2.4
41	2j	27	ALA	2.4
50	2s	31	ILE	2.4
7	2H	38	SER	2.4
7	2H	48	GLY	2.4
33	1b	97	TRP	2.4
47	1p	48	TRP	2.4
52	2u	2	GLY	2.4
1	1A	2896	C	2.3
22	20	3	HIS	2.3
54	2w	3	C	2.3
54	2w	13	C	2.3
57	1y	13	C	2.3
57	2y	48	C	2.3
35	1d	110	PHE	2.3
41	2j	54	PHE	2.3
1	1A	882	G	2.3
1	1A	1173	G	2.3
1	1A	2894	G	2.3
1	2A	880	G	2.3
32	2a	1010	G	2.3
34	1c	184	TYR	2.3
40	2i	92	TYR	2.3
52	1u	18	TYR	2.3
50	2s	18	LYS	2.3
50	2s	42	PRO	2.3
8	1I	41	GLU	2.3
12	2Q	6	ARG	2.3
20	2Y	45	VAL	2.3
33	2b	15	VAL	2.3
33	2b	112	VAL	2.3
34	1c	55	VAL	2.3
50	1s	11	VAL	2.3
1	1A	1045	A	2.3
1	2A	878	A	2.3

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Mol	Chain	Res	Type	RSRZ
2	2B	120	A	2.3
16	1U	117	GLN	2.3
20	2Y	44	ILE	2.3
32	2a	1251	A	2.3
32	2a	1503	A	2.3
33	2b	127	ILE	2.3
51	1t	63	ILE	2.3
1	1A	12	U	2.3
7	2H	120	GLY	2.3
36	2e	23	GLY	2.3
57	2y	45	U	2.3
17	2V	71	LEU	2.3
33	2b	140	HIS	2.3
37	2f	21	LEU	2.3
22	20	45	PHE	2.3
45	2n	37	PHE	2.3
51	1t	64	ASP	2.3
1	2A	2789	C	2.3
32	1a	1039	C	2.3
32	1a	1137	C	2.3
32	2a	1249	C	2.3
57	1y	48	C	2.3
57	2y	56	C	2.3
6	2G	118	ARG	2.3
7	2H	21	PRO	2.3
7	2H	29	PRO	2.3
40	2i	98	PRO	2.3
41	2j	66	ARG	2.3
7	2H	44	VAL	2.3
8	2I	136	VAL	2.3
20	2Y	49	VAL	2.3
21	2Z	139	VAL	2.3
25	13	60	GLU	2.3
32	2a	1253	G	2.3
34	2c	137	ALA	2.3
34	2c	152	ILE	2.3
41	2j	23	ILE	2.3
32	2a	1256	A	2.3
26	24	66	SER	2.3
33	1b	38	GLY	2.3
45	1n	60	SER	2.3
50	1s	26	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
50	2s	8	GLY	2.3
34	1c	87	LEU	2.3
45	2n	49	HIS	2.3
1	1A	271(L)	U	2.3
1	1A	1026	U	2.3
32	1a	1040	U	2.3
20	2Y	28	LYS	2.3
40	2i	118	LYS	2.3
44	1m	27	LYS	2.3
33	2b	48	MET	2.3
1	2A	2108	C	2.3
8	1I	113	ARG	2.3
40	1i	9	ARG	2.3
33	2b	148	TYR	2.3
7	2H	49	VAL	2.3
1	2A	892	G	2.3
57	2y	70	G	2.3
21	2Z	76	LEU	2.3
40	2i	67	GLY	2.3
40	2i	96	LEU	2.3
51	1t	24	LEU	2.3
1	1A	1174	A	2.3
1	2A	2171	A	2.3
32	2a	977	A	2.3
40	1i	7	THR	2.3
21	1Z	104	PHE	2.3
51	2t	74	LYS	2.3
34	1c	18	TRP	2.3
57	2y	47	U	2.3
21	2Z	140	ASP	2.3
39	2h	4	ASP	2.3
41	2j	73	ASP	2.3
41	2j	86	MET	2.3
15	1T	115	ARG	2.3
33	2b	36	ARG	2.3
7	2H	10	PRO	2.3
8	2I	134	PRO	2.3
39	2h	72	PRO	2.3
1	2A	2183	C	2.3
7	2H	72	ILE	2.3
8	2I	145	VAL	2.3
21	2Z	161	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
31	29	16	VAL	2.3
32	1a	1006	C	2.3
32	1a	1019	C	2.3
33	2b	200	ILE	2.3
41	2j	72	VAL	2.3
43	1l	55	VAL	2.3
57	1y	75	C	2.3
12	2Q	117	ALA	2.3
36	1e	95	ALA	2.3
44	1m	5	ALA	2.3
11	1P	44	GLY	2.2
27	25	58	LEU	2.2
33	2b	138	LEU	2.2
34	2c	178	LEU	2.2
39	2h	2	LEU	2.2
41	1j	62	HIS	2.2
45	2n	47	LEU	2.2
45	2n	51	GLY	2.2
50	1s	71	LEU	2.2
1	1A	1091	G	2.2
1	1A	2148	G	2.2
1	1A	2156	G	2.2
1	2A	100	G	2.2
7	2H	13	LYS	2.2
45	2n	16	PHE	2.2
1	2A	528	A	2.2
19	1X	68	ARG	2.2
24	22	51	ARG	2.2
38	1g	78	ARG	2.2
35	2d	154	ASN	2.2
57	1y	45	U	2.2
57	2y	66	U	2.2
15	2T	128	GLU	2.2
21	2Z	145	GLU	2.2
34	2c	28	GLN	2.2
8	1I	107	VAL	2.2
34	2c	23	TYR	2.2
34	2c	99	VAL	2.2
34	2c	124	ILE	2.2
34	2c	193	TYR	2.2
40	2i	53	VAL	2.2
40	2i	62	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
44	2m	21	TYR	2.2
48	2q	23	VAL	2.2
1	1A	1080	C	2.2
1	1A	2177	C	2.2
33	1b	140	HIS	2.2
33	1b	145	LEU	2.2
33	2b	187	LEU	2.2
51	1t	62	LEU	2.2
21	2Z	156	LYS	2.2
33	2b	55	PHE	2.2
40	1i	101	PHE	2.2
7	1H	3	ARG	2.2
11	2P	77	ARG	2.2
41	1j	29	ARG	2.2
47	1p	81	ARG	2.2
1	1A	1089	G	2.2
1	1A	2100	G	2.2
1	1A	2106	G	2.2
1	1A	2157	G	2.2
1	2A	1114	G	2.2
1	2A	2807	G	2.2
6	2G	49	ASP	2.2
32	2a	998	G	2.2
20	2Y	66	PRO	2.2
1	1A	2132	U	2.2
1	2A	2176	A	2.2
46	1o	19	PRO	2.2
1	2A	2895	U	2.2
54	2w	14	A	2.2
51	1t	60	GLU	2.2
24	22	70	GLN	2.2
38	2g	9	VAL	2.2
40	2i	81	ILE	2.2
48	2q	9	VAL	2.2
40	2i	125	TYR	2.2
51	2t	68	LYS	2.2
50	2s	26	GLY	2.2
24	22	1	MET	2.2
32	2a	995	C	2.2
32	2a	1029	C	2.2
35	1d	137	SER	2.2
48	1q	99	SER	2.2

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Mol	Chain	Res	Type	RSRZ
7	2H	39	PRO	2.2
20	2Y	53	PRO	2.2
34	2c	19	GLU	2.2
38	1g	8	GLU	2.2
44	1m	106	ASN	2.2
1	1A	2127	G	2.2
1	2A	157	U	2.2
1	2A	1113	U	2.2
32	1a	1446	U	2.2
54	1w	47	U	2.2
8	1I	19	VAL	2.2
8	2I	79	ILE	2.2
16	2U	88	ILE	2.2
29	17	46	VAL	2.2
41	2j	94	VAL	2.2
51	2t	63	ILE	2.2
8	1I	45	LYS	2.2
33	2b	161	ALA	2.2
35	1d	138	TYR	2.2
45	2n	20	ALA	2.2
51	2t	94	ALA	2.2
6	2G	53	LEU	2.2
33	2b	10	LEU	2.2
10	2O	112	MET	2.2
3	2D	263	ARG	2.2
6	2G	51	ARG	2.2
8	2I	86	THR	2.2
15	2T	108	ARG	2.2
15	2T	115	ARG	2.2
21	2Z	79	ARG	2.2
25	23	29	ARG	2.2
36	2e	25	ARG	2.2
41	1j	79	ARG	2.2
47	2p	28	ARG	2.2
21	1Z	166	SER	2.2
51	1t	11	SER	2.2
1	1A	271(J)	C	2.2
1	2A	893	C	2.2
32	2a	1277	C	2.2
6	1G	26	GLN	2.2
6	1G	137	GLU	2.2
16	2U	117	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	1A	1083	U	2.2
1	2A	2122	U	2.2
1	2A	2808	U	2.2
26	14	50	VAL	2.2
31	29	3	VAL	2.2
31	29	25	VAL	2.2
32	2a	1219	U	2.2
33	2b	42	ILE	2.2
34	2c	77	ILE	2.2
41	1j	75	ILE	2.2
33	2b	164	VAL	2.2
1	1A	545	G	2.2
1	1A	2893	G	2.2
1	2A	229	A	2.2
4	2E	28	ALA	2.2
32	1a	160	A	2.2
32	2a	1009	G	2.2
32	2a	1123	A	2.2
32	2a	1224	G	2.2
32	2a	1287	A	2.2
34	2c	60	ALA	2.2
36	1e	48	ALA	2.2
40	1i	76	ALA	2.2
57	1y	7	A	2.2
57	2y	22	G	2.2
57	2y	71	G	2.2
5	2F	20	LEU	2.1
14	1S	48	LEU	2.1
35	2d	157	LEU	2.1
44	2m	70	LEU	2.1
47	1p	38	TYR	2.1
21	2Z	106	GLY	2.1
5	1F	17	ARG	2.1
29	17	41	ARG	2.1
35	2d	47	ARG	2.1
38	2g	79	ARG	2.1
52	2u	9	ARG	2.1
33	2b	192	SER	2.1
34	2c	20	SER	2.1
40	2i	37	PHE	2.1
20	2Y	82	PRO	2.1
32	2a	1223	C	2.1

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Mol	Chain	Res	Type	RSRZ
57	1y	49	C	2.1
57	1y	68	C	2.1
57	2y	75	C	2.1
18	2W	60	ASN	2.1
34	1c	14	ILE	2.1
41	1j	55	LYS	2.1
7	2H	50	VAL	2.1
7	2H	125	VAL	2.1
15	2T	30	VAL	2.1
34	2c	198	VAL	2.1
32	1a	182	U	2.1
32	2a	1148	U	2.1
33	1b	186	ALA	2.1
33	2b	118	LEU	2.1
40	2i	15	ALA	2.1
50	1s	5	LEU	2.1
1	1A	878	A	2.1
1	2A	1508	A	2.1
7	2H	157	TYR	2.1
32	1a	197	A	2.1
32	2a	969	A	2.1
32	2a	1248	A	2.1
34	2c	29	TYR	2.1
21	2Z	122	ARG	2.1
38	2g	55	GLY	2.1
1	1A	2154	G	2.1
1	2A	2181	G	2.1
1	2A	2894	G	2.1
32	2a	1022	G	2.1
32	2a	1120	G	2.1
34	2c	15	THR	2.1
40	2i	18	PHE	2.1
6	2G	54	GLU	2.1
8	1I	117	GLU	2.1
26	24	30	GLU	2.1
33	1b	126	GLU	2.1
6	1G	147	ASP	2.1
36	1e	117	ASP	2.1
45	2n	17	LYS	2.1
49	2r	84	LYS	2.1
50	2s	53	ASN	2.1
32	1a	345	C	2.1

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Mol	Chain	Res	Type	RSRZ
33	2b	172	ILE	2.1
33	2b	185	ILE	2.1
54	2w	67	C	2.1
5	1F	6	VAL	2.1
12	2Q	52	VAL	2.1
34	2c	70	VAL	2.1
8	2I	55	ALA	2.1
17	2V	20	LEU	2.1
33	1b	29	ALA	2.1
33	2b	154	LEU	2.1
33	2b	171	ALA	2.1
36	1e	138	ALA	2.1
40	1i	50	LEU	2.1
50	2s	24	ALA	2.1
26	24	55	ARG	2.1
29	27	23	ARG	2.1
32	1a	1020	U	2.1
32	2a	1025	U	2.1
32	2a	1125	U	2.1
33	1b	130	ARG	2.1
45	2n	31	ARG	2.1
51	1t	8	ARG	2.1
8	2I	34	GLY	2.1
45	2n	55	GLY	2.1
40	2i	88	TYR	2.1
44	2m	23	TYR	2.1
44	2m	87	TYR	2.1
1	2A	1847	A	2.1
8	2I	108	THR	2.1
50	2s	79	THR	2.1
46	2o	19	PRO	2.1
1	2A	879	G	2.1
32	2a	1011	G	2.1
32	2a	1042	G	2.1
32	2a	1131	G	2.1
7	2H	58	GLU	2.1
17	2V	56	SER	2.1
54	1w	15	G	2.1
11	2P	38	GLN	2.1
21	1Z	2	GLU	2.1
33	2b	143	GLU	2.1
40	2i	3	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
14	2S	11	LYS	2.1
35	1d	86	LYS	2.1
8	1I	38	LEU	2.1
8	2I	107	VAL	2.1
9	1N	9	VAL	2.1
34	1c	47	LEU	2.1
34	2c	52	LEU	2.1
40	2i	86	VAL	2.1
42	1k	14	VAL	2.1
43	2l	84	LEU	2.1
1	2A	889	C	2.1
1	2A	898	C	2.1
7	2H	20	ALA	2.1
32	1a	479	C	2.1
32	2a	1116	C	2.1
7	2H	51	ARG	2.1
7	2H	96	ALA	2.1
15	2T	111	ARG	2.1
21	2Z	51	ALA	2.1
34	2c	92	ALA	2.1
38	1g	2	ALA	2.1
40	2i	119	ALA	2.1
42	2k	89	ALA	2.1
55	1x	69	C	2.1
21	2Z	81	ARG	2.1
43	2l	97	ARG	2.1
46	2o	88	ARG	2.1
48	2q	75	ARG	2.1
7	2H	135	GLY	2.1
12	2Q	33	GLY	2.1
21	2Z	160	GLY	2.1
32	1a	65	U	2.1
32	1a	90	U	2.1
38	1g	26	PHE	2.1
41	2j	41	PRO	2.1
50	2s	48	THR	2.1
14	2S	83	LYS	2.1
32	1a	143	A	2.1
33	2b	135	GLN	2.1
37	1f	27	GLN	2.1
44	2m	65	LYS	2.1
54	1w	7	A	2.1

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Mol	Chain	Res	Type	RSRZ
57	1y	58	A	2.1
1	1A	1099	G	2.1
1	1A	2182	G	2.1
32	2a	630	G	2.1
32	2a	993	G	2.1
39	1h	80	ILE	2.1
40	2i	58	HIS	2.1
57	2y	65	G	2.1
12	2Q	1	MET	2.1
14	2S	61	ASN	2.1
21	1Z	120	ILE	2.1
40	2i	63	ILE	2.1
41	1j	76	ASN	2.1
42	2k	36	ASP	2.1
50	1s	40	ILE	2.1
8	2I	75	LEU	2.0
39	2h	53	VAL	2.0
40	2i	109	VAL	2.0
41	1j	85	LEU	2.0
6	2G	21	ARG	2.0
44	1m	3	ARG	2.0
44	2m	11	ARG	2.0
10	2O	11	ALA	2.0
33	1b	13	ALA	2.0
40	2i	43	ALA	2.0
45	2n	59	ALA	2.0
49	2r	60	ALA	2.0
26	24	19	GLY	2.0
32	1a	848	C	2.0
41	2j	93	GLY	2.0
54	1w	3	C	2.0
57	1y	43	C	2.0
57	2y	4	C	2.0
57	2y	43	C	2.0
21	2Z	99	TYR	2.0
26	24	25	TYR	2.0
34	2c	48	TYR	2.0
48	2q	95	TYR	2.0
47	1p	80	PHE	2.0
12	2Q	141	GLN	2.0
20	1Y	91	GLU	2.0
23	21	83	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
33	2b	35	GLU	2.0
40	1i	12	GLU	2.0
40	1i	35	GLU	2.0
21	1Z	149	SER	2.0
1	1A	229	A	2.0
1	2A	655	A	2.0
1	2A	901	A	2.0
1	2A	2892	A	2.0
32	2a	1447	A	2.0
33	2b	208	ILE	2.0
33	2b	211	ILE	2.0
34	2c	202	ILE	2.0
35	1d	70	ILE	2.0
39	2h	100	ILE	2.0
44	2m	106	ASN	2.0
6	2G	133	LEU	2.0
21	2Z	150	LEU	2.0
35	2d	155	LEU	2.0
38	1g	12	LEU	2.0
39	1h	2	LEU	2.0
5	2F	183	VAL	2.0
8	1I	142	VAL	2.0
14	2S	14	VAL	2.0
21	1Z	139	VAL	2.0
43	2l	19	ARG	2.0
44	2m	53	VAL	2.0
47	1p	21	VAL	2.0
52	1u	15	ARG	2.0
1	1A	275	G	2.0
1	1A	881	G	2.0
1	1A	1055	G	2.0
1	1A	1537	G	2.0
1	2A	271(M)	G	2.0
32	1a	306	G	2.0
54	1w	44	G	2.0
57	1y	69	G	2.0
5	2F	21	ALA	2.0
42	1k	15	ALA	2.0
51	2t	47	GLY	2.0
44	2m	64	TRP	2.0
34	1c	135	LYS	2.0
38	2g	35	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	2A	271(J)	C	2.0
1	2A	614(A)	U	2.0
1	2A	2132	U	2.0
32	2a	1008	C	2.0
32	2a	1363	C	2.0
33	2b	125	PRO	2.0
54	2w	4	C	2.0
55	1x	68	C	2.0
57	1y	25	C	2.0
9	2N	75	TYR	2.0
33	1b	190	THR	2.0
33	1b	231	GLU	2.0
33	2b	86	GLU	2.0
33	2b	199	TYR	2.0
34	1c	23	TYR	2.0
34	2c	184	TYR	2.0
34	2c	192	THR	2.0
40	1i	59	PHE	2.0
41	2j	48	THR	2.0
42	1k	75	TYR	2.0
42	2k	125	PHE	2.0
47	1p	22	THR	2.0
47	1p	16	HIS	2.0
33	2b	162	ILE	2.0
34	2c	39	ILE	2.0
41	1j	74	ILE	2.0
15	2T	103	ARG	2.0
36	2e	18	ARG	2.0
38	2g	115	ARG	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
57	4SU	2y	8	20/21	0.33	0.19	97,104,109,125	0
57	PSU	1y	55	20/21	0.47	0.18	98,101,103,116	0
57	5MU	2y	54	21/22	0.48	0.18	96,100,108,126	0
57	G7M	2y	46	24/25	0.50	0.16	91,99,107,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	G7M	1y	46	24/25	0.51	0.18	95,99,103,112	0
57	MIA	2y	37	22/30	0.51	0.18	89,98,112,126	0
57	4SU	1y	8	20/21	0.56	0.16	98,100,110,115	0
57	PSU	2y	55	20/21	0.59	0.15	94,99,102,107	0
57	5MU	1y	54	21/22	0.60	0.17	93,97,101,116	0
57	MIA	1y	37	22/30	0.62	0.19	89,96,105,116	0
57	PSU	1y	39	20/21	0.66	0.15	88,94,106,106	0
57	PSU	2y	39	20/21	0.69	0.14	91,97,105,115	0
57	PSU	2y	32	20/21	0.71	0.14	93,97,103,116	0
54	G7M	2w	46	24/25	0.71	0.15	88,96,107,121	0
57	PSU	1y	32	20/21	0.73	0.16	90,93,105,108	0
54	G7M	1w	46	24/25	0.73	0.14	79,86,100,116	0
54	4SU	2w	8	20/21	0.82	0.12	91,94,108,111	0
54	PSU	2w	55	20/21	0.83	0.11	84,86,95,101	0
56	FME	1z	1	10/11	0.85	0.22	61,66,74,77	0
54	4SU	1w	8	20/21	0.86	0.14	82,88,93,97	0
54	PSU	1w	55	20/21	0.86	0.12	60,73,84,85	0
56	FME	2z	1	10/11	0.86	0.28	70,75,82,82	0
54	5MU	2w	54	21/22	0.88	0.11	75,83,86,92	0
55	PSU	1x	55	20/21	0.88	0.10	63,68,82,85	0
55	PSU	2x	55	20/21	0.88	0.11	74,79,86,88	0
54	MIA	2w	37	25/30	0.89	0.14	63,75,83,105	0
55	4SU	2x	8	20/21	0.89	0.13	79,82,85,87	0
32	2MG	2a	1207	24/25	0.89	0.12	74,84,86,88	0
54	MIA	1w	37	29/30	0.89	0.18	56,63,77,92	0
55	5MU	2x	54	21/22	0.90	0.13	76,81,85,88	0
55	5MU	1x	54	21/22	0.91	0.11	66,70,75,81	0
54	PSU	2w	32	20/21	0.91	0.12	75,82,86,89	0
1	5MU	2A	1915	21/22	0.92	0.10	62,66,70,73	0
32	PSU	2a	516	20/21	0.93	0.10	60,73,77,78	0
32	G7M	2a	527	24/25	0.93	0.12	61,68,71,74	0
54	PSU	1w	32	20/21	0.93	0.11	59,65,74,75	0
32	2MG	1a	1207	24/25	0.93	0.10	70,73,77,80	0
1	PSU	2A	1917	20/21	0.93	0.10	57,64,71,75	0
55	5MC	1x	32	21/22	0.93	0.13	56,60,66,68	0
55	5MC	2x	32	21/22	0.93	0.12	68,72,76,77	0
55	4SU	1x	8	20/21	0.94	0.10	62,68,70,71	0
54	PSU	2w	39	20/21	0.94	0.11	68,79,86,89	0
32	M2G	2a	966	25/26	0.94	0.13	61,67,76,80	0
32	5MC	2a	967	21/22	0.94	0.12	62,69,75,82	0
43	0TD	1l	92	10/11	0.94	0.11	51,56,58,71	0
32	5MC	2a	1400	21/22	0.94	0.13	64,69,76,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	4OC	2a	1402	22/23	0.94	0.11	56,61,64,68	0
43	0TD	2l	92	10/11	0.94	0.10	64,67,70,75	0
1	5MC	2A	1962	21/22	0.94	0.10	43,52,60,68	0
54	5MU	1w	54	21/22	0.94	0.09	52,63,67,69	0
32	G7M	1a	527	24/25	0.94	0.10	49,56,61,63	0
32	5MC	1a	967	21/22	0.95	0.10	49,56,62,63	0
32	PSU	1a	516	20/21	0.95	0.07	55,61,66,67	0
1	PSU	1A	1917	20/21	0.95	0.08	52,56,60,61	0
32	M2G	1a	966	25/26	0.95	0.11	51,55,63,66	0
1	OMC	2A	1920	21/22	0.95	0.09	49,60,64,67	0
32	5MC	2a	1404	21/22	0.95	0.10	47,55,59,63	0
32	UR3	2a	1498	21/22	0.95	0.11	53,58,62,63	0
32	MA6	2a	1518	24/25	0.95	0.10	53,63,69,70	0
32	MA6	2a	1519	24/25	0.96	0.11	55,62,65,66	0
1	5MU	1A	1915	21/22	0.96	0.09	47,56,60,61	0
55	8AN	2x	76	22/23	0.96	0.09	41,48,54,61	0
54	PSU	1w	39	20/21	0.96	0.09	61,66,76,78	0
32	5MC	1a	1407	21/22	0.96	0.09	42,46,49,52	0
54	F3N	2w	76	33/34	0.96	0.10	41,47,51,52	0
1	5MC	1A	1942	21/22	0.96	0.09	35,45,49,56	0
1	5MC	2A	1942	21/22	0.96	0.09	53,59,65,71	0
32	5MC	2a	1407	21/22	0.96	0.08	51,57,65,68	0
1	2MU	2A	2552	21/23	0.96	0.09	39,50,54,57	0
55	8AN	1x	76	22/23	0.96	0.08	22,30,37,48	0
32	MA6	1a	1519	24/25	0.96	0.09	40,46,53,56	0
32	4OC	1a	1402	22/23	0.97	0.09	44,50,52,53	0
32	5MC	1a	1400	21/22	0.97	0.10	49,56,59,63	0
32	MA6	1a	1518	24/25	0.97	0.08	39,45,49,51	0
1	PSU	1A	1911	20/21	0.97	0.06	43,51,58,58	0
1	PSU	2A	2605	20/21	0.97	0.08	36,43,50,52	0
1	PSU	2A	1911	20/21	0.97	0.08	53,58,63,63	0
1	5MU	2A	1939	21/22	0.97	0.07	35,43,49,51	0
32	5MC	1a	1404	21/22	0.98	0.07	38,45,49,50	0
1	OMG	2A	2251	24/25	0.98	0.07	39,46,49,58	0
1	8AH	2A	2503	24/25	0.98	0.09	39,44,48,52	0
1	2MU	1A	2552	21/23	0.98	0.06	25,32,35,37	0
1	5MU	1A	1939	21/22	0.98	0.07	25,33,37,39	0
1	PSU	1A	2605	20/21	0.98	0.06	27,32,34,35	0
32	UR3	1a	1498	21/22	0.98	0.07	39,45,50,52	0
54	F3N	1w	76	33/34	0.98	0.07	24,29,34,36	0
1	OMC	1A	1920	21/22	0.98	0.06	39,49,52,55	0
1	5MC	1A	1962	21/22	0.99	0.05	31,40,43,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	8AH	1A	2503	24/25	0.99	0.06	21,29,33,37	0
1	OMG	1A	2251	24/25	0.99	0.06	25,29,31,33	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3395	1/1	0.36	0.25	88,88,88,88	0
58	MG	1A	4028	1/1	0.48	0.25	83,83,83,83	0
58	MG	2a	1798	1/1	0.49	0.29	92,92,92,92	0
58	MG	2v	102	1/1	0.52	0.38	87,87,87,87	0
58	MG	1a	1729	1/1	0.59	0.23	78,78,78,78	0
58	MG	2A	3277	1/1	0.60	0.20	77,77,77,77	0
58	MG	1x	109	1/1	0.60	0.19	95,95,95,95	0
58	MG	2A	3561	1/1	0.61	0.26	79,79,79,79	0
58	MG	2A	3259	1/1	0.61	0.32	82,82,82,82	0
58	MG	2A	3265	1/1	0.61	0.41	85,85,85,85	0
58	MG	1A	3748	1/1	0.62	0.22	71,71,71,71	0
58	MG	1B	222	1/1	0.62	0.30	84,84,84,84	0
58	MG	1W	206	1/1	0.62	0.35	56,56,56,56	0
58	MG	2a	1771	1/1	0.63	0.26	77,77,77,77	0
58	MG	2a	1665	1/1	0.64	0.25	86,86,86,86	0
58	MG	1A	3487	1/1	0.65	0.22	70,70,70,70	0
58	MG	1A	3761	1/1	0.66	0.35	79,79,79,79	0
58	MG	2A	3512	1/1	0.67	0.22	71,71,71,71	0
58	MG	2a	1610	1/1	0.67	0.28	84,84,84,84	0
58	MG	1a	1666	1/1	0.68	0.28	77,77,77,77	0
58	MG	1A	3746	1/1	0.68	0.20	74,74,74,74	0
58	MG	1A	3899	1/1	0.69	0.29	81,81,81,81	0
58	MG	1A	3782	1/1	0.69	0.23	78,78,78,78	0
58	MG	1A	3829	1/1	0.69	0.23	40,40,40,40	0
58	MG	2A	3628	1/1	0.70	0.27	84,84,84,84	0
58	MG	2A	3706	1/1	0.70	0.20	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3946	1/1	0.70	0.12	86,86,86,86	0
58	MG	1a	1724	1/1	0.70	0.24	81,81,81,81	0
58	MG	1A	3656	1/1	0.70	0.23	59,59,59,59	0
58	MG	1A	3670	1/1	0.70	0.24	71,71,71,71	0
58	MG	2l	202	1/1	0.70	0.28	74,74,74,74	0
58	MG	1A	3926	1/1	0.70	0.20	73,73,73,73	0
58	MG	2U	202	1/1	0.71	0.12	83,83,83,83	0
58	MG	2W	201	1/1	0.71	0.25	74,74,74,74	0
58	MG	1A	3663	1/1	0.71	0.32	67,67,67,67	0
58	MG	2A	3606	1/1	0.71	0.24	80,80,80,80	0
58	MG	2a	1691	1/1	0.71	0.32	82,82,82,82	0
58	MG	1A	3947	1/1	0.71	0.16	85,85,85,85	0
58	MG	2a	1782	1/1	0.71	0.26	82,82,82,82	0
58	MG	2A	3649	1/1	0.71	0.23	72,72,72,72	0
58	MG	1A	4009	1/1	0.71	0.18	60,60,60,60	0
58	MG	2B	210	1/1	0.71	0.27	83,83,83,83	0
58	MG	1a	1795	1/1	0.72	0.16	88,88,88,88	0
58	MG	1A	3847	1/1	0.72	0.22	62,62,62,62	0
58	MG	1A	4036	1/1	0.72	0.16	58,58,58,58	0
58	MG	2A	3261	1/1	0.72	0.33	76,76,76,76	0
58	MG	1A	4027	1/1	0.72	0.22	80,80,80,80	0
58	MG	1O	206	1/1	0.72	0.32	76,76,76,76	0
58	MG	2A	3659	1/1	0.73	0.20	53,53,53,53	0
58	MG	1A	3956	1/1	0.73	0.17	59,59,59,59	0
58	MG	2A	3366	1/1	0.73	0.14	73,73,73,73	0
58	MG	2E	302	1/1	0.73	0.14	71,71,71,71	0
58	MG	2A	3392	1/1	0.73	0.22	74,74,74,74	0
58	MG	1w	101	1/1	0.73	0.31	82,82,82,82	0
58	MG	2A	3407	1/1	0.73	0.21	73,73,73,73	0
58	MG	1A	3260	1/1	0.73	0.42	72,72,72,72	0
58	MG	2A	3248	1/1	0.73	0.31	79,79,79,79	0
58	MG	2A	3595	1/1	0.73	0.27	54,54,54,54	0
58	MG	2A	3605	1/1	0.73	0.17	87,87,87,87	0
58	MG	1A	4092	1/1	0.73	0.26	81,81,81,81	0
58	MG	1A	3327	1/1	0.73	0.37	77,77,77,77	0
58	MG	1E	310	1/1	0.73	0.22	72,72,72,72	0
58	MG	1A	3736	1/1	0.74	0.32	91,91,91,91	0
58	MG	2A	3274	1/1	0.74	0.27	81,81,81,81	0
58	MG	2A	3604	1/1	0.74	0.17	83,83,83,83	0
58	MG	1A	3532	1/1	0.74	0.27	58,58,58,58	0
58	MG	2A	3284	1/1	0.74	0.24	68,68,68,68	0
58	MG	1A	3155	1/1	0.74	0.39	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3044	1/1	0.74	0.37	79,79,79,79	0
58	MG	1A	3969	1/1	0.74	0.14	53,53,53,53	0
58	MG	1A	3975	1/1	0.74	0.30	73,73,73,73	0
58	MG	2A	3800	1/1	0.74	0.17	70,70,70,70	0
58	MG	1A	3979	1/1	0.74	0.16	68,68,68,68	0
58	MG	1A	3783	1/1	0.75	0.20	71,71,71,71	0
58	MG	1A	3972	1/1	0.75	0.16	63,63,63,63	0
58	MG	2a	1721	1/1	0.75	0.43	80,80,80,80	0
58	MG	2a	1756	1/1	0.75	0.22	64,64,64,64	0
58	MG	1A	3685	1/1	0.75	0.13	66,66,66,66	0
58	MG	2A	3634	1/1	0.75	0.19	82,82,82,82	0
58	MG	1S	203	1/1	0.75	0.12	77,77,77,77	0
58	MG	2j	201	1/1	0.75	0.19	83,83,83,83	0
58	MG	2A	3080	1/1	0.75	0.27	90,90,90,90	0
58	MG	2A	3665	1/1	0.75	0.19	76,76,76,76	0
58	MG	2A	3171	1/1	0.76	0.20	78,78,78,78	0
58	MG	2A	3178	1/1	0.76	0.28	78,78,78,78	0
58	MG	2A	3222	1/1	0.76	0.29	85,85,85,85	0
58	MG	1A	3658	1/1	0.76	0.26	69,69,69,69	0
58	MG	2A	3573	1/1	0.76	0.24	85,85,85,85	0
58	MG	1A	3539	1/1	0.76	0.13	80,80,80,80	0
58	MG	1a	1809	1/1	0.76	0.13	82,82,82,82	0
58	MG	14	101	1/1	0.76	0.26	87,87,87,87	0
58	MG	1a	1634	1/1	0.76	0.29	81,81,81,81	0
58	MG	1A	3853	1/1	0.76	0.15	57,57,57,57	0
58	MG	2a	1764	1/1	0.76	0.27	78,78,78,78	0
58	MG	1A	3986	1/1	0.76	0.20	45,45,45,45	0
58	MG	2A	3289	1/1	0.76	0.14	85,85,85,85	0
58	MG	2A	3325	1/1	0.76	0.12	85,85,85,85	0
58	MG	2A	3086	1/1	0.76	0.23	82,82,82,82	0
58	MG	2A	3089	1/1	0.76	0.28	85,85,85,85	0
58	MG	2A	3770	1/1	0.76	0.23	96,96,96,96	0
58	MG	2A	3635	1/1	0.77	0.18	67,67,67,67	0
58	MG	2A	3826	1/1	0.77	0.12	75,75,75,75	0
58	MG	2A	3636	1/1	0.77	0.23	80,80,80,80	0
58	MG	2a	1768	1/1	0.77	0.26	75,75,75,75	0
58	MG	2A	3308	1/1	0.77	0.39	79,79,79,79	0
58	MG	1A	3483	1/1	0.77	0.24	59,59,59,59	0
58	MG	1A	3200	1/1	0.77	0.11	71,71,71,71	0
58	MG	2a	1804	1/1	0.77	0.19	79,79,79,79	0
58	MG	2A	3697	1/1	0.77	0.14	75,75,75,75	0
58	MG	1A	3940	1/1	0.77	0.14	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3307	1/1	0.77	0.36	80,80,80,80	0
58	MG	1a	1730	1/1	0.78	0.24	78,78,78,78	0
58	MG	2A	3815	1/1	0.78	0.17	77,77,77,77	0
58	MG	2A	3504	1/1	0.78	0.25	77,77,77,77	0
58	MG	2A	3230	1/1	0.78	0.33	76,76,76,76	0
58	MG	2A	3246	1/1	0.78	0.16	63,63,63,63	0
58	MG	1A	4084	1/1	0.78	0.17	69,69,69,69	0
58	MG	10	109	1/1	0.78	0.28	72,72,72,72	0
58	MG	1l	201	1/1	0.78	0.12	81,81,81,81	0
58	MG	1A	3993	1/1	0.78	0.14	80,80,80,80	0
58	MG	1w	103	1/1	0.78	0.29	87,87,87,87	0
58	MG	2a	1714	1/1	0.78	0.31	69,69,69,69	0
58	MG	2a	1719	1/1	0.78	0.37	82,82,82,82	0
58	MG	1A	3024	1/1	0.78	0.26	64,64,64,64	0
58	MG	2a	1725	1/1	0.78	0.23	82,82,82,82	0
58	MG	1a	1657	1/1	0.78	0.27	83,83,83,83	0
58	MG	1A	3788	1/1	0.78	0.19	77,77,77,77	0
58	MG	1a	1690	1/1	0.78	0.28	79,79,79,79	0
58	MG	1a	1706	1/1	0.78	0.30	79,79,79,79	0
58	MG	2a	1775	1/1	0.78	0.26	67,67,67,67	0
58	MG	2A	3115	1/1	0.78	0.22	71,71,71,71	0
58	MG	1A	3964	1/1	0.78	0.10	72,72,72,72	0
58	MG	2A	3691	1/1	0.78	0.15	84,84,84,84	0
58	MG	2A	3378	1/1	0.78	0.20	78,78,78,78	0
58	MG	1A	3754	1/1	0.78	0.27	69,69,69,69	0
58	MG	2l	204	1/1	0.78	0.19	69,69,69,69	0
58	MG	2A	3219	1/1	0.78	0.33	85,85,85,85	0
58	MG	2A	3772	1/1	0.79	0.21	65,65,65,65	0
58	MG	2A	3253	1/1	0.79	0.30	79,79,79,79	0
58	MG	1A	3773	1/1	0.79	0.19	59,59,59,59	0
58	MG	2A	3546	1/1	0.79	0.17	50,50,50,50	0
58	MG	2B	205	1/1	0.79	0.28	72,72,72,72	0
58	MG	1A	3861	1/1	0.79	0.14	33,33,33,33	0
58	MG	2A	3088	1/1	0.79	0.25	78,78,78,78	0
58	MG	2A	3582	1/1	0.79	0.20	63,63,63,63	0
58	MG	2A	3583	1/1	0.79	0.29	83,83,83,83	0
58	MG	2A	3589	1/1	0.79	0.20	65,65,65,65	0
58	MG	1A	4106	1/1	0.79	0.26	66,66,66,66	0
58	MG	2a	1678	1/1	0.79	0.24	88,88,88,88	0
58	MG	1a	1734	1/1	0.79	0.25	76,76,76,76	0
58	MG	2a	1704	1/1	0.79	0.38	78,78,78,78	0
58	MG	1a	1608	1/1	0.79	0.23	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3971	1/1	0.79	0.17	63,63,63,63	0
58	MG	2A	3624	1/1	0.79	0.15	60,60,60,60	0
58	MG	2A	3187	1/1	0.79	0.28	76,76,76,76	0
58	MG	2a	1747	1/1	0.79	0.13	83,83,83,83	0
58	MG	2A	3217	1/1	0.79	0.51	82,82,82,82	0
58	MG	1B	229	1/1	0.79	0.14	79,79,79,79	0
58	MG	1A	3470	1/1	0.79	0.19	70,70,70,70	0
58	MG	2A	3229	1/1	0.79	0.34	72,72,72,72	0
58	MG	2A	3653	1/1	0.79	0.21	51,51,51,51	0
58	MG	1a	1679	1/1	0.79	0.38	81,81,81,81	0
58	MG	2a	1790	1/1	0.79	0.20	88,88,88,88	0
58	MG	1A	3948	1/1	0.79	0.20	59,59,59,59	0
58	MG	1A	3549	1/1	0.79	0.14	63,63,63,63	0
58	MG	2a	1822	1/1	0.79	0.24	74,74,74,74	0
58	MG	2A	3481	1/1	0.79	0.17	62,62,62,62	0
58	MG	2A	3487	1/1	0.79	0.18	86,86,86,86	0
58	MG	2A	3717	1/1	0.79	0.18	46,46,46,46	0
58	MG	2A	3498	1/1	0.79	0.28	73,73,73,73	0
58	MG	2x	106	1/1	0.79	0.42	80,80,80,80	0
58	MG	1A	3384	1/1	0.80	0.17	62,62,62,62	0
58	MG	1A	3905	1/1	0.80	0.11	58,58,58,58	0
58	MG	2A	3642	1/1	0.80	0.26	75,75,75,75	0
58	MG	2a	1703	1/1	0.80	0.30	74,74,74,74	0
58	MG	1a	1601	1/1	0.80	0.16	76,76,76,76	0
58	MG	1A	3730	1/1	0.80	0.12	74,74,74,74	0
58	MG	1a	1749	1/1	0.80	0.24	76,76,76,76	0
58	MG	1a	1770	1/1	0.80	0.17	58,58,58,58	0
58	MG	2A	3160	1/1	0.80	0.16	67,67,67,67	0
58	MG	1A	4017	1/1	0.80	0.14	64,64,64,64	0
58	MG	2A	3553	1/1	0.80	0.32	73,73,73,73	0
58	MG	2A	3172	1/1	0.80	0.20	68,68,68,68	0
58	MG	2A	3278	1/1	0.80	0.16	81,81,81,81	0
58	MG	2A	3771	1/1	0.80	0.32	72,72,72,72	0
58	MG	2A	3173	1/1	0.80	0.20	79,79,79,79	0
58	MG	1A	3601	1/1	0.80	0.21	59,59,59,59	0
58	MG	2a	1784	1/1	0.80	0.18	80,80,80,80	0
58	MG	1a	1821	1/1	0.80	0.13	79,79,79,79	0
58	MG	1F	314	1/1	0.80	0.24	65,65,65,65	0
58	MG	1A	3215	1/1	0.80	0.24	63,63,63,63	0
58	MG	2A	3327	1/1	0.80	0.12	74,74,74,74	0
58	MG	2a	1832	1/1	0.80	0.18	90,90,90,90	0
58	MG	2A	3333	1/1	0.80	0.26	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3220	1/1	0.80	0.13	84,84,84,84	0
58	MG	1A	3673	1/1	0.80	0.19	76,76,76,76	0
58	MG	2v	101	1/1	0.80	0.23	65,65,65,65	0
58	MG	1A	3871	1/1	0.80	0.12	38,38,38,38	0
58	MG	2a	1617	1/1	0.80	0.18	73,73,73,73	0
58	MG	2a	1634	1/1	0.81	0.27	74,74,74,74	0
58	MG	2A	3254	1/1	0.81	0.27	63,63,63,63	0
58	MG	2A	3464	1/1	0.81	0.22	55,55,55,55	0
58	MG	1a	1785	1/1	0.81	0.29	71,71,71,71	0
58	MG	2A	3162	1/1	0.81	0.28	71,71,71,71	0
58	MG	1A	4000	1/1	0.81	0.18	40,40,40,40	0
58	MG	1A	3869	1/1	0.81	0.13	66,66,66,66	0
58	MG	1A	3453	1/1	0.81	0.15	67,67,67,67	0
58	MG	1A	3889	1/1	0.81	0.10	69,69,69,69	0
58	MG	2A	3185	1/1	0.81	0.29	85,85,85,85	0
58	MG	1A	3174	1/1	0.81	0.20	71,71,71,71	0
58	MG	2A	3716	1/1	0.81	0.11	82,82,82,82	0
58	MG	2A	3562	1/1	0.81	0.23	76,76,76,76	0
58	MG	1A	4035	1/1	0.81	0.18	66,66,66,66	0
58	MG	1A	3952	1/1	0.81	0.16	48,48,48,48	0
58	MG	2A	3320	1/1	0.81	0.27	80,80,80,80	0
58	MG	1A	3980	1/1	0.81	0.16	53,53,53,53	0
58	MG	1A	3792	1/1	0.81	0.14	64,64,64,64	0
58	MG	2a	1789	1/1	0.81	0.22	71,71,71,71	0
58	MG	2A	3602	1/1	0.81	0.29	78,78,78,78	0
58	MG	1A	3805	1/1	0.81	0.14	62,62,62,62	0
58	MG	2B	207	1/1	0.81	0.23	72,72,72,72	0
58	MG	1B	207	1/1	0.81	0.14	75,75,75,75	0
58	MG	2a	1824	1/1	0.81	0.13	70,70,70,70	0
58	MG	2B	216	1/1	0.81	0.17	85,85,85,85	0
58	MG	2a	1841	1/1	0.81	0.10	87,87,87,87	0
58	MG	1a	1755	1/1	0.81	0.12	73,73,73,73	0
58	MG	2A	3610	1/1	0.81	0.15	69,69,69,69	0
58	MG	2A	3382	1/1	0.81	0.18	75,75,75,75	0
58	MG	2a	1606	1/1	0.81	0.39	73,73,73,73	0
58	MG	1a	1624	1/1	0.81	0.29	74,74,74,74	0
58	MG	2A	3139	1/1	0.81	0.21	78,78,78,78	0
58	MG	2F	302	1/1	0.82	0.18	78,78,78,78	0
58	MG	2A	3609	1/1	0.82	0.12	43,43,43,43	0
58	MG	1A	3397	1/1	0.82	0.21	51,51,51,51	0
58	MG	1A	3416	1/1	0.82	0.18	70,70,70,70	0
58	MG	1A	3937	1/1	0.82	0.18	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3776	1/1	0.82	0.19	66,66,66,66	0
58	MG	1A	3780	1/1	0.82	0.11	47,47,47,47	0
58	MG	2A	3497	1/1	0.82	0.25	77,77,77,77	0
58	MG	1a	1811	1/1	0.82	0.14	76,76,76,76	0
58	MG	2a	1679	1/1	0.82	0.15	64,64,64,64	0
58	MG	2a	1689	1/1	0.82	0.20	86,86,86,86	0
58	MG	2A	3643	1/1	0.82	0.25	69,69,69,69	0
58	MG	1B	221	1/1	0.82	0.15	69,69,69,69	0
58	MG	2A	3652	1/1	0.82	0.14	76,76,76,76	0
58	MG	2a	1712	1/1	0.82	0.22	84,84,84,84	0
58	MG	2A	3511	1/1	0.82	0.21	77,77,77,77	0
58	MG	1a	1824	1/1	0.82	0.14	87,87,87,87	0
58	MG	2A	3525	1/1	0.82	0.26	77,77,77,77	0
58	MG	2A	3530	1/1	0.82	0.18	73,73,73,73	0
58	MG	1A	3781	1/1	0.82	0.16	63,63,63,63	0
58	MG	1A	3294	1/1	0.82	0.22	59,59,59,59	0
58	MG	2a	1762	1/1	0.82	0.14	66,66,66,66	0
58	MG	1A	3493	1/1	0.82	0.20	71,71,71,71	0
58	MG	1A	3643	1/1	0.82	0.12	50,50,50,50	0
58	MG	2A	3745	1/1	0.82	0.13	80,80,80,80	0
58	MG	2a	1772	1/1	0.82	0.20	81,81,81,81	0
58	MG	2A	3566	1/1	0.82	0.17	75,75,75,75	0
58	MG	2A	3022	1/1	0.82	0.21	78,78,78,78	0
58	MG	1A	3963	1/1	0.82	0.13	62,62,62,62	0
58	MG	1A	3890	1/1	0.82	0.25	74,74,74,74	0
58	MG	2A	3805	1/1	0.82	0.17	59,59,59,59	0
58	MG	2A	3812	1/1	0.82	0.18	74,74,74,74	0
58	MG	2a	1800	1/1	0.82	0.20	67,67,67,67	0
58	MG	2A	3813	1/1	0.82	0.10	90,90,90,90	0
58	MG	2A	3587	1/1	0.82	0.18	80,80,80,80	0
58	MG	2A	3821	1/1	0.82	0.12	71,71,71,71	0
58	MG	1T	203	1/1	0.82	0.29	67,67,67,67	0
58	MG	2a	1837	1/1	0.82	0.21	78,78,78,78	0
58	MG	2A	3353	1/1	0.82	0.30	70,70,70,70	0
58	MG	2A	3239	1/1	0.82	0.35	88,88,88,88	0
58	MG	2B	208	1/1	0.82	0.27	76,76,76,76	0
58	MG	2B	209	1/1	0.82	0.13	77,77,77,77	0
58	MG	1A	3965	1/1	0.82	0.11	77,77,77,77	0
58	MG	1A	3681	1/1	0.82	0.15	70,70,70,70	0
58	MG	2w	102	1/1	0.82	0.18	86,86,86,86	0
58	MG	2A	3251	1/1	0.82	0.26	76,76,76,76	0
58	MG	2A	3250	1/1	0.83	0.21	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1a	1664	1/1	0.83	0.24	72,72,72,72	0
58	MG	2F	308	1/1	0.83	0.12	69,69,69,69	0
58	MG	1R	203	1/1	0.83	0.25	44,44,44,44	0
58	MG	2A	3447	1/1	0.83	0.18	69,69,69,69	0
58	MG	2A	3625	1/1	0.83	0.12	79,79,79,79	0
58	MG	2A	3461	1/1	0.83	0.16	72,72,72,72	0
58	MG	2A	3633	1/1	0.83	0.21	70,70,70,70	0
58	MG	2a	1630	1/1	0.83	0.17	79,79,79,79	0
58	MG	1A	3064	1/1	0.83	0.15	56,56,56,56	0
58	MG	1a	1680	1/1	0.83	0.29	75,75,75,75	0
58	MG	2a	1670	1/1	0.83	0.25	75,75,75,75	0
58	MG	2A	3486	1/1	0.83	0.12	68,68,68,68	0
58	MG	1A	3458	1/1	0.83	0.24	77,77,77,77	0
58	MG	1a	1699	1/1	0.83	0.22	82,82,82,82	0
58	MG	2A	3266	1/1	0.83	0.21	72,72,72,72	0
58	MG	2A	3651	1/1	0.83	0.24	90,90,90,90	0
58	MG	1A	3994	1/1	0.83	0.20	70,70,70,70	0
58	MG	2a	1711	1/1	0.83	0.27	72,72,72,72	0
58	MG	2A	3505	1/1	0.83	0.22	69,69,69,69	0
58	MG	1A	3545	1/1	0.83	0.13	61,61,61,61	0
58	MG	2a	1718	1/1	0.83	0.37	70,70,70,70	0
58	MG	2A	3661	1/1	0.83	0.25	71,71,71,71	0
58	MG	1A	3179	1/1	0.83	0.16	58,58,58,58	0
58	MG	2a	1723	1/1	0.83	0.14	72,72,72,72	0
58	MG	2A	3519	1/1	0.83	0.16	48,48,48,48	0
58	MG	2A	3520	1/1	0.83	0.21	76,76,76,76	0
58	MG	2A	3004	1/1	0.83	0.44	81,81,81,81	0
58	MG	2A	3288	1/1	0.83	0.13	72,72,72,72	0
58	MG	2A	3191	1/1	0.83	0.25	73,73,73,73	0
58	MG	2a	1766	1/1	0.83	0.34	71,71,71,71	0
58	MG	2A	3735	1/1	0.83	0.18	50,50,50,50	0
58	MG	2A	3552	1/1	0.83	0.16	67,67,67,67	0
58	MG	2A	3754	1/1	0.83	0.15	46,46,46,46	0
58	MG	2a	1774	1/1	0.83	0.44	83,83,83,83	0
58	MG	2A	3762	1/1	0.83	0.28	76,76,76,76	0
58	MG	2A	3204	1/1	0.83	0.26	68,68,68,68	0
58	MG	2A	3556	1/1	0.83	0.20	65,65,65,65	0
58	MG	2A	3558	1/1	0.83	0.16	71,71,71,71	0
58	MG	2A	3781	1/1	0.83	0.09	83,83,83,83	0
58	MG	2A	3017	1/1	0.83	0.16	60,60,60,60	0
58	MG	2A	3313	1/1	0.83	0.17	78,78,78,78	0
58	MG	2A	3807	1/1	0.83	0.21	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3246	1/1	0.83	0.12	77,77,77,77	0
58	MG	1A	3197	1/1	0.83	0.17	58,58,58,58	0
58	MG	2A	3071	1/1	0.83	0.17	64,64,64,64	0
58	MG	1A	3717	1/1	0.83	0.12	26,26,26,26	0
58	MG	1A	3954	1/1	0.83	0.10	49,49,49,49	0
58	MG	2A	3588	1/1	0.83	0.22	60,60,60,60	0
58	MG	2A	3356	1/1	0.83	0.25	71,71,71,71	0
58	MG	2A	3365	1/1	0.83	0.25	75,75,75,75	0
58	MG	1a	1656	1/1	0.83	0.16	63,63,63,63	0
58	MG	1A	3282	1/1	0.83	0.39	62,62,62,62	0
58	MG	2A	3102	1/1	0.83	0.29	74,74,74,74	0
58	MG	2D	304	1/1	0.83	0.40	67,67,67,67	0
58	MG	1x	103	1/1	0.84	0.12	60,60,60,60	0
58	MG	25	101	1/1	0.84	0.30	66,66,66,66	0
58	MG	1A	3960	1/1	0.84	0.11	66,66,66,66	0
58	MG	1B	230	1/1	0.84	0.25	83,83,83,83	0
58	MG	2a	1612	1/1	0.84	0.16	74,74,74,74	0
58	MG	1E	306	1/1	0.84	0.32	57,57,57,57	0
58	MG	2a	1620	1/1	0.84	0.29	72,72,72,72	0
58	MG	1A	3446	1/1	0.84	0.16	64,64,64,64	0
58	MG	2A	3030	1/1	0.84	0.23	70,70,70,70	0
58	MG	1A	3743	1/1	0.84	0.11	27,27,27,27	0
58	MG	2a	1668	1/1	0.84	0.24	67,67,67,67	0
58	MG	2A	3062	1/1	0.84	0.15	66,66,66,66	0
58	MG	1a	1696	1/1	0.84	0.20	87,87,87,87	0
58	MG	1A	4019	1/1	0.84	0.11	30,30,30,30	0
58	MG	2A	3082	1/1	0.84	0.26	63,63,63,63	0
58	MG	1A	3494	1/1	0.84	0.14	80,80,80,80	0
58	MG	2a	1692	1/1	0.84	0.27	73,73,73,73	0
58	MG	2A	3509	1/1	0.84	0.28	69,69,69,69	0
58	MG	1A	3356	1/1	0.84	0.30	77,77,77,77	0
58	MG	1A	4034	1/1	0.84	0.25	79,79,79,79	0
58	MG	2A	3276	1/1	0.84	0.25	76,76,76,76	0
58	MG	2A	3708	1/1	0.84	0.24	80,80,80,80	0
58	MG	2A	3711	1/1	0.84	0.18	66,66,66,66	0
58	MG	2A	3095	1/1	0.84	0.13	65,65,65,65	0
58	MG	1U	212	1/1	0.84	0.19	67,67,67,67	0
58	MG	1U	214	1/1	0.84	0.54	81,81,81,81	0
58	MG	2A	3136	1/1	0.84	0.22	69,69,69,69	0
58	MG	2a	1746	1/1	0.84	0.19	75,75,75,75	0
58	MG	1a	1746	1/1	0.84	0.14	61,61,61,61	0
58	MG	2A	3290	1/1	0.84	0.07	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3766	1/1	0.84	0.10	61,61,61,61	0
58	MG	2A	3295	1/1	0.84	0.17	59,59,59,59	0
58	MG	2a	1765	1/1	0.84	0.24	68,68,68,68	0
58	MG	2A	3298	1/1	0.84	0.23	71,71,71,71	0
58	MG	2A	3302	1/1	0.84	0.27	83,83,83,83	0
58	MG	2A	3303	1/1	0.84	0.23	58,58,58,58	0
58	MG	2A	3304	1/1	0.84	0.34	67,67,67,67	0
58	MG	1A	3092	1/1	0.84	0.28	71,71,71,71	0
58	MG	1a	1754	1/1	0.84	0.16	66,66,66,66	0
58	MG	1Y	201	1/1	0.84	0.15	76,76,76,76	0
58	MG	1A	3841	1/1	0.84	0.23	82,82,82,82	0
58	MG	2A	3814	1/1	0.84	0.17	69,69,69,69	0
58	MG	1A	4053	1/1	0.84	0.19	71,71,71,71	0
58	MG	1A	3462	1/1	0.84	0.15	63,63,63,63	0
58	MG	1A	3059	1/1	0.84	0.34	67,67,67,67	0
58	MG	2A	3601	1/1	0.84	0.19	63,63,63,63	0
58	MG	2A	3337	1/1	0.84	0.23	60,60,60,60	0
58	MG	1a	1621	1/1	0.84	0.15	54,54,54,54	0
58	MG	1A	3037	1/1	0.84	0.21	70,70,70,70	0
58	MG	1A	3687	1/1	0.84	0.12	64,64,64,64	0
58	MG	2B	212	1/1	0.84	0.11	78,78,78,78	0
58	MG	1a	1655	1/1	0.84	0.14	76,76,76,76	0
58	MG	2B	219	1/1	0.84	0.21	78,78,78,78	0
58	MG	1v	101	1/1	0.84	0.24	80,80,80,80	0
58	MG	2q	201	1/1	0.84	0.20	79,79,79,79	0
58	MG	2A	3611	1/1	0.84	0.31	70,70,70,70	0
58	MG	1A	3617	1/1	0.84	0.11	42,42,42,42	0
58	MG	2A	3390	1/1	0.84	0.24	79,79,79,79	0
58	MG	2x	105	1/1	0.84	0.26	86,86,86,86	0
58	MG	1A	3430	1/1	0.84	0.16	74,74,74,74	0
58	MG	2A	3321	1/1	0.85	0.17	77,77,77,77	0
58	MG	1A	3311	1/1	0.85	0.18	59,59,59,59	0
58	MG	2V	201	1/1	0.85	0.37	54,54,54,54	0
58	MG	1a	1728	1/1	0.85	0.19	78,78,78,78	0
58	MG	20	101	1/1	0.85	0.47	73,73,73,73	0
58	MG	20	102	1/1	0.85	0.27	74,74,74,74	0
58	MG	2A	3142	1/1	0.85	0.25	63,63,63,63	0
58	MG	1A	3319	1/1	0.85	0.14	68,68,68,68	0
58	MG	1A	3984	1/1	0.85	0.13	59,59,59,59	0
58	MG	1A	3172	1/1	0.85	0.29	62,62,62,62	0
58	MG	1Q	205	1/1	0.85	0.19	63,63,63,63	0
58	MG	1A	3778	1/1	0.85	0.17	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1622	1/1	0.85	0.29	66,66,66,66	0
58	MG	2a	1626	1/1	0.85	0.16	66,66,66,66	0
58	MG	1A	3917	1/1	0.85	0.13	76,76,76,76	0
58	MG	1A	3920	1/1	0.85	0.12	79,79,79,79	0
58	MG	2a	1637	1/1	0.85	0.19	75,75,75,75	0
58	MG	2A	3387	1/1	0.85	0.12	67,67,67,67	0
58	MG	2a	1666	1/1	0.85	0.42	77,77,77,77	0
58	MG	1a	1757	1/1	0.85	0.23	86,86,86,86	0
58	MG	1T	204	1/1	0.85	0.13	65,65,65,65	0
58	MG	1A	3674	1/1	0.85	0.17	68,68,68,68	0
58	MG	1A	3333	1/1	0.85	0.13	66,66,66,66	0
58	MG	2A	3412	1/1	0.85	0.15	78,78,78,78	0
58	MG	1a	1802	1/1	0.85	0.12	70,70,70,70	0
58	MG	2A	3454	1/1	0.85	0.21	65,65,65,65	0
58	MG	2a	1694	1/1	0.85	0.38	75,75,75,75	0
58	MG	1A	3342	1/1	0.85	0.18	61,61,61,61	0
58	MG	1A	3686	1/1	0.85	0.15	55,55,55,55	0
58	MG	2a	1706	1/1	0.85	0.47	81,81,81,81	0
58	MG	2A	3678	1/1	0.85	0.18	67,67,67,67	0
58	MG	1a	1812	1/1	0.85	0.25	90,90,90,90	0
58	MG	1a	1818	1/1	0.85	0.13	74,74,74,74	0
58	MG	2A	3235	1/1	0.85	0.18	83,83,83,83	0
58	MG	1A	3786	1/1	0.85	0.24	66,66,66,66	0
58	MG	1A	3345	1/1	0.85	0.18	58,58,58,58	0
58	MG	18	104	1/1	0.85	0.21	73,73,73,73	0
58	MG	1A	3791	1/1	0.85	0.14	66,66,66,66	0
58	MG	1A	3696	1/1	0.85	0.11	43,43,43,43	0
58	MG	1w	102	1/1	0.85	0.17	69,69,69,69	0
58	MG	1A	3558	1/1	0.85	0.12	39,39,39,39	0
58	MG	1w	105	1/1	0.85	0.16	80,80,80,80	0
58	MG	1w	108	1/1	0.85	0.17	87,87,87,87	0
58	MG	1a	1623	1/1	0.85	0.29	75,75,75,75	0
58	MG	1A	4055	1/1	0.85	0.18	73,73,73,73	0
58	MG	2A	3273	1/1	0.85	0.14	71,71,71,71	0
58	MG	2a	1770	1/1	0.85	0.19	77,77,77,77	0
58	MG	1A	4060	1/1	0.85	0.15	64,64,64,64	0
58	MG	2A	3005	1/1	0.85	0.33	70,70,70,70	0
58	MG	1a	1636	1/1	0.85	0.18	76,76,76,76	0
58	MG	1A	3347	1/1	0.85	0.45	59,59,59,59	0
58	MG	2a	1776	1/1	0.85	0.26	79,79,79,79	0
58	MG	2A	3560	1/1	0.85	0.18	58,58,58,58	0
58	MG	1A	3734	1/1	0.85	0.10	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1786	1/1	0.85	0.26	71,71,71,71	0
58	MG	2a	1787	1/1	0.85	0.15	75,75,75,75	0
58	MG	1A	3187	1/1	0.85	0.33	72,72,72,72	0
58	MG	2A	3055	1/1	0.85	0.36	74,74,74,74	0
58	MG	2a	1794	1/1	0.85	0.26	72,72,72,72	0
58	MG	1B	202	1/1	0.85	0.24	59,59,59,59	0
58	MG	2A	3825	1/1	0.85	0.12	63,63,63,63	0
58	MG	2A	3576	1/1	0.85	0.18	63,63,63,63	0
58	MG	1A	3638	1/1	0.85	0.11	29,29,29,29	0
58	MG	1a	1668	1/1	0.85	0.28	68,68,68,68	0
58	MG	1B	210	1/1	0.85	0.24	64,64,64,64	0
58	MG	1A	3381	1/1	0.85	0.30	72,72,72,72	0
58	MG	1A	3862	1/1	0.85	0.14	42,42,42,42	0
58	MG	2B	211	1/1	0.85	0.25	76,76,76,76	0
58	MG	2A	3593	1/1	0.85	0.15	66,66,66,66	0
58	MG	2B	213	1/1	0.85	0.25	76,76,76,76	0
58	MG	2n	101	1/1	0.85	0.17	74,74,74,74	0
58	MG	1A	3251	1/1	0.85	0.13	70,70,70,70	0
58	MG	2A	3600	1/1	0.85	0.22	62,62,62,62	0
58	MG	1A	3488	1/1	0.85	0.23	68,68,68,68	0
58	MG	1a	1703	1/1	0.85	0.37	69,69,69,69	0
58	MG	2w	103	1/1	0.85	0.09	98,98,98,98	0
58	MG	2x	101	1/1	0.85	0.16	76,76,76,76	0
58	MG	2E	306	1/1	0.85	0.28	73,73,73,73	0
58	MG	1D	310	1/1	0.85	0.22	49,49,49,49	0
58	MG	1A	3237	1/1	0.86	0.16	69,69,69,69	0
58	MG	1A	3803	1/1	0.86	0.19	62,62,62,62	0
58	MG	2E	305	1/1	0.86	0.19	76,76,76,76	0
58	MG	2A	3267	1/1	0.86	0.32	60,60,60,60	0
58	MG	1E	311	1/1	0.86	0.22	49,49,49,49	0
58	MG	1a	1693	1/1	0.86	0.22	64,64,64,64	0
58	MG	2A	3038	1/1	0.86	0.22	75,75,75,75	0
58	MG	1F	312	1/1	0.86	0.21	42,42,42,42	0
58	MG	2A	3047	1/1	0.86	0.17	68,68,68,68	0
58	MG	1A	3924	1/1	0.86	0.11	73,73,73,73	0
58	MG	2A	3057	1/1	0.86	0.14	58,58,58,58	0
58	MG	1A	3995	1/1	0.86	0.08	20,20,20,20	0
58	MG	2a	1602	1/1	0.86	0.11	77,77,77,77	0
58	MG	1A	3283	1/1	0.86	0.19	68,68,68,68	0
58	MG	2a	1607	1/1	0.86	0.17	75,75,75,75	0
58	MG	2A	3077	1/1	0.86	0.18	73,73,73,73	0
58	MG	1a	1722	1/1	0.86	0.33	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1a	1723	1/1	0.86	0.15	71,71,71,71	0
58	MG	1A	4006	1/1	0.86	0.13	50,50,50,50	0
58	MG	1A	3929	1/1	0.86	0.12	42,42,42,42	0
58	MG	2A	3305	1/1	0.86	0.11	76,76,76,76	0
58	MG	1T	202	1/1	0.86	0.24	72,72,72,72	0
58	MG	2a	1631	1/1	0.86	0.15	77,77,77,77	0
58	MG	2A	3090	1/1	0.86	0.32	72,72,72,72	0
58	MG	1A	3933	1/1	0.86	0.10	38,38,38,38	0
58	MG	2a	1642	1/1	0.86	0.29	75,75,75,75	0
58	MG	2a	1650	1/1	0.86	0.18	70,70,70,70	0
58	MG	2A	3098	1/1	0.86	0.11	76,76,76,76	0
58	MG	1A	3757	1/1	0.86	0.13	68,68,68,68	0
58	MG	2A	3108	1/1	0.86	0.25	79,79,79,79	0
58	MG	2A	3113	1/1	0.86	0.10	64,64,64,64	0
58	MG	2a	1671	1/1	0.86	0.21	78,78,78,78	0
58	MG	2a	1674	1/1	0.86	0.32	74,74,74,74	0
58	MG	2a	1676	1/1	0.86	0.18	63,63,63,63	0
58	MG	1a	1740	1/1	0.86	0.19	85,85,85,85	0
58	MG	2A	3637	1/1	0.86	0.17	77,77,77,77	0
58	MG	2A	3336	1/1	0.86	0.26	47,47,47,47	0
58	MG	1A	3469	1/1	0.86	0.26	73,73,73,73	0
58	MG	1A	3409	1/1	0.86	0.19	57,57,57,57	0
58	MG	1A	3848	1/1	0.86	0.22	65,65,65,65	0
58	MG	2A	3358	1/1	0.86	0.33	67,67,67,67	0
58	MG	2A	3149	1/1	0.86	0.17	60,60,60,60	0
58	MG	2A	3154	1/1	0.86	0.09	69,69,69,69	0
58	MG	2a	1708	1/1	0.86	0.18	80,80,80,80	0
58	MG	1A	3852	1/1	0.86	0.22	68,68,68,68	0
58	MG	1A	3135	1/1	0.86	0.18	52,52,52,52	0
58	MG	2A	3676	1/1	0.86	0.14	63,63,63,63	0
58	MG	2a	1717	1/1	0.86	0.30	70,70,70,70	0
58	MG	1a	1760	1/1	0.86	0.11	83,83,83,83	0
58	MG	2A	3686	1/1	0.86	0.20	83,83,83,83	0
58	MG	1a	1767	1/1	0.86	0.12	58,58,58,58	0
58	MG	10	110	1/1	0.86	0.20	70,70,70,70	0
58	MG	2A	3177	1/1	0.86	0.20	73,73,73,73	0
58	MG	2a	1733	1/1	0.86	0.08	92,92,92,92	0
58	MG	10	112	1/1	0.86	0.14	78,78,78,78	0
58	MG	2A	3183	1/1	0.86	0.14	64,64,64,64	0
58	MG	2A	3421	1/1	0.86	0.26	65,65,65,65	0
58	MG	2a	1759	1/1	0.86	0.20	73,73,73,73	0
58	MG	2A	3427	1/1	0.86	0.17	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3719	1/1	0.86	0.12	54,54,54,54	0
58	MG	11	105	1/1	0.86	0.14	59,59,59,59	0
58	MG	1A	4040	1/1	0.86	0.12	71,71,71,71	0
58	MG	1A	3422	1/1	0.86	0.19	69,69,69,69	0
58	MG	2A	3197	1/1	0.86	0.18	58,58,58,58	0
58	MG	2A	3765	1/1	0.86	0.20	76,76,76,76	0
58	MG	2A	3478	1/1	0.86	0.23	76,76,76,76	0
58	MG	2A	3769	1/1	0.86	0.21	58,58,58,58	0
58	MG	2A	3198	1/1	0.86	0.18	76,76,76,76	0
58	MG	1A	3702	1/1	0.86	0.23	72,72,72,72	0
58	MG	2a	1778	1/1	0.86	0.25	62,62,62,62	0
58	MG	2A	3206	1/1	0.86	0.30	69,69,69,69	0
58	MG	2A	3212	1/1	0.86	0.17	61,61,61,61	0
58	MG	1A	3427	1/1	0.86	0.17	71,71,71,71	0
58	MG	1A	3248	1/1	0.86	0.09	45,45,45,45	0
58	MG	1A	3434	1/1	0.86	0.28	71,71,71,71	0
58	MG	2A	3808	1/1	0.86	0.18	87,87,87,87	0
58	MG	1A	3529	1/1	0.86	0.22	66,66,66,66	0
58	MG	2a	1797	1/1	0.86	0.13	78,78,78,78	0
58	MG	1A	3967	1/1	0.86	0.13	87,87,87,87	0
58	MG	1A	3894	1/1	0.86	0.11	74,74,74,74	0
58	MG	1A	3897	1/1	0.86	0.10	79,79,79,79	0
58	MG	2a	1817	1/1	0.86	0.12	59,59,59,59	0
58	MG	2A	3816	1/1	0.86	0.16	77,77,77,77	0
58	MG	2A	3819	1/1	0.86	0.21	73,73,73,73	0
58	MG	2A	3236	1/1	0.86	0.24	81,81,81,81	0
58	MG	2a	1835	1/1	0.86	0.16	69,69,69,69	0
58	MG	2a	1836	1/1	0.86	0.16	81,81,81,81	0
58	MG	2A	3823	1/1	0.86	0.14	66,66,66,66	0
58	MG	1A	3058	1/1	0.86	0.15	60,60,60,60	0
58	MG	2A	3242	1/1	0.86	0.31	78,78,78,78	0
58	MG	2B	202	1/1	0.86	0.23	81,81,81,81	0
58	MG	2A	3534	1/1	0.86	0.17	46,46,46,46	0
58	MG	1A	3027	1/1	0.86	0.17	42,42,42,42	0
58	MG	1a	1659	1/1	0.86	0.12	66,66,66,66	0
58	MG	1A	3907	1/1	0.86	0.12	61,61,61,61	0
58	MG	1A	3912	1/1	0.86	0.18	64,64,64,64	0
58	MG	1x	104	1/1	0.86	0.21	73,73,73,73	0
58	MG	1A	3916	1/1	0.86	0.13	79,79,79,79	0
58	MG	1x	110	1/1	0.86	0.28	72,72,72,72	0
58	MG	1a	1672	1/1	0.86	0.22	74,74,74,74	0
58	MG	2A	3565	1/1	0.86	0.22	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3640	1/1	0.87	0.12	64,64,64,64	0
58	MG	2A	3028	1/1	0.87	0.13	72,72,72,72	0
58	MG	1A	4059	1/1	0.87	0.12	58,58,58,58	0
58	MG	1a	1725	1/1	0.87	0.18	58,58,58,58	0
58	MG	1A	3610	1/1	0.87	0.12	52,52,52,52	0
58	MG	1A	3895	1/1	0.87	0.11	70,70,70,70	0
58	MG	2A	3223	1/1	0.87	0.31	72,72,72,72	0
58	MG	2a	1638	1/1	0.87	0.23	56,56,56,56	0
58	MG	2a	1641	1/1	0.87	0.22	74,74,74,74	0
58	MG	2A	3227	1/1	0.87	0.20	68,68,68,68	0
58	MG	2a	1649	1/1	0.87	0.25	67,67,67,67	0
58	MG	2A	3415	1/1	0.87	0.15	50,50,50,50	0
58	MG	2a	1663	1/1	0.87	0.18	76,76,76,76	0
58	MG	1A	3489	1/1	0.87	0.30	65,65,65,65	0
58	MG	1A	4098	1/1	0.87	0.15	64,64,64,64	0
58	MG	2A	3443	1/1	0.87	0.12	59,59,59,59	0
58	MG	1A	3285	1/1	0.87	0.11	63,63,63,63	0
58	MG	1A	4107	1/1	0.87	0.20	53,53,53,53	0
58	MG	2A	3074	1/1	0.87	0.21	70,70,70,70	0
58	MG	2A	3698	1/1	0.87	0.13	64,64,64,64	0
58	MG	1A	3904	1/1	0.87	0.10	38,38,38,38	0
58	MG	2A	3079	1/1	0.87	0.15	72,72,72,72	0
58	MG	2A	3710	1/1	0.87	0.12	65,65,65,65	0
58	MG	1a	1602	1/1	0.87	0.12	56,56,56,56	0
58	MG	1a	1606	1/1	0.87	0.10	70,70,70,70	0
58	MG	2a	1693	1/1	0.87	0.38	74,74,74,74	0
58	MG	1A	3361	1/1	0.87	0.14	65,65,65,65	0
58	MG	2a	1695	1/1	0.87	0.15	76,76,76,76	0
58	MG	2a	1700	1/1	0.87	0.10	66,66,66,66	0
58	MG	2A	3489	1/1	0.87	0.15	65,65,65,65	0
58	MG	1A	3906	1/1	0.87	0.12	39,39,39,39	0
58	MG	2A	3742	1/1	0.87	0.11	72,72,72,72	0
58	MG	1B	214	1/1	0.87	0.14	74,74,74,74	0
58	MG	2a	1710	1/1	0.87	0.31	73,73,73,73	0
58	MG	2A	3501	1/1	0.87	0.14	80,80,80,80	0
58	MG	1A	3794	1/1	0.87	0.12	62,62,62,62	0
58	MG	2A	3092	1/1	0.87	0.35	67,67,67,67	0
58	MG	2A	3507	1/1	0.87	0.28	79,79,79,79	0
58	MG	1a	1625	1/1	0.87	0.15	69,69,69,69	0
58	MG	1A	3799	1/1	0.87	0.11	75,75,75,75	0
58	MG	2A	3101	1/1	0.87	0.24	61,61,61,61	0
58	MG	2a	1722	1/1	0.87	0.14	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3518	1/1	0.87	0.11	41,41,41,41	0
58	MG	2a	1724	1/1	0.87	0.16	76,76,76,76	0
58	MG	1A	3738	1/1	0.87	0.12	53,53,53,53	0
58	MG	2A	3785	1/1	0.87	0.14	58,58,58,58	0
58	MG	1a	1653	1/1	0.87	0.29	71,71,71,71	0
58	MG	1A	3497	1/1	0.87	0.21	62,62,62,62	0
58	MG	1A	3825	1/1	0.87	0.23	72,72,72,72	0
58	MG	2A	3133	1/1	0.87	0.30	67,67,67,67	0
58	MG	2A	3810	1/1	0.87	0.14	58,58,58,58	0
58	MG	2A	3281	1/1	0.87	0.15	66,66,66,66	0
58	MG	2A	3548	1/1	0.87	0.16	62,62,62,62	0
58	MG	1A	3506	1/1	0.87	0.18	63,63,63,63	0
58	MG	1A	3522	1/1	0.87	0.27	68,68,68,68	0
58	MG	1A	3927	1/1	0.87	0.22	64,64,64,64	0
58	MG	2A	3146	1/1	0.87	0.16	69,69,69,69	0
58	MG	2A	3294	1/1	0.87	0.16	75,75,75,75	0
58	MG	1b	301	1/1	0.87	0.20	78,78,78,78	0
58	MG	1A	3846	1/1	0.87	0.11	57,57,57,57	0
58	MG	2A	3301	1/1	0.87	0.21	66,66,66,66	0
58	MG	2B	201	1/1	0.87	0.41	80,80,80,80	0
58	MG	2A	3156	1/1	0.87	0.27	76,76,76,76	0
58	MG	2A	3157	1/1	0.87	0.20	78,78,78,78	0
58	MG	2A	3575	1/1	0.87	0.20	58,58,58,58	0
58	MG	1A	3667	1/1	0.87	0.14	56,56,56,56	0
58	MG	1a	1670	1/1	0.87	0.24	73,73,73,73	0
58	MG	2A	3306	1/1	0.87	0.27	62,62,62,62	0
58	MG	1A	3281	1/1	0.87	0.11	49,49,49,49	0
58	MG	1P	206	1/1	0.87	0.18	57,57,57,57	0
58	MG	1A	3295	1/1	0.87	0.13	60,60,60,60	0
58	MG	2B	215	1/1	0.87	0.12	77,77,77,77	0
58	MG	2A	3315	1/1	0.87	0.18	81,81,81,81	0
58	MG	2A	3316	1/1	0.87	0.27	78,78,78,78	0
58	MG	1A	3533	1/1	0.87	0.16	68,68,68,68	0
58	MG	2E	301	1/1	0.87	0.19	68,68,68,68	0
58	MG	1A	3480	1/1	0.87	0.18	87,87,87,87	0
58	MG	2A	3181	1/1	0.87	0.12	70,70,70,70	0
58	MG	1A	3006	1/1	0.87	0.26	67,67,67,67	0
58	MG	2A	3328	1/1	0.87	0.13	72,72,72,72	0
58	MG	1x	106	1/1	0.87	0.20	72,72,72,72	0
58	MG	1A	3486	1/1	0.87	0.24	49,49,49,49	0
58	MG	1A	3277	1/1	0.87	0.10	62,62,62,62	0
58	MG	2A	3347	1/1	0.87	0.36	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3349	1/1	0.87	0.25	63,63,63,63	0
58	MG	2A	3196	1/1	0.87	0.22	75,75,75,75	0
58	MG	1A	3888	1/1	0.87	0.10	34,34,34,34	0
58	MG	2A	3631	1/1	0.87	0.14	65,65,65,65	0
58	MG	1a	1713	1/1	0.87	0.18	77,77,77,77	0
58	MG	2A	3360	1/1	0.87	0.39	84,84,84,84	0
58	MG	2A	3200	1/1	0.87	0.13	54,54,54,54	0
58	MG	1A	3597	1/1	0.87	0.12	59,59,59,59	0
58	MG	1A	3414	1/1	0.87	0.15	61,61,61,61	0
58	MG	1a	1756	1/1	0.88	0.11	78,78,78,78	0
58	MG	1A	3428	1/1	0.88	0.15	73,73,73,73	0
58	MG	2A	3299	1/1	0.88	0.14	72,72,72,72	0
58	MG	2A	3570	1/1	0.88	0.11	69,69,69,69	0
58	MG	2A	3571	1/1	0.88	0.16	65,65,65,65	0
58	MG	1A	3022	1/1	0.88	0.29	69,69,69,69	0
58	MG	2A	3574	1/1	0.88	0.12	49,49,49,49	0
58	MG	2A	3128	1/1	0.88	0.14	52,52,52,52	0
58	MG	1A	4072	1/1	0.88	0.17	74,74,74,74	0
58	MG	1A	3865	1/1	0.88	0.09	41,41,41,41	0
58	MG	2A	3138	1/1	0.88	0.28	63,63,63,63	0
58	MG	1A	3224	1/1	0.88	0.15	67,67,67,67	0
58	MG	1A	3142	1/1	0.88	0.18	44,44,44,44	0
58	MG	1a	1611	1/1	0.88	0.27	79,79,79,79	0
58	MG	27	103	1/1	0.88	0.19	74,74,74,74	0
58	MG	2A	3591	1/1	0.88	0.19	64,64,64,64	0
58	MG	2A	3309	1/1	0.88	0.25	62,62,62,62	0
58	MG	1a	1806	1/1	0.88	0.12	74,74,74,74	0
58	MG	2a	1609	1/1	0.88	0.39	73,73,73,73	0
58	MG	1A	4100	1/1	0.88	0.13	52,52,52,52	0
58	MG	2a	1611	1/1	0.88	0.16	77,77,77,77	0
58	MG	1A	3242	1/1	0.88	0.13	61,61,61,61	0
58	MG	2a	1614	1/1	0.88	0.25	70,70,70,70	0
58	MG	2A	3319	1/1	0.88	0.21	67,67,67,67	0
58	MG	2A	3603	1/1	0.88	0.10	64,64,64,64	0
58	MG	2a	1621	1/1	0.88	0.65	85,85,85,85	0
58	MG	1A	3677	1/1	0.88	0.08	49,49,49,49	0
58	MG	1A	4109	1/1	0.88	0.13	71,71,71,71	0
58	MG	2a	1627	1/1	0.88	0.18	72,72,72,72	0
58	MG	2A	3323	1/1	0.88	0.16	79,79,79,79	0
58	MG	1a	1628	1/1	0.88	0.20	50,50,50,50	0
58	MG	2a	1632	1/1	0.88	0.24	79,79,79,79	0
58	MG	1A	3086	1/1	0.88	0.17	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3682	1/1	0.88	0.15	70,70,70,70	0
58	MG	2A	3621	1/1	0.88	0.18	66,66,66,66	0
58	MG	1e	201	1/1	0.88	0.12	81,81,81,81	0
58	MG	1a	1638	1/1	0.88	0.23	65,65,65,65	0
58	MG	1n	103	1/1	0.88	0.10	85,85,85,85	0
58	MG	1t	201	1/1	0.88	0.18	63,63,63,63	0
58	MG	2a	1656	1/1	0.88	0.16	68,68,68,68	0
58	MG	1a	1650	1/1	0.88	0.14	71,71,71,71	0
58	MG	2A	3352	1/1	0.88	0.26	78,78,78,78	0
58	MG	1A	3460	1/1	0.88	0.21	84,84,84,84	0
58	MG	2a	1667	1/1	0.88	0.24	64,64,64,64	0
58	MG	1A	3368	1/1	0.88	0.25	58,58,58,58	0
58	MG	1A	3373	1/1	0.88	0.18	63,63,63,63	0
58	MG	1A	3160	1/1	0.88	0.23	60,60,60,60	0
58	MG	1B	223	1/1	0.88	0.11	60,60,60,60	0
58	MG	1A	3587	1/1	0.88	0.20	56,56,56,56	0
58	MG	1A	3797	1/1	0.88	0.22	59,59,59,59	0
58	MG	1A	3713	1/1	0.88	0.16	41,41,41,41	0
58	MG	2a	1686	1/1	0.88	0.19	75,75,75,75	0
58	MG	2A	3384	1/1	0.88	0.29	73,73,73,73	0
58	MG	1A	3296	1/1	0.88	0.38	67,67,67,67	0
58	MG	2A	3389	1/1	0.88	0.15	62,62,62,62	0
58	MG	2A	3207	1/1	0.88	0.18	82,82,82,82	0
58	MG	1a	1671	1/1	0.88	0.21	73,73,73,73	0
58	MG	2A	3668	1/1	0.88	0.15	72,72,72,72	0
58	MG	2A	3674	1/1	0.88	0.11	71,71,71,71	0
58	MG	1x	111	1/1	0.88	0.10	49,49,49,49	0
58	MG	1A	3297	1/1	0.88	0.25	65,65,65,65	0
58	MG	2A	3685	1/1	0.88	0.13	69,69,69,69	0
58	MG	2A	3409	1/1	0.88	0.20	69,69,69,69	0
58	MG	2A	3687	1/1	0.88	0.10	75,75,75,75	0
58	MG	1a	1673	1/1	0.88	0.17	71,71,71,71	0
58	MG	2A	3413	1/1	0.88	0.11	57,57,57,57	0
58	MG	2A	3007	1/1	0.88	0.17	56,56,56,56	0
58	MG	2A	3702	1/1	0.88	0.11	65,65,65,65	0
58	MG	1A	3808	1/1	0.88	0.15	61,61,61,61	0
58	MG	2A	3226	1/1	0.88	0.26	63,63,63,63	0
58	MG	2A	3441	1/1	0.88	0.36	69,69,69,69	0
58	MG	1A	4003	1/1	0.88	0.09	39,39,39,39	0
58	MG	2A	3228	1/1	0.88	0.16	67,67,67,67	0
58	MG	2A	3449	1/1	0.88	0.13	46,46,46,46	0
58	MG	2A	3023	1/1	0.88	0.21	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1730	1/1	0.88	0.13	80,80,80,80	0
58	MG	1A	3813	1/1	0.88	0.11	47,47,47,47	0
58	MG	1a	1691	1/1	0.88	0.31	69,69,69,69	0
58	MG	2A	3467	1/1	0.88	0.20	58,58,58,58	0
58	MG	2a	1754	1/1	0.88	0.33	79,79,79,79	0
58	MG	2A	3749	1/1	0.88	0.16	67,67,67,67	0
58	MG	2A	3750	1/1	0.88	0.32	74,74,74,74	0
58	MG	2a	1760	1/1	0.88	0.18	73,73,73,73	0
58	MG	1A	3822	1/1	0.88	0.15	46,46,46,46	0
58	MG	2a	1763	1/1	0.88	0.21	75,75,75,75	0
58	MG	2A	3480	1/1	0.88	0.22	73,73,73,73	0
58	MG	2A	3764	1/1	0.88	0.15	63,63,63,63	0
58	MG	1A	4014	1/1	0.88	0.16	58,58,58,58	0
58	MG	1A	3301	1/1	0.88	0.37	73,73,73,73	0
58	MG	2A	3048	1/1	0.88	0.17	72,72,72,72	0
58	MG	1A	4018	1/1	0.88	0.15	44,44,44,44	0
58	MG	1R	205	1/1	0.88	0.15	61,61,61,61	0
58	MG	1A	3199	1/1	0.88	0.12	61,61,61,61	0
58	MG	2A	3773	1/1	0.88	0.13	71,71,71,71	0
58	MG	2A	3063	1/1	0.88	0.19	67,67,67,67	0
58	MG	2A	3782	1/1	0.88	0.12	62,62,62,62	0
58	MG	2a	1781	1/1	0.88	0.24	70,70,70,70	0
58	MG	1a	1721	1/1	0.88	0.10	71,71,71,71	0
58	MG	2A	3793	1/1	0.88	0.12	80,80,80,80	0
58	MG	2A	3073	1/1	0.88	0.15	66,66,66,66	0
58	MG	1A	4026	1/1	0.88	0.13	59,59,59,59	0
58	MG	1A	3835	1/1	0.88	0.11	54,54,54,54	0
58	MG	2A	3510	1/1	0.88	0.11	72,72,72,72	0
58	MG	2a	1793	1/1	0.88	0.10	65,65,65,65	0
58	MG	1A	3631	1/1	0.88	0.11	49,49,49,49	0
58	MG	1A	4029	1/1	0.88	0.14	68,68,68,68	0
58	MG	2A	3516	1/1	0.88	0.13	72,72,72,72	0
58	MG	2A	3271	1/1	0.88	0.16	66,66,66,66	0
58	MG	1A	3844	1/1	0.88	0.16	54,54,54,54	0
58	MG	2a	1808	1/1	0.88	0.15	69,69,69,69	0
58	MG	2a	1809	1/1	0.88	0.10	75,75,75,75	0
58	MG	1W	202	1/1	0.88	0.23	65,65,65,65	0
58	MG	2A	3521	1/1	0.88	0.15	61,61,61,61	0
58	MG	2A	3524	1/1	0.88	0.16	57,57,57,57	0
58	MG	1A	3254	1/1	0.88	0.15	65,65,65,65	0
58	MG	1A	3025	1/1	0.88	0.30	77,77,77,77	0
58	MG	2A	3531	1/1	0.88	0.22	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3425	1/1	0.88	0.22	53,53,53,53	0
58	MG	2A	3280	1/1	0.88	0.17	69,69,69,69	0
58	MG	2B	203	1/1	0.88	0.28	69,69,69,69	0
58	MG	1A	4044	1/1	0.88	0.17	57,57,57,57	0
58	MG	2A	3550	1/1	0.88	0.16	75,75,75,75	0
58	MG	2A	3551	1/1	0.88	0.18	66,66,66,66	0
58	MG	1A	3657	1/1	0.88	0.20	62,62,62,62	0
58	MG	2A	3286	1/1	0.88	0.16	73,73,73,73	0
58	MG	1a	1751	1/1	0.88	0.12	68,68,68,68	0
58	MG	2A	3557	1/1	0.88	0.24	78,78,78,78	0
58	MG	11	104	1/1	0.88	0.16	68,68,68,68	0
58	MG	1A	3209	1/1	0.88	0.12	57,57,57,57	0
58	MG	2A	3104	1/1	0.88	0.26	63,63,63,63	0
58	MG	2B	217	1/1	0.88	0.29	74,74,74,74	0
58	MG	2x	108	1/1	0.88	0.16	61,61,61,61	0
58	MG	2A	3581	1/1	0.89	0.17	71,71,71,71	0
58	MG	1A	3714	1/1	0.89	0.13	48,48,48,48	0
58	MG	1a	1819	1/1	0.89	0.23	81,81,81,81	0
58	MG	2R	201	1/1	0.89	0.19	70,70,70,70	0
58	MG	2T	201	1/1	0.89	0.14	69,69,69,69	0
58	MG	1a	1820	1/1	0.89	0.15	83,83,83,83	0
58	MG	1A	3569	1/1	0.89	0.13	39,39,39,39	0
58	MG	1a	1822	1/1	0.89	0.14	77,77,77,77	0
58	MG	2A	3322	1/1	0.89	0.24	77,77,77,77	0
58	MG	1a	1631	1/1	0.89	0.22	79,79,79,79	0
58	MG	2A	3168	1/1	0.89	0.21	67,67,67,67	0
58	MG	1A	3339	1/1	0.89	0.20	57,57,57,57	0
58	MG	27	104	1/1	0.89	0.15	70,70,70,70	0
58	MG	1A	4108	1/1	0.89	0.18	70,70,70,70	0
58	MG	2a	1603	1/1	0.89	0.25	68,68,68,68	0
58	MG	2A	3331	1/1	0.89	0.10	72,72,72,72	0
58	MG	1a	1637	1/1	0.89	0.25	59,59,59,59	0
58	MG	2A	3335	1/1	0.89	0.28	63,63,63,63	0
58	MG	2A	3175	1/1	0.89	0.13	66,66,66,66	0
58	MG	1A	3591	1/1	0.89	0.17	76,76,76,76	0
58	MG	2A	3343	1/1	0.89	0.17	70,70,70,70	0
58	MG	2A	3345	1/1	0.89	0.37	79,79,79,79	0
58	MG	2a	1616	1/1	0.89	0.27	75,75,75,75	0
58	MG	1A	3481	1/1	0.89	0.13	62,62,62,62	0
58	MG	2a	1618	1/1	0.89	0.36	75,75,75,75	0
58	MG	2A	3619	1/1	0.89	0.12	74,74,74,74	0
58	MG	1A	3259	1/1	0.89	0.30	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3350	1/1	0.89	0.31	65,65,65,65	0
58	MG	2a	1623	1/1	0.89	0.22	67,67,67,67	0
58	MG	2a	1624	1/1	0.89	0.29	76,76,76,76	0
58	MG	2A	3351	1/1	0.89	0.32	63,63,63,63	0
58	MG	1A	3603	1/1	0.89	0.14	60,60,60,60	0
58	MG	2a	1629	1/1	0.89	0.38	73,73,73,73	0
58	MG	1A	3130	1/1	0.89	0.17	56,56,56,56	0
58	MG	1A	3346	1/1	0.89	0.22	67,67,67,67	0
58	MG	1A	3049	1/1	0.89	0.16	57,57,57,57	0
58	MG	1w	106	1/1	0.89	0.14	82,82,82,82	0
58	MG	2a	1635	1/1	0.89	0.16	82,82,82,82	0
58	MG	1A	3977	1/1	0.89	0.08	46,46,46,46	0
58	MG	1A	3015	1/1	0.89	0.24	55,55,55,55	0
58	MG	2a	1639	1/1	0.89	0.14	76,76,76,76	0
58	MG	2A	3639	1/1	0.89	0.11	69,69,69,69	0
58	MG	2A	3372	1/1	0.89	0.15	60,60,60,60	0
58	MG	1A	3307	1/1	0.89	0.13	51,51,51,51	0
58	MG	2A	3380	1/1	0.89	0.32	74,74,74,74	0
58	MG	2A	3644	1/1	0.89	0.13	68,68,68,68	0
58	MG	2a	1657	1/1	0.89	0.21	67,67,67,67	0
58	MG	2a	1661	1/1	0.89	0.17	58,58,58,58	0
58	MG	2A	3646	1/1	0.89	0.14	64,64,64,64	0
58	MG	1B	233	1/1	0.89	0.12	67,67,67,67	0
58	MG	1B	236	1/1	0.89	0.11	57,57,57,57	0
58	MG	1A	3763	1/1	0.89	0.09	53,53,53,53	0
58	MG	1A	3772	1/1	0.89	0.14	55,55,55,55	0
58	MG	2a	1669	1/1	0.89	0.25	66,66,66,66	0
58	MG	2A	3213	1/1	0.89	0.15	64,64,64,64	0
58	MG	1x	114	1/1	0.89	0.26	70,70,70,70	0
58	MG	2a	1673	1/1	0.89	0.10	63,63,63,63	0
58	MG	1a	1676	1/1	0.89	0.11	72,72,72,72	0
58	MG	2A	3401	1/1	0.89	0.35	72,72,72,72	0
58	MG	2A	3671	1/1	0.89	0.20	52,52,52,52	0
58	MG	1A	3653	1/1	0.89	0.11	34,34,34,34	0
58	MG	2A	3675	1/1	0.89	0.17	76,76,76,76	0
58	MG	2A	3006	1/1	0.89	0.30	66,66,66,66	0
58	MG	2A	3410	1/1	0.89	0.20	75,75,75,75	0
58	MG	1A	3655	1/1	0.89	0.17	45,45,45,45	0
58	MG	2A	3224	1/1	0.89	0.13	56,56,56,56	0
58	MG	2A	3414	1/1	0.89	0.11	58,58,58,58	0
58	MG	1a	1687	1/1	0.89	0.16	69,69,69,69	0
58	MG	2a	1696	1/1	0.89	0.25	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3696	1/1	0.89	0.21	82,82,82,82	0
58	MG	2A	3021	1/1	0.89	0.27	58,58,58,58	0
58	MG	1F	310	1/1	0.89	0.16	62,62,62,62	0
58	MG	2A	3439	1/1	0.89	0.12	38,38,38,38	0
58	MG	2a	1707	1/1	0.89	0.34	68,68,68,68	0
58	MG	2A	3703	1/1	0.89	0.15	71,71,71,71	0
58	MG	2A	3704	1/1	0.89	0.14	68,68,68,68	0
58	MG	2A	3705	1/1	0.89	0.12	69,69,69,69	0
58	MG	1A	3046	1/1	0.89	0.15	55,55,55,55	0
58	MG	2a	1713	1/1	0.89	0.26	63,63,63,63	0
58	MG	1A	3996	1/1	0.89	0.19	73,73,73,73	0
58	MG	2A	3232	1/1	0.89	0.15	66,66,66,66	0
58	MG	1A	3218	1/1	0.89	0.20	67,67,67,67	0
58	MG	2A	3714	1/1	0.89	0.16	63,63,63,63	0
58	MG	1P	205	1/1	0.89	0.18	53,53,53,53	0
58	MG	2A	3237	1/1	0.89	0.12	71,71,71,71	0
58	MG	1A	3898	1/1	0.89	0.09	54,54,54,54	0
58	MG	2A	3240	1/1	0.89	0.15	60,60,60,60	0
58	MG	2A	3739	1/1	0.89	0.15	55,55,55,55	0
58	MG	2A	3474	1/1	0.89	0.14	44,44,44,44	0
58	MG	2A	3743	1/1	0.89	0.09	67,67,67,67	0
58	MG	2a	1744	1/1	0.89	0.13	77,77,77,77	0
58	MG	1a	1705	1/1	0.89	0.27	69,69,69,69	0
58	MG	2A	3243	1/1	0.89	0.11	74,74,74,74	0
58	MG	1A	3377	1/1	0.89	0.26	71,71,71,71	0
58	MG	2A	3485	1/1	0.89	0.15	59,59,59,59	0
58	MG	2A	3052	1/1	0.89	0.10	51,51,51,51	0
58	MG	2A	3053	1/1	0.89	0.14	80,80,80,80	0
58	MG	1A	3661	1/1	0.89	0.19	60,60,60,60	0
58	MG	2A	3495	1/1	0.89	0.24	70,70,70,70	0
58	MG	2A	3767	1/1	0.89	0.18	82,82,82,82	0
58	MG	2A	3252	1/1	0.89	0.16	74,74,74,74	0
58	MG	1A	3514	1/1	0.89	0.12	40,40,40,40	0
58	MG	1A	4015	1/1	0.89	0.13	53,53,53,53	0
58	MG	1A	3519	1/1	0.89	0.10	61,61,61,61	0
58	MG	1A	3668	1/1	0.89	0.17	45,45,45,45	0
58	MG	2A	3262	1/1	0.89	0.21	63,63,63,63	0
58	MG	2A	3508	1/1	0.89	0.18	72,72,72,72	0
58	MG	1A	3790	1/1	0.89	0.16	55,55,55,55	0
58	MG	1A	3253	1/1	0.89	0.21	66,66,66,66	0
58	MG	1A	3095	1/1	0.89	0.18	51,51,51,51	0
58	MG	1A	3385	1/1	0.89	0.27	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3272	1/1	0.89	0.25	78,78,78,78	0
58	MG	1a	1733	1/1	0.89	0.13	62,62,62,62	0
58	MG	1A	3464	1/1	0.89	0.19	63,63,63,63	0
58	MG	2A	3085	1/1	0.89	0.20	69,69,69,69	0
58	MG	1A	3465	1/1	0.89	0.16	48,48,48,48	0
58	MG	1A	3542	1/1	0.89	0.15	69,69,69,69	0
58	MG	1a	1747	1/1	0.89	0.11	69,69,69,69	0
58	MG	1A	3544	1/1	0.89	0.35	68,68,68,68	0
58	MG	2A	3818	1/1	0.89	0.16	70,70,70,70	0
58	MG	1A	3334	1/1	0.89	0.21	65,65,65,65	0
58	MG	2A	3820	1/1	0.89	0.28	79,79,79,79	0
58	MG	1A	3337	1/1	0.89	0.11	57,57,57,57	0
58	MG	2a	1807	1/1	0.89	0.11	78,78,78,78	0
58	MG	2A	3287	1/1	0.89	0.13	63,63,63,63	0
58	MG	1A	4051	1/1	0.89	0.10	68,68,68,68	0
58	MG	1A	3939	1/1	0.89	0.12	56,56,56,56	0
58	MG	2A	3827	1/1	0.89	0.17	70,70,70,70	0
58	MG	2a	1823	1/1	0.89	0.19	79,79,79,79	0
58	MG	16	102	1/1	0.89	0.18	53,53,53,53	0
58	MG	2a	1827	1/1	0.89	0.19	74,74,74,74	0
58	MG	1A	3814	1/1	0.89	0.23	51,51,51,51	0
58	MG	1A	3816	1/1	0.89	0.22	39,39,39,39	0
58	MG	1a	1769	1/1	0.89	0.12	70,70,70,70	0
58	MG	1A	3550	1/1	0.89	0.23	55,55,55,55	0
58	MG	2A	3300	1/1	0.89	0.16	69,69,69,69	0
58	MG	1a	1604	1/1	0.89	0.18	74,74,74,74	0
58	MG	2A	3131	1/1	0.89	0.21	69,69,69,69	0
58	MG	2A	3132	1/1	0.89	0.24	68,68,68,68	0
58	MG	1A	3473	1/1	0.89	0.40	47,47,47,47	0
58	MG	1A	4083	1/1	0.89	0.13	62,62,62,62	0
58	MG	2A	3568	1/1	0.89	0.13	71,71,71,71	0
58	MG	1A	3703	1/1	0.89	0.12	51,51,51,51	0
58	MG	2v	103	1/1	0.89	0.26	72,72,72,72	0
58	MG	2w	101	1/1	0.89	0.11	86,86,86,86	0
58	MG	1A	4089	1/1	0.89	0.17	72,72,72,72	0
58	MG	2A	3140	1/1	0.89	0.17	70,70,70,70	0
58	MG	1A	3565	1/1	0.89	0.09	12,12,12,12	0
58	MG	2x	102	1/1	0.89	0.20	49,49,49,49	0
58	MG	2x	103	1/1	0.89	0.45	77,77,77,77	0
58	MG	2A	3312	1/1	0.89	0.24	79,79,79,79	0
58	MG	1A	3955	1/1	0.89	0.09	50,50,50,50	0
58	MG	2A	3580	1/1	0.89	0.14	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3004	1/1	0.90	0.13	37,37,37,37	0
58	MG	1A	3611	1/1	0.90	0.11	53,53,53,53	0
58	MG	1A	3936	1/1	0.90	0.14	74,74,74,74	0
58	MG	1a	1778	1/1	0.90	0.17	87,87,87,87	0
58	MG	1a	1784	1/1	0.90	0.14	77,77,77,77	0
58	MG	1A	4047	1/1	0.90	0.14	57,57,57,57	0
58	MG	1a	1789	1/1	0.90	0.14	73,73,73,73	0
58	MG	2a	1604	1/1	0.90	0.28	75,75,75,75	0
58	MG	2A	3612	1/1	0.90	0.26	65,65,65,65	0
58	MG	2A	3158	1/1	0.90	0.23	65,65,65,65	0
58	MG	2A	3620	1/1	0.90	0.15	59,59,59,59	0
58	MG	1a	1794	1/1	0.90	0.25	69,69,69,69	0
58	MG	1A	3818	1/1	0.90	0.15	41,41,41,41	0
58	MG	1a	1796	1/1	0.90	0.24	68,68,68,68	0
58	MG	1A	3613	1/1	0.90	0.10	35,35,35,35	0
58	MG	1A	3387	1/1	0.90	0.14	64,64,64,64	0
58	MG	1a	1808	1/1	0.90	0.19	75,75,75,75	0
58	MG	2A	3174	1/1	0.90	0.36	76,76,76,76	0
58	MG	1A	3942	1/1	0.90	0.32	33,33,33,33	0
58	MG	2A	3176	1/1	0.90	0.28	81,81,81,81	0
58	MG	1a	1810	1/1	0.90	0.17	73,73,73,73	0
58	MG	2A	3638	1/1	0.90	0.21	75,75,75,75	0
58	MG	1A	3826	1/1	0.90	0.12	39,39,39,39	0
58	MG	2A	3179	1/1	0.90	0.11	66,66,66,66	0
58	MG	1A	4062	1/1	0.90	0.09	65,65,65,65	0
58	MG	2A	3371	1/1	0.90	0.13	57,57,57,57	0
58	MG	1A	3388	1/1	0.90	0.19	63,63,63,63	0
58	MG	1A	4080	1/1	0.90	0.13	77,77,77,77	0
58	MG	2A	3186	1/1	0.90	0.39	77,77,77,77	0
58	MG	1A	3521	1/1	0.90	0.30	67,67,67,67	0
58	MG	1a	1614	1/1	0.90	0.14	76,76,76,76	0
58	MG	2A	3194	1/1	0.90	0.10	67,67,67,67	0
58	MG	2A	3656	1/1	0.90	0.11	43,43,43,43	0
58	MG	2A	3657	1/1	0.90	0.23	60,60,60,60	0
58	MG	1a	1618	1/1	0.90	0.14	60,60,60,60	0
58	MG	1A	3840	1/1	0.90	0.10	26,26,26,26	0
58	MG	1A	3087	1/1	0.90	0.16	77,77,77,77	0
58	MG	2A	3394	1/1	0.90	0.33	69,69,69,69	0
58	MG	1A	3843	1/1	0.90	0.23	40,40,40,40	0
58	MG	2A	3202	1/1	0.90	0.36	55,55,55,55	0
58	MG	2a	1658	1/1	0.90	0.22	58,58,58,58	0
58	MG	2a	1659	1/1	0.90	0.30	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1660	1/1	0.90	0.16	60,60,60,60	0
58	MG	2A	3405	1/1	0.90	0.12	54,54,54,54	0
58	MG	1A	4094	1/1	0.90	0.10	57,57,57,57	0
58	MG	2A	3205	1/1	0.90	0.21	76,76,76,76	0
58	MG	2A	3679	1/1	0.90	0.15	77,77,77,77	0
58	MG	1l	202	1/1	0.90	0.15	62,62,62,62	0
58	MG	1n	101	1/1	0.90	0.13	59,59,59,59	0
58	MG	1A	3744	1/1	0.90	0.11	48,48,48,48	0
58	MG	1A	3647	1/1	0.90	0.17	57,57,57,57	0
58	MG	2A	3692	1/1	0.90	0.08	51,51,51,51	0
58	MG	2A	3694	1/1	0.90	0.15	72,72,72,72	0
58	MG	1A	3527	1/1	0.90	0.12	44,44,44,44	0
58	MG	1A	3398	1/1	0.90	0.17	55,55,55,55	0
58	MG	2a	1677	1/1	0.90	0.22	80,80,80,80	0
58	MG	1A	3258	1/1	0.90	0.30	67,67,67,67	0
58	MG	2A	3438	1/1	0.90	0.22	65,65,65,65	0
58	MG	2A	3221	1/1	0.90	0.11	75,75,75,75	0
58	MG	1A	3413	1/1	0.90	0.23	47,47,47,47	0
58	MG	1w	104	1/1	0.90	0.14	67,67,67,67	0
58	MG	1a	1639	1/1	0.90	0.17	70,70,70,70	0
58	MG	2A	3225	1/1	0.90	0.11	68,68,68,68	0
58	MG	1a	1640	1/1	0.90	0.25	63,63,63,63	0
58	MG	1a	1643	1/1	0.90	0.15	67,67,67,67	0
58	MG	1a	1645	1/1	0.90	0.16	58,58,58,58	0
58	MG	2a	1699	1/1	0.90	0.24	72,72,72,72	0
58	MG	2A	3715	1/1	0.90	0.13	66,66,66,66	0
58	MG	1A	3855	1/1	0.90	0.09	61,61,61,61	0
58	MG	1A	3314	1/1	0.90	0.19	65,65,65,65	0
58	MG	2A	3231	1/1	0.90	0.26	72,72,72,72	0
58	MG	2A	3723	1/1	0.90	0.21	67,67,67,67	0
58	MG	2A	3726	1/1	0.90	0.11	63,63,63,63	0
58	MG	1A	3290	1/1	0.90	0.29	60,60,60,60	0
58	MG	2A	3736	1/1	0.90	0.12	65,65,65,65	0
58	MG	1A	3864	1/1	0.90	0.20	64,64,64,64	0
58	MG	1B	215	1/1	0.90	0.12	64,64,64,64	0
58	MG	1A	3479	1/1	0.90	0.09	79,79,79,79	0
58	MG	1A	3420	1/1	0.90	0.12	60,60,60,60	0
58	MG	2A	3748	1/1	0.90	0.09	67,67,67,67	0
58	MG	1A	3325	1/1	0.90	0.15	70,70,70,70	0
58	MG	2a	1720	1/1	0.90	0.38	71,71,71,71	0
58	MG	1A	3981	1/1	0.90	0.07	39,39,39,39	0
58	MG	1A	3362	1/1	0.90	0.34	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1B	232	1/1	0.90	0.13	73,73,73,73	0
58	MG	1A	3426	1/1	0.90	0.15	56,56,56,56	0
58	MG	1A	3293	1/1	0.90	0.16	65,65,65,65	0
58	MG	1A	3891	1/1	0.90	0.09	71,71,71,71	0
58	MG	2a	1731	1/1	0.90	0.18	70,70,70,70	0
58	MG	1A	3134	1/1	0.90	0.11	56,56,56,56	0
58	MG	1A	3785	1/1	0.90	0.08	48,48,48,48	0
58	MG	1A	3998	1/1	0.90	0.15	56,56,56,56	0
58	MG	1A	3585	1/1	0.90	0.12	58,58,58,58	0
58	MG	2a	1753	1/1	0.90	0.12	69,69,69,69	0
58	MG	1A	3171	1/1	0.90	0.15	42,42,42,42	0
58	MG	1A	3017	1/1	0.90	0.17	54,54,54,54	0
58	MG	2A	3776	1/1	0.90	0.17	70,70,70,70	0
58	MG	2A	3049	1/1	0.90	0.13	68,68,68,68	0
58	MG	2a	1761	1/1	0.90	0.28	65,65,65,65	0
58	MG	2A	3051	1/1	0.90	0.19	59,59,59,59	0
58	MG	2A	3783	1/1	0.90	0.16	80,80,80,80	0
58	MG	1a	1695	1/1	0.90	0.21	56,56,56,56	0
58	MG	2A	3788	1/1	0.90	0.14	65,65,65,65	0
58	MG	1F	315	1/1	0.90	0.21	57,57,57,57	0
58	MG	2a	1767	1/1	0.90	0.21	62,62,62,62	0
58	MG	2A	3795	1/1	0.90	0.07	81,81,81,81	0
58	MG	1G	202	1/1	0.90	0.16	68,68,68,68	0
58	MG	2A	3803	1/1	0.90	0.11	42,42,42,42	0
58	MG	2A	3056	1/1	0.90	0.27	71,71,71,71	0
58	MG	1a	1702	1/1	0.90	0.11	83,83,83,83	0
58	MG	2A	3059	1/1	0.90	0.14	66,66,66,66	0
58	MG	1I	201	1/1	0.90	0.10	67,67,67,67	0
58	MG	2A	3533	1/1	0.90	0.15	65,65,65,65	0
58	MG	1N	204	1/1	0.90	0.24	52,52,52,52	0
58	MG	2A	3540	1/1	0.90	0.22	51,51,51,51	0
58	MG	2A	3070	1/1	0.90	0.20	61,61,61,61	0
58	MG	1O	201	1/1	0.90	0.13	72,72,72,72	0
58	MG	2A	3549	1/1	0.90	0.16	49,49,49,49	0
58	MG	1a	1712	1/1	0.90	0.20	68,68,68,68	0
58	MG	1O	205	1/1	0.90	0.11	68,68,68,68	0
58	MG	1a	1715	1/1	0.90	0.13	67,67,67,67	0
58	MG	1a	1720	1/1	0.90	0.28	72,72,72,72	0
58	MG	1A	3902	1/1	0.90	0.17	72,72,72,72	0
58	MG	1A	4010	1/1	0.90	0.09	22,22,22,22	0
58	MG	1A	3252	1/1	0.90	0.17	73,73,73,73	0
58	MG	2A	3559	1/1	0.90	0.17	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3451	1/1	0.90	0.16	68,68,68,68	0
58	MG	2A	3296	1/1	0.90	0.15	60,60,60,60	0
58	MG	1A	3689	1/1	0.90	0.11	30,30,30,30	0
58	MG	1A	3602	1/1	0.90	0.10	51,51,51,51	0
58	MG	2a	1820	1/1	0.90	0.11	67,67,67,67	0
58	MG	1R	206	1/1	0.90	0.09	75,75,75,75	0
58	MG	1A	3503	1/1	0.90	0.28	56,56,56,56	0
58	MG	2A	3094	1/1	0.90	0.07	82,82,82,82	0
58	MG	2a	1825	1/1	0.90	0.13	77,77,77,77	0
58	MG	1A	4024	1/1	0.90	0.20	65,65,65,65	0
58	MG	1A	3802	1/1	0.90	0.10	41,41,41,41	0
58	MG	1A	3606	1/1	0.90	0.07	31,31,31,31	0
58	MG	1a	1744	1/1	0.90	0.33	74,74,74,74	0
58	MG	1U	204	1/1	0.90	0.21	42,42,42,42	0
58	MG	2A	3105	1/1	0.90	0.18	73,73,73,73	0
58	MG	1A	3705	1/1	0.90	0.10	24,24,24,24	0
58	MG	2B	220	1/1	0.90	0.11	74,74,74,74	0
58	MG	1a	1748	1/1	0.90	0.20	73,73,73,73	0
58	MG	1A	3708	1/1	0.90	0.13	28,28,28,28	0
58	MG	2A	3314	1/1	0.90	0.30	78,78,78,78	0
58	MG	2t	201	1/1	0.90	0.19	66,66,66,66	0
58	MG	1V	208	1/1	0.90	0.12	55,55,55,55	0
58	MG	1A	4030	1/1	0.90	0.12	61,61,61,61	0
58	MG	2A	3317	1/1	0.90	0.21	70,70,70,70	0
58	MG	2A	3592	1/1	0.90	0.11	59,59,59,59	0
58	MG	2G	201	1/1	0.90	0.18	73,73,73,73	0
58	MG	2O	201	1/1	0.90	0.24	65,65,65,65	0
58	MG	1W	205	1/1	0.90	0.13	32,32,32,32	0
58	MG	1A	4031	1/1	0.90	0.12	73,73,73,73	0
58	MG	2T	202	1/1	0.90	0.16	73,73,73,73	0
58	MG	1A	3810	1/1	0.90	0.09	47,47,47,47	0
58	MG	1A	3608	1/1	0.90	0.07	30,30,30,30	0
58	MG	1a	1766	1/1	0.90	0.17	60,60,60,60	0
58	MG	2A	3332	1/1	0.91	0.15	51,51,51,51	0
58	MG	1A	4004	1/1	0.91	0.11	65,65,65,65	0
58	MG	2Y	201	1/1	0.91	0.23	69,69,69,69	0
58	MG	2A	3334	1/1	0.91	0.25	60,60,60,60	0
58	MG	1A	3173	1/1	0.91	0.18	58,58,58,58	0
58	MG	23	101	1/1	0.91	0.22	67,67,67,67	0
58	MG	1A	3421	1/1	0.91	0.16	50,50,50,50	0
58	MG	26	102	1/1	0.91	0.11	66,66,66,66	0
58	MG	27	102	1/1	0.91	0.10	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3250	1/1	0.91	0.19	49,49,49,49	0
58	MG	2A	3340	1/1	0.91	0.29	71,71,71,71	0
58	MG	28	101	1/1	0.91	0.25	58,58,58,58	0
58	MG	2A	3618	1/1	0.91	0.17	63,63,63,63	0
58	MG	2A	3342	1/1	0.91	0.34	67,67,67,67	0
58	MG	1a	1658	1/1	0.91	0.09	68,68,68,68	0
58	MG	1E	313	1/1	0.91	0.07	38,38,38,38	0
58	MG	2A	3622	1/1	0.91	0.16	58,58,58,58	0
58	MG	1F	304	1/1	0.91	0.14	63,63,63,63	0
58	MG	1A	3801	1/1	0.91	0.12	35,35,35,35	0
58	MG	1F	311	1/1	0.91	0.10	65,65,65,65	0
58	MG	2A	3630	1/1	0.91	0.11	59,59,59,59	0
58	MG	1A	3348	1/1	0.91	0.12	59,59,59,59	0
58	MG	1A	4016	1/1	0.91	0.17	70,70,70,70	0
58	MG	1A	3109	1/1	0.91	0.16	60,60,60,60	0
58	MG	2A	3355	1/1	0.91	0.25	57,57,57,57	0
58	MG	2a	1619	1/1	0.91	0.34	63,63,63,63	0
58	MG	1A	3177	1/1	0.91	0.14	51,51,51,51	0
58	MG	2A	3357	1/1	0.91	0.42	77,77,77,77	0
58	MG	1A	3918	1/1	0.91	0.07	81,81,81,81	0
58	MG	2A	3359	1/1	0.91	0.25	59,59,59,59	0
58	MG	1a	1678	1/1	0.91	0.34	61,61,61,61	0
58	MG	2a	1625	1/1	0.91	0.30	70,70,70,70	0
58	MG	2A	3641	1/1	0.91	0.13	45,45,45,45	0
58	MG	2A	3362	1/1	0.91	0.11	50,50,50,50	0
58	MG	2A	3193	1/1	0.91	0.27	72,72,72,72	0
58	MG	1A	3919	1/1	0.91	0.11	52,52,52,52	0
58	MG	2A	3367	1/1	0.91	0.23	58,58,58,58	0
58	MG	1A	3704	1/1	0.91	0.17	60,60,60,60	0
58	MG	2a	1633	1/1	0.91	0.08	63,63,63,63	0
58	MG	1w	107	1/1	0.91	0.11	59,59,59,59	0
58	MG	1a	1681	1/1	0.91	0.20	70,70,70,70	0
58	MG	1x	101	1/1	0.91	0.31	70,70,70,70	0
58	MG	2A	3654	1/1	0.91	0.11	66,66,66,66	0
58	MG	1x	102	1/1	0.91	0.26	73,73,73,73	0
58	MG	2a	1640	1/1	0.91	0.09	69,69,69,69	0
58	MG	1a	1682	1/1	0.91	0.22	69,69,69,69	0
58	MG	2A	3658	1/1	0.91	0.38	58,58,58,58	0
58	MG	1a	1683	1/1	0.91	0.37	67,67,67,67	0
58	MG	1a	1684	1/1	0.91	0.24	58,58,58,58	0
58	MG	2A	3664	1/1	0.91	0.17	77,77,77,77	0
58	MG	1A	3298	1/1	0.91	0.23	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3666	1/1	0.91	0.21	67,67,67,67	0
58	MG	2A	3209	1/1	0.91	0.15	54,54,54,54	0
58	MG	2A	3393	1/1	0.91	0.15	71,71,71,71	0
58	MG	2A	3673	1/1	0.91	0.25	63,63,63,63	0
58	MG	1a	1689	1/1	0.91	0.22	60,60,60,60	0
58	MG	1A	3363	1/1	0.91	0.15	69,69,69,69	0
58	MG	2A	3400	1/1	0.91	0.10	60,60,60,60	0
58	MG	1x	113	1/1	0.91	0.21	71,71,71,71	0
58	MG	2A	3218	1/1	0.91	0.45	86,86,86,86	0
58	MG	1A	3505	1/1	0.91	0.10	58,58,58,58	0
58	MG	1A	3928	1/1	0.91	0.08	34,34,34,34	0
58	MG	1A	3018	1/1	0.91	0.13	54,54,54,54	0
58	MG	2a	1672	1/1	0.91	0.14	64,64,64,64	0
58	MG	1A	3509	1/1	0.91	0.10	65,65,65,65	0
58	MG	1A	3719	1/1	0.91	0.09	20,20,20,20	0
58	MG	2A	3008	1/1	0.91	0.23	66,66,66,66	0
58	MG	2A	3695	1/1	0.91	0.13	59,59,59,59	0
58	MG	1a	1700	1/1	0.91	0.19	63,63,63,63	0
58	MG	1A	3372	1/1	0.91	0.11	53,53,53,53	0
58	MG	1S	201	1/1	0.91	0.29	59,59,59,59	0
58	MG	1A	3518	1/1	0.91	0.18	73,73,73,73	0
58	MG	1A	3131	1/1	0.91	0.18	44,44,44,44	0
58	MG	1A	3633	1/1	0.91	0.11	65,65,65,65	0
58	MG	1A	3374	1/1	0.91	0.18	65,65,65,65	0
58	MG	2A	3445	1/1	0.91	0.13	61,61,61,61	0
58	MG	1A	3084	1/1	0.91	0.22	69,69,69,69	0
58	MG	2A	3045	1/1	0.91	0.09	47,47,47,47	0
58	MG	2A	3450	1/1	0.91	0.08	56,56,56,56	0
58	MG	1a	1716	1/1	0.91	0.10	62,62,62,62	0
58	MG	2a	1702	1/1	0.91	0.24	59,59,59,59	0
58	MG	1A	3745	1/1	0.91	0.08	50,50,50,50	0
58	MG	1A	3085	1/1	0.91	0.16	68,68,68,68	0
58	MG	2a	1705	1/1	0.91	0.25	68,68,68,68	0
58	MG	1A	3014	1/1	0.91	0.17	50,50,50,50	0
58	MG	2A	3241	1/1	0.91	0.15	62,62,62,62	0
58	MG	1A	3264	1/1	0.91	0.16	63,63,63,63	0
58	MG	1A	4067	1/1	0.91	0.13	61,61,61,61	0
58	MG	2A	3732	1/1	0.91	0.10	56,56,56,56	0
58	MG	2A	3054	1/1	0.91	0.09	74,74,74,74	0
58	MG	2A	3484	1/1	0.91	0.13	46,46,46,46	0
58	MG	1A	3149	1/1	0.91	0.12	61,61,61,61	0
58	MG	2a	1715	1/1	0.91	0.33	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1X	103	1/1	0.91	0.21	47,47,47,47	0
58	MG	1A	3759	1/1	0.91	0.17	70,70,70,70	0
58	MG	10	104	1/1	0.91	0.11	49,49,49,49	0
58	MG	2A	3493	1/1	0.91	0.13	62,62,62,62	0
58	MG	1A	4081	1/1	0.91	0.14	47,47,47,47	0
58	MG	1A	3961	1/1	0.91	0.12	78,78,78,78	0
58	MG	2A	3255	1/1	0.91	0.18	72,72,72,72	0
58	MG	2A	3760	1/1	0.91	0.14	69,69,69,69	0
58	MG	2A	3257	1/1	0.91	0.21	71,71,71,71	0
58	MG	2A	3068	1/1	0.91	0.16	62,62,62,62	0
58	MG	1a	1737	1/1	0.91	0.28	67,67,67,67	0
58	MG	1A	3056	1/1	0.91	0.14	54,54,54,54	0
58	MG	2a	1735	1/1	0.91	0.11	86,86,86,86	0
58	MG	2a	1738	1/1	0.91	0.23	60,60,60,60	0
58	MG	2A	3263	1/1	0.91	0.15	67,67,67,67	0
58	MG	2A	3264	1/1	0.91	0.18	61,61,61,61	0
58	MG	1a	1743	1/1	0.91	0.13	66,66,66,66	0
58	MG	1A	3540	1/1	0.91	0.29	67,67,67,67	0
58	MG	1A	3770	1/1	0.91	0.07	41,41,41,41	0
58	MG	2a	1755	1/1	0.91	0.24	66,66,66,66	0
58	MG	2A	3269	1/1	0.91	0.17	60,60,60,60	0
58	MG	1A	3659	1/1	0.91	0.12	50,50,50,50	0
58	MG	2A	3777	1/1	0.91	0.12	70,70,70,70	0
58	MG	2A	3779	1/1	0.91	0.16	61,61,61,61	0
58	MG	15	108	1/1	0.91	0.13	64,64,64,64	0
58	MG	1A	3660	1/1	0.91	0.08	67,67,67,67	0
58	MG	2A	3083	1/1	0.91	0.10	51,51,51,51	0
58	MG	1A	3159	1/1	0.91	0.18	37,37,37,37	0
58	MG	1a	1752	1/1	0.91	0.27	60,60,60,60	0
58	MG	2A	3789	1/1	0.91	0.12	69,69,69,69	0
58	MG	19	101	1/1	0.91	0.28	60,60,60,60	0
58	MG	1A	4102	1/1	0.91	0.15	83,83,83,83	0
58	MG	1A	3543	1/1	0.91	0.12	66,66,66,66	0
58	MG	2A	3282	1/1	0.91	0.14	72,72,72,72	0
58	MG	2A	3804	1/1	0.91	0.10	63,63,63,63	0
58	MG	2A	3283	1/1	0.91	0.10	58,58,58,58	0
58	MG	2A	3545	1/1	0.91	0.16	65,65,65,65	0
58	MG	1A	3779	1/1	0.91	0.21	53,53,53,53	0
58	MG	2a	1779	1/1	0.91	0.16	71,71,71,71	0
58	MG	1A	3877	1/1	0.91	0.11	75,75,75,75	0
58	MG	1a	1761	1/1	0.91	0.11	70,70,70,70	0
58	MG	1a	1607	1/1	0.91	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3882	1/1	0.91	0.13	59,59,59,59	0
58	MG	1B	201	1/1	0.91	0.17	66,66,66,66	0
58	MG	2A	3292	1/1	0.91	0.18	68,68,68,68	0
58	MG	2A	3555	1/1	0.91	0.20	52,52,52,52	0
58	MG	2a	1792	1/1	0.91	0.24	72,72,72,72	0
58	MG	1A	3335	1/1	0.91	0.14	67,67,67,67	0
58	MG	1a	1771	1/1	0.91	0.13	52,52,52,52	0
58	MG	1B	204	1/1	0.91	0.35	73,73,73,73	0
58	MG	1a	1781	1/1	0.91	0.09	72,72,72,72	0
58	MG	2A	3824	1/1	0.91	0.22	68,68,68,68	0
58	MG	1A	3478	1/1	0.91	0.12	62,62,62,62	0
58	MG	1A	3038	1/1	0.91	0.09	38,38,38,38	0
58	MG	1a	1788	1/1	0.91	0.14	61,61,61,61	0
58	MG	1B	213	1/1	0.91	0.23	69,69,69,69	0
58	MG	2a	1813	1/1	0.91	0.20	75,75,75,75	0
58	MG	1A	3672	1/1	0.91	0.12	57,57,57,57	0
58	MG	2a	1819	1/1	0.91	0.22	76,76,76,76	0
58	MG	1A	3987	1/1	0.91	0.08	32,32,32,32	0
58	MG	2A	3137	1/1	0.91	0.23	56,56,56,56	0
58	MG	1B	219	1/1	0.91	0.16	52,52,52,52	0
58	MG	1a	1798	1/1	0.91	0.22	73,73,73,73	0
58	MG	1a	1799	1/1	0.91	0.09	66,66,66,66	0
58	MG	1a	1633	1/1	0.91	0.38	70,70,70,70	0
58	MG	2A	3145	1/1	0.91	0.14	68,68,68,68	0
58	MG	2A	3577	1/1	0.91	0.19	74,74,74,74	0
58	MG	2A	3578	1/1	0.91	0.28	45,45,45,45	0
58	MG	2A	3579	1/1	0.91	0.12	56,56,56,56	0
58	MG	1A	3163	1/1	0.91	0.10	52,52,52,52	0
58	MG	2d	302	1/1	0.91	0.21	68,68,68,68	0
58	MG	1A	3557	1/1	0.91	0.14	63,63,63,63	0
58	MG	2A	3150	1/1	0.91	0.15	76,76,76,76	0
58	MG	2l	203	1/1	0.91	0.12	74,74,74,74	0
58	MG	1A	3043	1/1	0.91	0.10	42,42,42,42	0
58	MG	2A	3155	1/1	0.91	0.20	78,78,78,78	0
58	MG	1A	3482	1/1	0.91	0.13	61,61,61,61	0
58	MG	1A	3096	1/1	0.91	0.29	58,58,58,58	0
58	MG	2A	3590	1/1	0.91	0.20	78,78,78,78	0
58	MG	1A	3999	1/1	0.91	0.15	64,64,64,64	0
58	MG	2A	3159	1/1	0.91	0.09	70,70,70,70	0
58	MG	2F	304	1/1	0.91	0.12	60,60,60,60	0
58	MG	2F	306	1/1	0.91	0.13	54,54,54,54	0
58	MG	1A	3573	1/1	0.91	0.08	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3324	1/1	0.91	0.12	82,82,82,82	0
58	MG	2A	3598	1/1	0.91	0.11	71,71,71,71	0
58	MG	1B	235	1/1	0.91	0.24	76,76,76,76	0
58	MG	2x	104	1/1	0.91	0.09	68,68,68,68	0
58	MG	2A	3164	1/1	0.91	0.10	59,59,59,59	0
58	MG	2A	3166	1/1	0.91	0.13	53,53,53,53	0
58	MG	2x	107	1/1	0.91	0.09	57,57,57,57	0
58	MG	1A	3903	1/1	0.91	0.09	51,51,51,51	0
59	K	2A	3368	1/1	0.91	0.13	73,73,73,73	0
58	MG	1a	1805	1/1	0.92	0.09	76,76,76,76	0
58	MG	1A	4096	1/1	0.92	0.11	53,53,53,53	0
58	MG	2A	3339	1/1	0.92	0.36	72,72,72,72	0
58	MG	1A	3459	1/1	0.92	0.08	63,63,63,63	0
58	MG	1A	3340	1/1	0.92	0.25	54,54,54,54	0
58	MG	2A	3613	1/1	0.92	0.13	67,67,67,67	0
58	MG	2A	3617	1/1	0.92	0.09	43,43,43,43	0
58	MG	1A	3088	1/1	0.92	0.24	50,50,50,50	0
58	MG	2A	3344	1/1	0.92	0.15	65,65,65,65	0
58	MG	1A	4103	1/1	0.92	0.08	58,58,58,58	0
58	MG	1A	3391	1/1	0.92	0.13	72,72,72,72	0
58	MG	1A	3676	1/1	0.92	0.07	47,47,47,47	0
58	MG	1A	3235	1/1	0.92	0.18	58,58,58,58	0
58	MG	1A	3680	1/1	0.92	0.09	69,69,69,69	0
58	MG	2A	3626	1/1	0.92	0.12	47,47,47,47	0
58	MG	1A	4110	1/1	0.92	0.14	57,57,57,57	0
58	MG	1A	4112	1/1	0.92	0.16	55,55,55,55	0
58	MG	1A	3194	1/1	0.92	0.11	65,65,65,65	0
58	MG	1A	3553	1/1	0.92	0.11	65,65,65,65	0
58	MG	2A	3180	1/1	0.92	0.10	78,78,78,78	0
58	MG	1A	3401	1/1	0.92	0.10	60,60,60,60	0
58	MG	1e	202	1/1	0.92	0.22	63,63,63,63	0
58	MG	2A	3184	1/1	0.92	0.34	68,68,68,68	0
58	MG	1A	3402	1/1	0.92	0.17	59,59,59,59	0
58	MG	1A	3562	1/1	0.92	0.17	59,59,59,59	0
58	MG	1a	1652	1/1	0.92	0.20	62,62,62,62	0
58	MG	2A	3189	1/1	0.92	0.37	71,71,71,71	0
58	MG	2A	3190	1/1	0.92	0.12	64,64,64,64	0
58	MG	1A	3815	1/1	0.92	0.10	45,45,45,45	0
58	MG	2A	3373	1/1	0.92	0.15	70,70,70,70	0
58	MG	2A	3645	1/1	0.92	0.07	81,81,81,81	0
58	MG	1A	3958	1/1	0.92	0.11	51,51,51,51	0
58	MG	2a	1628	1/1	0.92	0.13	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3477	1/1	0.92	0.13	64,64,64,64	0
58	MG	1B	218	1/1	0.92	0.09	57,57,57,57	0
58	MG	1A	3695	1/1	0.92	0.15	47,47,47,47	0
58	MG	2A	3386	1/1	0.92	0.23	66,66,66,66	0
58	MG	1A	3568	1/1	0.92	0.11	64,64,64,64	0
58	MG	1a	1663	1/1	0.92	0.12	70,70,70,70	0
58	MG	1A	3823	1/1	0.92	0.16	38,38,38,38	0
58	MG	2a	1636	1/1	0.92	0.34	77,77,77,77	0
58	MG	1a	1665	1/1	0.92	0.32	80,80,80,80	0
58	MG	1A	3405	1/1	0.92	0.10	73,73,73,73	0
58	MG	1A	3406	1/1	0.92	0.12	50,50,50,50	0
58	MG	1A	3828	1/1	0.92	0.11	43,43,43,43	0
58	MG	2A	3399	1/1	0.92	0.21	54,54,54,54	0
58	MG	1A	3238	1/1	0.92	0.26	67,67,67,67	0
58	MG	2A	3667	1/1	0.92	0.19	63,63,63,63	0
58	MG	2A	3210	1/1	0.92	0.15	64,64,64,64	0
58	MG	2a	1655	1/1	0.92	0.19	58,58,58,58	0
58	MG	1A	3831	1/1	0.92	0.14	40,40,40,40	0
58	MG	1A	3832	1/1	0.92	0.10	33,33,33,33	0
58	MG	1A	3410	1/1	0.92	0.25	47,47,47,47	0
58	MG	1A	3836	1/1	0.92	0.10	36,36,36,36	0
58	MG	1A	3838	1/1	0.92	0.09	29,29,29,29	0
58	MG	1E	308	1/1	0.92	0.07	26,26,26,26	0
58	MG	2a	1662	1/1	0.92	0.28	57,57,57,57	0
58	MG	1x	112	1/1	0.92	0.08	71,71,71,71	0
58	MG	1A	3706	1/1	0.92	0.12	50,50,50,50	0
58	MG	2A	3416	1/1	0.92	0.22	66,66,66,66	0
58	MG	1A	3154	1/1	0.92	0.28	61,61,61,61	0
58	MG	2A	3688	1/1	0.92	0.08	38,38,38,38	0
58	MG	2A	3001	1/1	0.92	0.34	69,69,69,69	0
58	MG	2A	3431	1/1	0.92	0.08	74,74,74,74	0
58	MG	2A	3433	1/1	0.92	0.14	70,70,70,70	0
58	MG	2A	3434	1/1	0.92	0.09	42,42,42,42	0
58	MG	2A	3003	1/1	0.92	0.19	56,56,56,56	0
58	MG	1A	3278	1/1	0.92	0.07	45,45,45,45	0
58	MG	2A	3440	1/1	0.92	0.12	71,71,71,71	0
58	MG	2A	3700	1/1	0.92	0.14	60,60,60,60	0
58	MG	1A	3415	1/1	0.92	0.19	50,50,50,50	0
58	MG	1a	1686	1/1	0.92	0.11	63,63,63,63	0
58	MG	2a	1682	1/1	0.92	0.20	72,72,72,72	0
58	MG	1F	306	1/1	0.92	0.15	43,43,43,43	0
58	MG	2a	1687	1/1	0.92	0.32	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1688	1/1	0.92	0.31	64,64,64,64	0
58	MG	1a	1688	1/1	0.92	0.20	62,62,62,62	0
58	MG	1A	3845	1/1	0.92	0.12	34,34,34,34	0
58	MG	2A	3707	1/1	0.92	0.12	69,69,69,69	0
58	MG	1A	3716	1/1	0.92	0.08	37,37,37,37	0
58	MG	2A	3709	1/1	0.92	0.11	92,92,92,92	0
58	MG	2A	3451	1/1	0.92	0.12	51,51,51,51	0
58	MG	1A	3312	1/1	0.92	0.16	60,60,60,60	0
58	MG	2A	3460	1/1	0.92	0.15	52,52,52,52	0
58	MG	1A	3417	1/1	0.92	0.17	66,66,66,66	0
58	MG	1a	1694	1/1	0.92	0.18	67,67,67,67	0
58	MG	1A	3722	1/1	0.92	0.19	67,67,67,67	0
58	MG	2A	3718	1/1	0.92	0.09	44,44,44,44	0
58	MG	2A	3471	1/1	0.92	0.11	65,65,65,65	0
58	MG	1A	3726	1/1	0.92	0.12	36,36,36,36	0
58	MG	2A	3475	1/1	0.92	0.10	47,47,47,47	0
58	MG	2A	3039	1/1	0.92	0.16	60,60,60,60	0
58	MG	2A	3042	1/1	0.92	0.15	51,51,51,51	0
58	MG	1G	203	1/1	0.92	0.14	72,72,72,72	0
58	MG	2A	3737	1/1	0.92	0.09	43,43,43,43	0
58	MG	1A	3727	1/1	0.92	0.11	61,61,61,61	0
58	MG	2A	3046	1/1	0.92	0.25	77,77,77,77	0
58	MG	2A	3249	1/1	0.92	0.12	73,73,73,73	0
58	MG	2a	1716	1/1	0.92	0.22	66,66,66,66	0
58	MG	1A	3419	1/1	0.92	0.13	59,59,59,59	0
58	MG	1A	3492	1/1	0.92	0.13	66,66,66,66	0
58	MG	2A	3490	1/1	0.92	0.25	60,60,60,60	0
58	MG	1A	3863	1/1	0.92	0.14	39,39,39,39	0
58	MG	1A	3245	1/1	0.92	0.15	58,58,58,58	0
58	MG	2A	3755	1/1	0.92	0.11	65,65,65,65	0
58	MG	1a	1707	1/1	0.92	0.12	70,70,70,70	0
58	MG	2A	3761	1/1	0.92	0.10	58,58,58,58	0
58	MG	1a	1708	1/1	0.92	0.13	55,55,55,55	0
58	MG	1a	1709	1/1	0.92	0.12	75,75,75,75	0
58	MG	2A	3503	1/1	0.92	0.22	62,62,62,62	0
58	MG	1A	3055	1/1	0.92	0.12	54,54,54,54	0
58	MG	2A	3260	1/1	0.92	0.14	64,64,64,64	0
58	MG	2a	1737	1/1	0.92	0.10	53,53,53,53	0
58	MG	2A	3506	1/1	0.92	0.10	45,45,45,45	0
58	MG	1A	4011	1/1	0.92	0.14	73,73,73,73	0
58	MG	1Q	204	1/1	0.92	0.17	72,72,72,72	0
58	MG	1A	3742	1/1	0.92	0.15	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1751	1/1	0.92	0.17	60,60,60,60	0
58	MG	1A	3870	1/1	0.92	0.09	66,66,66,66	0
58	MG	2A	3774	1/1	0.92	0.14	64,64,64,64	0
58	MG	2A	3775	1/1	0.92	0.13	73,73,73,73	0
58	MG	1A	3118	1/1	0.92	0.25	44,44,44,44	0
58	MG	2a	1757	1/1	0.92	0.16	57,57,57,57	0
58	MG	1A	3502	1/1	0.92	0.21	45,45,45,45	0
58	MG	1A	3618	1/1	0.92	0.09	45,45,45,45	0
58	MG	2A	3268	1/1	0.92	0.13	68,68,68,68	0
58	MG	1A	3883	1/1	0.92	0.08	44,44,44,44	0
58	MG	1A	3885	1/1	0.92	0.11	71,71,71,71	0
58	MG	1A	3175	1/1	0.92	0.11	77,77,77,77	0
58	MG	2A	3522	1/1	0.92	0.23	52,52,52,52	0
58	MG	1A	3330	1/1	0.92	0.09	59,59,59,59	0
58	MG	1U	203	1/1	0.92	0.19	56,56,56,56	0
58	MG	2A	3526	1/1	0.92	0.14	66,66,66,66	0
58	MG	2A	3797	1/1	0.92	0.08	74,74,74,74	0
58	MG	2A	3528	1/1	0.92	0.10	50,50,50,50	0
58	MG	1a	1731	1/1	0.92	0.10	64,64,64,64	0
58	MG	1A	3749	1/1	0.92	0.07	25,25,25,25	0
58	MG	1A	3750	1/1	0.92	0.08	21,21,21,21	0
58	MG	2A	3084	1/1	0.92	0.16	54,54,54,54	0
58	MG	1A	3636	1/1	0.92	0.13	34,34,34,34	0
58	MG	1A	3755	1/1	0.92	0.10	52,52,52,52	0
58	MG	1W	201	1/1	0.92	0.27	63,63,63,63	0
58	MG	1A	3637	1/1	0.92	0.13	30,30,30,30	0
58	MG	2a	1783	1/1	0.92	0.16	71,71,71,71	0
58	MG	1A	3082	1/1	0.92	0.11	46,46,46,46	0
58	MG	1A	3760	1/1	0.92	0.14	32,32,32,32	0
58	MG	1A	3640	1/1	0.92	0.10	67,67,67,67	0
58	MG	1X	104	1/1	0.92	0.12	49,49,49,49	0
58	MG	1A	3376	1/1	0.92	0.15	51,51,51,51	0
58	MG	2A	3099	1/1	0.92	0.24	69,69,69,69	0
58	MG	1A	3645	1/1	0.92	0.11	33,33,33,33	0
58	MG	2A	3822	1/1	0.92	0.14	56,56,56,56	0
58	MG	10	105	1/1	0.92	0.27	62,62,62,62	0
58	MG	1A	3291	1/1	0.92	0.14	58,58,58,58	0
58	MG	1A	3649	1/1	0.92	0.10	29,29,29,29	0
58	MG	1A	3433	1/1	0.92	0.14	57,57,57,57	0
58	MG	2A	3110	1/1	0.92	0.29	71,71,71,71	0
58	MG	1a	1759	1/1	0.92	0.08	81,81,81,81	0
58	MG	1A	3911	1/1	0.92	0.13	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1810	1/1	0.92	0.15	73,73,73,73	0
58	MG	2a	1811	1/1	0.92	0.14	64,64,64,64	0
58	MG	2A	3118	1/1	0.92	0.18	64,64,64,64	0
58	MG	2A	3121	1/1	0.92	0.11	52,52,52,52	0
58	MG	2A	3123	1/1	0.92	0.25	50,50,50,50	0
58	MG	2A	3126	1/1	0.92	0.28	54,54,54,54	0
58	MG	2A	3127	1/1	0.92	0.25	66,66,66,66	0
58	MG	1A	3216	1/1	0.92	0.14	51,51,51,51	0
58	MG	1a	1762	1/1	0.92	0.09	62,62,62,62	0
58	MG	2A	3311	1/1	0.92	0.30	70,70,70,70	0
58	MG	1A	3439	1/1	0.92	0.18	52,52,52,52	0
58	MG	2a	1828	1/1	0.92	0.12	69,69,69,69	0
58	MG	2B	214	1/1	0.92	0.22	71,71,71,71	0
58	MG	1A	3443	1/1	0.92	0.26	40,40,40,40	0
58	MG	1A	4068	1/1	0.92	0.19	71,71,71,71	0
58	MG	18	101	1/1	0.92	0.20	62,62,62,62	0
58	MG	1A	4071	1/1	0.92	0.15	65,65,65,65	0
58	MG	1A	3382	1/1	0.92	0.19	49,49,49,49	0
58	MG	2D	301	1/1	0.92	0.19	51,51,51,51	0
58	MG	2A	3318	1/1	0.92	0.10	65,65,65,65	0
58	MG	2A	3585	1/1	0.92	0.10	49,49,49,49	0
58	MG	1A	4078	1/1	0.92	0.06	81,81,81,81	0
58	MG	1A	3383	1/1	0.92	0.15	70,70,70,70	0
58	MG	1A	3530	1/1	0.92	0.19	46,46,46,46	0
58	MG	2F	301	1/1	0.92	0.20	52,52,52,52	0
58	MG	1a	1786	1/1	0.92	0.10	78,78,78,78	0
58	MG	2F	303	1/1	0.92	0.09	71,71,71,71	0
58	MG	1A	3452	1/1	0.92	0.12	55,55,55,55	0
58	MG	1A	3217	1/1	0.92	0.17	40,40,40,40	0
58	MG	2A	3151	1/1	0.92	0.45	72,72,72,72	0
58	MG	2A	3152	1/1	0.92	0.14	53,53,53,53	0
58	MG	1A	3664	1/1	0.92	0.14	47,47,47,47	0
58	MG	2P	201	1/1	0.92	0.13	61,61,61,61	0
58	MG	2Q	202	1/1	0.92	0.16	56,56,56,56	0
58	MG	2A	3329	1/1	0.92	0.07	69,69,69,69	0
58	MG	1a	1610	1/1	0.92	0.15	55,55,55,55	0
58	MG	1A	3455	1/1	0.92	0.21	35,35,35,35	0
58	MG	1A	3144	1/1	0.92	0.14	42,42,42,42	0
58	MG	1a	1615	1/1	0.92	0.21	67,67,67,67	0
58	MG	1A	4095	1/1	0.92	0.12	51,51,51,51	0
58	MG	1A	3126	1/1	0.93	0.12	51,51,51,51	0
58	MG	2A	3663	1/1	0.93	0.09	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1a	1714	1/1	0.93	0.12	59,59,59,59	0
58	MG	2a	1613	1/1	0.93	0.18	81,81,81,81	0
58	MG	1S	202	1/1	0.93	0.15	62,62,62,62	0
58	MG	2a	1615	1/1	0.93	0.14	62,62,62,62	0
58	MG	1A	3476	1/1	0.93	0.10	56,56,56,56	0
58	MG	1a	1718	1/1	0.93	0.13	46,46,46,46	0
58	MG	2A	3442	1/1	0.93	0.12	60,60,60,60	0
58	MG	2A	3669	1/1	0.93	0.09	46,46,46,46	0
58	MG	1A	3774	1/1	0.93	0.22	54,54,54,54	0
58	MG	1A	3775	1/1	0.93	0.17	63,63,63,63	0
58	MG	1A	3666	1/1	0.93	0.20	55,55,55,55	0
58	MG	1A	3552	1/1	0.93	0.10	43,43,43,43	0
58	MG	1A	3900	1/1	0.93	0.12	58,58,58,58	0
58	MG	1A	3901	1/1	0.93	0.08	52,52,52,52	0
58	MG	2A	3452	1/1	0.93	0.10	53,53,53,53	0
58	MG	1A	4043	1/1	0.93	0.10	58,58,58,58	0
58	MG	1A	3317	1/1	0.93	0.18	57,57,57,57	0
58	MG	1A	3556	1/1	0.93	0.09	37,37,37,37	0
58	MG	1A	4048	1/1	0.93	0.13	52,52,52,52	0
58	MG	2A	3689	1/1	0.93	0.13	63,63,63,63	0
58	MG	2A	3690	1/1	0.93	0.10	69,69,69,69	0
58	MG	1A	4050	1/1	0.93	0.12	66,66,66,66	0
58	MG	2A	3075	1/1	0.93	0.09	62,62,62,62	0
58	MG	1A	3671	1/1	0.93	0.07	52,52,52,52	0
58	MG	1A	3369	1/1	0.93	0.18	52,52,52,52	0
58	MG	2A	3476	1/1	0.93	0.06	41,41,41,41	0
58	MG	2A	3477	1/1	0.93	0.26	66,66,66,66	0
58	MG	1a	1739	1/1	0.93	0.24	77,77,77,77	0
58	MG	1A	3370	1/1	0.93	0.09	49,49,49,49	0
58	MG	1A	3559	1/1	0.93	0.12	64,64,64,64	0
58	MG	2A	3482	1/1	0.93	0.17	52,52,52,52	0
58	MG	2a	1643	1/1	0.93	0.21	57,57,57,57	0
58	MG	2a	1648	1/1	0.93	0.20	65,65,65,65	0
58	MG	1A	3193	1/1	0.93	0.14	43,43,43,43	0
58	MG	1A	3284	1/1	0.93	0.09	61,61,61,61	0
58	MG	10	107	1/1	0.93	0.10	63,63,63,63	0
58	MG	10	108	1/1	0.93	0.09	49,49,49,49	0
58	MG	1A	3915	1/1	0.93	0.15	66,66,66,66	0
58	MG	1A	3326	1/1	0.93	0.11	58,58,58,58	0
58	MG	2A	3491	1/1	0.93	0.17	70,70,70,70	0
58	MG	1A	3050	1/1	0.93	0.10	58,58,58,58	0
58	MG	1A	3572	1/1	0.93	0.12	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	4073	1/1	0.93	0.09	44,44,44,44	0
58	MG	1A	4076	1/1	0.93	0.26	41,41,41,41	0
58	MG	1A	4077	1/1	0.93	0.19	35,35,35,35	0
58	MG	1A	3793	1/1	0.93	0.12	55,55,55,55	0
58	MG	1A	3424	1/1	0.93	0.20	62,62,62,62	0
58	MG	1A	3578	1/1	0.93	0.06	45,45,45,45	0
58	MG	2A	3724	1/1	0.93	0.10	49,49,49,49	0
58	MG	1A	3798	1/1	0.93	0.12	63,63,63,63	0
58	MG	1A	3328	1/1	0.93	0.14	72,72,72,72	0
58	MG	2A	3109	1/1	0.93	0.23	70,70,70,70	0
58	MG	1A	4087	1/1	0.93	0.15	65,65,65,65	0
58	MG	2A	3112	1/1	0.93	0.10	54,54,54,54	0
58	MG	2a	1675	1/1	0.93	0.18	71,71,71,71	0
58	MG	2A	3738	1/1	0.93	0.08	61,61,61,61	0
58	MG	1a	1603	1/1	0.93	0.14	63,63,63,63	0
58	MG	2A	3291	1/1	0.93	0.13	72,72,72,72	0
58	MG	1A	3378	1/1	0.93	0.08	55,55,55,55	0
58	MG	2a	1681	1/1	0.93	0.34	69,69,69,69	0
58	MG	2A	3517	1/1	0.93	0.12	71,71,71,71	0
58	MG	2a	1685	1/1	0.93	0.20	58,58,58,58	0
58	MG	2A	3746	1/1	0.93	0.09	39,39,39,39	0
58	MG	2A	3747	1/1	0.93	0.09	81,81,81,81	0
58	MG	2A	3117	1/1	0.93	0.13	52,52,52,52	0
58	MG	1a	1605	1/1	0.93	0.17	68,68,68,68	0
58	MG	2a	1690	1/1	0.93	0.10	73,73,73,73	0
58	MG	1a	1772	1/1	0.93	0.09	70,70,70,70	0
58	MG	2A	3751	1/1	0.93	0.08	55,55,55,55	0
58	MG	1A	3693	1/1	0.93	0.17	56,56,56,56	0
58	MG	1A	4093	1/1	0.93	0.11	66,66,66,66	0
58	MG	2A	3756	1/1	0.93	0.14	50,50,50,50	0
58	MG	1A	3590	1/1	0.93	0.12	63,63,63,63	0
58	MG	1A	3934	1/1	0.93	0.14	64,64,64,64	0
58	MG	1A	3804	1/1	0.93	0.22	41,41,41,41	0
58	MG	2a	1701	1/1	0.93	0.28	64,64,64,64	0
58	MG	2A	3527	1/1	0.93	0.13	79,79,79,79	0
58	MG	1A	3287	1/1	0.93	0.24	59,59,59,59	0
58	MG	1A	3699	1/1	0.93	0.11	53,53,53,53	0
58	MG	2A	3134	1/1	0.93	0.19	47,47,47,47	0
58	MG	2A	3768	1/1	0.93	0.19	62,62,62,62	0
58	MG	1A	3701	1/1	0.93	0.09	32,32,32,32	0
58	MG	1A	3812	1/1	0.93	0.10	58,58,58,58	0
58	MG	2A	3537	1/1	0.93	0.11	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3490	1/1	0.93	0.10	58,58,58,58	0
58	MG	1A	3491	1/1	0.93	0.13	57,57,57,57	0
58	MG	1A	3099	1/1	0.93	0.29	46,46,46,46	0
58	MG	1a	1627	1/1	0.93	0.30	66,66,66,66	0
58	MG	1A	3229	1/1	0.93	0.09	47,47,47,47	0
58	MG	1a	1629	1/1	0.93	0.14	55,55,55,55	0
58	MG	2A	3147	1/1	0.93	0.24	67,67,67,67	0
58	MG	2A	3780	1/1	0.93	0.11	56,56,56,56	0
58	MG	1a	1630	1/1	0.93	0.40	70,70,70,70	0
58	MG	1A	3198	1/1	0.93	0.12	45,45,45,45	0
58	MG	1A	3819	1/1	0.93	0.14	41,41,41,41	0
58	MG	1A	3607	1/1	0.93	0.07	34,34,34,34	0
58	MG	1A	3710	1/1	0.93	0.08	34,34,34,34	0
58	MG	1a	1814	1/1	0.93	0.10	66,66,66,66	0
58	MG	2A	3792	1/1	0.93	0.10	66,66,66,66	0
58	MG	2a	1728	1/1	0.93	0.16	78,78,78,78	0
58	MG	1a	1816	1/1	0.93	0.08	69,69,69,69	0
58	MG	2A	3794	1/1	0.93	0.08	66,66,66,66	0
58	MG	1A	3255	1/1	0.93	0.06	54,54,54,54	0
58	MG	1A	3436	1/1	0.93	0.26	66,66,66,66	0
58	MG	2a	1736	1/1	0.93	0.14	73,73,73,73	0
58	MG	1B	209	1/1	0.93	0.11	49,49,49,49	0
58	MG	2A	3326	1/1	0.93	0.13	76,76,76,76	0
58	MG	2a	1742	1/1	0.93	0.13	49,49,49,49	0
58	MG	1A	3386	1/1	0.93	0.15	59,59,59,59	0
58	MG	1a	1642	1/1	0.93	0.20	64,64,64,64	0
58	MG	1B	212	1/1	0.93	0.27	69,69,69,69	0
58	MG	2A	3165	1/1	0.93	0.26	68,68,68,68	0
58	MG	1a	1825	1/1	0.93	0.09	83,83,83,83	0
58	MG	1A	3441	1/1	0.93	0.17	46,46,46,46	0
58	MG	1A	3236	1/1	0.93	0.28	62,62,62,62	0
58	MG	1A	3720	1/1	0.93	0.07	33,33,33,33	0
58	MG	1A	3968	1/1	0.93	0.11	57,57,57,57	0
58	MG	1a	1654	1/1	0.93	0.08	68,68,68,68	0
58	MG	1A	3133	1/1	0.93	0.10	52,52,52,52	0
58	MG	1A	3725	1/1	0.93	0.07	26,26,26,26	0
58	MG	1A	3621	1/1	0.93	0.05	30,30,30,30	0
58	MG	1A	3626	1/1	0.93	0.11	62,62,62,62	0
58	MG	1B	226	1/1	0.93	0.12	63,63,63,63	0
58	MG	1B	228	1/1	0.93	0.08	47,47,47,47	0
58	MG	1A	3976	1/1	0.93	0.14	52,52,52,52	0
58	MG	2A	3348	1/1	0.93	0.18	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3182	1/1	0.93	0.11	64,64,64,64	0
58	MG	1A	3629	1/1	0.93	0.16	69,69,69,69	0
58	MG	1A	3513	1/1	0.93	0.10	52,52,52,52	0
58	MG	1A	3447	1/1	0.93	0.11	60,60,60,60	0
58	MG	1A	3450	1/1	0.93	0.12	56,56,56,56	0
58	MG	2B	204	1/1	0.93	0.20	68,68,68,68	0
58	MG	2A	3354	1/1	0.93	0.17	49,49,49,49	0
58	MG	1A	3983	1/1	0.93	0.07	53,53,53,53	0
58	MG	1B	237	1/1	0.93	0.11	49,49,49,49	0
58	MG	1D	308	1/1	0.93	0.17	52,52,52,52	0
58	MG	1A	3390	1/1	0.93	0.14	63,63,63,63	0
58	MG	1A	3053	1/1	0.93	0.22	51,51,51,51	0
58	MG	1A	3393	1/1	0.93	0.13	46,46,46,46	0
58	MG	2A	3361	1/1	0.93	0.17	63,63,63,63	0
58	MG	2A	3195	1/1	0.93	0.33	51,51,51,51	0
58	MG	1x	107	1/1	0.93	0.20	60,60,60,60	0
58	MG	1x	108	1/1	0.93	0.16	32,32,32,32	0
58	MG	1A	3240	1/1	0.93	0.08	62,62,62,62	0
58	MG	1A	3644	1/1	0.93	0.09	40,40,40,40	0
58	MG	1A	3747	1/1	0.93	0.12	52,52,52,52	0
58	MG	2A	3616	1/1	0.93	0.11	41,41,41,41	0
58	MG	1A	3857	1/1	0.93	0.14	45,45,45,45	0
58	MG	2D	306	1/1	0.93	0.23	64,64,64,64	0
58	MG	2a	1801	1/1	0.93	0.07	88,88,88,88	0
58	MG	2A	3374	1/1	0.93	0.26	65,65,65,65	0
58	MG	1A	3266	1/1	0.93	0.18	58,58,58,58	0
58	MG	2E	304	1/1	0.93	0.09	45,45,45,45	0
58	MG	2A	3379	1/1	0.93	0.34	57,57,57,57	0
58	MG	1A	3304	1/1	0.93	0.13	61,61,61,61	0
58	MG	2E	307	1/1	0.93	0.12	53,53,53,53	0
58	MG	2E	308	1/1	0.93	0.14	75,75,75,75	0
58	MG	2a	1816	1/1	0.93	0.16	83,83,83,83	0
58	MG	1A	3531	1/1	0.93	0.19	60,60,60,60	0
58	MG	2a	1818	1/1	0.93	0.11	67,67,67,67	0
58	MG	1A	4002	1/1	0.93	0.06	21,21,21,21	0
58	MG	2A	3385	1/1	0.93	0.12	50,50,50,50	0
58	MG	1A	3202	1/1	0.93	0.17	57,57,57,57	0
58	MG	2F	305	1/1	0.93	0.12	60,60,60,60	0
58	MG	1A	3351	1/1	0.93	0.19	41,41,41,41	0
58	MG	2F	307	1/1	0.93	0.28	55,55,55,55	0
58	MG	1A	3354	1/1	0.93	0.14	58,58,58,58	0
58	MG	1A	3758	1/1	0.93	0.14	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3309	1/1	0.93	0.15	48,48,48,48	0
58	MG	2A	3014	1/1	0.93	0.11	48,48,48,48	0
58	MG	1N	202	1/1	0.93	0.10	52,52,52,52	0
58	MG	2A	3018	1/1	0.93	0.11	43,43,43,43	0
58	MG	2A	3396	1/1	0.93	0.13	72,72,72,72	0
58	MG	2d	301	1/1	0.93	0.09	71,71,71,71	0
58	MG	1A	3872	1/1	0.93	0.10	57,57,57,57	0
58	MG	2e	201	1/1	0.93	0.07	81,81,81,81	0
58	MG	1A	3468	1/1	0.93	0.28	57,57,57,57	0
58	MG	1A	3878	1/1	0.93	0.07	81,81,81,81	0
58	MG	2A	3027	1/1	0.93	0.29	62,62,62,62	0
58	MG	1a	1701	1/1	0.93	0.14	82,82,82,82	0
58	MG	1A	3007	1/1	0.93	0.10	45,45,45,45	0
58	MG	1A	3119	1/1	0.93	0.21	64,64,64,64	0
58	MG	21	101	1/1	0.93	0.35	56,56,56,56	0
58	MG	1a	1704	1/1	0.93	0.33	71,71,71,71	0
58	MG	2A	3040	1/1	0.93	0.24	77,77,77,77	0
58	MG	2A	3647	1/1	0.93	0.11	66,66,66,66	0
58	MG	1A	3884	1/1	0.93	0.06	66,66,66,66	0
58	MG	1A	3764	1/1	0.93	0.07	44,44,44,44	0
58	MG	2A	3234	1/1	0.93	0.10	72,72,72,72	0
58	MG	2A	3420	1/1	0.93	0.13	27,27,27,27	0
58	MG	28	103	1/1	0.93	0.23	56,56,56,56	0
58	MG	1A	4021	1/1	0.93	0.20	56,56,56,56	0
58	MG	2A	3655	1/1	0.93	0.10	59,59,59,59	0
58	MG	2A	3422	1/1	0.93	0.21	49,49,49,49	0
58	MG	2a	1605	1/1	0.93	0.26	75,75,75,75	0
58	MG	1A	3769	1/1	0.93	0.09	42,42,42,42	0
58	MG	1A	3472	1/1	0.93	0.30	39,39,39,39	0
58	MG	1A	3771	1/1	0.93	0.07	54,54,54,54	0
58	MG	2A	3437	1/1	0.94	0.10	64,64,64,64	0
58	MG	1A	4086	1/1	0.94	0.10	79,79,79,79	0
58	MG	2A	3050	1/1	0.94	0.12	57,57,57,57	0
58	MG	2A	3238	1/1	0.94	0.33	76,76,76,76	0
58	MG	2A	3670	1/1	0.94	0.17	51,51,51,51	0
58	MG	1A	3839	1/1	0.94	0.07	34,34,34,34	0
58	MG	2A	3672	1/1	0.94	0.17	67,67,67,67	0
58	MG	1a	1727	1/1	0.94	0.10	44,44,44,44	0
58	MG	1A	4088	1/1	0.94	0.16	43,43,43,43	0
58	MG	1A	3262	1/1	0.94	0.17	60,60,60,60	0
58	MG	1A	4090	1/1	0.94	0.12	49,49,49,49	0
58	MG	2A	3245	1/1	0.94	0.23	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3457	1/1	0.94	0.23	45,45,45,45	0
58	MG	2A	3247	1/1	0.94	0.19	70,70,70,70	0
58	MG	1A	3211	1/1	0.94	0.17	49,49,49,49	0
58	MG	2A	3453	1/1	0.94	0.14	55,55,55,55	0
58	MG	1A	3959	1/1	0.94	0.10	53,53,53,53	0
58	MG	13	103	1/1	0.94	0.12	57,57,57,57	0
58	MG	1A	3105	1/1	0.94	0.06	40,40,40,40	0
58	MG	2A	3463	1/1	0.94	0.14	40,40,40,40	0
58	MG	2A	3066	1/1	0.94	0.07	55,55,55,55	0
58	MG	15	102	1/1	0.94	0.20	47,47,47,47	0
58	MG	2A	3069	1/1	0.94	0.21	63,63,63,63	0
58	MG	15	106	1/1	0.94	0.24	44,44,44,44	0
58	MG	1A	3269	1/1	0.94	0.14	41,41,41,41	0
58	MG	2A	3258	1/1	0.94	0.38	69,69,69,69	0
58	MG	2A	3072	1/1	0.94	0.17	54,54,54,54	0
58	MG	2A	3701	1/1	0.94	0.12	59,59,59,59	0
58	MG	16	101	1/1	0.94	0.09	67,67,67,67	0
58	MG	2A	3479	1/1	0.94	0.07	47,47,47,47	0
58	MG	1A	3756	1/1	0.94	0.10	57,57,57,57	0
58	MG	17	101	1/1	0.94	0.13	42,42,42,42	0
58	MG	2a	1647	1/1	0.94	0.22	74,74,74,74	0
58	MG	1A	3332	1/1	0.94	0.08	52,52,52,52	0
58	MG	2A	3078	1/1	0.94	0.11	59,59,59,59	0
58	MG	1A	3548	1/1	0.94	0.43	69,69,69,69	0
58	MG	2a	1652	1/1	0.94	0.10	54,54,54,54	0
58	MG	2a	1654	1/1	0.94	0.22	65,65,65,65	0
58	MG	1A	3850	1/1	0.94	0.14	40,40,40,40	0
58	MG	1a	1753	1/1	0.94	0.10	63,63,63,63	0
58	MG	1A	4105	1/1	0.94	0.07	40,40,40,40	0
58	MG	2A	3713	1/1	0.94	0.06	62,62,62,62	0
58	MG	1A	3156	1/1	0.94	0.14	47,47,47,47	0
58	MG	1A	3106	1/1	0.94	0.23	56,56,56,56	0
58	MG	1A	3279	1/1	0.94	0.11	54,54,54,54	0
58	MG	2A	3087	1/1	0.94	0.11	64,64,64,64	0
58	MG	1a	1758	1/1	0.94	0.12	70,70,70,70	0
58	MG	1A	3856	1/1	0.94	0.12	49,49,49,49	0
58	MG	2A	3721	1/1	0.94	0.08	41,41,41,41	0
58	MG	2A	3500	1/1	0.94	0.10	54,54,54,54	0
58	MG	1A	3077	1/1	0.94	0.29	53,53,53,53	0
58	MG	1A	3858	1/1	0.94	0.14	39,39,39,39	0
58	MG	2A	3093	1/1	0.94	0.12	64,64,64,64	0
58	MG	2A	3734	1/1	0.94	0.07	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3554	1/1	0.94	0.12	36,36,36,36	0
58	MG	1A	3767	1/1	0.94	0.09	31,31,31,31	0
58	MG	1B	203	1/1	0.94	0.09	56,56,56,56	0
58	MG	1a	1613	1/1	0.94	0.15	68,68,68,68	0
58	MG	1A	3555	1/1	0.94	0.08	41,41,41,41	0
58	MG	1A	3399	1/1	0.94	0.09	61,61,61,61	0
58	MG	1A	3982	1/1	0.94	0.15	53,53,53,53	0
58	MG	1a	1775	1/1	0.94	0.07	66,66,66,66	0
58	MG	2a	1680	1/1	0.94	0.15	57,57,57,57	0
58	MG	2A	3515	1/1	0.94	0.11	59,59,59,59	0
58	MG	1A	3110	1/1	0.94	0.10	45,45,45,45	0
58	MG	1A	3866	1/1	0.94	0.09	78,78,78,78	0
58	MG	1a	1783	1/1	0.94	0.08	89,89,89,89	0
58	MG	2A	3293	1/1	0.94	0.09	60,60,60,60	0
58	MG	2A	3111	1/1	0.94	0.14	63,63,63,63	0
58	MG	1A	3113	1/1	0.94	0.18	51,51,51,51	0
58	MG	1A	3002	1/1	0.94	0.08	53,53,53,53	0
58	MG	2A	3523	1/1	0.94	0.08	47,47,47,47	0
58	MG	2A	3297	1/1	0.94	0.15	61,61,61,61	0
58	MG	2A	3114	1/1	0.94	0.27	65,65,65,65	0
58	MG	1a	1626	1/1	0.94	0.20	67,67,67,67	0
58	MG	1a	1787	1/1	0.94	0.08	83,83,83,83	0
58	MG	1A	3988	1/1	0.94	0.06	45,45,45,45	0
58	MG	2a	1697	1/1	0.94	0.13	65,65,65,65	0
58	MG	1A	3992	1/1	0.94	0.09	31,31,31,31	0
58	MG	1A	3560	1/1	0.94	0.07	43,43,43,43	0
58	MG	2A	3125	1/1	0.94	0.18	71,71,71,71	0
58	MG	1A	3343	1/1	0.94	0.17	46,46,46,46	0
58	MG	2A	3536	1/1	0.94	0.10	47,47,47,47	0
58	MG	1A	3875	1/1	0.94	0.08	49,49,49,49	0
58	MG	2A	3538	1/1	0.94	0.12	57,57,57,57	0
58	MG	1A	3344	1/1	0.94	0.17	45,45,45,45	0
58	MG	2A	3542	1/1	0.94	0.08	51,51,51,51	0
58	MG	2A	3129	1/1	0.94	0.15	45,45,45,45	0
58	MG	1B	224	1/1	0.94	0.15	60,60,60,60	0
58	MG	2A	3547	1/1	0.94	0.11	58,58,58,58	0
58	MG	2A	3778	1/1	0.94	0.10	74,74,74,74	0
58	MG	1a	1801	1/1	0.94	0.12	64,64,64,64	0
58	MG	1A	3997	1/1	0.94	0.13	66,66,66,66	0
58	MG	1B	227	1/1	0.94	0.10	56,56,56,56	0
58	MG	1A	3777	1/1	0.94	0.09	60,60,60,60	0
58	MG	1A	3083	1/1	0.94	0.16	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3121	1/1	0.94	0.11	71,71,71,71	0
58	MG	1A	3032	1/1	0.94	0.08	50,50,50,50	0
58	MG	1A	3051	1/1	0.94	0.10	53,53,53,53	0
58	MG	2A	3791	1/1	0.94	0.15	66,66,66,66	0
58	MG	1A	3684	1/1	0.94	0.07	60,60,60,60	0
58	MG	2A	3143	1/1	0.94	0.11	43,43,43,43	0
58	MG	2A	3144	1/1	0.94	0.20	57,57,57,57	0
58	MG	1a	1646	1/1	0.94	0.20	63,63,63,63	0
58	MG	1A	3576	1/1	0.94	0.09	59,59,59,59	0
58	MG	1A	3784	1/1	0.94	0.09	56,56,56,56	0
58	MG	2A	3564	1/1	0.94	0.15	63,63,63,63	0
58	MG	1A	3350	1/1	0.94	0.10	50,50,50,50	0
58	MG	1A	3893	1/1	0.94	0.10	56,56,56,56	0
58	MG	2A	3567	1/1	0.94	0.13	69,69,69,69	0
58	MG	1A	3020	1/1	0.94	0.10	54,54,54,54	0
58	MG	1A	3418	1/1	0.94	0.10	52,52,52,52	0
58	MG	2a	1741	1/1	0.94	0.14	81,81,81,81	0
58	MG	2A	3811	1/1	0.94	0.07	50,50,50,50	0
58	MG	1A	3243	1/1	0.94	0.17	56,56,56,56	0
58	MG	2A	3572	1/1	0.94	0.10	67,67,67,67	0
58	MG	1A	3184	1/1	0.94	0.35	41,41,41,41	0
58	MG	2a	1748	1/1	0.94	0.16	83,83,83,83	0
58	MG	2a	1750	1/1	0.94	0.17	77,77,77,77	0
58	MG	1A	3593	1/1	0.94	0.07	35,35,35,35	0
58	MG	2a	1752	1/1	0.94	0.12	57,57,57,57	0
58	MG	1d	301	1/1	0.94	0.07	69,69,69,69	0
58	MG	2A	3817	1/1	0.94	0.09	78,78,78,78	0
58	MG	1a	1660	1/1	0.94	0.13	70,70,70,70	0
58	MG	1a	1662	1/1	0.94	0.28	66,66,66,66	0
58	MG	1A	3357	1/1	0.94	0.21	50,50,50,50	0
58	MG	1A	3600	1/1	0.94	0.10	51,51,51,51	0
58	MG	1A	3359	1/1	0.94	0.27	34,34,34,34	0
58	MG	1A	3005	1/1	0.94	0.15	45,45,45,45	0
58	MG	1A	3247	1/1	0.94	0.17	37,37,37,37	0
58	MG	1a	1669	1/1	0.94	0.08	47,47,47,47	0
58	MG	2A	3169	1/1	0.94	0.12	64,64,64,64	0
58	MG	2A	3586	1/1	0.94	0.18	55,55,55,55	0
58	MG	1A	3190	1/1	0.94	0.08	44,44,44,44	0
58	MG	1A	3299	1/1	0.94	0.06	36,36,36,36	0
58	MG	1A	3041	1/1	0.94	0.09	41,41,41,41	0
58	MG	2a	1769	1/1	0.94	0.15	64,64,64,64	0
58	MG	1A	3908	1/1	0.94	0.16	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1a	1674	1/1	0.94	0.37	66,66,66,66	0
58	MG	2B	206	1/1	0.94	0.11	78,78,78,78	0
58	MG	2a	1773	1/1	0.94	0.19	81,81,81,81	0
58	MG	1a	1675	1/1	0.94	0.25	64,64,64,64	0
58	MG	1H	201	1/1	0.94	0.22	70,70,70,70	0
58	MG	2A	3594	1/1	0.94	0.11	56,56,56,56	0
58	MG	1A	3609	1/1	0.94	0.06	30,30,30,30	0
58	MG	2A	3596	1/1	0.94	0.09	83,83,83,83	0
58	MG	1N	201	1/1	0.94	0.14	41,41,41,41	0
58	MG	1A	3016	1/1	0.94	0.11	57,57,57,57	0
58	MG	1A	3432	1/1	0.94	0.17	52,52,52,52	0
58	MG	1A	3139	1/1	0.94	0.18	49,49,49,49	0
58	MG	1x	105	1/1	0.94	0.20	62,62,62,62	0
58	MG	1A	3141	1/1	0.94	0.17	46,46,46,46	0
58	MG	2a	1788	1/1	0.94	0.15	72,72,72,72	0
58	MG	1A	3718	1/1	0.94	0.07	60,60,60,60	0
58	MG	1a	1685	1/1	0.94	0.08	54,54,54,54	0
58	MG	2A	3608	1/1	0.94	0.12	61,61,61,61	0
58	MG	1A	4045	1/1	0.94	0.14	68,68,68,68	0
58	MG	2A	3364	1/1	0.94	0.34	51,51,51,51	0
58	MG	2a	1796	1/1	0.94	0.14	75,75,75,75	0
58	MG	1A	3093	1/1	0.94	0.14	71,71,71,71	0
58	MG	1A	3375	1/1	0.94	0.13	53,53,53,53	0
58	MG	1A	3923	1/1	0.94	0.07	77,77,77,77	0
58	MG	1Q	206	1/1	0.94	0.16	57,57,57,57	0
58	MG	1Q	207	1/1	0.94	0.10	50,50,50,50	0
58	MG	1A	3516	1/1	0.94	0.19	39,39,39,39	0
58	MG	2A	3002	1/1	0.94	0.47	71,71,71,71	0
58	MG	2E	309	1/1	0.94	0.12	77,77,77,77	0
58	MG	2A	3377	1/1	0.94	0.12	80,80,80,80	0
58	MG	1A	4052	1/1	0.94	0.08	58,58,58,58	0
58	MG	2a	1812	1/1	0.94	0.08	53,53,53,53	0
58	MG	1A	3925	1/1	0.94	0.12	73,73,73,73	0
58	MG	2A	3199	1/1	0.94	0.13	57,57,57,57	0
58	MG	2A	3381	1/1	0.94	0.11	33,33,33,33	0
58	MG	1A	3009	1/1	0.94	0.06	27,27,27,27	0
58	MG	1A	3442	1/1	0.94	0.25	46,46,46,46	0
58	MG	1A	3256	1/1	0.94	0.13	39,39,39,39	0
58	MG	1A	3445	1/1	0.94	0.13	54,54,54,54	0
58	MG	2A	3010	1/1	0.94	0.10	60,60,60,60	0
58	MG	2A	3011	1/1	0.94	0.12	61,61,61,61	0
58	MG	2P	202	1/1	0.94	0.10	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1826	1/1	0.94	0.19	58,58,58,58	0
58	MG	2A	3208	1/1	0.94	0.10	60,60,60,60	0
58	MG	2A	3391	1/1	0.94	0.12	55,55,55,55	0
58	MG	2a	1831	1/1	0.94	0.24	74,74,74,74	0
58	MG	2R	202	1/1	0.94	0.14	54,54,54,54	0
58	MG	1A	4065	1/1	0.94	0.07	28,28,28,28	0
58	MG	2A	3015	1/1	0.94	0.12	52,52,52,52	0
58	MG	2U	201	1/1	0.94	0.20	57,57,57,57	0
58	MG	2a	1839	1/1	0.94	0.14	70,70,70,70	0
58	MG	1A	4066	1/1	0.94	0.08	69,69,69,69	0
58	MG	1A	3047	1/1	0.94	0.17	35,35,35,35	0
58	MG	2V	202	1/1	0.94	0.16	67,67,67,67	0
58	MG	2A	3214	1/1	0.94	0.13	61,61,61,61	0
58	MG	2e	202	1/1	0.94	0.12	84,84,84,84	0
58	MG	2X	101	1/1	0.94	0.06	71,71,71,71	0
58	MG	2A	3215	1/1	0.94	0.12	67,67,67,67	0
58	MG	1A	3379	1/1	0.94	0.10	54,54,54,54	0
58	MG	1U	205	1/1	0.94	0.13	54,54,54,54	0
58	MG	1A	3827	1/1	0.94	0.06	39,39,39,39	0
58	MG	2n	102	1/1	0.94	0.07	79,79,79,79	0
58	MG	2p	101	1/1	0.94	0.33	76,76,76,76	0
58	MG	1A	3639	1/1	0.94	0.11	36,36,36,36	0
58	MG	1A	3205	1/1	0.94	0.12	48,48,48,48	0
58	MG	2A	3648	1/1	0.94	0.21	57,57,57,57	0
58	MG	1A	4075	1/1	0.94	0.25	35,35,35,35	0
58	MG	2A	3031	1/1	0.94	0.14	49,49,49,49	0
58	MG	2A	3037	1/1	0.94	0.12	56,56,56,56	0
58	MG	1A	3320	1/1	0.94	0.19	51,51,51,51	0
58	MG	1A	3322	1/1	0.94	0.15	42,42,42,42	0
58	MG	1A	3945	1/1	0.94	0.06	58,58,58,58	0
58	MG	2A	3041	1/1	0.94	0.14	59,59,59,59	0
58	MG	1A	3833	1/1	0.94	0.09	39,39,39,39	0
58	MG	1A	3074	1/1	0.94	0.15	61,61,61,61	0
58	MG	1A	3646	1/1	0.94	0.10	26,26,26,26	0
58	MG	2A	3429	1/1	0.94	0.09	58,58,58,58	0
58	MG	1Z	301	1/1	0.94	0.08	64,64,64,64	0
58	MG	1Z	303	1/1	0.94	0.09	67,67,67,67	0
58	MG	1A	3535	1/1	0.94	0.34	53,53,53,53	0
58	MG	1A	4069	1/1	0.95	0.09	54,54,54,54	0
58	MG	2A	3502	1/1	0.95	0.14	56,56,56,56	0
58	MG	1a	1667	1/1	0.95	0.30	71,71,71,71	0
58	MG	1A	3950	1/1	0.95	0.06	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1a	1823	1/1	0.95	0.08	69,69,69,69	0
58	MG	2A	3130	1/1	0.95	0.15	58,58,58,58	0
58	MG	1A	3244	1/1	0.95	0.12	31,31,31,31	0
58	MG	1A	3652	1/1	0.95	0.06	31,31,31,31	0
58	MG	1A	3206	1/1	0.95	0.13	53,53,53,53	0
58	MG	1A	3551	1/1	0.95	0.09	33,33,33,33	0
58	MG	2A	3722	1/1	0.95	0.12	57,57,57,57	0
58	MG	1A	3138	1/1	0.95	0.09	41,41,41,41	0
58	MG	1A	3180	1/1	0.95	0.23	49,49,49,49	0
58	MG	2A	3725	1/1	0.95	0.14	56,56,56,56	0
58	MG	2A	3514	1/1	0.95	0.15	48,48,48,48	0
58	MG	1k	3100	1/1	0.95	0.15	55,55,55,55	0
58	MG	1A	4079	1/1	0.95	0.16	36,36,36,36	0
58	MG	1A	3331	1/1	0.95	0.09	63,63,63,63	0
58	MG	1m	3001	1/1	0.95	0.08	66,66,66,66	0
58	MG	1T	201	1/1	0.95	0.12	66,66,66,66	0
58	MG	1n	102	1/1	0.95	0.17	70,70,70,70	0
58	MG	1A	3212	1/1	0.95	0.13	53,53,53,53	0
58	MG	1r	101	1/1	0.95	0.06	81,81,81,81	0
58	MG	1A	3183	1/1	0.95	0.08	53,53,53,53	0
58	MG	1A	3157	1/1	0.95	0.15	42,42,42,42	0
58	MG	1A	3186	1/1	0.95	0.20	40,40,40,40	0
58	MG	1A	3031	1/1	0.95	0.13	36,36,36,36	0
58	MG	2a	1664	1/1	0.95	0.23	47,47,47,47	0
58	MG	1A	3765	1/1	0.95	0.06	30,30,30,30	0
58	MG	1U	210	1/1	0.95	0.14	33,33,33,33	0
58	MG	1A	3222	1/1	0.95	0.08	58,58,58,58	0
58	MG	1U	213	1/1	0.95	0.16	39,39,39,39	0
58	MG	1A	3970	1/1	0.95	0.07	53,53,53,53	0
58	MG	1V	203	1/1	0.95	0.29	48,48,48,48	0
58	MG	2A	3535	1/1	0.95	0.13	59,59,59,59	0
58	MG	2A	3757	1/1	0.95	0.10	54,54,54,54	0
58	MG	2A	3758	1/1	0.95	0.10	54,54,54,54	0
58	MG	2A	3759	1/1	0.95	0.08	72,72,72,72	0
58	MG	1A	3768	1/1	0.95	0.06	39,39,39,39	0
58	MG	1A	3223	1/1	0.95	0.23	59,59,59,59	0
58	MG	1A	3563	1/1	0.95	0.09	30,30,30,30	0
58	MG	2A	3763	1/1	0.95	0.10	65,65,65,65	0
58	MG	1A	3435	1/1	0.95	0.18	56,56,56,56	0
58	MG	1A	3341	1/1	0.95	0.21	43,43,43,43	0
58	MG	1A	3437	1/1	0.95	0.08	52,52,52,52	0
58	MG	2A	3167	1/1	0.95	0.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1683	1/1	0.95	0.17	65,65,65,65	0
58	MG	1A	3438	1/1	0.95	0.14	58,58,58,58	0
58	MG	1X	106	1/1	0.95	0.10	61,61,61,61	0
58	MG	1A	3129	1/1	0.95	0.16	57,57,57,57	0
58	MG	1A	3574	1/1	0.95	0.11	56,56,56,56	0
58	MG	1A	3226	1/1	0.95	0.11	56,56,56,56	0
58	MG	10	102	1/1	0.95	0.09	59,59,59,59	0
58	MG	1A	3495	1/1	0.95	0.13	54,54,54,54	0
58	MG	1A	3001	1/1	0.95	0.14	48,48,48,48	0
58	MG	1A	3586	1/1	0.95	0.10	41,41,41,41	0
58	MG	2A	3338	1/1	0.95	0.28	64,64,64,64	0
58	MG	1A	3500	1/1	0.95	0.15	38,38,38,38	0
58	MG	1A	3588	1/1	0.95	0.10	27,27,27,27	0
58	MG	2A	3341	1/1	0.95	0.28	68,68,68,68	0
58	MG	1A	3501	1/1	0.95	0.43	56,56,56,56	0
58	MG	10	111	1/1	0.95	0.10	60,60,60,60	0
58	MG	1A	3887	1/1	0.95	0.10	30,30,30,30	0
58	MG	11	102	1/1	0.95	0.09	48,48,48,48	0
58	MG	2A	3786	1/1	0.95	0.12	62,62,62,62	0
58	MG	2A	3346	1/1	0.95	0.28	64,64,64,64	0
58	MG	1A	3300	1/1	0.95	0.14	58,58,58,58	0
58	MG	2A	3790	1/1	0.95	0.08	53,53,53,53	0
58	MG	1A	3444	1/1	0.95	0.08	58,58,58,58	0
58	MG	13	102	1/1	0.95	0.14	44,44,44,44	0
58	MG	1A	3691	1/1	0.95	0.12	33,33,33,33	0
58	MG	2A	3188	1/1	0.95	0.21	49,49,49,49	0
58	MG	1B	206	1/1	0.95	0.10	52,52,52,52	0
58	MG	2A	3796	1/1	0.95	0.07	56,56,56,56	0
58	MG	2A	3016	1/1	0.95	0.27	54,54,54,54	0
58	MG	1A	3692	1/1	0.95	0.05	24,24,24,24	0
58	MG	2A	3192	1/1	0.95	0.37	56,56,56,56	0
58	MG	1A	3789	1/1	0.95	0.08	70,70,70,70	0
58	MG	1A	3230	1/1	0.95	0.11	34,34,34,34	0
58	MG	1B	211	1/1	0.95	0.11	60,60,60,60	0
58	MG	1A	3261	1/1	0.95	0.07	44,44,44,44	0
58	MG	2A	3809	1/1	0.95	0.06	65,65,65,65	0
58	MG	1A	3306	1/1	0.95	0.12	45,45,45,45	0
58	MG	17	104	1/1	0.95	0.13	67,67,67,67	0
58	MG	2A	3029	1/1	0.95	0.24	52,52,52,52	0
58	MG	2A	3363	1/1	0.95	0.16	70,70,70,70	0
58	MG	2a	1727	1/1	0.95	0.06	82,82,82,82	0
58	MG	1A	3697	1/1	0.95	0.09	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1729	1/1	0.95	0.08	74,74,74,74	0
58	MG	1a	1732	1/1	0.95	0.07	56,56,56,56	0
58	MG	2A	3203	1/1	0.95	0.16	49,49,49,49	0
58	MG	2A	3032	1/1	0.95	0.18	53,53,53,53	0
58	MG	2A	3034	1/1	0.95	0.16	44,44,44,44	0
58	MG	18	103	1/1	0.95	0.13	60,60,60,60	0
58	MG	1A	3448	1/1	0.95	0.20	59,59,59,59	0
58	MG	1A	3349	1/1	0.95	0.26	40,40,40,40	0
58	MG	2A	3375	1/1	0.95	0.33	57,57,57,57	0
58	MG	1a	1738	1/1	0.95	0.07	59,59,59,59	0
58	MG	1A	3233	1/1	0.95	0.16	50,50,50,50	0
58	MG	2a	1745	1/1	0.95	0.10	76,76,76,76	0
58	MG	2A	3597	1/1	0.95	0.07	35,35,35,35	0
58	MG	2A	3211	1/1	0.95	0.19	51,51,51,51	0
58	MG	1A	3308	1/1	0.95	0.11	56,56,56,56	0
58	MG	2A	3043	1/1	0.95	0.09	34,34,34,34	0
58	MG	1A	3404	1/1	0.95	0.13	70,70,70,70	0
58	MG	1A	3063	1/1	0.95	0.07	35,35,35,35	0
58	MG	1a	1745	1/1	0.95	0.07	60,60,60,60	0
58	MG	1A	3456	1/1	0.95	0.13	36,36,36,36	0
58	MG	1A	3523	1/1	0.95	0.10	56,56,56,56	0
58	MG	1A	3525	1/1	0.95	0.13	48,48,48,48	0
58	MG	1A	3616	1/1	0.95	0.13	44,44,44,44	0
58	MG	1a	1609	1/1	0.95	0.07	62,62,62,62	0
58	MG	1A	3909	1/1	0.95	0.09	47,47,47,47	0
58	MG	1A	4022	1/1	0.95	0.13	62,62,62,62	0
58	MG	1B	231	1/1	0.95	0.10	82,82,82,82	0
58	MG	2A	3614	1/1	0.95	0.11	61,61,61,61	0
58	MG	1A	3526	1/1	0.95	0.20	54,54,54,54	0
58	MG	1A	3715	1/1	0.95	0.12	35,35,35,35	0
58	MG	2A	3398	1/1	0.95	0.12	60,60,60,60	0
58	MG	1a	1616	1/1	0.95	0.07	70,70,70,70	0
58	MG	2B	218	1/1	0.95	0.10	87,87,87,87	0
58	MG	1A	3914	1/1	0.95	0.12	62,62,62,62	0
58	MG	2A	3060	1/1	0.95	0.12	55,55,55,55	0
58	MG	2A	3402	1/1	0.95	0.14	77,77,77,77	0
58	MG	2D	302	1/1	0.95	0.10	39,39,39,39	0
58	MG	2A	3404	1/1	0.95	0.17	63,63,63,63	0
58	MG	2A	3061	1/1	0.95	0.10	60,60,60,60	0
58	MG	1A	3310	1/1	0.95	0.15	60,60,60,60	0
58	MG	2A	3233	1/1	0.95	0.09	57,57,57,57	0
58	MG	1A	3407	1/1	0.95	0.16	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3411	1/1	0.95	0.10	49,49,49,49	0
58	MG	2a	1780	1/1	0.95	0.28	60,60,60,60	0
58	MG	2A	3064	1/1	0.95	0.14	47,47,47,47	0
58	MG	1A	3622	1/1	0.95	0.13	31,31,31,31	0
58	MG	1A	3624	1/1	0.95	0.04	31,31,31,31	0
58	MG	1a	1764	1/1	0.95	0.09	73,73,73,73	0
58	MG	1a	1765	1/1	0.95	0.07	73,73,73,73	0
58	MG	2A	3419	1/1	0.95	0.15	58,58,58,58	0
58	MG	1E	302	1/1	0.95	0.20	47,47,47,47	0
58	MG	1A	4033	1/1	0.95	0.20	49,49,49,49	0
58	MG	1A	3817	1/1	0.95	0.05	45,45,45,45	0
58	MG	2A	3424	1/1	0.95	0.10	54,54,54,54	0
58	MG	1A	3145	1/1	0.95	0.17	44,44,44,44	0
58	MG	1A	3921	1/1	0.95	0.07	66,66,66,66	0
58	MG	1E	312	1/1	0.95	0.10	57,57,57,57	0
58	MG	2A	3432	1/1	0.95	0.07	54,54,54,54	0
58	MG	1A	3146	1/1	0.95	0.07	49,49,49,49	0
58	MG	1a	1776	1/1	0.95	0.11	60,60,60,60	0
58	MG	2A	3436	1/1	0.95	0.10	46,46,46,46	0
58	MG	2a	1803	1/1	0.95	0.07	77,77,77,77	0
58	MG	1A	4041	1/1	0.95	0.09	41,41,41,41	0
58	MG	1a	1635	1/1	0.95	0.15	55,55,55,55	0
58	MG	1A	3821	1/1	0.95	0.33	43,43,43,43	0
58	MG	1A	3461	1/1	0.95	0.10	72,72,72,72	0
58	MG	2T	204	1/1	0.95	0.15	70,70,70,70	0
58	MG	1A	3275	1/1	0.95	0.18	54,54,54,54	0
58	MG	1A	3634	1/1	0.95	0.06	41,41,41,41	0
58	MG	1F	313	1/1	0.95	0.09	54,54,54,54	0
58	MG	2a	1814	1/1	0.95	0.08	76,76,76,76	0
58	MG	2A	3444	1/1	0.95	0.16	55,55,55,55	0
58	MG	2A	3256	1/1	0.95	0.09	67,67,67,67	0
58	MG	2A	3660	1/1	0.95	0.19	71,71,71,71	0
58	MG	2A	3446	1/1	0.95	0.10	48,48,48,48	0
58	MG	1a	1641	1/1	0.95	0.16	69,69,69,69	0
58	MG	1A	3729	1/1	0.95	0.10	33,33,33,33	0
58	MG	1a	1790	1/1	0.95	0.07	57,57,57,57	0
58	MG	2A	3091	1/1	0.95	0.14	35,35,35,35	0
58	MG	1a	1791	1/1	0.95	0.12	66,66,66,66	0
58	MG	25	102	1/1	0.95	0.13	60,60,60,60	0
58	MG	26	101	1/1	0.95	0.26	68,68,68,68	0
58	MG	1a	1792	1/1	0.95	0.07	56,56,56,56	0
58	MG	2a	1830	1/1	0.95	0.11	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3463	1/1	0.95	0.16	45,45,45,45	0
58	MG	1A	3316	1/1	0.95	0.09	49,49,49,49	0
58	MG	2A	3096	1/1	0.95	0.14	63,63,63,63	0
58	MG	2A	3462	1/1	0.95	0.12	52,52,52,52	0
58	MG	1A	3080	1/1	0.95	0.28	45,45,45,45	0
58	MG	2a	1601	1/1	0.95	0.09	62,62,62,62	0
58	MG	1G	204	1/1	0.95	0.10	68,68,68,68	0
58	MG	2A	3465	1/1	0.95	0.08	58,58,58,58	0
58	MG	1A	3467	1/1	0.95	0.07	57,57,57,57	0
58	MG	2A	3469	1/1	0.95	0.09	59,59,59,59	0
58	MG	2A	3470	1/1	0.95	0.07	41,41,41,41	0
58	MG	2A	3684	1/1	0.95	0.09	56,56,56,56	0
58	MG	1A	3739	1/1	0.95	0.07	51,51,51,51	0
58	MG	2A	3270	1/1	0.95	0.11	63,63,63,63	0
58	MG	1A	4058	1/1	0.95	0.15	58,58,58,58	0
58	MG	1a	1803	1/1	0.95	0.07	75,75,75,75	0
58	MG	2A	3107	1/1	0.95	0.14	45,45,45,45	0
58	MG	1a	1804	1/1	0.95	0.07	63,63,63,63	0
58	MG	2A	3275	1/1	0.95	0.13	56,56,56,56	0
58	MG	1A	3122	1/1	0.95	0.15	54,54,54,54	0
58	MG	1A	3642	1/1	0.95	0.10	49,49,49,49	0
58	MG	1A	3176	1/1	0.95	0.10	45,45,45,45	0
58	MG	2A	3279	1/1	0.95	0.30	59,59,59,59	0
58	MG	1O	202	1/1	0.95	0.21	52,52,52,52	0
58	MG	1O	204	1/1	0.95	0.11	57,57,57,57	0
58	MG	1A	3280	1/1	0.95	0.10	52,52,52,52	0
58	MG	2A	3488	1/1	0.95	0.15	40,40,40,40	0
58	MG	1a	1661	1/1	0.95	0.27	62,62,62,62	0
58	MG	1A	3546	1/1	0.95	0.13	43,43,43,43	0
58	MG	2A	3285	1/1	0.95	0.11	62,62,62,62	0
58	MG	1P	202	1/1	0.95	0.29	38,38,38,38	0
58	MG	1a	1817	1/1	0.95	0.07	81,81,81,81	0
58	MG	1A	3547	1/1	0.95	0.27	57,57,57,57	0
58	MG	2A	3124	1/1	0.95	0.12	47,47,47,47	0
58	MG	1A	3124	1/1	0.95	0.10	47,47,47,47	0
58	MG	2A	3141	1/1	0.96	0.11	57,57,57,57	0
58	MG	2A	3513	1/1	0.96	0.06	67,67,67,67	0
58	MG	1A	3913	1/1	0.96	0.11	53,53,53,53	0
58	MG	1A	3806	1/1	0.96	0.13	50,50,50,50	0
58	MG	2A	3729	1/1	0.96	0.04	71,71,71,71	0
58	MG	1A	3807	1/1	0.96	0.10	53,53,53,53	0
58	MG	1A	4039	1/1	0.96	0.06	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1644	1/1	0.96	0.17	59,59,59,59	0
58	MG	1f	201	1/1	0.96	0.12	51,51,51,51	0
58	MG	1A	3196	1/1	0.96	0.11	47,47,47,47	0
58	MG	1A	3394	1/1	0.96	0.11	59,59,59,59	0
58	MG	1A	3811	1/1	0.96	0.07	30,30,30,30	0
58	MG	1A	3395	1/1	0.96	0.12	52,52,52,52	0
58	MG	2a	1653	1/1	0.96	0.22	57,57,57,57	0
58	MG	1A	3454	1/1	0.96	0.21	60,60,60,60	0
58	MG	1A	3028	1/1	0.96	0.18	35,35,35,35	0
58	MG	1A	3102	1/1	0.96	0.18	35,35,35,35	0
58	MG	1A	4049	1/1	0.96	0.08	56,56,56,56	0
58	MG	1A	3127	1/1	0.96	0.21	34,34,34,34	0
58	MG	1A	3400	1/1	0.96	0.22	39,39,39,39	0
58	MG	1A	3103	1/1	0.96	0.15	38,38,38,38	0
58	MG	1A	3201	1/1	0.96	0.07	45,45,45,45	0
58	MG	1A	3628	1/1	0.96	0.07	30,30,30,30	0
58	MG	2A	3752	1/1	0.96	0.06	49,49,49,49	0
58	MG	2A	3330	1/1	0.96	0.15	55,55,55,55	0
58	MG	2A	3163	1/1	0.96	0.18	65,65,65,65	0
58	MG	1A	3536	1/1	0.96	0.22	46,46,46,46	0
58	MG	1A	3931	1/1	0.96	0.09	26,26,26,26	0
58	MG	1A	3403	1/1	0.96	0.12	57,57,57,57	0
58	MG	1a	1677	1/1	0.96	0.21	56,56,56,56	0
58	MG	1A	3249	1/1	0.96	0.07	36,36,36,36	0
58	MG	2A	3543	1/1	0.96	0.08	54,54,54,54	0
58	MG	1A	4064	1/1	0.96	0.07	60,60,60,60	0
58	MG	2A	3170	1/1	0.96	0.05	56,56,56,56	0
58	MG	1A	3935	1/1	0.96	0.10	53,53,53,53	0
58	MG	1R	202	1/1	0.96	0.07	31,31,31,31	0
58	MG	1A	3033	1/1	0.96	0.08	47,47,47,47	0
58	MG	1R	204	1/1	0.96	0.07	53,53,53,53	0
58	MG	1A	3635	1/1	0.96	0.09	36,36,36,36	0
58	MG	1A	3073	1/1	0.96	0.07	27,27,27,27	0
58	MG	1A	3168	1/1	0.96	0.12	43,43,43,43	0
58	MG	2A	3554	1/1	0.96	0.21	55,55,55,55	0
58	MG	1A	3941	1/1	0.96	0.06	19,19,19,19	0
58	MG	1A	3408	1/1	0.96	0.11	54,54,54,54	0
58	MG	1A	3208	1/1	0.96	0.13	41,41,41,41	0
58	MG	1A	4074	1/1	0.96	0.14	53,53,53,53	0
58	MG	1A	3737	1/1	0.96	0.08	53,53,53,53	0
58	MG	1A	3107	1/1	0.96	0.25	32,32,32,32	0
58	MG	1A	3641	1/1	0.96	0.10	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3949	1/1	0.96	0.06	39,39,39,39	0
58	MG	2A	3563	1/1	0.96	0.16	70,70,70,70	0
58	MG	1A	3352	1/1	0.96	0.09	58,58,58,58	0
58	MG	1U	206	1/1	0.96	0.19	45,45,45,45	0
58	MG	1U	208	1/1	0.96	0.18	43,43,43,43	0
58	MG	2A	3784	1/1	0.96	0.05	77,77,77,77	0
58	MG	1U	209	1/1	0.96	0.27	41,41,41,41	0
58	MG	1A	3210	1/1	0.96	0.14	42,42,42,42	0
58	MG	2a	1698	1/1	0.96	0.17	55,55,55,55	0
58	MG	2A	3569	1/1	0.96	0.05	38,38,38,38	0
58	MG	1A	3953	1/1	0.96	0.06	32,32,32,32	0
58	MG	1A	4082	1/1	0.96	0.07	63,63,63,63	0
58	MG	1A	3108	1/1	0.96	0.14	40,40,40,40	0
58	MG	2A	3012	1/1	0.96	0.07	51,51,51,51	0
58	MG	1A	3474	1/1	0.96	0.28	53,53,53,53	0
58	MG	1V	206	1/1	0.96	0.26	60,60,60,60	0
58	MG	1A	4085	1/1	0.96	0.22	43,43,43,43	0
58	MG	1A	3842	1/1	0.96	0.05	42,42,42,42	0
58	MG	1a	1711	1/1	0.96	0.28	60,60,60,60	0
58	MG	2A	3798	1/1	0.96	0.08	71,71,71,71	0
58	MG	2A	3799	1/1	0.96	0.06	82,82,82,82	0
58	MG	2A	3369	1/1	0.96	0.19	58,58,58,58	0
58	MG	1A	3052	1/1	0.96	0.09	44,44,44,44	0
58	MG	2A	3201	1/1	0.96	0.15	46,46,46,46	0
58	MG	1W	204	1/1	0.96	0.15	44,44,44,44	0
58	MG	1A	3136	1/1	0.96	0.21	39,39,39,39	0
58	MG	2A	3584	1/1	0.96	0.14	65,65,65,65	0
58	MG	2A	3024	1/1	0.96	0.08	56,56,56,56	0
58	MG	2A	3376	1/1	0.96	0.08	50,50,50,50	0
58	MG	1A	3648	1/1	0.96	0.08	37,37,37,37	0
58	MG	1X	101	1/1	0.96	0.22	50,50,50,50	0
58	MG	1A	3360	1/1	0.96	0.17	36,36,36,36	0
58	MG	1A	3075	1/1	0.96	0.09	43,43,43,43	0
58	MG	1A	3112	1/1	0.96	0.16	45,45,45,45	0
58	MG	1A	3313	1/1	0.96	0.12	44,44,44,44	0
58	MG	2A	3033	1/1	0.96	0.08	50,50,50,50	0
58	MG	1A	3966	1/1	0.96	0.08	61,61,61,61	0
58	MG	1A	3851	1/1	0.96	0.26	30,30,30,30	0
58	MG	1A	4097	1/1	0.96	0.05	44,44,44,44	0
58	MG	2A	3388	1/1	0.96	0.05	38,38,38,38	0
58	MG	1A	3364	1/1	0.96	0.09	56,56,56,56	0
58	MG	2A	3216	1/1	0.96	0.11	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	4099	1/1	0.96	0.11	56,56,56,56	0
58	MG	10	106	1/1	0.96	0.11	57,57,57,57	0
58	MG	1A	3423	1/1	0.96	0.14	67,67,67,67	0
58	MG	2a	1740	1/1	0.96	0.05	66,66,66,66	0
58	MG	1A	4101	1/1	0.96	0.16	51,51,51,51	0
58	MG	1A	3484	1/1	0.96	0.23	44,44,44,44	0
58	MG	1A	3076	1/1	0.96	0.23	37,37,37,37	0
58	MG	1A	3178	1/1	0.96	0.20	46,46,46,46	0
58	MG	1a	1735	1/1	0.96	0.19	47,47,47,47	0
58	MG	1a	1736	1/1	0.96	0.10	56,56,56,56	0
58	MG	1A	3023	1/1	0.96	0.16	38,38,38,38	0
58	MG	2a	1749	1/1	0.96	0.12	66,66,66,66	0
58	MG	11	101	1/1	0.96	0.39	44,44,44,44	0
58	MG	2A	3403	1/1	0.96	0.27	56,56,56,56	0
58	MG	1A	3762	1/1	0.96	0.26	36,36,36,36	0
58	MG	11	103	1/1	0.96	0.06	40,40,40,40	0
58	MG	1a	1742	1/1	0.96	0.06	51,51,51,51	0
58	MG	1A	3662	1/1	0.96	0.05	19,19,19,19	0
58	MG	1A	3978	1/1	0.96	0.07	52,52,52,52	0
58	MG	12	102	1/1	0.96	0.07	54,54,54,54	0
58	MG	2a	1758	1/1	0.96	0.11	76,76,76,76	0
58	MG	1A	3318	1/1	0.96	0.17	54,54,54,54	0
58	MG	1A	3143	1/1	0.96	0.09	49,49,49,49	0
58	MG	1A	3571	1/1	0.96	0.09	32,32,32,32	0
58	MG	1A	3429	1/1	0.96	0.10	38,38,38,38	0
58	MG	15	103	1/1	0.96	0.23	37,37,37,37	0
58	MG	2A	3627	1/1	0.96	0.19	52,52,52,52	0
58	MG	2A	3417	1/1	0.96	0.11	70,70,70,70	0
58	MG	2A	3418	1/1	0.96	0.11	46,46,46,46	0
58	MG	1A	3868	1/1	0.96	0.06	52,52,52,52	0
58	MG	2D	305	1/1	0.96	0.12	68,68,68,68	0
58	MG	15	107	1/1	0.96	0.12	41,41,41,41	0
58	MG	1A	3270	1/1	0.96	0.29	45,45,45,45	0
58	MG	1A	3431	1/1	0.96	0.12	42,42,42,42	0
58	MG	1A	3271	1/1	0.96	0.18	37,37,37,37	0
58	MG	2A	3244	1/1	0.96	0.30	63,63,63,63	0
58	MG	1B	208	1/1	0.96	0.17	68,68,68,68	0
58	MG	2A	3430	1/1	0.96	0.08	51,51,51,51	0
58	MG	17	102	1/1	0.96	0.27	37,37,37,37	0
58	MG	2a	1777	1/1	0.96	0.26	67,67,67,67	0
58	MG	1A	3324	1/1	0.96	0.11	46,46,46,46	0
58	MG	1A	3989	1/1	0.96	0.05	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3990	1/1	0.96	0.06	50,50,50,50	0
58	MG	1A	3991	1/1	0.96	0.07	54,54,54,54	0
58	MG	1A	3579	1/1	0.96	0.05	24,24,24,24	0
58	MG	1A	3580	1/1	0.96	0.08	31,31,31,31	0
58	MG	1A	3675	1/1	0.96	0.15	65,65,65,65	0
58	MG	1B	216	1/1	0.96	0.06	68,68,68,68	0
58	MG	1A	3581	1/1	0.96	0.10	30,30,30,30	0
58	MG	2A	3650	1/1	0.96	0.07	58,58,58,58	0
58	MG	1A	3582	1/1	0.96	0.11	60,60,60,60	0
58	MG	1A	3679	1/1	0.96	0.06	29,29,29,29	0
58	MG	2a	1791	1/1	0.96	0.06	62,62,62,62	0
58	MG	1A	3584	1/1	0.96	0.04	23,23,23,23	0
58	MG	2Q	201	1/1	0.96	0.09	63,63,63,63	0
58	MG	1A	3225	1/1	0.96	0.26	56,56,56,56	0
58	MG	1A	3060	1/1	0.96	0.26	56,56,56,56	0
58	MG	1a	1777	1/1	0.96	0.08	49,49,49,49	0
58	MG	1B	225	1/1	0.96	0.10	59,59,59,59	0
58	MG	1A	3120	1/1	0.96	0.08	52,52,52,52	0
58	MG	2T	203	1/1	0.96	0.10	60,60,60,60	0
58	MG	1A	3380	1/1	0.96	0.21	49,49,49,49	0
58	MG	1A	3081	1/1	0.96	0.06	35,35,35,35	0
58	MG	1A	3147	1/1	0.96	0.23	38,38,38,38	0
58	MG	1A	4007	1/1	0.96	0.11	19,19,19,19	0
58	MG	2A	3456	1/1	0.96	0.09	50,50,50,50	0
58	MG	2A	3457	1/1	0.96	0.10	64,64,64,64	0
58	MG	1A	3688	1/1	0.96	0.06	60,60,60,60	0
58	MG	2X	102	1/1	0.96	0.09	53,53,53,53	0
58	MG	1A	3189	1/1	0.96	0.20	41,41,41,41	0
58	MG	2A	3097	1/1	0.96	0.10	44,44,44,44	0
58	MG	1A	3896	1/1	0.96	0.12	58,58,58,58	0
58	MG	1A	3690	1/1	0.96	0.08	41,41,41,41	0
58	MG	2A	3100	1/1	0.96	0.17	48,48,48,48	0
58	MG	2A	3466	1/1	0.96	0.11	39,39,39,39	0
58	MG	1A	3594	1/1	0.96	0.06	36,36,36,36	0
58	MG	2A	3468	1/1	0.96	0.07	58,58,58,58	0
58	MG	1A	3148	1/1	0.96	0.07	45,45,45,45	0
58	MG	27	101	1/1	0.96	0.19	52,52,52,52	0
58	MG	1D	301	1/1	0.96	0.09	53,53,53,53	0
58	MG	2A	3677	1/1	0.96	0.08	59,59,59,59	0
58	MG	1D	302	1/1	0.96	0.14	45,45,45,45	0
58	MG	2A	3472	1/1	0.96	0.09	46,46,46,46	0
58	MG	2A	3683	1/1	0.96	0.05	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1D	304	1/1	0.96	0.09	44,44,44,44	0
58	MG	1a	1797	1/1	0.96	0.17	65,65,65,65	0
58	MG	1D	306	1/1	0.96	0.24	42,42,42,42	0
58	MG	1D	307	1/1	0.96	0.11	55,55,55,55	0
58	MG	1a	1800	1/1	0.96	0.06	71,71,71,71	0
58	MG	2a	1838	1/1	0.96	0.15	72,72,72,72	0
58	MG	1A	3598	1/1	0.96	0.10	57,57,57,57	0
58	MG	1D	309	1/1	0.96	0.19	37,37,37,37	0
58	MG	1A	3694	1/1	0.96	0.09	69,69,69,69	0
58	MG	1D	311	1/1	0.96	0.12	60,60,60,60	0
58	MG	1A	3192	1/1	0.96	0.10	44,44,44,44	0
58	MG	1A	3795	1/1	0.96	0.23	55,55,55,55	0
58	MG	2A	3120	1/1	0.96	0.23	51,51,51,51	0
58	MG	1A	3062	1/1	0.96	0.24	61,61,61,61	0
58	MG	2A	3122	1/1	0.96	0.10	60,60,60,60	0
58	MG	1E	309	1/1	0.96	0.09	33,33,33,33	0
58	MG	1A	3515	1/1	0.96	0.20	42,42,42,42	0
58	MG	1A	3698	1/1	0.96	0.05	44,44,44,44	0
58	MG	2A	3492	1/1	0.96	0.11	59,59,59,59	0
58	MG	1A	3239	1/1	0.96	0.12	47,47,47,47	0
58	MG	1a	1813	1/1	0.96	0.07	74,74,74,74	0
58	MG	2A	3496	1/1	0.96	0.09	71,71,71,71	0
58	MG	1a	1644	1/1	0.96	0.14	62,62,62,62	0
58	MG	1a	1815	1/1	0.96	0.09	78,78,78,78	0
58	MG	1A	3123	1/1	0.96	0.09	44,44,44,44	0
58	MG	1F	301	1/1	0.96	0.14	43,43,43,43	0
58	MG	1a	1647	1/1	0.96	0.08	53,53,53,53	0
58	MG	1A	3389	1/1	0.96	0.10	60,60,60,60	0
58	MG	1a	1651	1/1	0.96	0.08	50,50,50,50	0
58	MG	2A	3135	1/1	0.96	0.12	42,42,42,42	0
58	MG	1A	3910	1/1	0.96	0.06	41,41,41,41	0
58	MG	1F	308	1/1	0.96	0.09	34,34,34,34	0
58	MG	1A	3338	1/1	0.96	0.16	43,43,43,43	0
58	MG	1A	4032	1/1	0.96	0.11	59,59,59,59	0
58	MG	1A	3195	1/1	0.96	0.09	27,27,27,27	0
59	K	1A	3504	1/1	0.96	0.10	69,69,69,69	0
58	MG	2A	3310	1/1	0.96	0.07	54,54,54,54	0
58	MG	2A	3058	1/1	0.97	0.08	38,38,38,38	0
58	MG	1A	3066	1/1	0.97	0.09	17,17,17,17	0
58	MG	1A	3070	1/1	0.97	0.03	28,28,28,28	0
58	MG	1A	3507	1/1	0.97	0.20	34,34,34,34	0
58	MG	1A	3683	1/1	0.97	0.06	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3508	1/1	0.97	0.05	23,23,23,23	0
58	MG	1A	3592	1/1	0.97	0.12	28,28,28,28	0
58	MG	1A	3213	1/1	0.97	0.07	47,47,47,47	0
58	MG	2A	3397	1/1	0.97	0.10	49,49,49,49	0
58	MG	2A	3067	1/1	0.97	0.14	37,37,37,37	0
58	MG	1A	4025	1/1	0.97	0.10	46,46,46,46	0
58	MG	1A	3440	1/1	0.97	0.08	46,46,46,46	0
58	MG	1A	3596	1/1	0.97	0.05	35,35,35,35	0
58	MG	1A	3071	1/1	0.97	0.17	51,51,51,51	0
58	MG	1A	3323	1/1	0.97	0.24	39,39,39,39	0
58	MG	1A	3599	1/1	0.97	0.07	41,41,41,41	0
58	MG	1A	3044	1/1	0.97	0.14	41,41,41,41	0
58	MG	2A	3787	1/1	0.97	0.07	65,65,65,65	0
58	MG	1A	3796	1/1	0.97	0.12	23,23,23,23	0
58	MG	2A	3408	1/1	0.97	0.06	66,66,66,66	0
58	MG	2A	3076	1/1	0.97	0.06	47,47,47,47	0
58	MG	1E	305	1/1	0.97	0.19	41,41,41,41	0
58	MG	1A	3268	1/1	0.97	0.18	36,36,36,36	0
58	MG	1E	307	1/1	0.97	0.12	35,35,35,35	0
58	MG	2a	1684	1/1	0.97	0.14	51,51,51,51	0
58	MG	1A	3137	1/1	0.97	0.16	39,39,39,39	0
58	MG	1a	1617	1/1	0.97	0.07	52,52,52,52	0
58	MG	1A	3520	1/1	0.97	0.13	41,41,41,41	0
58	MG	1a	1619	1/1	0.97	0.07	51,51,51,51	0
58	MG	1a	1620	1/1	0.97	0.05	56,56,56,56	0
58	MG	1A	3800	1/1	0.97	0.10	30,30,30,30	0
58	MG	1a	1622	1/1	0.97	0.06	49,49,49,49	0
58	MG	1A	4038	1/1	0.97	0.09	35,35,35,35	0
58	MG	1A	3605	1/1	0.97	0.11	40,40,40,40	0
58	MG	1A	3111	1/1	0.97	0.30	51,51,51,51	0
58	MG	2A	3806	1/1	0.97	0.06	52,52,52,52	0
58	MG	1A	3219	1/1	0.97	0.09	39,39,39,39	0
58	MG	2A	3425	1/1	0.97	0.19	59,59,59,59	0
58	MG	2A	3426	1/1	0.97	0.09	49,49,49,49	0
58	MG	1A	3329	1/1	0.97	0.08	41,41,41,41	0
58	MG	1A	3449	1/1	0.97	0.15	47,47,47,47	0
58	MG	1F	307	1/1	0.97	0.12	45,45,45,45	0
58	MG	1a	1793	1/1	0.97	0.05	64,64,64,64	0
58	MG	1A	3273	1/1	0.97	0.21	36,36,36,36	0
58	MG	1F	309	1/1	0.97	0.14	35,35,35,35	0
58	MG	1A	3274	1/1	0.97	0.17	50,50,50,50	0
58	MG	1A	3091	1/1	0.97	0.07	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3614	1/1	0.97	0.05	33,33,33,33	0
58	MG	1A	3392	1/1	0.97	0.24	41,41,41,41	0
58	MG	2a	1709	1/1	0.97	0.14	54,54,54,54	0
58	MG	1A	3140	1/1	0.97	0.20	37,37,37,37	0
58	MG	2A	3103	1/1	0.97	0.23	54,54,54,54	0
58	MG	1A	3709	1/1	0.97	0.06	44,44,44,44	0
58	MG	1A	3030	1/1	0.97	0.14	34,34,34,34	0
58	MG	2A	3106	1/1	0.97	0.14	39,39,39,39	0
58	MG	1A	3711	1/1	0.97	0.07	46,46,46,46	0
58	MG	2A	3629	1/1	0.97	0.06	37,37,37,37	0
58	MG	1A	4056	1/1	0.97	0.06	77,77,77,77	0
58	MG	1A	3930	1/1	0.97	0.11	46,46,46,46	0
58	MG	1A	3712	1/1	0.97	0.07	32,32,32,32	0
58	MG	2A	3448	1/1	0.97	0.09	61,61,61,61	0
58	MG	1A	3932	1/1	0.97	0.10	37,37,37,37	0
58	MG	1A	4061	1/1	0.97	0.06	43,43,43,43	0
58	MG	1N	203	1/1	0.97	0.07	43,43,43,43	0
58	MG	1A	3619	1/1	0.97	0.09	32,32,32,32	0
58	MG	1A	4063	1/1	0.97	0.05	82,82,82,82	0
58	MG	2a	1726	1/1	0.97	0.08	64,64,64,64	0
58	MG	2A	3116	1/1	0.97	0.09	55,55,55,55	0
58	MG	2A	3455	1/1	0.97	0.07	45,45,45,45	0
58	MG	1A	3114	1/1	0.97	0.16	40,40,40,40	0
58	MG	1O	203	1/1	0.97	0.11	55,55,55,55	0
58	MG	2A	3458	1/1	0.97	0.09	40,40,40,40	0
58	MG	1A	3534	1/1	0.97	0.25	43,43,43,43	0
58	MG	2a	1734	1/1	0.97	0.09	71,71,71,71	0
58	MG	1A	3820	1/1	0.97	0.16	43,43,43,43	0
58	MG	1A	3623	1/1	0.97	0.05	27,27,27,27	0
58	MG	1A	3336	1/1	0.97	0.10	60,60,60,60	0
58	MG	1A	3625	1/1	0.97	0.04	31,31,31,31	0
58	MG	1A	3824	1/1	0.97	0.10	40,40,40,40	0
58	MG	1Q	201	1/1	0.97	0.15	40,40,40,40	0
58	MG	1Q	202	1/1	0.97	0.11	33,33,33,33	0
58	MG	1A	3181	1/1	0.97	0.12	39,39,39,39	0
58	MG	2D	303	1/1	0.97	0.31	44,44,44,44	0
58	MG	1A	3943	1/1	0.97	0.09	27,27,27,27	0
58	MG	1A	3627	1/1	0.97	0.09	57,57,57,57	0
58	MG	1a	1826	1/1	0.97	0.06	64,64,64,64	0
58	MG	1A	3538	1/1	0.97	0.29	44,44,44,44	0
58	MG	1R	201	1/1	0.97	0.32	45,45,45,45	0
58	MG	2E	303	1/1	0.97	0.14	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3724	1/1	0.97	0.05	36,36,36,36	0
58	MG	1A	3115	1/1	0.97	0.12	35,35,35,35	0
58	MG	1A	3117	1/1	0.97	0.25	42,42,42,42	0
58	MG	2A	3662	1/1	0.97	0.06	55,55,55,55	0
58	MG	1A	3231	1/1	0.97	0.07	41,41,41,41	0
58	MG	1A	3728	1/1	0.97	0.14	67,67,67,67	0
58	MG	1A	3834	1/1	0.97	0.10	54,54,54,54	0
58	MG	1A	3185	1/1	0.97	0.28	33,33,33,33	0
58	MG	1A	3057	1/1	0.97	0.14	40,40,40,40	0
58	MG	1A	3837	1/1	0.97	0.10	37,37,37,37	0
58	MG	1A	3957	1/1	0.97	0.07	45,45,45,45	0
58	MG	1A	3732	1/1	0.97	0.07	46,46,46,46	0
58	MG	1A	3733	1/1	0.97	0.03	38,38,38,38	0
58	MG	1U	202	1/1	0.97	0.21	44,44,44,44	0
58	MG	1A	3286	1/1	0.97	0.09	42,42,42,42	0
58	MG	2A	3148	1/1	0.97	0.11	53,53,53,53	0
58	MG	1A	3735	1/1	0.97	0.05	24,24,24,24	0
58	MG	1A	3962	1/1	0.97	0.06	67,67,67,67	0
58	MG	1A	3094	1/1	0.97	0.04	36,36,36,36	0
58	MG	2A	3494	1/1	0.97	0.09	42,42,42,42	0
58	MG	1U	207	1/1	0.97	0.27	41,41,41,41	0
58	MG	2A	3680	1/1	0.97	0.10	49,49,49,49	0
58	MG	2A	3681	1/1	0.97	0.04	72,72,72,72	0
58	MG	2A	3682	1/1	0.97	0.06	67,67,67,67	0
58	MG	2A	3153	1/1	0.97	0.10	55,55,55,55	0
58	MG	1A	3288	1/1	0.97	0.09	35,35,35,35	0
58	MG	1A	3188	1/1	0.97	0.05	41,41,41,41	0
58	MG	1A	3011	1/1	0.97	0.04	33,33,33,33	0
58	MG	1U	211	1/1	0.97	0.30	39,39,39,39	0
58	MG	1A	3740	1/1	0.97	0.05	22,22,22,22	0
58	MG	1A	3039	1/1	0.97	0.26	34,34,34,34	0
58	MG	2W	202	1/1	0.97	0.11	63,63,63,63	0
58	MG	1A	3097	1/1	0.97	0.11	39,39,39,39	0
58	MG	1V	201	1/1	0.97	0.11	35,35,35,35	0
58	MG	1A	3411	1/1	0.97	0.11	43,43,43,43	0
58	MG	2A	3693	1/1	0.97	0.06	64,64,64,64	0
58	MG	1V	204	1/1	0.97	0.32	37,37,37,37	0
58	MG	1A	3412	1/1	0.97	0.21	39,39,39,39	0
58	MG	1A	3241	1/1	0.97	0.20	60,60,60,60	0
58	MG	1a	1697	1/1	0.97	0.14	50,50,50,50	0
58	MG	1A	3151	1/1	0.97	0.09	35,35,35,35	0
58	MG	1A	3040	1/1	0.97	0.13	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3100	1/1	0.97	0.33	33,33,33,33	0
58	MG	1A	3061	1/1	0.97	0.17	48,48,48,48	0
58	MG	1A	3651	1/1	0.97	0.12	58,58,58,58	0
58	MG	1A	3026	1/1	0.97	0.26	35,35,35,35	0
58	MG	1X	102	1/1	0.97	0.06	48,48,48,48	0
58	MG	2a	1802	1/1	0.97	0.05	70,70,70,70	0
58	MG	1A	3158	1/1	0.97	0.08	36,36,36,36	0
58	MG	28	102	1/1	0.97	0.12	56,56,56,56	0
58	MG	1A	3561	1/1	0.97	0.06	47,47,47,47	0
58	MG	1A	4111	1/1	0.97	0.10	49,49,49,49	0
58	MG	1A	3303	1/1	0.97	0.23	34,34,34,34	0
58	MG	1a	1710	1/1	0.97	0.13	61,61,61,61	0
58	MG	1Y	202	1/1	0.97	0.22	52,52,52,52	0
58	MG	1A	3128	1/1	0.97	0.32	38,38,38,38	0
58	MG	1Z	302	1/1	0.97	0.07	58,58,58,58	0
58	MG	1A	3564	1/1	0.97	0.06	41,41,41,41	0
58	MG	2a	1608	1/1	0.97	0.25	66,66,66,66	0
58	MG	1A	3867	1/1	0.97	0.15	45,45,45,45	0
58	MG	1A	3104	1/1	0.97	0.13	40,40,40,40	0
58	MG	2A	3529	1/1	0.97	0.06	43,43,43,43	0
58	MG	1B	205	1/1	0.97	0.07	62,62,62,62	0
58	MG	2A	3720	1/1	0.97	0.13	50,50,50,50	0
58	MG	1a	1719	1/1	0.97	0.07	43,43,43,43	0
58	MG	2A	3532	1/1	0.97	0.08	50,50,50,50	0
58	MG	1A	3567	1/1	0.97	0.09	34,34,34,34	0
58	MG	1A	3162	1/1	0.97	0.13	44,44,44,44	0
58	MG	1A	3042	1/1	0.97	0.06	36,36,36,36	0
58	MG	1A	3366	1/1	0.97	0.09	34,34,34,34	0
58	MG	2a	1829	1/1	0.97	0.05	79,79,79,79	0
58	MG	2A	3727	1/1	0.97	0.07	47,47,47,47	0
58	MG	2A	3025	1/1	0.97	0.12	58,58,58,58	0
58	MG	1A	3874	1/1	0.97	0.06	44,44,44,44	0
58	MG	2A	3539	1/1	0.97	0.09	43,43,43,43	0
58	MG	1A	3766	1/1	0.97	0.07	33,33,33,33	0
58	MG	1a	1726	1/1	0.97	0.04	43,43,43,43	0
58	MG	1A	3367	1/1	0.97	0.14	33,33,33,33	0
58	MG	1A	3665	1/1	0.97	0.11	61,61,61,61	0
58	MG	2a	1840	1/1	0.97	0.12	60,60,60,60	0
58	MG	1A	3204	1/1	0.97	0.05	43,43,43,43	0
58	MG	2A	3741	1/1	0.97	0.08	78,78,78,78	0
58	MG	1A	3164	1/1	0.97	0.13	40,40,40,40	0
58	MG	1A	3165	1/1	0.97	0.37	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3744	1/1	0.97	0.05	71,71,71,71	0
58	MG	2A	3035	1/1	0.97	0.12	55,55,55,55	0
58	MG	2l	201	1/1	0.97	0.07	71,71,71,71	0
58	MG	2A	3036	1/1	0.97	0.14	35,35,35,35	0
58	MG	1B	217	1/1	0.97	0.15	59,59,59,59	0
58	MG	12	101	1/1	0.97	0.08	51,51,51,51	0
58	MG	1A	3371	1/1	0.97	0.06	46,46,46,46	0
58	MG	13	101	1/1	0.97	0.09	37,37,37,37	0
58	MG	1A	3886	1/1	0.97	0.06	51,51,51,51	0
58	MG	1B	220	1/1	0.97	0.06	44,44,44,44	0
58	MG	1A	3207	1/1	0.97	0.15	46,46,46,46	0
58	MG	15	101	1/1	0.97	0.31	38,38,38,38	0
58	MG	1A	3496	1/1	0.97	0.18	38,38,38,38	0
58	MG	1a	1741	1/1	0.97	0.06	59,59,59,59	0
58	MG	1A	3029	1/1	0.97	0.24	37,37,37,37	0
58	MG	15	105	1/1	0.97	0.22	45,45,45,45	0
58	MG	1A	3257	1/1	0.97	0.17	44,44,44,44	0
58	MG	1A	3583	1/1	0.97	0.07	39,39,39,39	0
58	MG	2a	1651	1/1	0.97	0.09	62,62,62,62	0
58	MG	1A	3315	1/1	0.97	0.10	66,66,66,66	0
58	MG	1A	3169	1/1	0.97	0.12	27,27,27,27	0
58	MG	2A	3383	1/1	0.97	0.07	49,49,49,49	0
58	MG	1A	4012	1/1	0.97	0.05	46,46,46,46	0
58	MG	1A	4013	1/1	0.97	0.10	41,41,41,41	0
58	MG	1A	3678	1/1	0.97	0.07	34,34,34,34	0
58	MG	17	103	1/1	0.97	0.09	40,40,40,40	0
58	MG	1A	3170	1/1	0.97	0.07	51,51,51,51	0
60	ZN	24	501	1/1	0.97	0.10	126,126,126,126	0
60	ZN	2n	103	1/1	0.97	0.06	97,97,97,97	0
58	MG	1A	3227	1/1	0.98	0.13	38,38,38,38	0
58	MG	1A	3809	1/1	0.98	0.05	51,51,51,51	0
58	MG	1V	202	1/1	0.98	0.24	35,35,35,35	0
58	MG	1A	4057	1/1	0.98	0.06	49,49,49,49	0
58	MG	2A	3623	1/1	0.98	0.05	59,59,59,59	0
58	MG	2A	3009	1/1	0.98	0.06	43,43,43,43	0
58	MG	1A	3228	1/1	0.98	0.17	32,32,32,32	0
58	MG	1V	205	1/1	0.98	0.07	34,34,34,34	0
58	MG	2a	1732	1/1	0.98	0.08	68,68,68,68	0
58	MG	1A	3153	1/1	0.98	0.25	39,39,39,39	0
58	MG	2A	3013	1/1	0.98	0.06	50,50,50,50	0
58	MG	1V	207	1/1	0.98	0.06	39,39,39,39	0
58	MG	1a	1648	1/1	0.98	0.15	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1a	1649	1/1	0.98	0.09	56,56,56,56	0
58	MG	1A	3498	1/1	0.98	0.10	35,35,35,35	0
58	MG	1A	3892	1/1	0.98	0.04	50,50,50,50	0
58	MG	2A	3019	1/1	0.98	0.09	56,56,56,56	0
58	MG	1A	3072	1/1	0.98	0.10	50,50,50,50	0
58	MG	2a	1743	1/1	0.98	0.05	77,77,77,77	0
58	MG	1W	203	1/1	0.98	0.16	39,39,39,39	0
58	MG	1D	303	1/1	0.98	0.05	21,21,21,21	0
58	MG	1A	3974	1/1	0.98	0.09	59,59,59,59	0
58	MG	1a	1768	1/1	0.98	0.05	75,75,75,75	0
58	MG	2A	3026	1/1	0.98	0.12	45,45,45,45	0
58	MG	1D	305	1/1	0.98	0.20	43,43,43,43	0
58	MG	1A	3116	1/1	0.98	0.23	37,37,37,37	0
58	MG	1A	3232	1/1	0.98	0.23	43,43,43,43	0
58	MG	1A	3203	1/1	0.98	0.17	39,39,39,39	0
58	MG	1A	3615	1/1	0.98	0.04	28,28,28,28	0
58	MG	1X	105	1/1	0.98	0.06	38,38,38,38	0
58	MG	1A	3302	1/1	0.98	0.15	35,35,35,35	0
58	MG	1A	3267	1/1	0.98	0.10	38,38,38,38	0
58	MG	1a	1780	1/1	0.98	0.05	57,57,57,57	0
58	MG	1A	3101	1/1	0.98	0.04	43,43,43,43	0
58	MG	1E	304	1/1	0.98	0.16	33,33,33,33	0
58	MG	1A	3751	1/1	0.98	0.05	51,51,51,51	0
58	MG	1A	3753	1/1	0.98	0.27	33,33,33,33	0
58	MG	10	101	1/1	0.98	0.08	54,54,54,54	0
58	MG	1A	3305	1/1	0.98	0.15	45,45,45,45	0
58	MG	10	103	1/1	0.98	0.06	50,50,50,50	0
58	MG	2A	3161	1/1	0.98	0.10	36,36,36,36	0
58	MG	1A	3985	1/1	0.98	0.09	33,33,33,33	0
58	MG	1A	3620	1/1	0.98	0.07	29,29,29,29	0
58	MG	1A	3008	1/1	0.98	0.10	29,29,29,29	0
58	MG	1A	3510	1/1	0.98	0.12	47,47,47,47	0
58	MG	2A	3406	1/1	0.98	0.04	68,68,68,68	0
58	MG	1A	3511	1/1	0.98	0.07	48,48,48,48	0
58	MG	2A	3801	1/1	0.98	0.07	67,67,67,67	0
58	MG	2A	3802	1/1	0.98	0.05	79,79,79,79	0
58	MG	1A	3512	1/1	0.98	0.42	46,46,46,46	0
58	MG	1A	3036	1/1	0.98	0.31	35,35,35,35	0
58	MG	1F	303	1/1	0.98	0.17	40,40,40,40	0
58	MG	1A	3830	1/1	0.98	0.04	29,29,29,29	0
58	MG	1F	305	1/1	0.98	0.09	36,36,36,36	0
58	MG	1A	3182	1/1	0.98	0.19	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3541	1/1	0.98	0.16	51,51,51,51	0
58	MG	1A	3566	1/1	0.98	0.07	44,44,44,44	0
58	MG	1A	3045	1/1	0.98	0.03	20,20,20,20	0
58	MG	2A	3544	1/1	0.98	0.11	52,52,52,52	0
58	MG	1A	3466	1/1	0.98	0.13	30,30,30,30	0
58	MG	2a	1785	1/1	0.98	0.04	81,81,81,81	0
58	MG	1A	3630	1/1	0.98	0.07	26,26,26,26	0
58	MG	2a	1645	1/1	0.98	0.12	50,50,50,50	0
58	MG	2a	1646	1/1	0.98	0.06	52,52,52,52	0
58	MG	1A	3517	1/1	0.98	0.27	43,43,43,43	0
58	MG	1A	3632	1/1	0.98	0.04	30,30,30,30	0
58	MG	1A	3570	1/1	0.98	0.06	37,37,37,37	0
58	MG	1A	3089	1/1	0.98	0.07	40,40,40,40	0
58	MG	1A	3065	1/1	0.98	0.12	31,31,31,31	0
58	MG	1G	201	1/1	0.98	0.10	42,42,42,42	0
58	MG	2a	1795	1/1	0.98	0.09	57,57,57,57	0
58	MG	1A	3276	1/1	0.98	0.07	30,30,30,30	0
58	MG	2A	3065	1/1	0.98	0.24	49,49,49,49	0
58	MG	1A	4005	1/1	0.98	0.06	49,49,49,49	0
58	MG	2a	1799	1/1	0.98	0.06	57,57,57,57	0
58	MG	2A	3428	1/1	0.98	0.06	48,48,48,48	0
58	MG	15	104	1/1	0.98	0.28	34,34,34,34	0
58	MG	1A	3922	1/1	0.98	0.04	43,43,43,43	0
58	MG	1A	3010	1/1	0.98	0.09	39,39,39,39	0
58	MG	1a	1698	1/1	0.98	0.09	42,42,42,42	0
58	MG	2a	1805	1/1	0.98	0.06	77,77,77,77	0
58	MG	1A	3078	1/1	0.98	0.14	31,31,31,31	0
58	MG	1A	3125	1/1	0.98	0.10	50,50,50,50	0
58	MG	1A	3524	1/1	0.98	0.14	51,51,51,51	0
58	MG	1A	3214	1/1	0.98	0.10	43,43,43,43	0
58	MG	1A	3475	1/1	0.98	0.24	38,38,38,38	0
58	MG	1A	3166	1/1	0.98	0.23	36,36,36,36	0
58	MG	1A	4104	1/1	0.98	0.06	33,33,33,33	0
58	MG	1A	3528	1/1	0.98	0.19	39,39,39,39	0
58	MG	2a	1815	1/1	0.98	0.06	63,63,63,63	0
58	MG	2A	3699	1/1	0.98	0.12	51,51,51,51	0
58	MG	1A	3355	1/1	0.98	0.11	60,60,60,60	0
58	MG	1A	3167	1/1	0.98	0.05	36,36,36,36	0
58	MG	2A	3081	1/1	0.98	0.08	49,49,49,49	0
58	MG	1A	3396	1/1	0.98	0.08	55,55,55,55	0
58	MG	2a	1821	1/1	0.98	0.04	88,88,88,88	0
58	MG	1P	201	1/1	0.98	0.30	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3067	1/1	0.98	0.26	35,35,35,35	0
58	MG	1P	204	1/1	0.98	0.19	39,39,39,39	0
58	MG	1A	4020	1/1	0.98	0.09	42,42,42,42	0
58	MG	1A	3358	1/1	0.98	0.20	32,32,32,32	0
58	MG	1A	3650	1/1	0.98	0.04	15,15,15,15	0
58	MG	1A	4023	1/1	0.98	0.21	60,60,60,60	0
58	MG	1a	1717	1/1	0.98	0.04	41,41,41,41	0
58	MG	2A	3712	1/1	0.98	0.06	57,57,57,57	0
58	MG	1Q	203	1/1	0.98	0.05	45,45,45,45	0
58	MG	1A	3589	1/1	0.98	0.06	15,15,15,15	0
58	MG	2a	1834	1/1	0.98	0.09	85,85,85,85	0
58	MG	1A	3860	1/1	0.98	0.04	39,39,39,39	0
58	MG	1A	3787	1/1	0.98	0.07	37,37,37,37	0
58	MG	1A	3068	1/1	0.98	0.04	18,18,18,18	0
58	MG	1A	3321	1/1	0.98	0.27	41,41,41,41	0
58	MG	1A	3654	1/1	0.98	0.07	47,47,47,47	0
58	MG	1A	3069	1/1	0.98	0.05	33,33,33,33	0
58	MG	1A	3537	1/1	0.98	0.07	49,49,49,49	0
58	MG	1A	3723	1/1	0.98	0.07	45,45,45,45	0
58	MG	1A	3220	1/1	0.98	0.09	33,33,33,33	0
58	MG	1A	3595	1/1	0.98	0.04	33,33,33,33	0
58	MG	1A	3221	1/1	0.98	0.20	32,32,32,32	0
58	MG	2f	201	1/1	0.98	0.05	45,45,45,45	0
58	MG	2f	202	1/1	0.98	0.04	82,82,82,82	0
58	MG	1A	3951	1/1	0.98	0.04	32,32,32,32	0
58	MG	1A	3019	1/1	0.98	0.06	26,26,26,26	0
58	MG	1A	3541	1/1	0.98	0.19	32,32,32,32	0
58	MG	2A	3731	1/1	0.98	0.05	64,64,64,64	0
58	MG	1A	3873	1/1	0.98	0.09	44,44,44,44	0
58	MG	2A	3733	1/1	0.98	0.10	68,68,68,68	0
58	MG	1A	3365	1/1	0.98	0.15	32,32,32,32	0
58	MG	2A	3599	1/1	0.98	0.04	64,64,64,64	0
58	MG	2A	3473	1/1	0.98	0.08	50,50,50,50	0
58	MG	1U	201	1/1	0.98	0.14	36,36,36,36	0
58	MG	1A	4042	1/1	0.98	0.05	58,58,58,58	0
58	MG	1A	3289	1/1	0.98	0.06	45,45,45,45	0
58	MG	2A	3740	1/1	0.98	0.07	37,37,37,37	0
58	MG	1A	3731	1/1	0.98	0.07	45,45,45,45	0
58	MG	1A	3098	1/1	0.98	0.04	33,33,33,33	0
58	MG	1A	3880	1/1	0.98	0.03	43,43,43,43	0
58	MG	2A	3607	1/1	0.98	0.04	68,68,68,68	0
58	MG	1a	1632	1/1	0.98	0.13	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3881	1/1	0.98	0.07	35,35,35,35	0
58	MG	1A	3048	1/1	0.98	0.13	30,30,30,30	0
58	MG	2A	3483	1/1	0.98	0.12	45,45,45,45	0
58	MG	1A	3132	1/1	0.98	0.04	15,15,15,15	0
58	MG	2A	3119	1/1	0.98	0.08	57,57,57,57	0
58	MG	1A	3604	1/1	0.98	0.04	45,45,45,45	0
58	MG	1A	3152	1/1	0.98	0.12	33,33,33,33	0
58	MG	2A	3753	1/1	0.98	0.05	50,50,50,50	0
60	ZN	14	102	1/1	0.98	0.11	110,110,110,110	0
60	ZN	2Y	202	1/1	0.98	0.05	96,96,96,96	0
58	MG	1A	3669	1/1	0.98	0.08	29,29,29,29	0
60	ZN	29	501	1/1	0.98	0.04	81,81,81,81	0
58	MG	1A	4054	1/1	0.98	0.05	60,60,60,60	0
61	SF4	1d	302	8/8	0.98	0.04	65,72,75,76	0
58	MG	1A	3707	1/1	0.99	0.09	48,48,48,48	0
58	MG	1E	301	1/1	0.99	0.17	34,34,34,34	0
58	MG	1A	3191	1/1	0.99	0.14	27,27,27,27	0
58	MG	1E	303	1/1	0.99	0.12	37,37,37,37	0
58	MG	18	102	1/1	0.99	0.11	43,43,43,43	0
58	MG	1A	3353	1/1	0.99	0.18	34,34,34,34	0
58	MG	1A	3854	1/1	0.99	0.07	54,54,54,54	0
58	MG	1a	1750	1/1	0.99	0.04	70,70,70,70	0
58	MG	1a	1807	1/1	0.99	0.04	70,70,70,70	0
58	MG	1A	3612	1/1	0.99	0.10	41,41,41,41	0
58	MG	2A	3728	1/1	0.99	0.05	46,46,46,46	0
58	MG	1A	3013	1/1	0.99	0.05	33,33,33,33	0
58	MG	2A	3730	1/1	0.99	0.04	50,50,50,50	0
58	MG	1A	4037	1/1	0.99	0.04	54,54,54,54	0
58	MG	1A	3003	1/1	0.99	0.06	27,27,27,27	0
58	MG	1A	3150	1/1	0.99	0.11	36,36,36,36	0
58	MG	1A	3859	1/1	0.99	0.07	33,33,33,33	0
58	MG	1A	4001	1/1	0.99	0.05	45,45,45,45	0
58	MG	1A	3741	1/1	0.99	0.06	26,26,26,26	0
58	MG	1A	3272	1/1	0.99	0.34	39,39,39,39	0
58	MG	1F	302	1/1	0.99	0.13	35,35,35,35	0
58	MG	1A	3485	1/1	0.99	0.25	39,39,39,39	0
58	MG	2a	1833	1/1	0.99	0.06	63,63,63,63	0
58	MG	1A	3161	1/1	0.99	0.11	18,18,18,18	0
58	MG	1a	1763	1/1	0.99	0.06	61,61,61,61	0
58	MG	2A	3423	1/1	0.99	0.06	45,45,45,45	0
58	MG	1A	4046	1/1	0.99	0.05	53,53,53,53	0
58	MG	1A	3079	1/1	0.99	0.19	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3021	1/1	0.99	0.07	17,17,17,17	0
58	MG	1A	4091	1/1	0.99	0.04	46,46,46,46	0
58	MG	1A	4008	1/1	0.99	0.11	35,35,35,35	0
58	MG	2A	3020	1/1	0.99	0.09	28,28,28,28	0
58	MG	2A	3370	1/1	0.99	0.09	27,27,27,27	0
58	MG	1A	3292	1/1	0.99	0.05	37,37,37,37	0
58	MG	1A	3575	1/1	0.99	0.09	30,30,30,30	0
58	MG	1A	3721	1/1	0.99	0.05	47,47,47,47	0
58	MG	1A	3973	1/1	0.99	0.04	29,29,29,29	0
58	MG	2A	3435	1/1	0.99	0.05	43,43,43,43	0
58	MG	1a	1773	1/1	0.99	0.07	66,66,66,66	0
58	MG	2A	3499	1/1	0.99	0.05	40,40,40,40	0
58	MG	1a	1774	1/1	0.99	0.03	54,54,54,54	0
58	MG	1A	3234	1/1	0.99	0.05	48,48,48,48	0
58	MG	1A	3938	1/1	0.99	0.03	43,43,43,43	0
58	MG	1A	3577	1/1	0.99	0.03	31,31,31,31	0
58	MG	1A	3752	1/1	0.99	0.04	30,30,30,30	0
58	MG	2A	3632	1/1	0.99	0.09	45,45,45,45	0
58	MG	1a	1779	1/1	0.99	0.03	69,69,69,69	0
58	MG	1A	3471	1/1	0.99	0.12	33,33,33,33	0
58	MG	1A	3034	1/1	0.99	0.06	26,26,26,26	0
58	MG	1a	1782	1/1	0.99	0.06	72,72,72,72	0
58	MG	1B	234	1/1	0.99	0.10	64,64,64,64	0
58	MG	1A	3090	1/1	0.99	0.11	23,23,23,23	0
58	MG	1A	3944	1/1	0.99	0.06	45,45,45,45	0
58	MG	1A	3700	1/1	0.99	0.06	26,26,26,26	0
58	MG	1A	3876	1/1	0.99	0.03	13,13,13,13	0
58	MG	1A	3263	1/1	0.99	0.17	33,33,33,33	0
58	MG	1A	3035	1/1	0.99	0.17	34,34,34,34	0
58	MG	1A	3879	1/1	0.99	0.07	40,40,40,40	0
58	MG	1A	3265	1/1	0.99	0.07	44,44,44,44	0
58	MG	1A	3054	1/1	0.99	0.11	27,27,27,27	0
58	MG	1A	3012	1/1	0.99	0.12	26,26,26,26	0
58	MG	1A	4070	1/1	0.99	0.04	74,74,74,74	0
58	MG	1A	3849	1/1	0.99	0.04	42,42,42,42	0
60	ZN	1Y	203	1/1	0.99	0.03	78,78,78,78	0
58	MG	2A	3459	1/1	0.99	0.10	38,38,38,38	0
60	ZN	15	109	1/1	0.99	0.03	50,50,50,50	0
60	ZN	1n	104	1/1	0.99	0.03	78,78,78,78	0
58	MG	2a	1806	1/1	0.99	0.03	66,66,66,66	0
58	MG	2a	1739	1/1	0.99	0.02	65,65,65,65	0
60	ZN	25	103	1/1	0.99	0.03	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3499	1/1	0.99	0.09	36,36,36,36	0
58	MG	1P	203	1/1	0.99	0.15	27,27,27,27	0
58	MG	1a	1692	1/1	0.99	0.10	44,44,44,44	0
61	SF4	2d	303	8/8	0.99	0.04	62,70,76,82	0
60	ZN	26	103	1/1	1.00	0.03	65,65,65,65	0
58	MG	2A	3615	1/1	1.00	0.04	39,39,39,39	0
58	MG	1a	1612	1/1	1.00	0.03	31,31,31,31	0
60	ZN	16	103	1/1	1.00	0.02	44,44,44,44	0
60	ZN	19	102	1/1	1.00	0.08	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.