Full wwPDB X-ray Structure Validation Report (i)

Mar 16, 2026 – 11:33 PM UTC

PDB ID	:	8VTV / pdb_00008vtv
Title	:	Crystal structure of the wild-type Thermus thermophilus 70S ribosome in complex with macrolone MCX-91, mRNA, aminoacylated A-site Phe-tRNAphe, aminoacylated P-site fMet-tRNAmet, and deacylated E-site tRNAphe at 2.55A resolution
Authors	:	Aleksandrova, E.V.; Ma, C.-X.; Klepacki, D.; Alizadeh, F.; Vazquez-Laslop, N.; Liang, J.-H.; Polikanov, Y.S.; Mankin, A.S.
Deposited on	:	2024-01-27
Resolution	:	2.55 Å(reported)

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

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

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

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

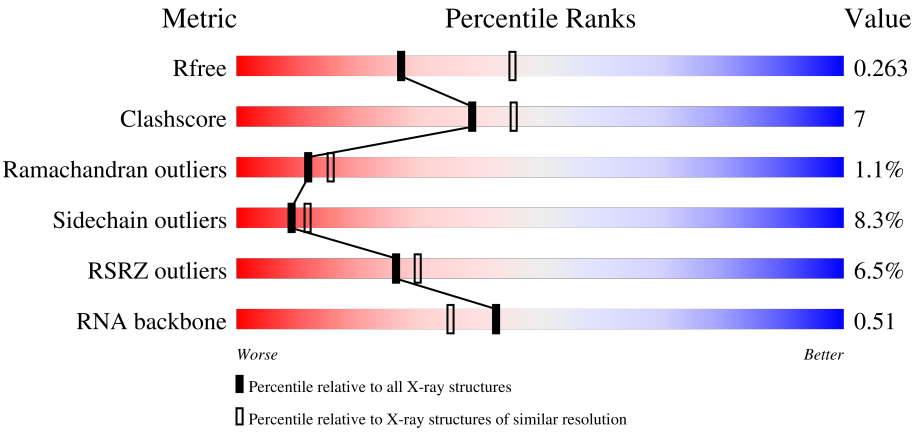
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	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 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1004 (2.54-2.54)
Clashscore	180529	1055 (2.54-2.54)
Ramachandran outliers	177936	1048 (2.54-2.54)
Sidechain outliers	177891	1048 (2.54-2.54)
RSRZ outliers	164620	1004 (2.54-2.54)
RNA backbone	3690	1040 (2.80-2.28)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	5% 71% 22% 5% •
1	2A	2915	5% 64% 26% 5% •

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

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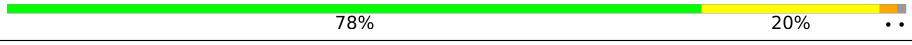
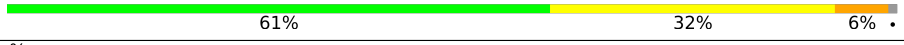
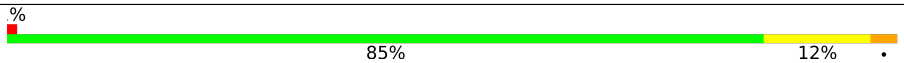
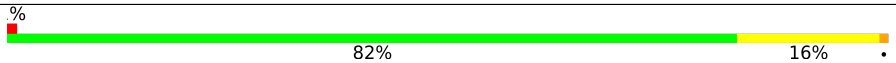
Mol	Chain	Length	Quality of chain
2	1B	121	
2	2B	121	
3	1D	276	
3	2D	276	
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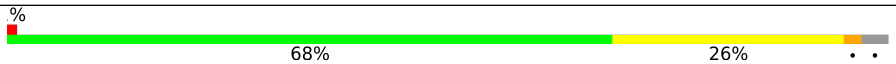
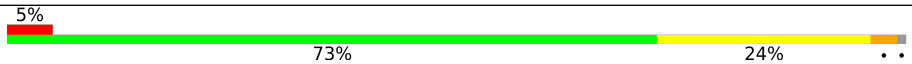
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
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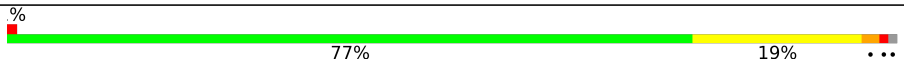
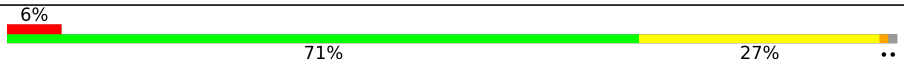
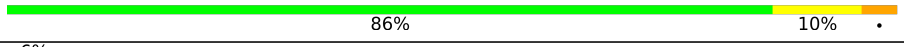
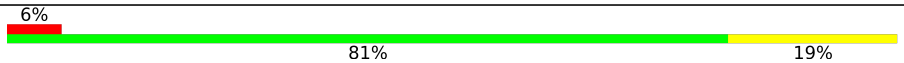
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
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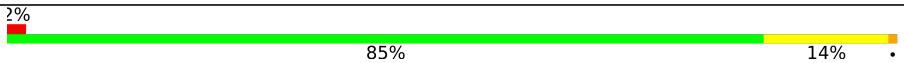
13	2R	118	
14	1S	112	

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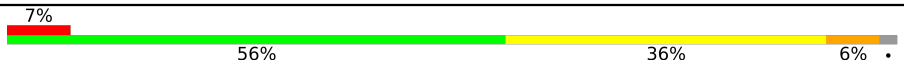
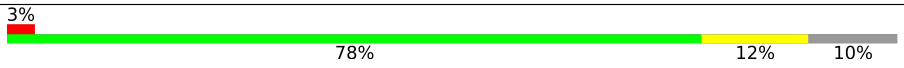
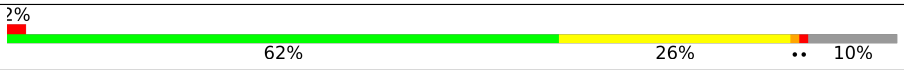
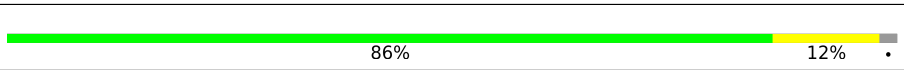
Mol	Chain	Length	Quality of chain
14	2S	112	
15	1T	146	
15	2T	146	
16	1U	118	
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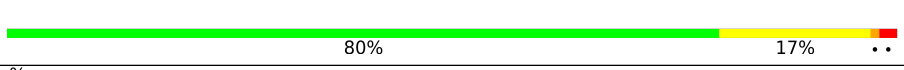
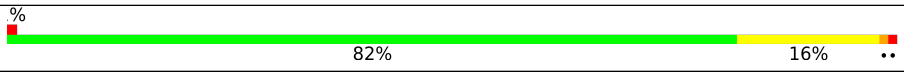
17	1V	101	
17	2V	101	
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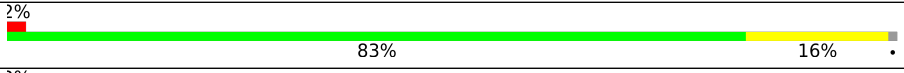
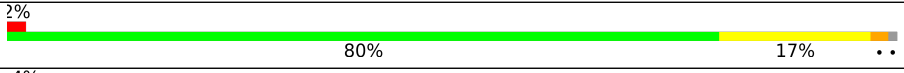
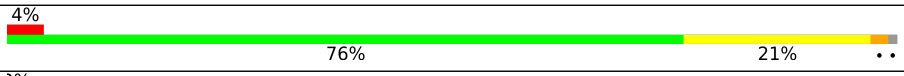
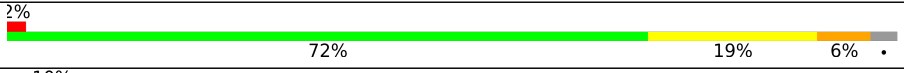
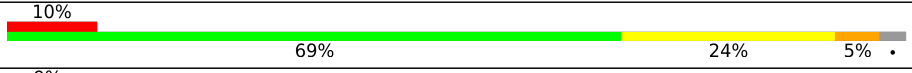
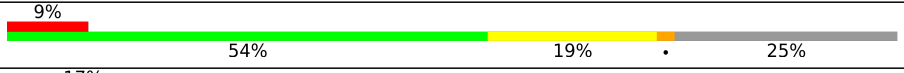
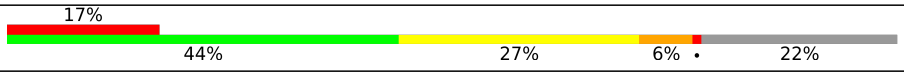
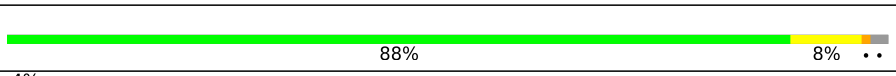
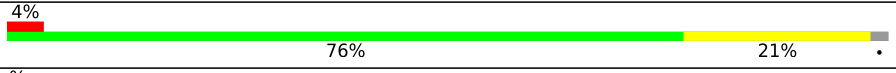
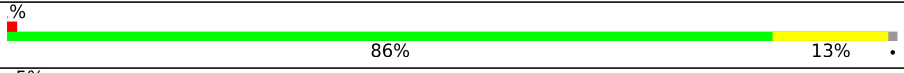
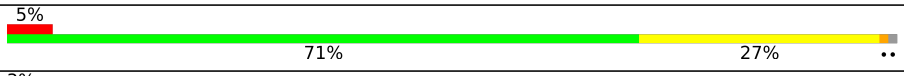
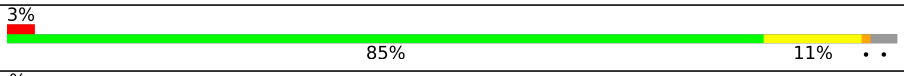
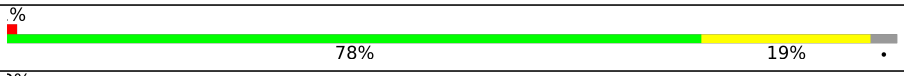
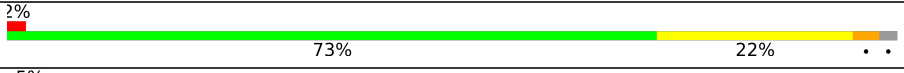
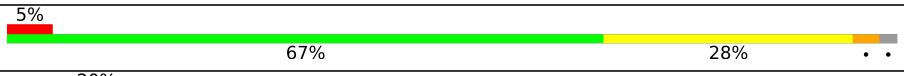
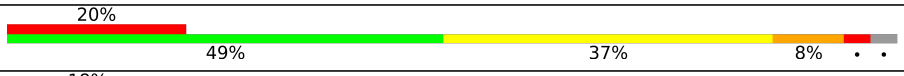
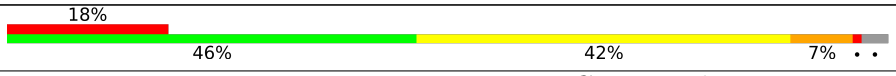
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	

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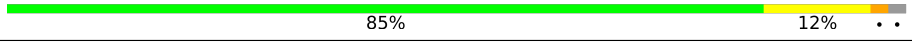
27	25	60	
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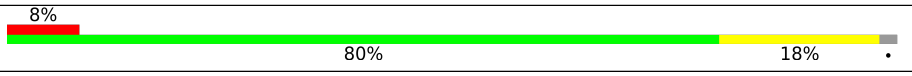
28	26	54	
29	17	49	
29	27	49	
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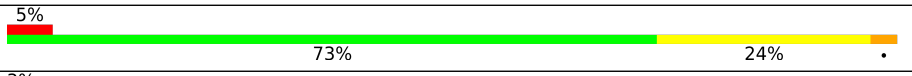
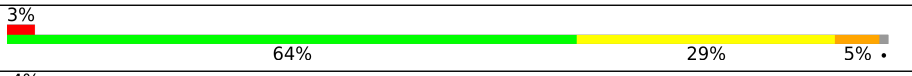
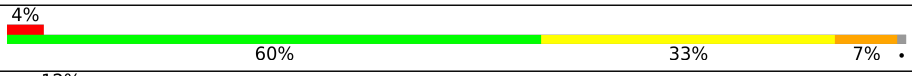
31	29	37	
32	1a	1521	
32	2a	1521	
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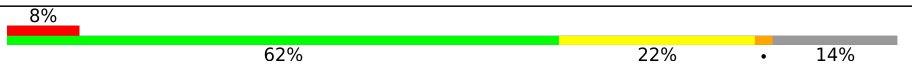
33	2b	256	
34	1c	239	
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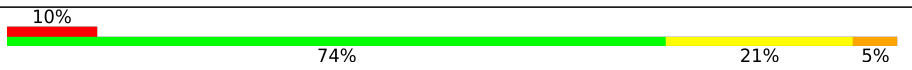
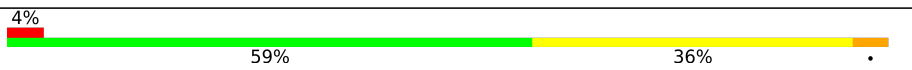
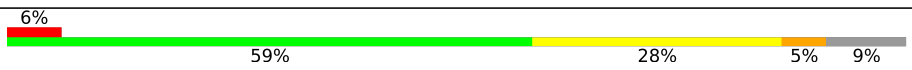
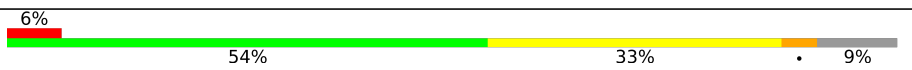
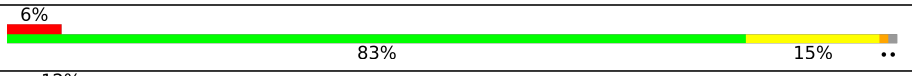
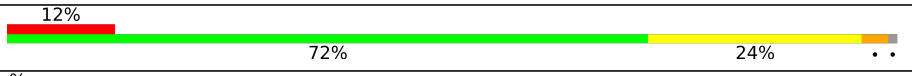
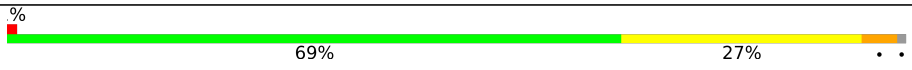
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	

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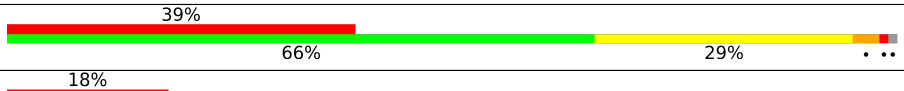
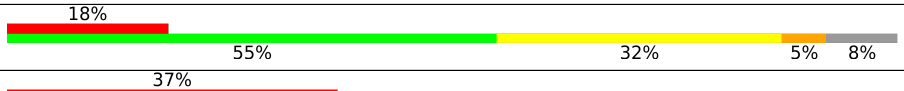
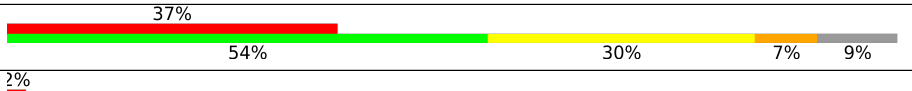
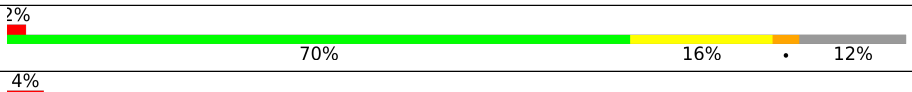
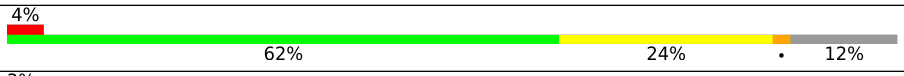
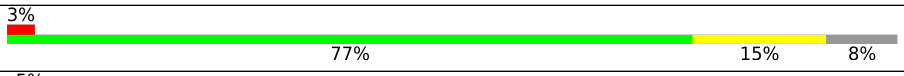
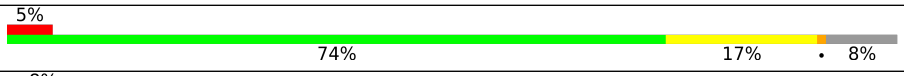
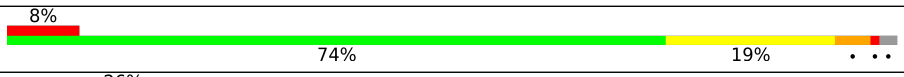
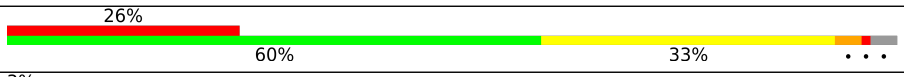
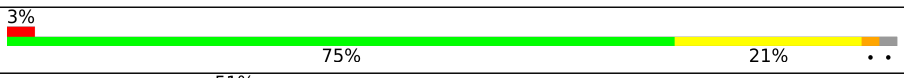
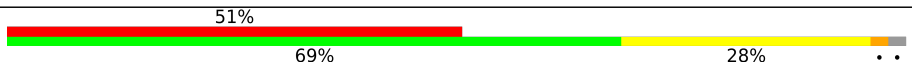
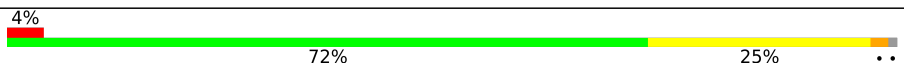
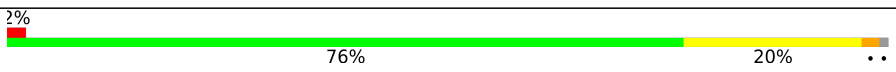
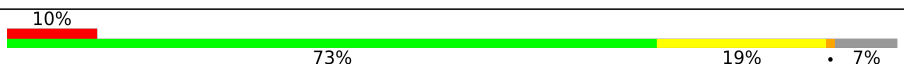
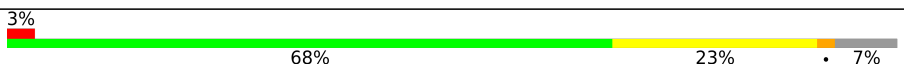
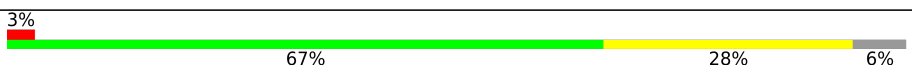
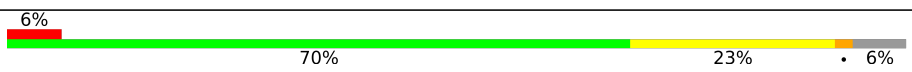
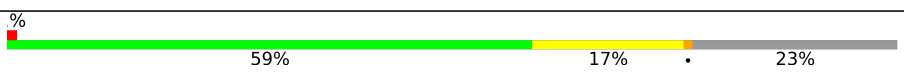
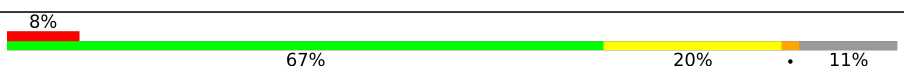
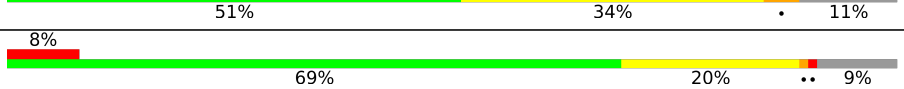
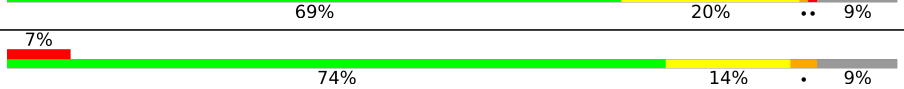
Mol	Chain	Length	Quality of chain
39	2h	138	
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	

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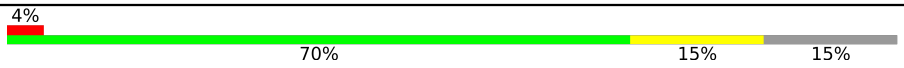
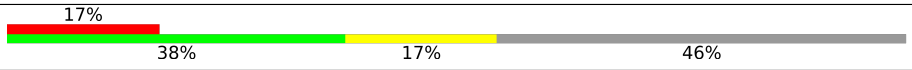
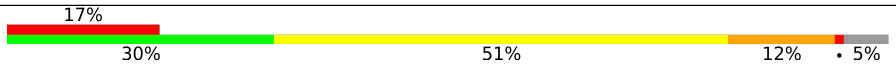
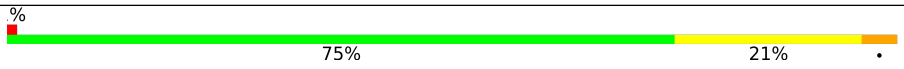
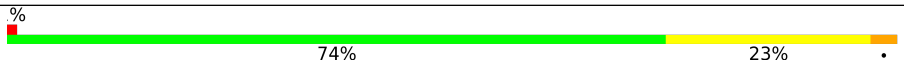
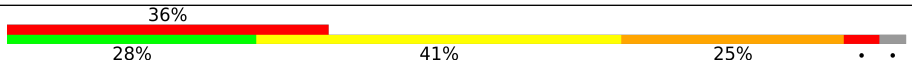
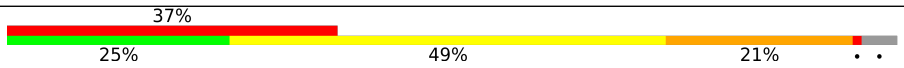
Mol	Chain	Length	Quality of chain
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	2y	76	

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 300368 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
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	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	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			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 Aminoacylated Phe-tRNAphe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1592	713	286	517	74	2			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1544	690	279	501	72	2			

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

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 RNA chain called Deacylated tRNAphe.

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

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1108	Total	Mg	0	0
			1108	1108		
57	1B	36	Total	Mg	0	0
			36	36		
57	1D	13	Total	Mg	0	0
			13	13		
57	1E	14	Total	Mg	0	0
			14	14		
57	1F	13	Total	Mg	0	0
			13	13		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1G	5	Total Mg 5 5	0	0
57	1I	1	Total Mg 1 1	0	0
57	1N	7	Total Mg 7 7	0	0
57	1O	5	Total Mg 5 5	0	0
57	1P	6	Total Mg 6 6	0	0
57	1Q	6	Total Mg 6 6	0	0
57	1R	5	Total Mg 5 5	0	0
57	1S	3	Total Mg 3 3	0	0
57	1T	2	Total Mg 2 2	0	0
57	1U	7	Total Mg 7 7	0	0
57	1V	8	Total Mg 8 8	0	0
57	1W	6	Total Mg 6 6	0	0
57	1X	8	Total Mg 8 8	0	0
57	1Y	2	Total Mg 2 2	0	0
57	1Z	3	Total Mg 3 3	0	0
57	10	9	Total Mg 9 9	0	0
57	11	4	Total Mg 4 4	0	0
57	12	2	Total Mg 2 2	0	0
57	13	4	Total Mg 4 4	0	0
57	14	1	Total Mg 1 1	0	0
57	15	8	Total Mg 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	16	3	Total Mg 3 3	0	0
57	17	4	Total Mg 4 4	0	0
57	18	3	Total Mg 3 3	0	0
57	19	2	Total Mg 2 2	0	0
57	1a	217	Total Mg 217 217	0	0
57	1b	1	Total Mg 1 1	0	0
57	1d	1	Total Mg 1 1	0	0
57	1e	2	Total Mg 2 2	0	0
57	1f	2	Total Mg 2 2	0	0
57	1h	1	Total Mg 1 1	0	0
57	1l	2	Total Mg 2 2	0	0
57	1m	2	Total Mg 2 2	0	0
57	1n	2	Total Mg 2 2	0	0
57	1q	1	Total Mg 1 1	0	0
57	1t	1	Total Mg 1 1	0	0
57	1v	1	Total Mg 1 1	0	0
57	1w	8	Total Mg 8 8	0	0
57	1x	14	Total Mg 14 14	0	0
57	1y	1	Total Mg 1 1	0	0
57	2A	861	Total Mg 861 861	0	0
57	2B	19	Total Mg 19 19	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2D	6	Total Mg 6 6	0	0
57	2E	7	Total Mg 7 7	0	0
57	2F	8	Total Mg 8 8	0	0
57	2G	1	Total Mg 1 1	0	0
57	2O	2	Total Mg 2 2	0	0
57	2P	2	Total Mg 2 2	0	0
57	2Q	2	Total Mg 2 2	0	0
57	2R	2	Total Mg 2 2	0	0
57	2S	1	Total Mg 1 1	0	0
57	2T	4	Total Mg 4 4	0	0
57	2U	2	Total Mg 2 2	0	0
57	2V	2	Total Mg 2 2	0	0
57	2W	2	Total Mg 2 2	0	0
57	2X	2	Total Mg 2 2	0	0
57	2Y	1	Total Mg 1 1	0	0
57	2Z	1	Total Mg 1 1	0	0
57	20	2	Total Mg 2 2	0	0
57	21	3	Total Mg 3 3	0	0
57	23	2	Total Mg 2 2	0	0
57	25	7	Total Mg 7 7	0	0
57	26	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	27	2	Total Mg 2 2	0	0
57	28	3	Total Mg 3 3	0	0
57	29	1	Total Mg 1 1	0	0
57	2a	238	Total Mg 238 238	0	0
57	2d	2	Total Mg 2 2	0	0
57	2e	1	Total Mg 1 1	0	0
57	2f	2	Total Mg 2 2	0	0
57	2g	1	Total Mg 1 1	0	0
57	2j	1	Total Mg 1 1	0	0
57	2l	3	Total Mg 3 3	0	0
57	2p	1	Total Mg 1 1	0	0
57	2q	2	Total Mg 2 2	0	0
57	2r	1	Total Mg 1 1	0	0
57	2t	1	Total Mg 1 1	0	0
57	2v	2	Total Mg 2 2	0	0
57	2w	7	Total Mg 7 7	0	0
57	2x	6	Total Mg 6 6	0	0
57	2y	4	Total Mg 4 4	0	0

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

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

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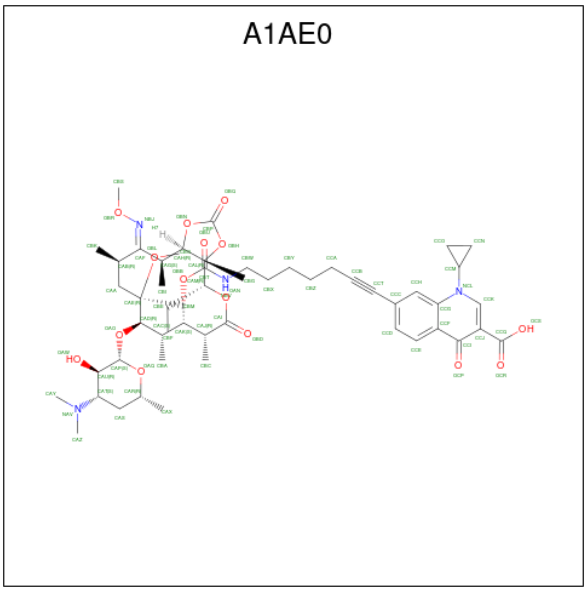
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	2A	1	Total K 1 1	0	0

- Molecule 59 is 1-cyclopropyl-7-{7-[({[(3aR,4R,7R,8S,9S,10R,11R,13R,14E,15S,15aR)-10-{[(2S,3R,4S,6R)-4-(dimethylamino)-3-hydroxy-6-methyloxan-2-yl]oxy}-4-ethyl-11-methoxy-14-(methoxyimino)-3a,7,9,11,13,15-hexamethyl-2,6-dioxododecahydro-2H,4H-[1,3]dioxolo[4,5-c]oxacyclotetradecin-8-yl]oxy}carbonyl)amino]hept-1-yn-1-yl}-4-oxo-1,4-dihydroquinoline-3-carboxylic acid (non-preferred name) (CCD ID: A1AE0) (formula: $C_{53}H_{76}N_4O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1	Total C N O 72 53 4 15	0	0
59	2A	1	Total C N O 72 53 4 15	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

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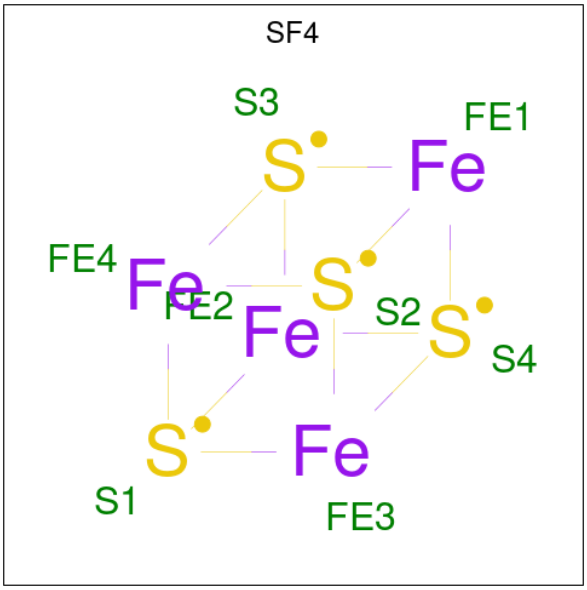
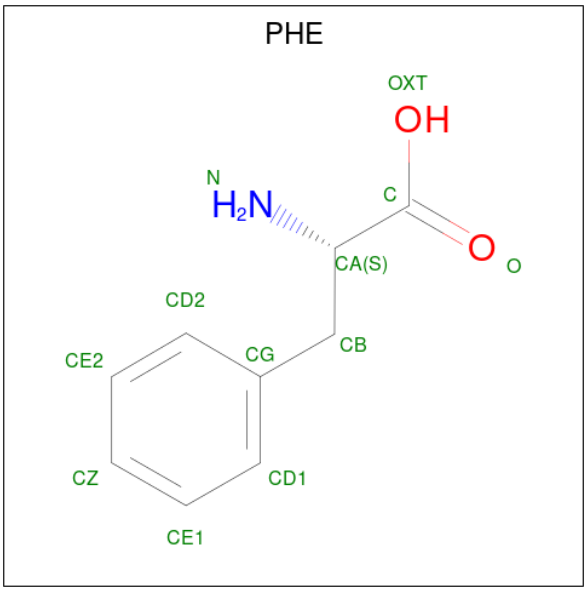
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	19	1	Total Zn 1 1	0	0
60	1n	1	Total Zn 1 1	0	0
60	2Y	1	Total Zn 1 1	0	0
60	24	1	Total Zn 1 1	0	0
60	25	1	Total Zn 1 1	0	0
60	26	1	Total Zn 1 1	0	0
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

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



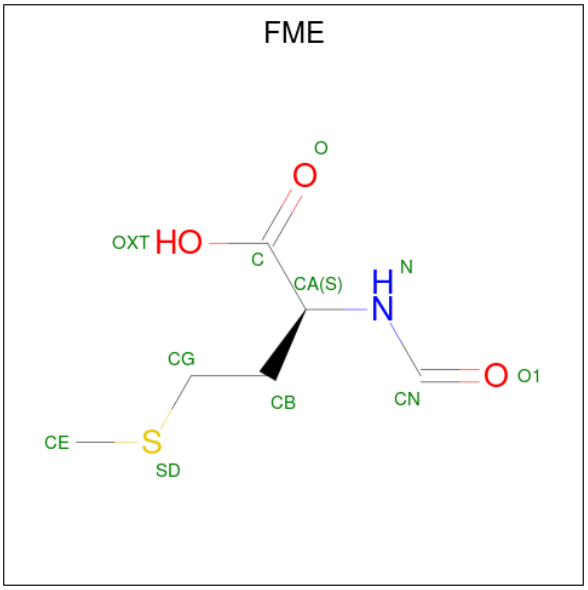
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1d	1	Total Fe S 8 4 4	0	0
61	2d	1	Total Fe S 8 4 4	0	0

- Molecule 62 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1w	1	Total C N O 11 9 1 1	0	0
62	2w	1	Total C N O 11 9 1 1	0	0

- Molecule 63 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1x	1	Total C N O S 10 6 1 2 1	0	0
63	2x	1	Total C N O S 10 6 1 2 1	0	0

- Molecule 64 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	1A	2019	Total O 2019 2019	0	0
64	1B	62	Total O 62 62	0	0
64	1D	27	Total O 27 27	0	0
64	1E	25	Total O 25 25	0	0
64	1F	18	Total O 18 18	0	0
64	1G	2	Total O 2 2	0	0
64	1H	2	Total O 2 2	0	0
64	1N	5	Total O 5 5	0	0
64	1O	6	Total O 6 6	0	0
64	1P	21	Total O 21 21	0	0
64	1Q	9	Total O 9 9	0	0
64	1R	11	Total O 11 11	0	0
64	1S	3	Total O 3 3	0	0
64	1T	7	Total O 7 7	0	0
64	1U	11	Total O 11 11	0	0
64	1V	7	Total O 7 7	0	0
64	1W	8	Total O 8 8	0	0
64	1X	4	Total O 4 4	0	0
64	1Y	3	Total O 3 3	0	0
64	1Z	1	Total O 1 1	0	0
64	10	11	Total O 11 11	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	11	12	Total O 12 12	0	0
64	12	4	Total O 4 4	0	0
64	13	5	Total O 5 5	0	0
64	14	1	Total O 1 1	0	0
64	15	6	Total O 6 6	0	0
64	16	3	Total O 3 3	0	0
64	17	7	Total O 7 7	0	0
64	18	12	Total O 12 12	0	0
64	1a	391	Total O 391 391	0	0
64	1b	1	Total O 1 1	0	0
64	1d	1	Total O 1 1	0	0
64	1e	1	Total O 1 1	0	0
64	1f	1	Total O 1 1	0	0
64	1g	1	Total O 1 1	0	0
64	1j	1	Total O 1 1	0	0
64	1l	5	Total O 5 5	0	0
64	1m	1	Total O 1 1	0	0
64	1n	1	Total O 1 1	0	0
64	1o	1	Total O 1 1	0	0
64	1p	1	Total O 1 1	0	0
64	1q	2	Total O 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	1t	1	Total O 1 1	0	0
64	1u	1	Total O 1 1	0	0
64	1v	5	Total O 5 5	0	0
64	1w	13	Total O 13 13	0	0
64	1x	12	Total O 12 12	0	0
64	1y	1	Total O 1 1	0	0
64	2A	1149	Total O 1149 1149	0	0
64	2B	20	Total O 20 20	0	0
64	2D	20	Total O 20 20	0	0
64	2E	14	Total O 14 14	0	0
64	2F	12	Total O 12 12	0	0
64	2I	1	Total O 1 1	0	0
64	2O	1	Total O 1 1	0	0
64	2P	12	Total O 12 12	0	0
64	2Q	1	Total O 1 1	0	0
64	2R	4	Total O 4 4	0	0
64	2T	5	Total O 5 5	0	0
64	2U	3	Total O 3 3	0	0
64	2W	3	Total O 3 3	0	0
64	2X	1	Total O 1 1	0	0
64	2Y	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	20	1	Total O 1 1	0	0
64	21	11	Total O 11 11	0	0
64	22	1	Total O 1 1	0	0
64	23	3	Total O 3 3	0	0
64	25	2	Total O 2 2	0	0
64	27	4	Total O 4 4	0	0
64	28	3	Total O 3 3	0	0
64	29	1	Total O 1 1	0	0
64	2a	288	Total O 288 288	0	0
64	2c	1	Total O 1 1	0	0
64	2d	3	Total O 3 3	0	0
64	2e	2	Total O 2 2	0	0
64	2j	1	Total O 1 1	0	0
64	2l	6	Total O 6 6	0	0
64	2n	1	Total O 1 1	0	0
64	2p	2	Total O 2 2	0	0
64	2q	1	Total O 1 1	0	0
64	2r	1	Total O 1 1	0	0
64	2t	2	Total O 2 2	0	0
64	2v	2	Total O 2 2	0	0
64	2w	3	Total O 3 3	0	0

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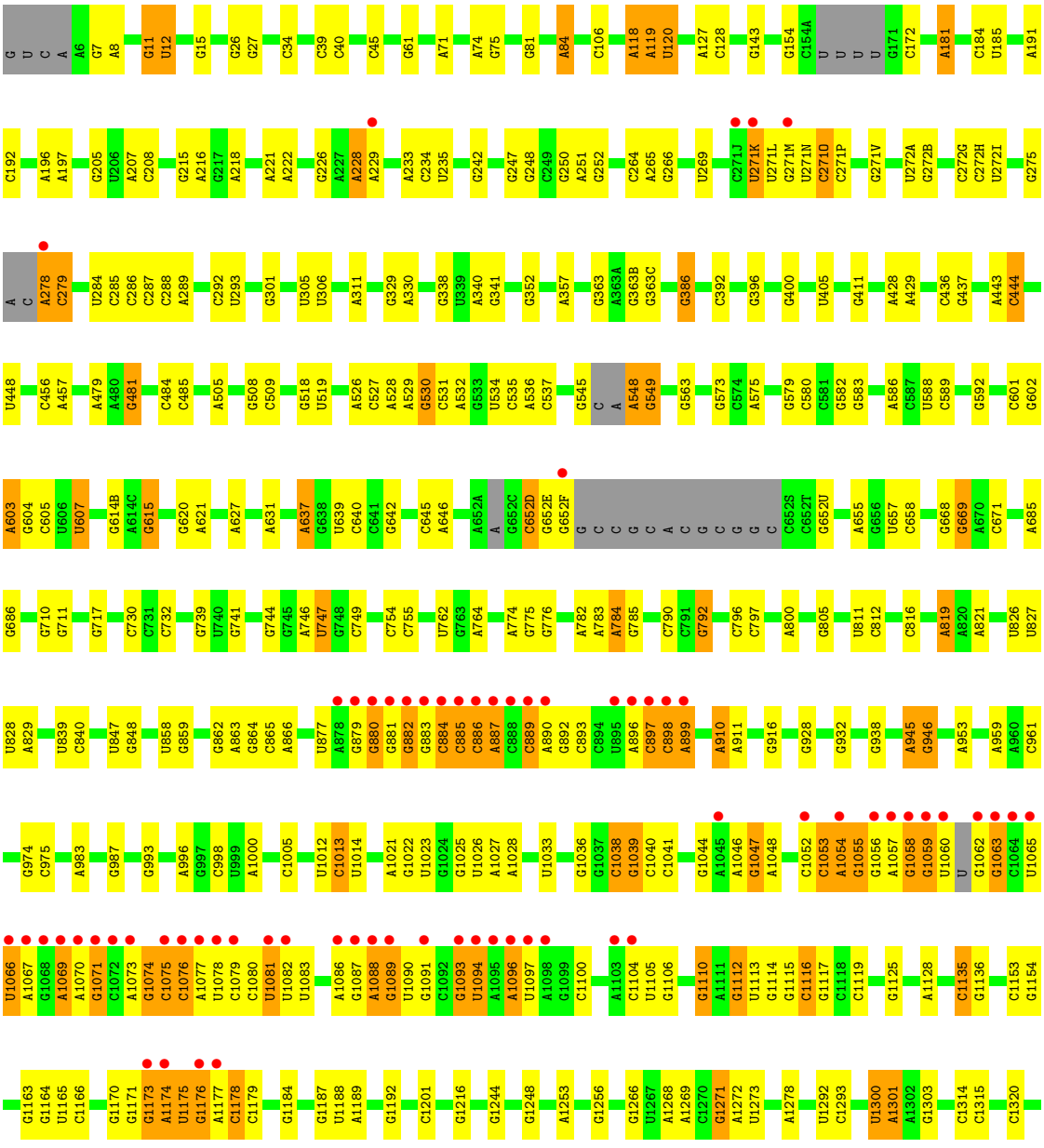
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	2x	9	Total O 9 9	0	0
64	2y	5	Total O 5 5	0	0

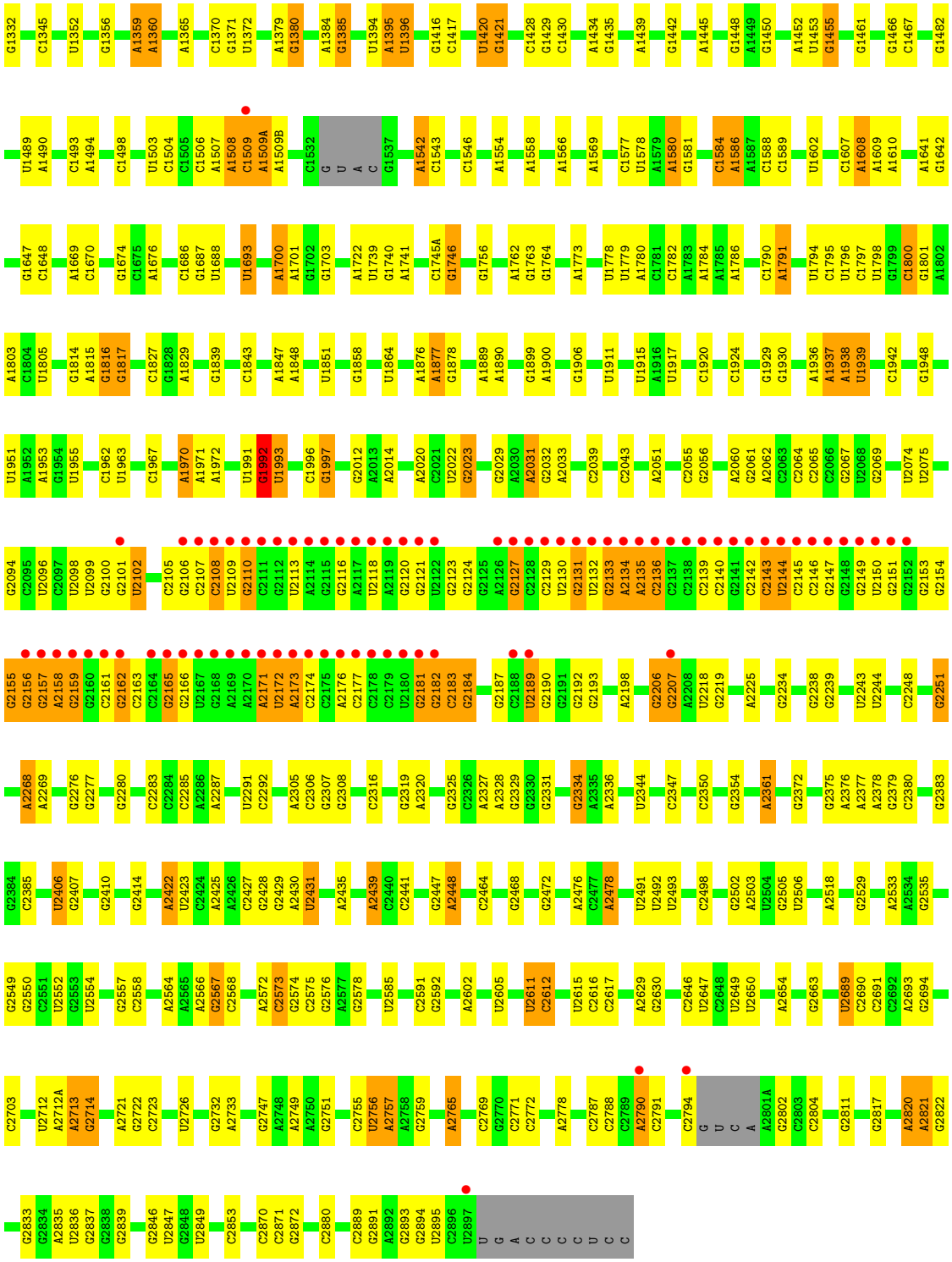
3 Residue-property plots (i)

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

• Molecule 1: 23S Ribosomal RNA

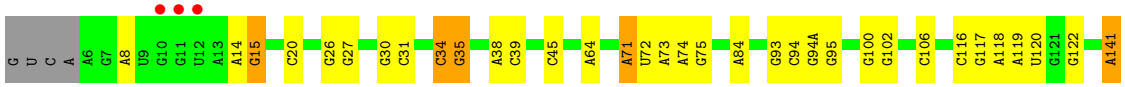
Chain 1A:

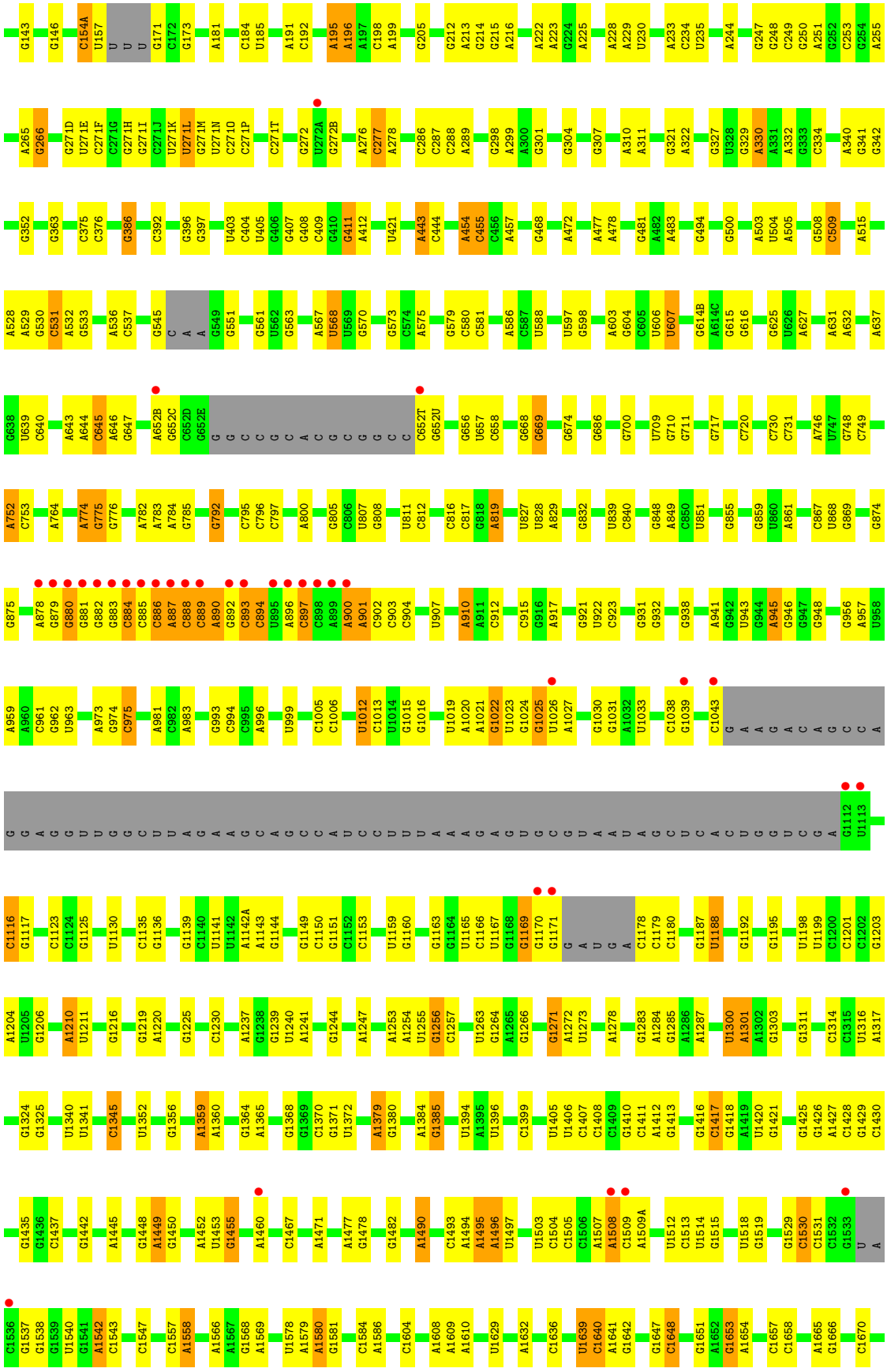


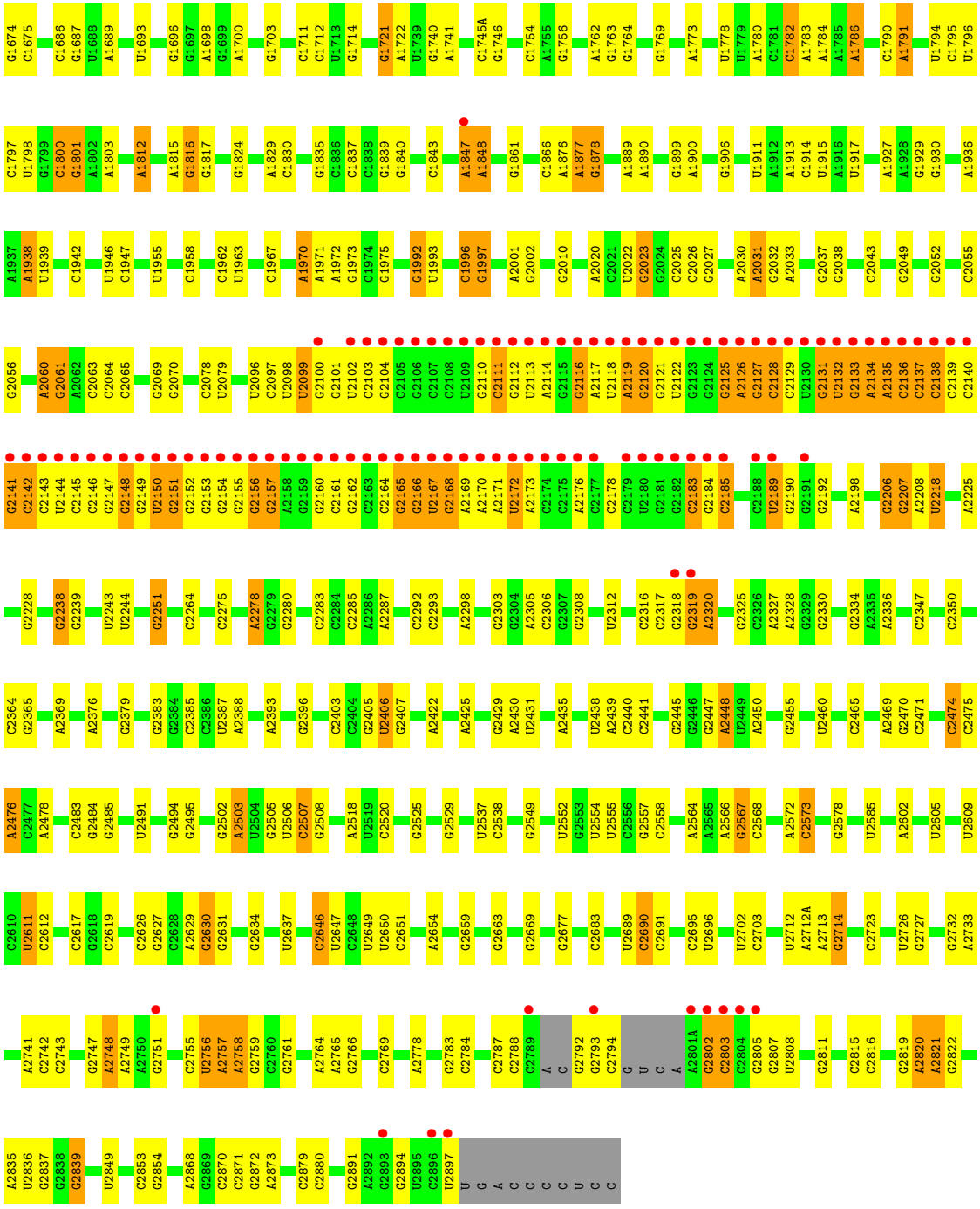


• Molecule 1: 23S Ribosomal RNA

Chain 2A:





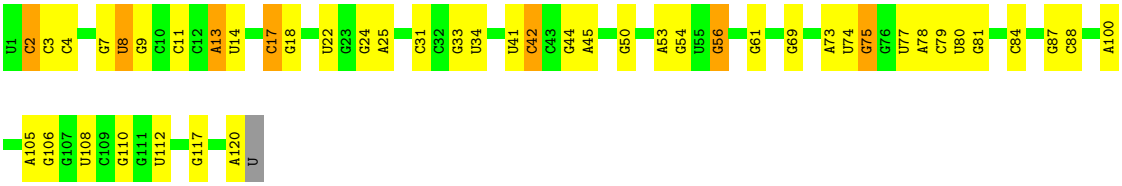


• Molecule 2: 5S Ribosomal RNA

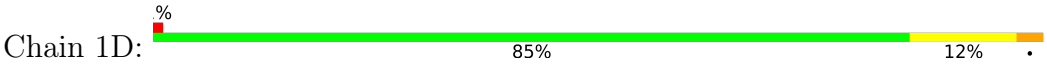
Chain 1B:

• Molecule 2: 5S Ribosomal RNA

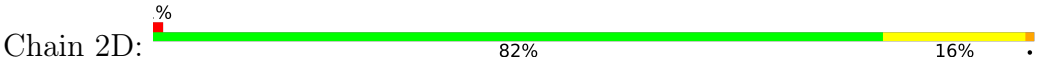
Chain 2B:

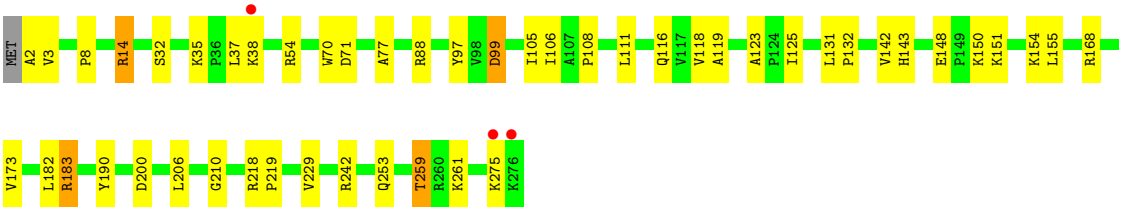


• Molecule 3: 50S ribosomal protein L2

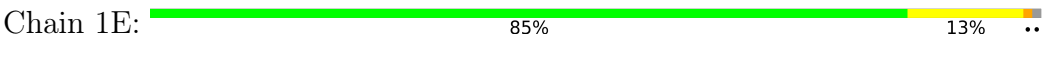


• Molecule 3: 50S ribosomal protein L2

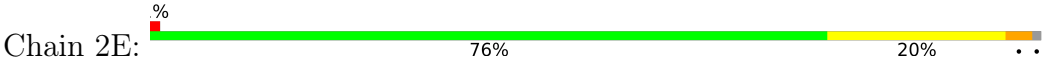


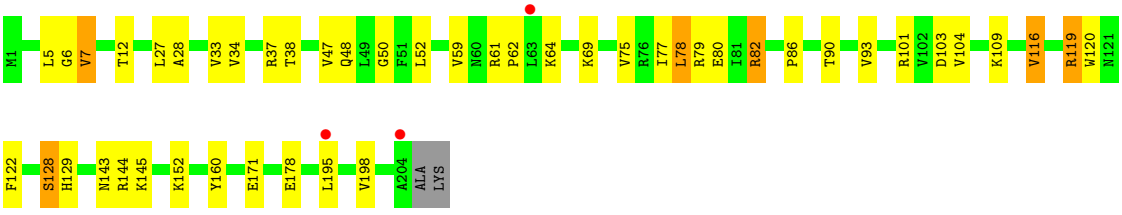


• Molecule 4: 50S ribosomal protein L3

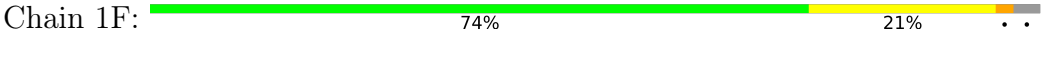


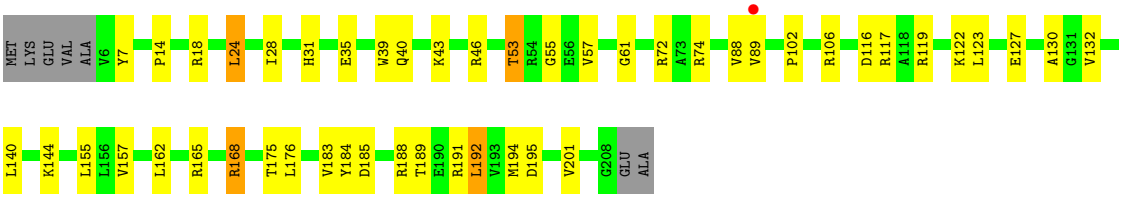
• Molecule 4: 50S ribosomal protein L3





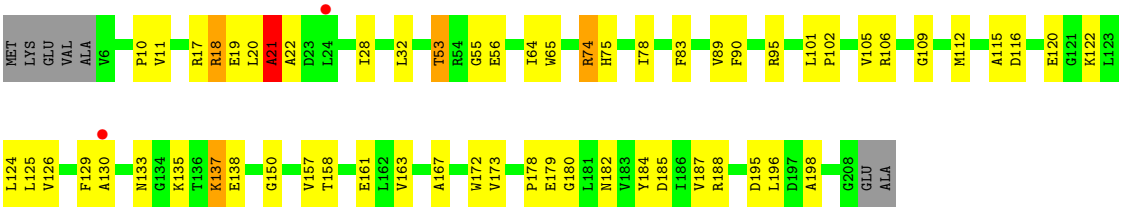
• Molecule 5: 50S ribosomal protein L4





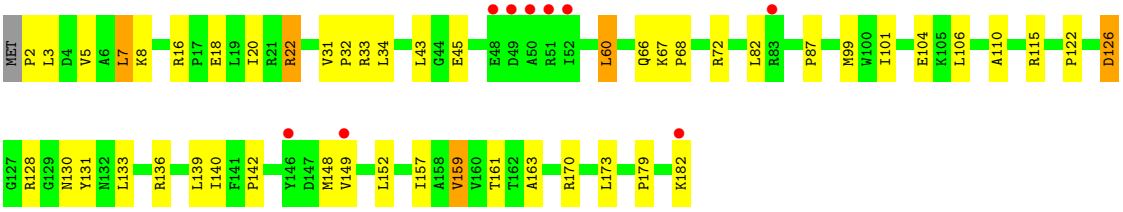
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



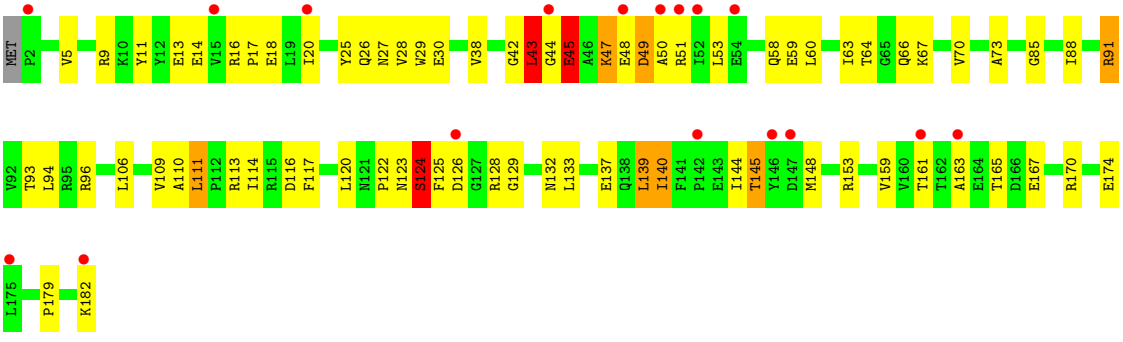
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



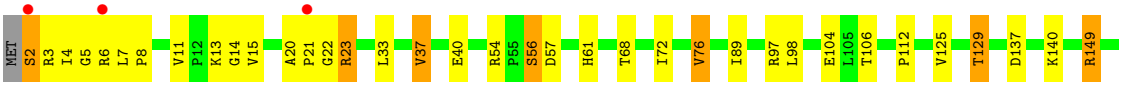
• Molecule 6: 50S ribosomal protein L5

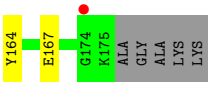
Chain 2G:



• Molecule 7: 50S ribosomal protein L6

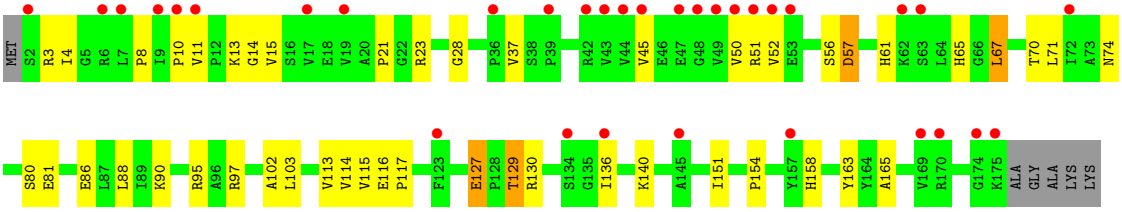
Chain 1H:





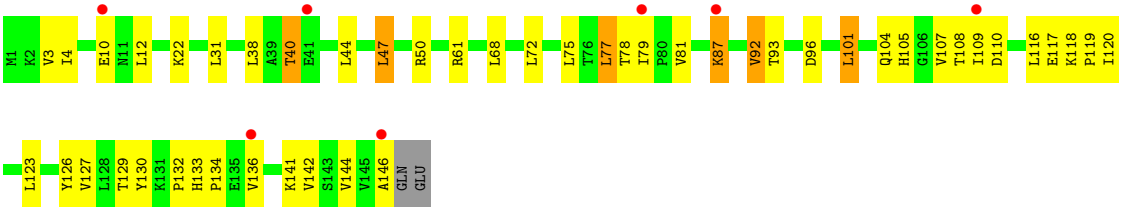
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



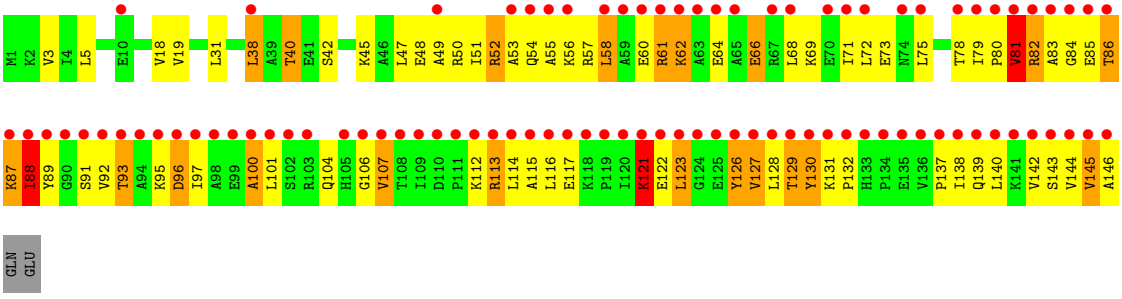
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



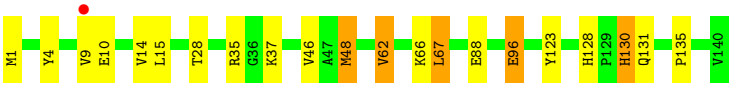
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



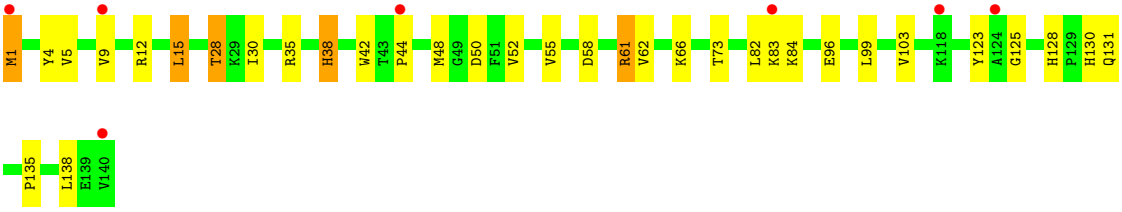
• Molecule 9: 50S ribosomal protein L13

Chain 1N:

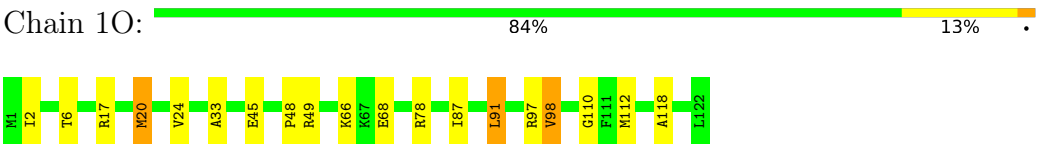


• Molecule 9: 50S ribosomal protein L13

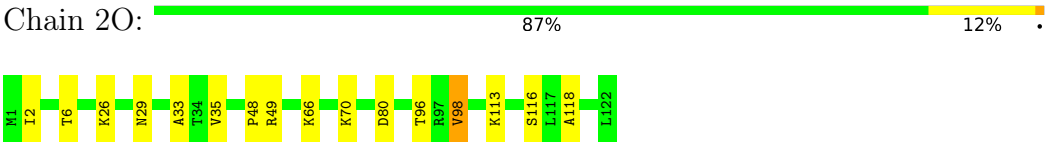
Chain 2N:



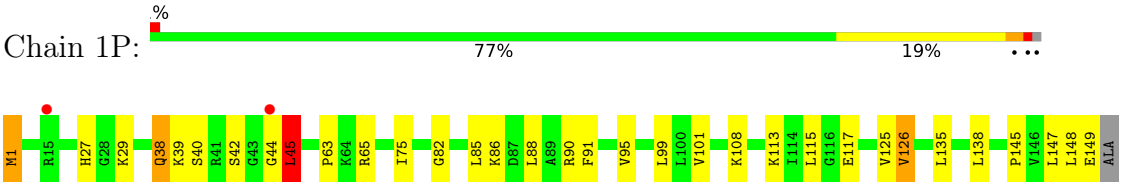
• Molecule 10: 50S ribosomal protein L14



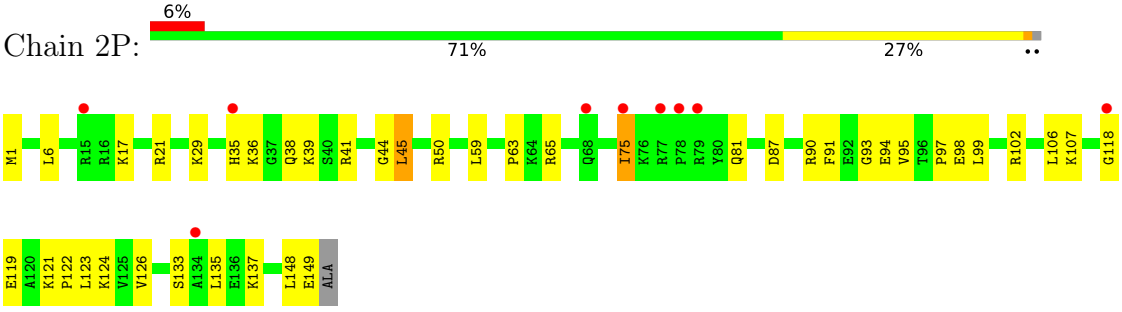
• Molecule 10: 50S ribosomal protein L14



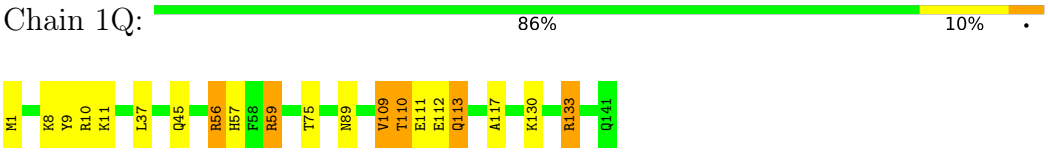
• Molecule 11: 50S ribosomal protein L15



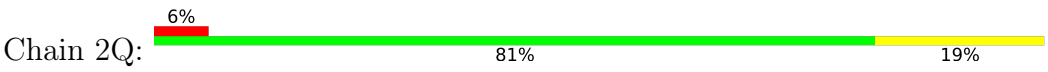
• Molecule 11: 50S ribosomal protein L15

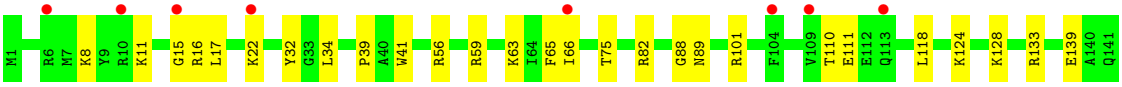


• Molecule 12: 50S ribosomal protein L16



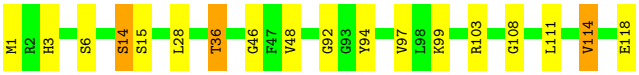
• Molecule 12: 50S ribosomal protein L16





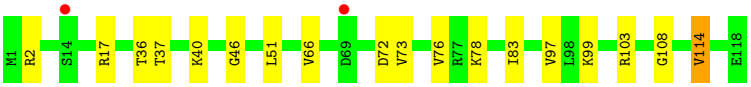
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



• Molecule 13: 50S ribosomal protein L17

Chain 2R:

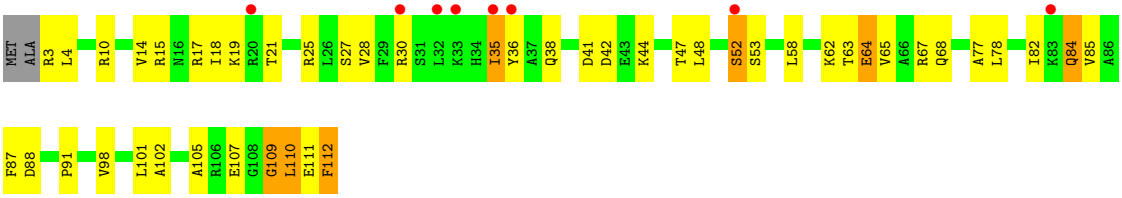


• Molecule 14: 50S ribosomal protein L18

Chain 1S:

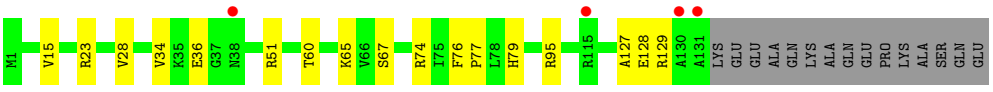
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



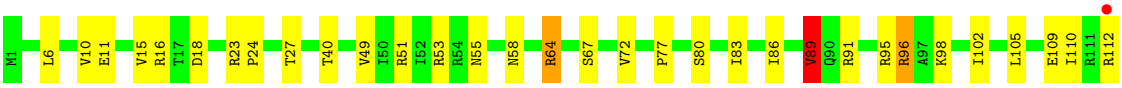
• Molecule 15: 50S ribosomal protein L19

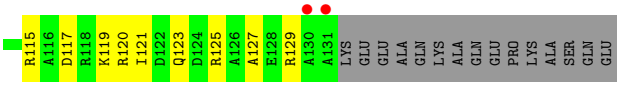
Chain 1T:



• Molecule 15: 50S ribosomal protein L19

Chain 2T:





• Molecule 16: 50S ribosomal protein L20

Chain 1U:

• Molecule 16: 50S ribosomal protein L20

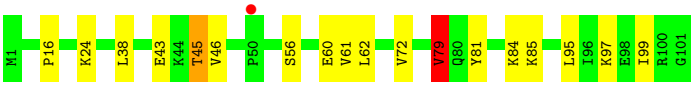
Chain 2U:

• Molecule 17: 50S ribosomal protein L21

Chain 1V:

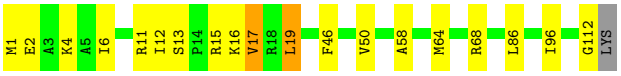
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



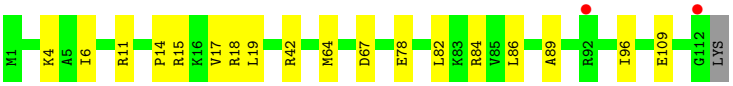
• Molecule 18: 50S ribosomal protein L22

Chain 1W:



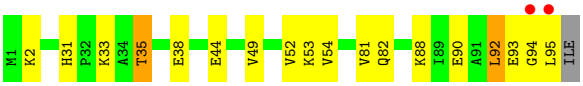
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



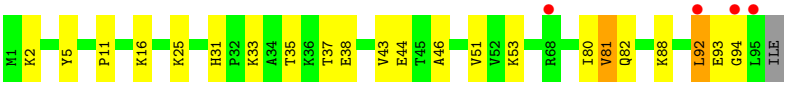
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



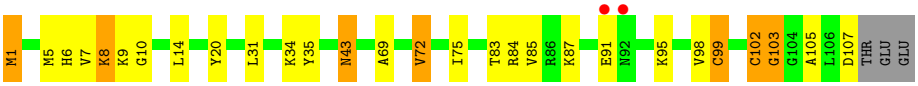
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



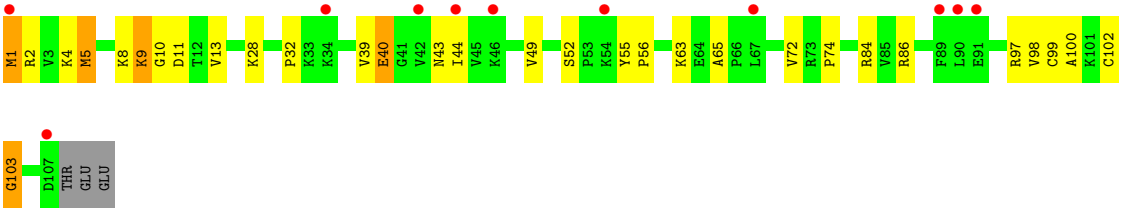
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



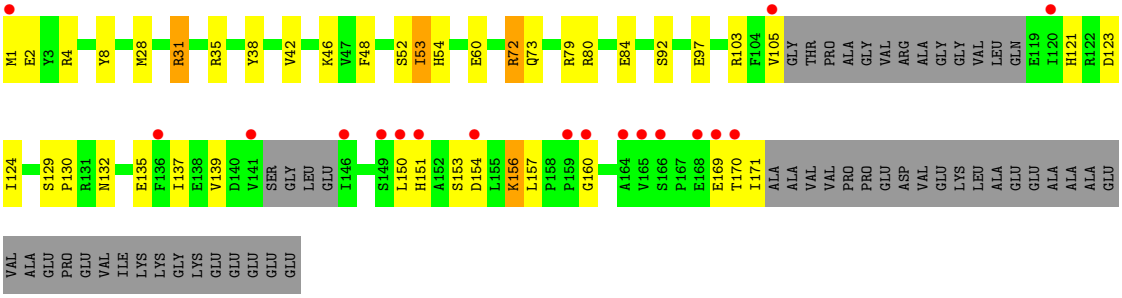
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



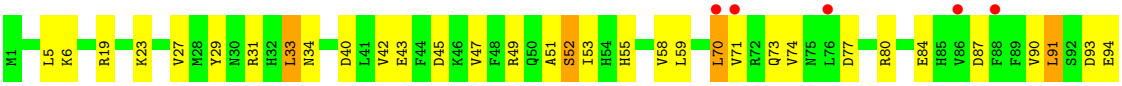
• Molecule 21: 50S ribosomal protein L25

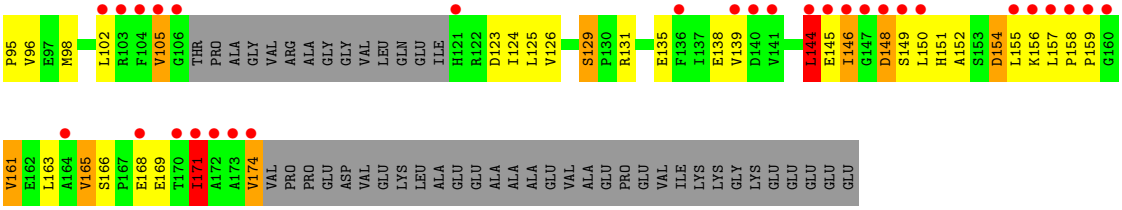
Chain 1Z:



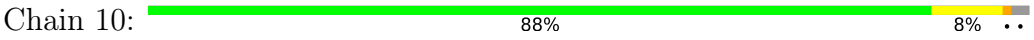
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:

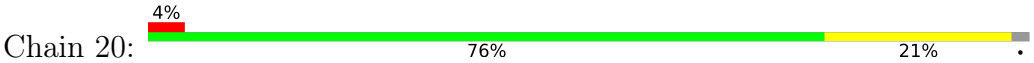


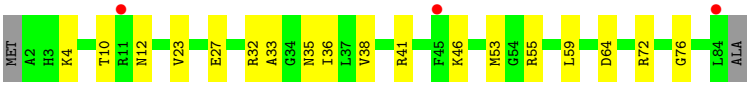


• Molecule 22: 50S ribosomal protein L27

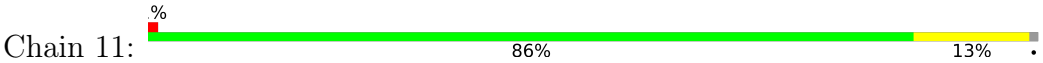


• Molecule 22: 50S ribosomal protein L27

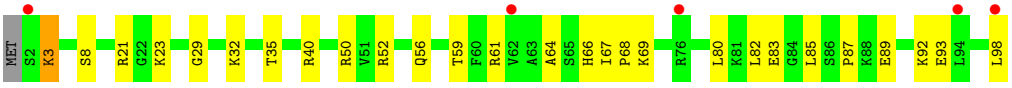




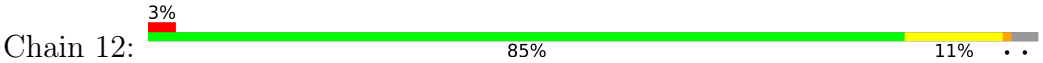
• Molecule 23: 50S ribosomal protein L28

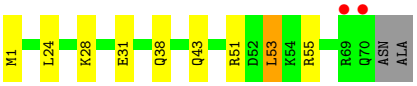


• Molecule 23: 50S ribosomal protein L28

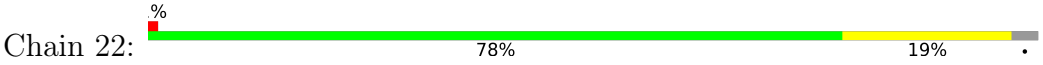


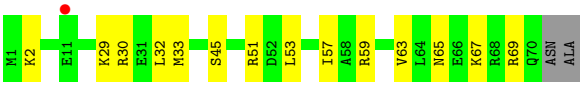
• Molecule 24: 50S ribosomal protein L29





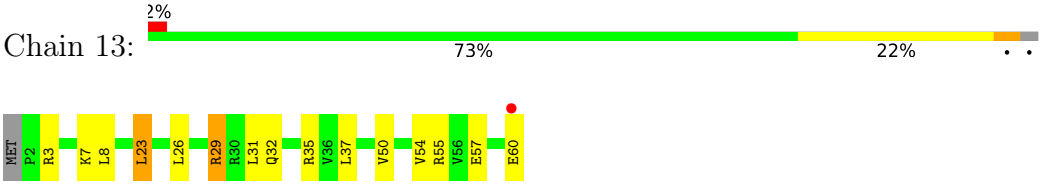
• Molecule 24: 50S ribosomal protein L29





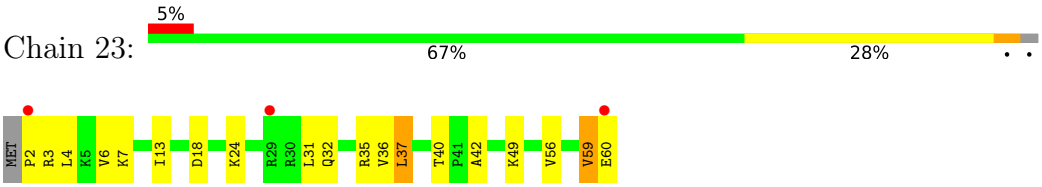
• Molecule 25: 50S ribosomal protein L30

Chain 13:



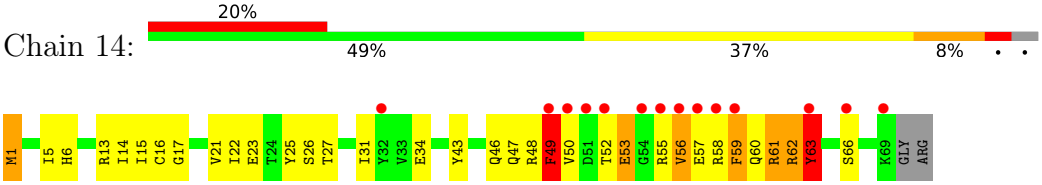
• Molecule 25: 50S ribosomal protein L30

Chain 23:



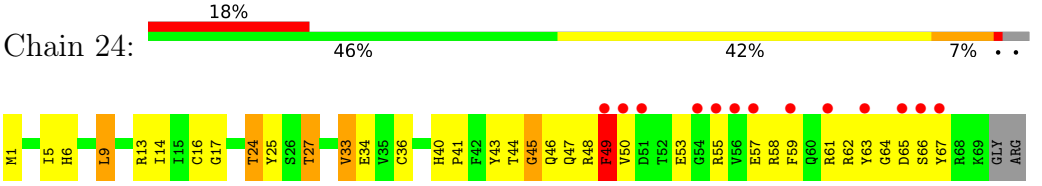
• Molecule 26: 50S ribosomal protein L31

Chain 14:



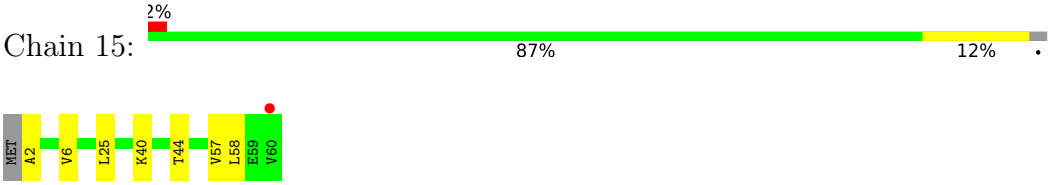
• Molecule 26: 50S ribosomal protein L31

Chain 24:



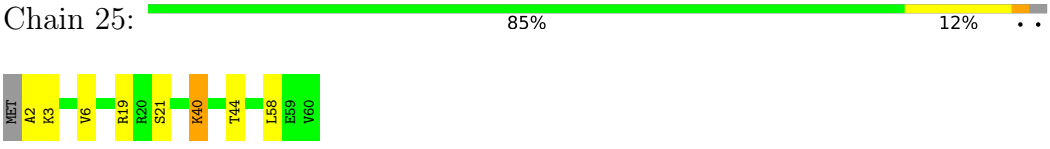
• Molecule 27: 50S ribosomal protein L32

Chain 15:



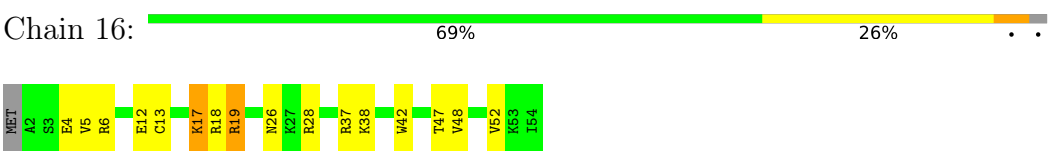
• Molecule 27: 50S ribosomal protein L32

Chain 25:



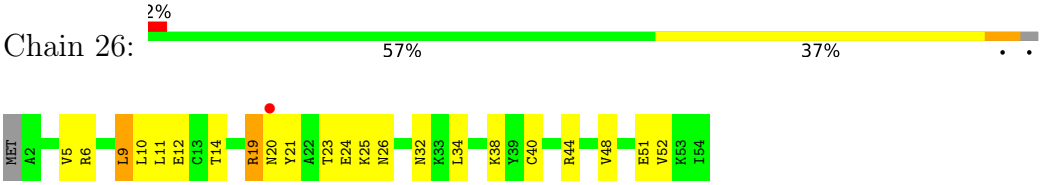
• Molecule 28: 50S ribosomal protein L33

Chain 16:



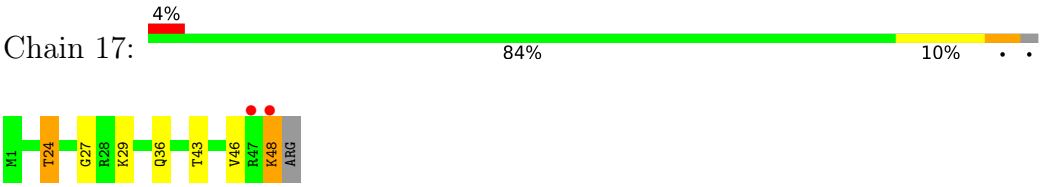
• Molecule 28: 50S ribosomal protein L33

Chain 26:



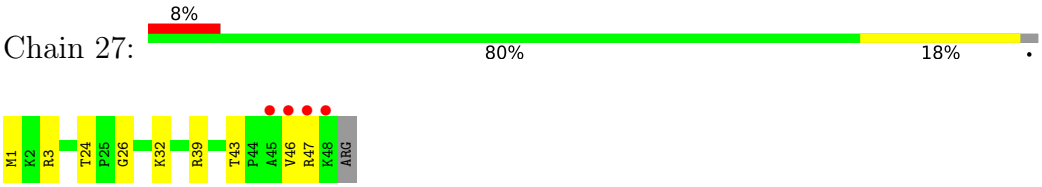
• Molecule 29: 50S ribosomal protein L34

Chain 17:



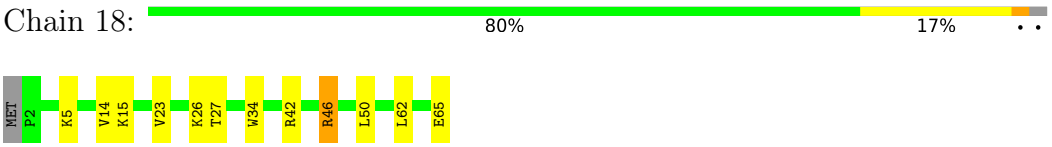
• Molecule 29: 50S ribosomal protein L34

Chain 27:



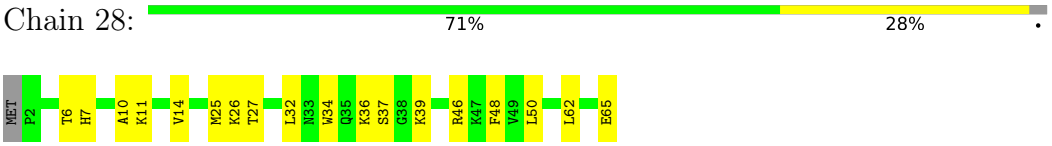
• Molecule 30: 50S ribosomal protein L35

Chain 18:



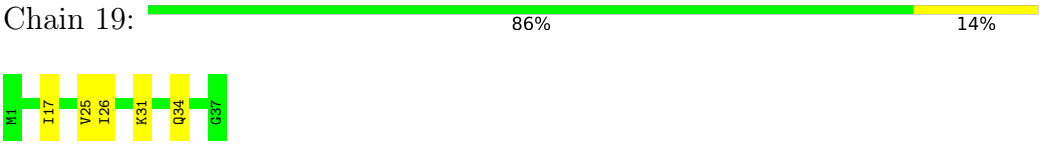
• Molecule 30: 50S ribosomal protein L35

Chain 28:



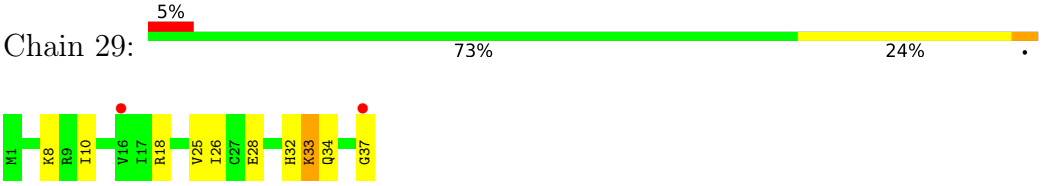
• Molecule 31: 50S ribosomal protein L36

Chain 19:



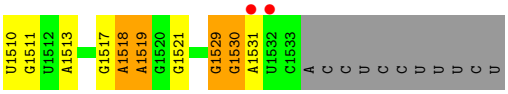
• Molecule 31: 50S ribosomal protein L36

Chain 29:



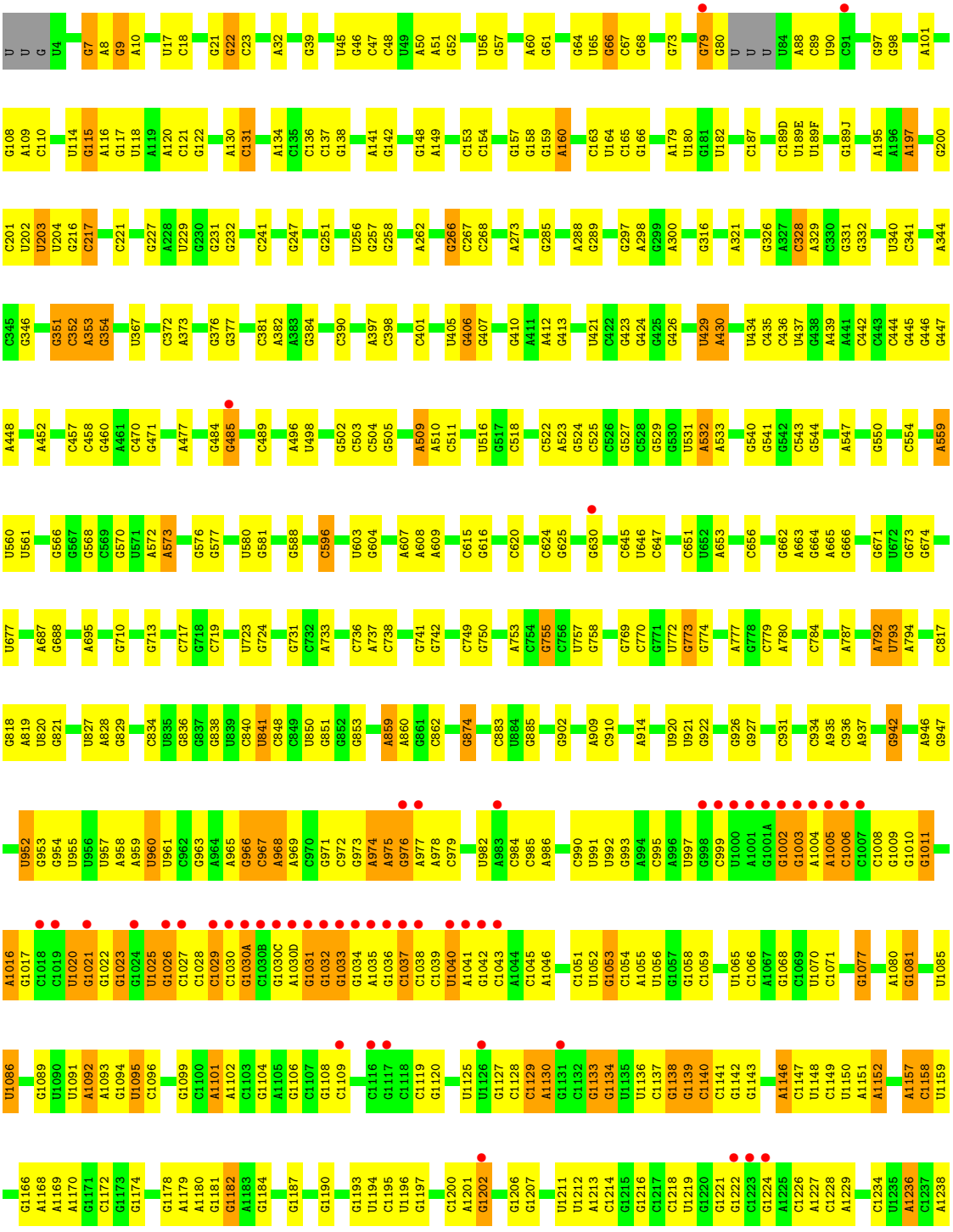
• Molecule 32: 16S Ribosomal RNA

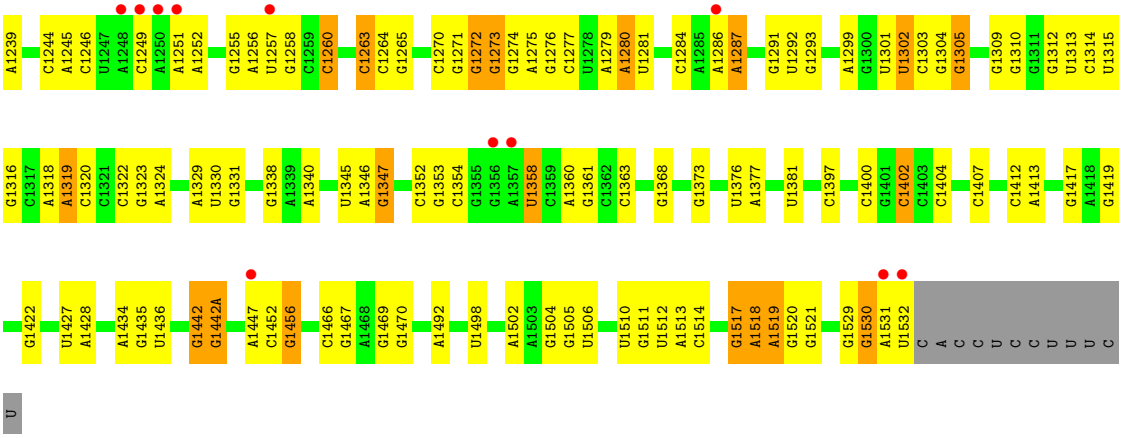
Chain 1a:



• Molecule 32: 16S Ribosomal RNA

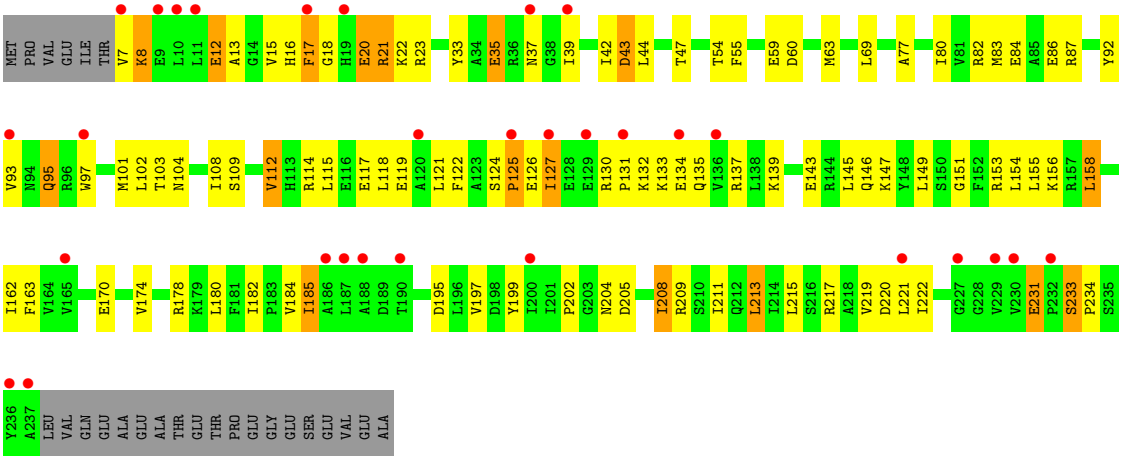
Chain 2a:





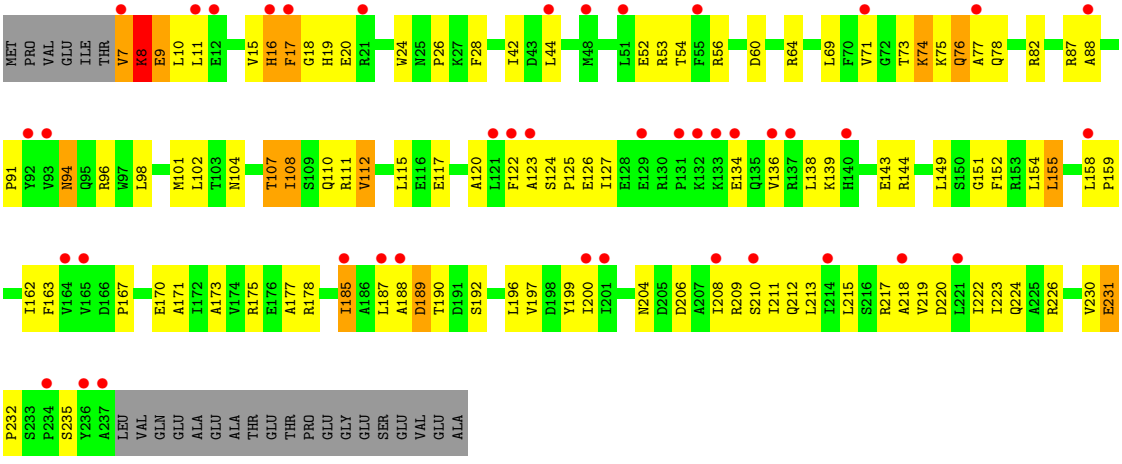
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



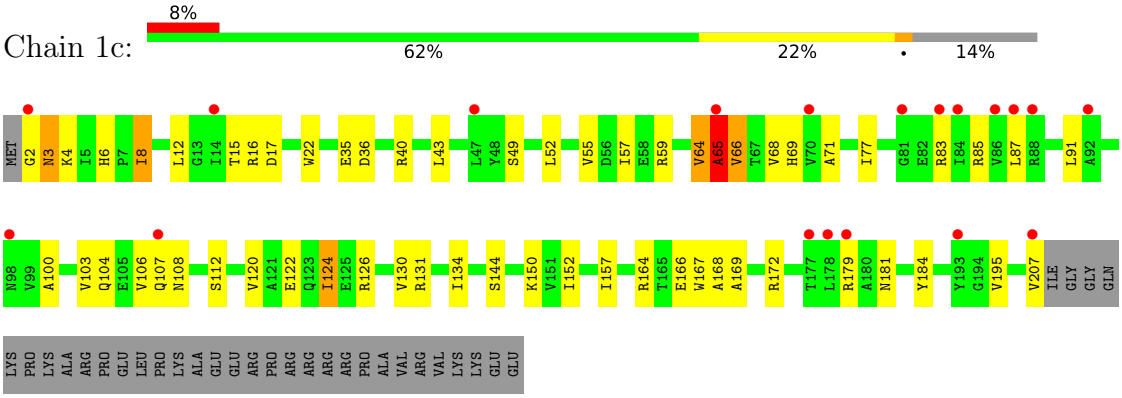
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



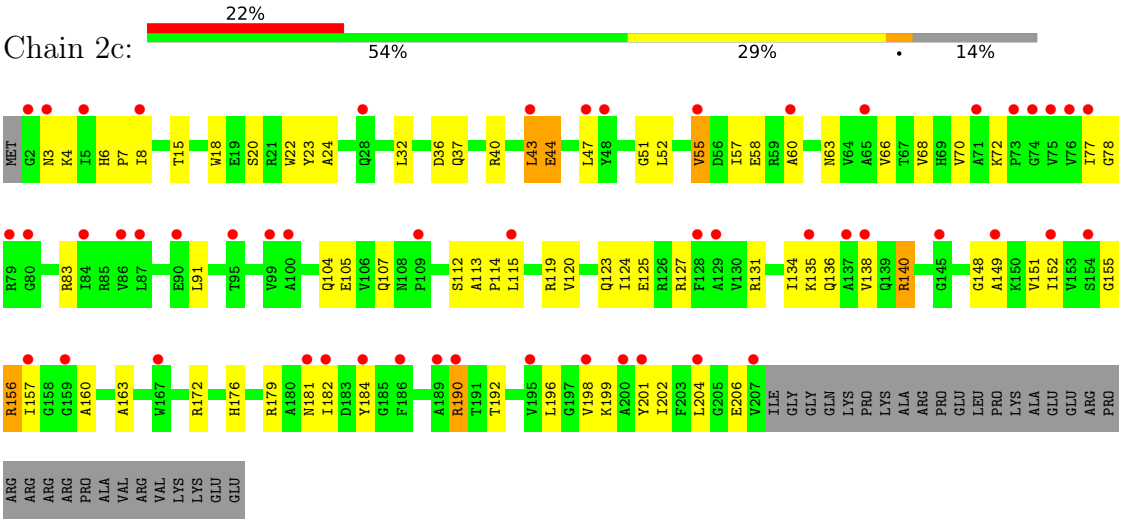
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



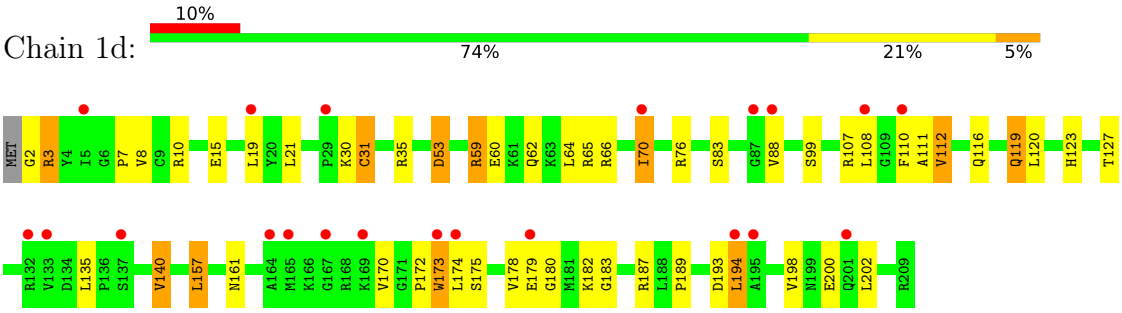
• Molecule 34: 30S ribosomal protein S3

Chain 2c:



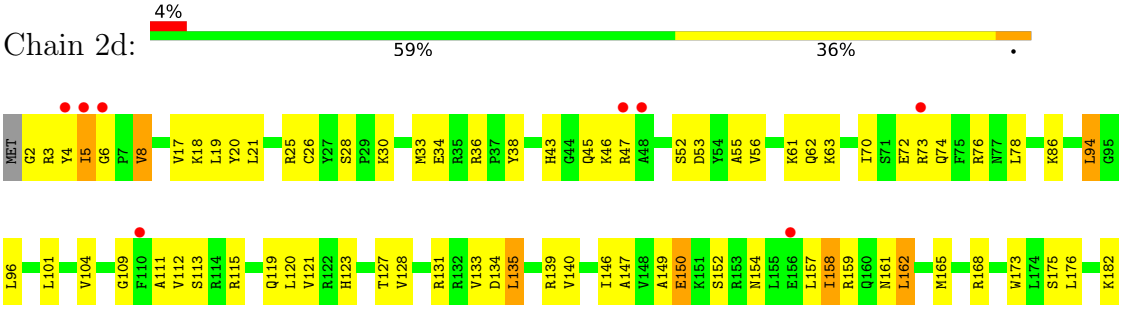
• Molecule 35: 30S ribosomal protein S4

Chain 1d:



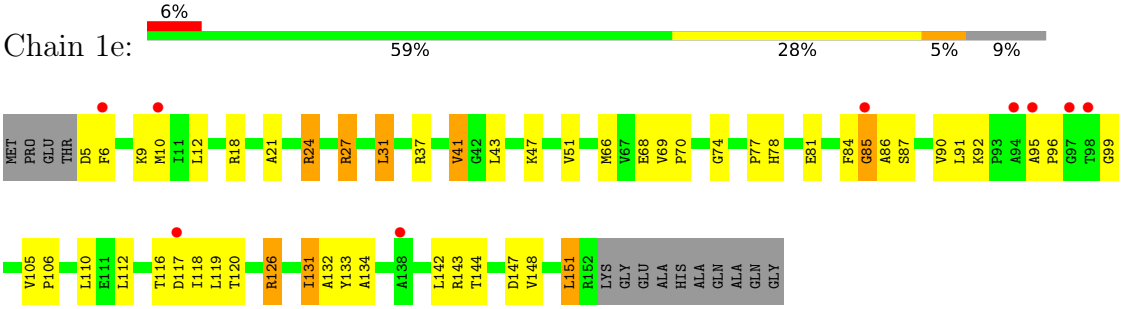
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



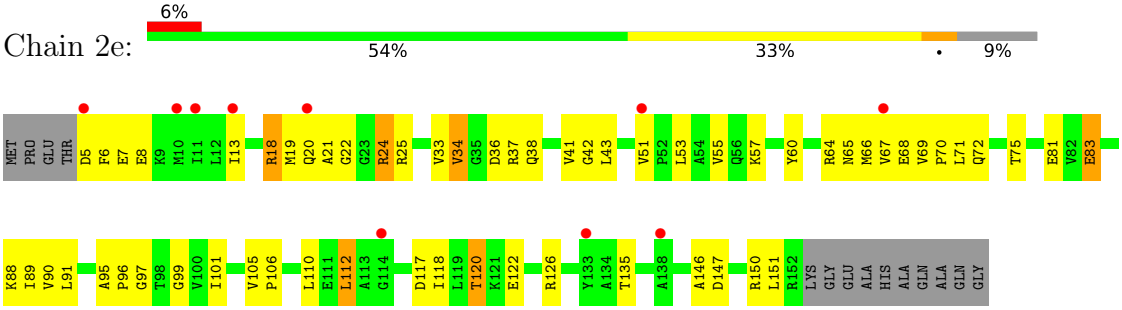
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



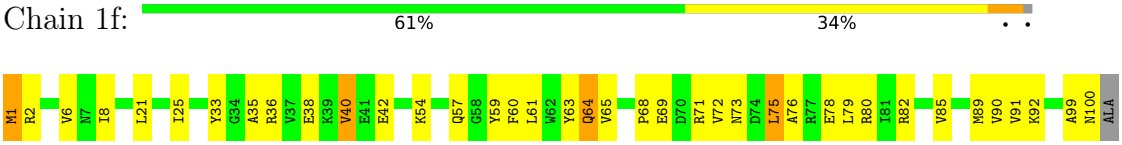
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



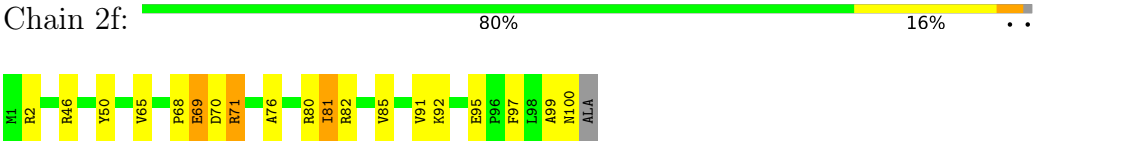
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



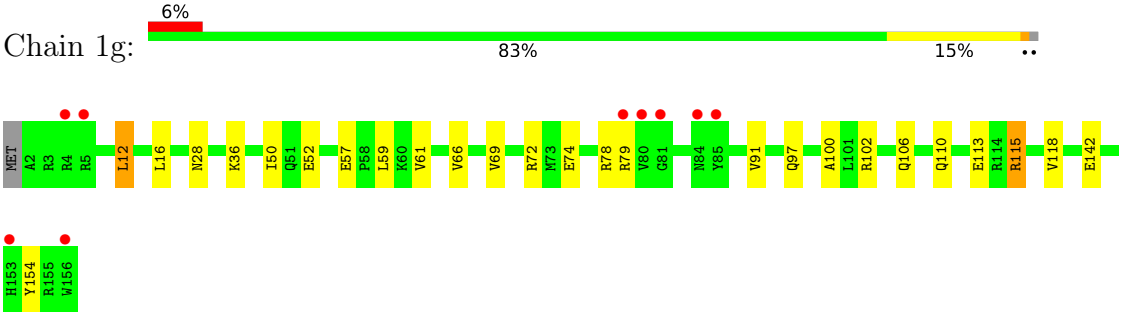
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



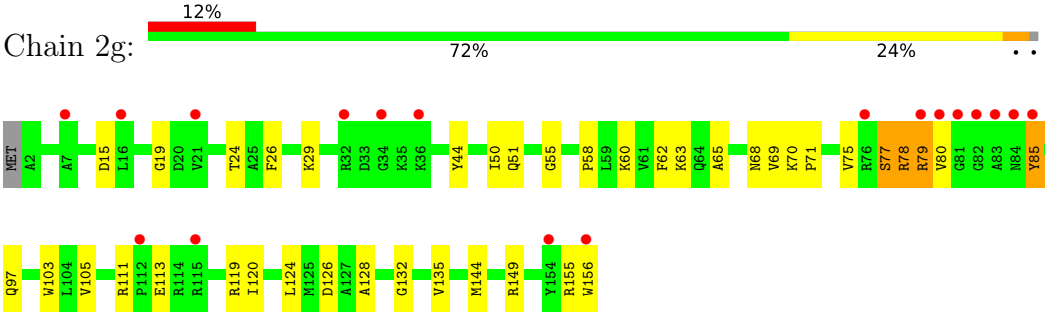
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



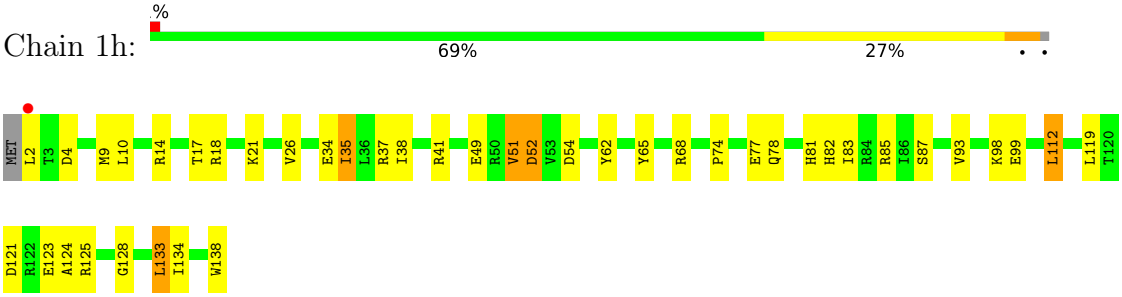
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



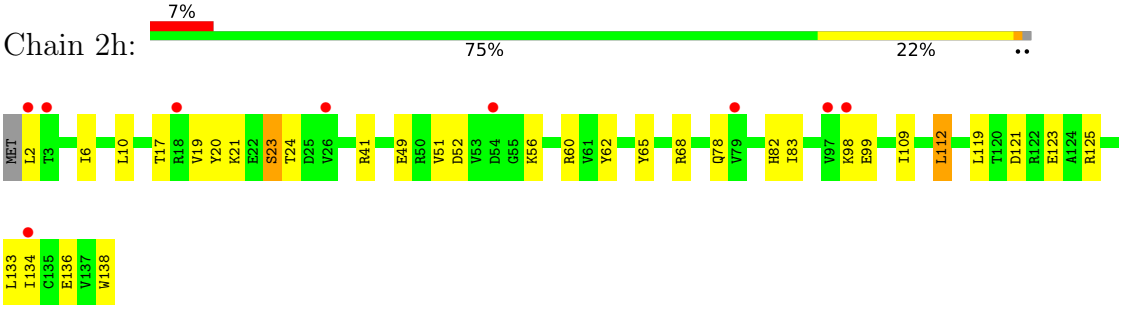
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



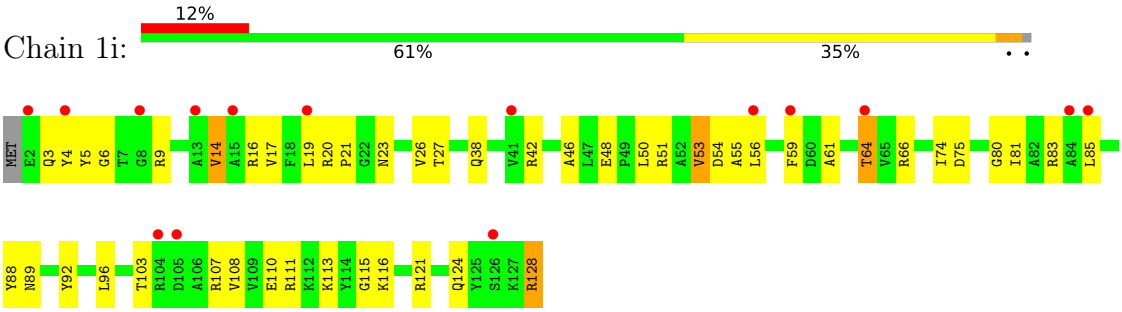
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



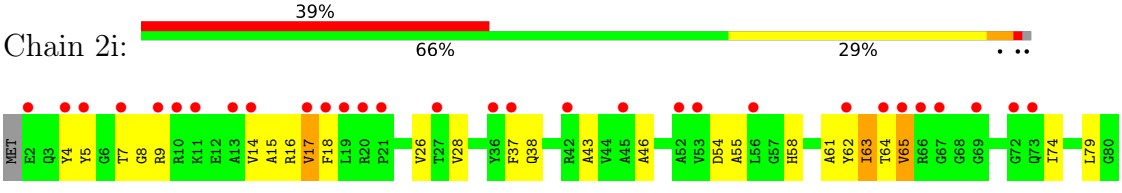
• Molecule 40: 30S ribosomal protein S9

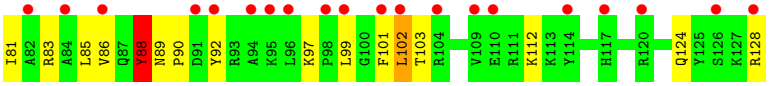
Chain 1i:



• Molecule 40: 30S ribosomal protein S9

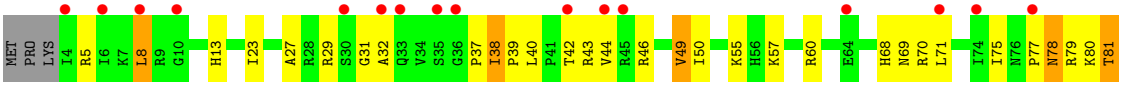
Chain 2i:





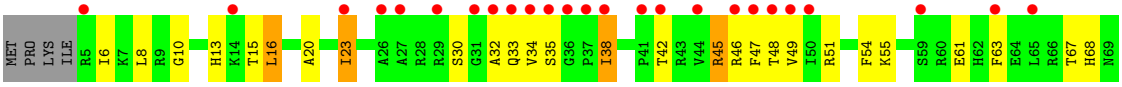
• Molecule 41: 30S ribosomal protein S10

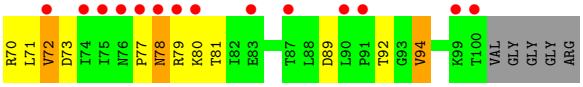
Chain 1j:



• Molecule 41: 30S ribosomal protein S10

Chain 2j:



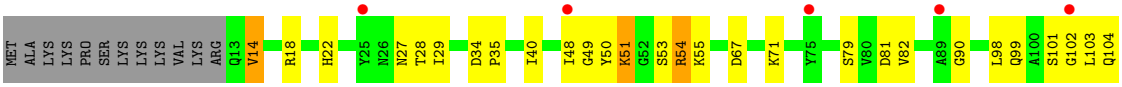


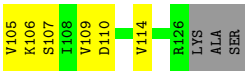
• Molecule 42: 30S ribosomal protein S11

Chain 1k:

• Molecule 42: 30S ribosomal protein S11

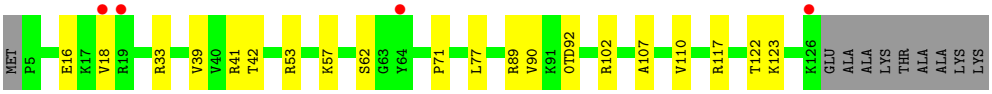
Chain 2k:



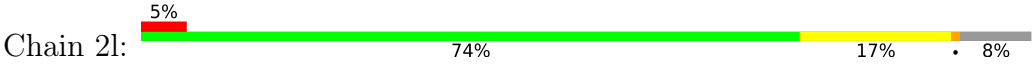


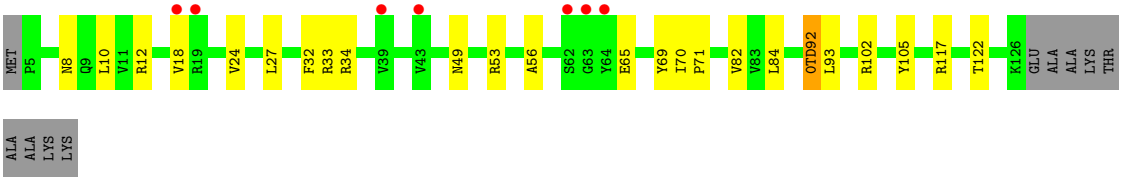
• Molecule 43: 30S ribosomal protein S12

Chain 1l:

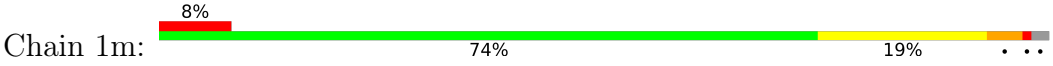


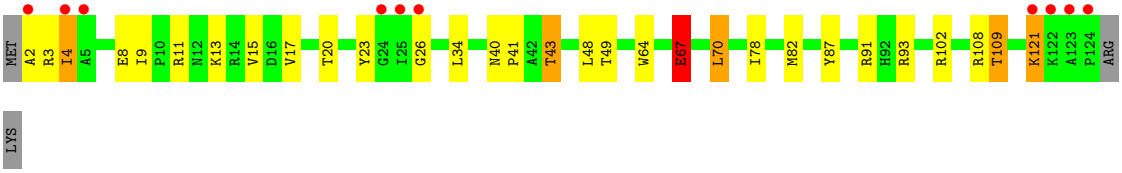
• Molecule 43: 30S ribosomal protein S12



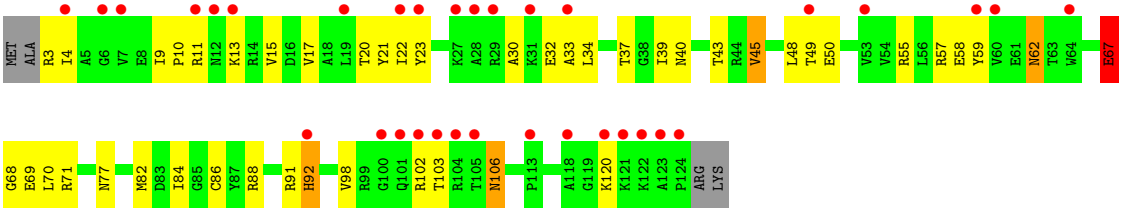


• Molecule 44: 30S ribosomal protein S13

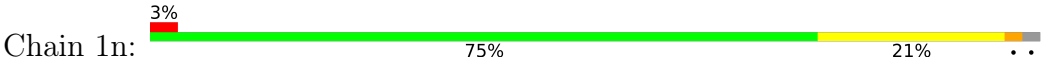


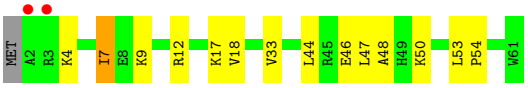


• Molecule 44: 30S ribosomal protein S13

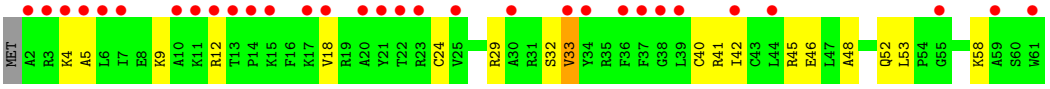


• Molecule 45: 30S ribosomal protein S14 type Z



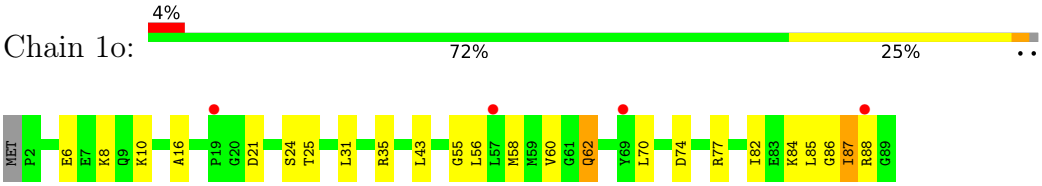


• Molecule 45: 30S ribosomal protein S14 type Z



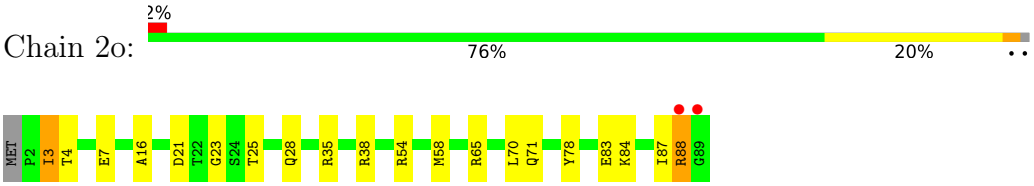
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



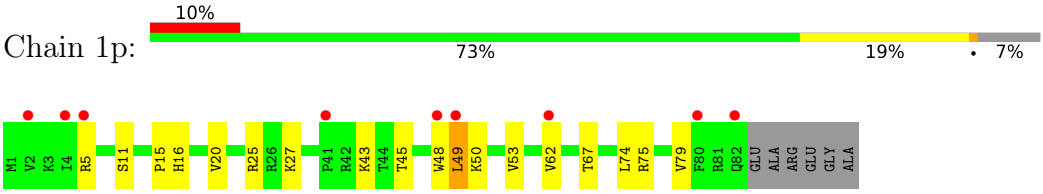
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



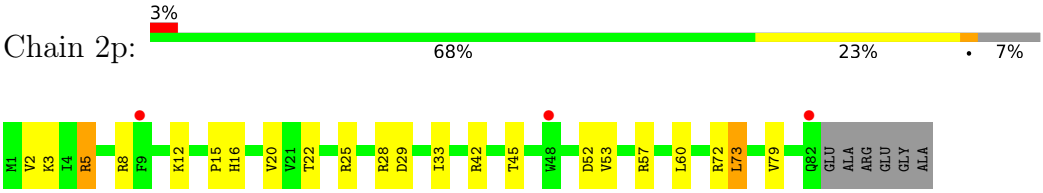
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



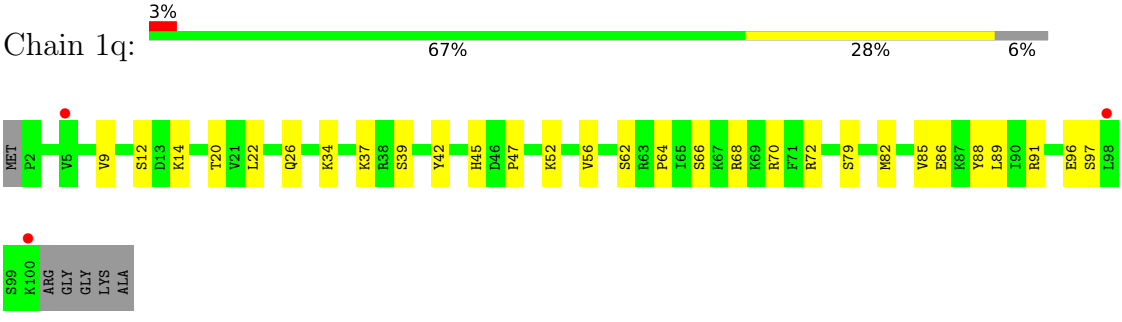
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



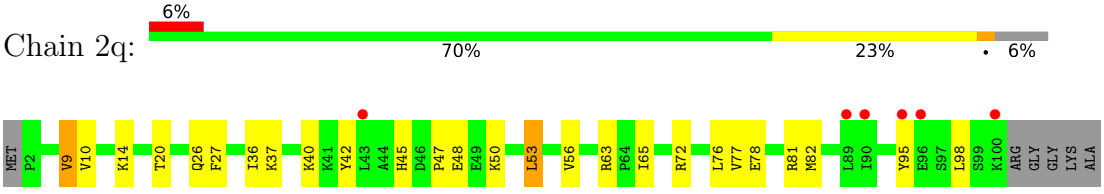
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



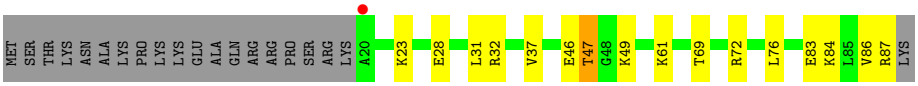
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



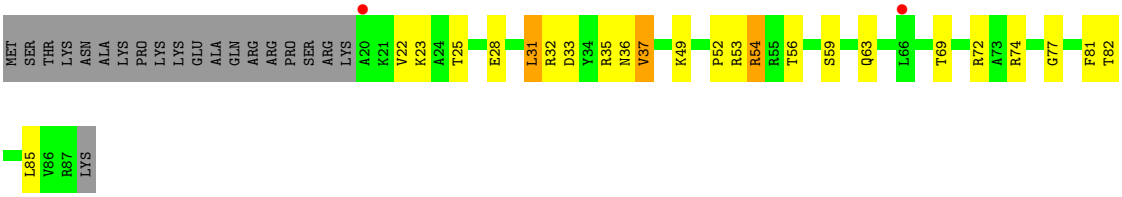
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



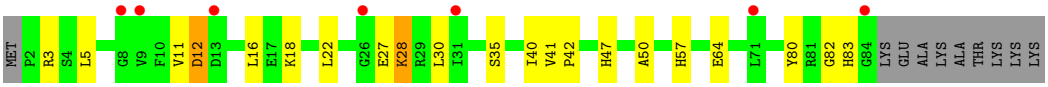
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



• Molecule 50: 30S ribosomal protein S19

Chain 1s:



• Molecule 50: 30S ribosomal protein S19

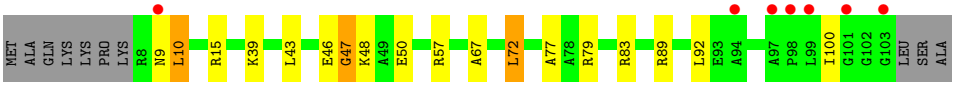
Chain 2s:

• Molecule 51: 30S ribosomal protein S20

Chain 1t:

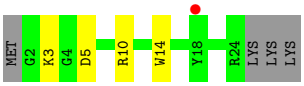
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



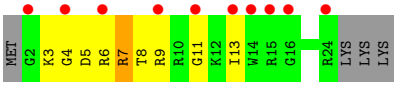
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



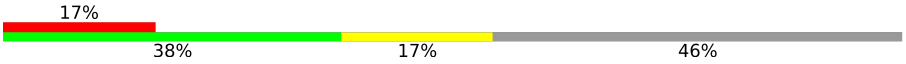
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



• Molecule 53: MF-mRNA

Chain 1v:

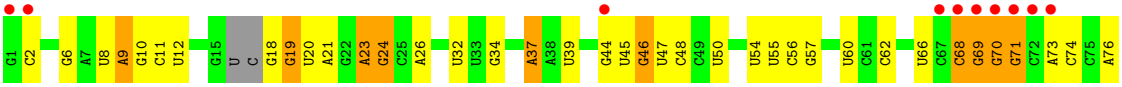


• Molecule 53: MF-mRNA

Chain 2v:

• Molecule 54: Aminoacylated Phe-tRNAphe

Chain 1w:

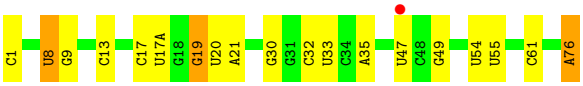


• Molecule 54: Aminoacylated Phe-tRNAphe

Chain 2w:

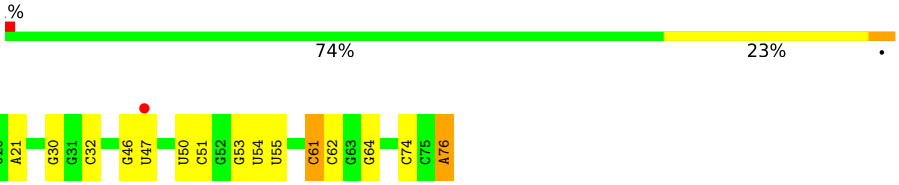
• Molecule 55: Aminoacylated fMet-tRNAmet

Chain 1x:



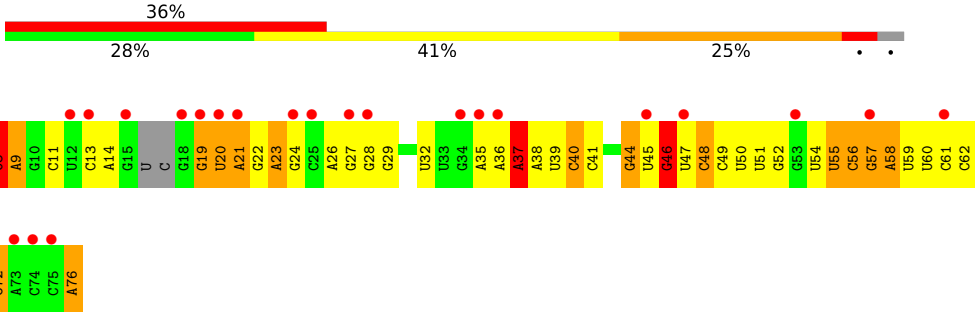
• Molecule 55: Aminoacylated fMet-tRNAmet

Chain 2x:



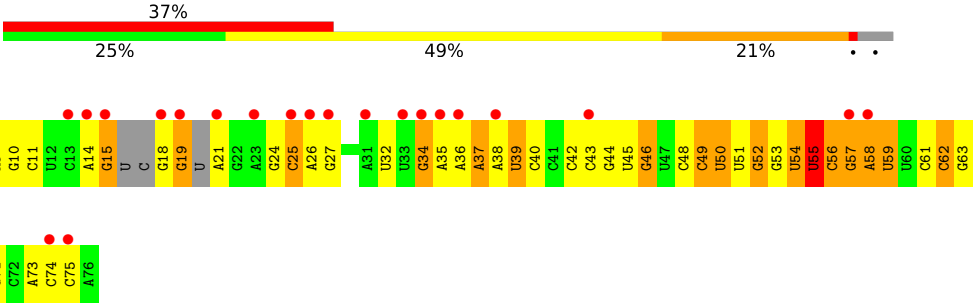
• Molecule 56: Deacylated tRNAphe

Chain 1y:



• Molecule 56: Deacylated tRNAphe

Chain 2y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	211.85Å 451.31Å 630.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.66 – 2.55 122.66 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.4 (122.66-2.55) 99.4 (122.66-2.55)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.220 , 0.262 0.222 , 0.263	Depositor DCC
R_{free} test set	96493 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	51.6	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	300368	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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: G7M, MIA, 8AN, K, 0TD, M2G, MA6, OMU, PSU, 2MA, SF4, OMC, 5MC, 4OC, 2MG, MG, UR3, A1AE0, FME, 4SU, ZN, 5MU, OMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1A	0.26	0/69011	0.46	2/107720 (0.0%)
1	2A	0.21	0/67295	0.40	2/105042 (0.0%)
2	1B	0.21	0/2882	0.39	0/4494
2	2B	0.19	0/2879	0.36	0/4487
3	1D	0.26	0/2186	0.52	0/2944
3	2D	0.22	0/2186	0.45	0/2944
4	1E	0.26	0/1592	0.52	1/2149 (0.0%)
4	2E	0.20	0/1592	0.43	0/2149
5	1F	0.26	0/1619	0.50	0/2193
5	2F	0.20	0/1615	0.48	2/2188 (0.1%)
6	1G	0.21	0/1448	0.43	0/1957
6	2G	0.18	0/1453	0.43	1/1963 (0.1%)
7	1H	0.22	0/1356	0.42	0/1834
7	2H	0.18	0/1356	0.35	0/1834
8	1I	0.18	0/1112	0.42	0/1514
8	2I	0.33	0/1079	0.69	1/1475 (0.1%)
9	1N	0.24	0/1144	0.49	1/1543 (0.1%)
9	2N	0.19	0/1144	0.40	0/1543
10	1O	0.25	0/943	0.47	0/1269
10	2O	0.19	0/943	0.41	0/1269
11	1P	0.26	0/1152	0.57	0/1533
11	2P	0.21	0/1152	0.48	0/1533
12	1Q	0.25	0/1143	0.46	0/1527
12	2Q	0.19	0/1143	0.41	0/1527
13	1R	0.29	0/982	0.51	0/1312
13	2R	0.21	0/982	0.46	0/1312
14	1S	0.23	0/883	0.49	0/1176
14	2S	0.21	0/880	0.46	0/1172
15	1T	0.24	0/1105	0.44	0/1477
15	2T	0.21	0/1097	0.49	1/1468 (0.1%)
16	1U	0.27	0/977	0.46	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	2U	0.20	0/977	0.39	0/1301
17	1V	0.24	0/782	0.48	0/1049
17	2V	0.20	0/782	0.42	0/1049
18	1W	0.27	0/897	0.46	0/1205
18	2W	0.22	0/897	0.41	0/1205
19	1X	0.26	0/764	0.51	0/1025
19	2X	0.21	0/764	0.48	0/1025
20	1Y	0.22	0/819	0.48	0/1095
20	2Y	0.20	0/819	0.39	0/1095
21	1Z	0.22	0/1267	0.46	0/1717
21	2Z	0.24	0/1299	0.50	1/1763 (0.1%)
22	10	0.27	0/662	0.49	0/881
22	20	0.20	0/662	0.45	0/881
23	11	0.23	0/762	0.42	0/1014
23	21	0.21	0/762	0.40	0/1014
24	12	0.24	0/590	0.43	0/781
24	22	0.18	0/590	0.39	0/781
25	13	0.25	0/474	0.47	0/635
25	23	0.19	0/469	0.44	0/630
26	14	0.23	0/565	0.56	0/761
26	24	0.24	0/545	0.47	0/737
27	15	0.25	0/469	0.50	0/635
27	25	0.20	0/469	0.42	0/635
28	16	0.24	0/460	0.42	0/613
28	26	0.22	0/456	0.46	0/608
29	17	0.30	0/426	0.53	0/561
29	27	0.25	0/426	0.51	0/561
30	18	0.26	0/525	0.47	0/691
30	28	0.20	0/525	0.41	0/691
31	19	0.26	0/310	0.49	0/407
31	29	0.19	0/310	0.45	0/407
32	1a	0.20	0/35795	0.38	0/55864
32	2a	0.19	0/35886	0.37	4/56005 (0.0%)
33	1b	0.20	0/1881	0.46	0/2542
33	2b	0.21	0/1860	0.46	0/2518
34	1c	0.20	0/1572	0.46	2/2126 (0.1%)
34	2c	0.20	0/1566	0.41	0/2119
35	1d	0.18	0/1685	0.42	0/2262
35	2d	0.20	0/1704	0.45	0/2284
36	1e	0.20	0/1145	0.45	0/1543
36	2e	0.21	0/1149	0.46	0/1548
37	1f	0.18	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	0.18	0/1250	0.39	0/1679
38	2g	0.18	0/1254	0.41	0/1683
39	1h	0.19	0/1108	0.42	0/1494
39	2h	0.18	0/1108	0.44	0/1494
40	1i	0.20	0/1002	0.51	0/1346
40	2i	0.21	0/997	0.46	0/1343
41	1j	0.22	0/722	0.45	0/982
41	2j	0.22	0/727	0.47	0/988
42	1k	0.19	0/844	0.42	0/1145
42	2k	0.17	0/848	0.38	0/1149
43	1l	0.21	0/937	0.41	0/1260
43	2l	0.19	0/937	0.40	0/1260
44	1m	0.20	0/969	0.47	0/1302
44	2m	0.19	0/961	0.45	0/1291
45	1n	0.20	0/501	0.43	0/664
45	2n	0.22	0/501	0.47	0/664
46	1o	0.19	0/739	0.38	0/985
46	2o	0.18	0/739	0.38	0/985
47	1p	0.22	0/697	0.45	0/939
47	2p	0.19	0/693	0.43	0/935
48	1q	0.20	0/836	0.39	0/1117
48	2q	0.18	0/836	0.40	0/1117
49	1r	0.19	0/560	0.41	0/746
49	2r	0.18	0/560	0.39	0/746
50	1s	0.18	0/667	0.47	0/900
50	2s	0.25	0/661	0.56	0/893
51	1t	0.19	0/730	0.47	0/965
51	2t	0.22	0/729	0.47	0/965
52	1u	0.18	0/203	0.42	0/266
52	2u	0.20	0/203	0.43	0/266
53	1v	0.20	0/310	0.35	0/480
53	2v	0.20	0/310	0.36	0/480
54	1w	0.29	1/1581 (0.1%)	0.43	0/2458
54	2w	0.30	2/1531 (0.1%)	0.41	0/2379
55	1x	0.26	1/1723 (0.1%)	0.40	0/2684
55	2x	0.26	1/1723 (0.1%)	0.40	0/2684
56	1y	0.32	2/1606 (0.1%)	0.40	0/2497
56	2y	0.32	2/1583 (0.1%)	0.44	0/2459
All	All	0.22	9/316636 (0.0%)	0.42	18/474041 (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	2b	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	1y	46	G7M	O3'-P	5.75	1.62	1.56
56	2y	8	4SU	O3'-P	5.68	1.61	1.56
55	2x	8	4SU	O3'-P	5.42	1.61	1.56
56	1y	8	4SU	O3'-P	5.38	1.61	1.56
54	2w	8	4SU	O3'-P	5.27	1.61	1.56
54	2w	46	G7M	O3'-P	5.18	1.61	1.56
55	1x	8	4SU	O3'-P	5.10	1.61	1.56
54	1w	46	G7M	O3'-P	5.08	1.61	1.56
56	2y	46	G7M	O3'-P	5.07	1.61	1.56

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2I	66	GLU	N-CA-C	-7.62	105.15	114.75
32	2a	1272	G	N1-C2-N2	-6.99	95.23	116.20
4	1E	34	VAL	N-CA-C	-6.88	106.08	112.96
1	1A	1992	G	C2'-C3'-O3'	6.78	119.66	109.50
1	2A	1992	G	C2'-C3'-O3'	6.38	119.07	109.50
21	2Z	105	VAL	N-CA-C	6.34	113.00	106.21
32	2a	1263	C	N1-C2-O2	6.22	137.57	118.90
15	2T	89	VAL	N-CA-C	-6.06	106.90	112.96
34	1c	65	ALA	CA-C-N	5.78	132.37	121.97
34	1c	65	ALA	C-N-CA	5.78	132.37	121.97
32	2a	1272	G	N3-C2-N2	5.73	137.08	119.90
9	1N	130	HIS	N-CA-C	-5.68	106.95	112.97
32	2a	1272	G	C5-C6-O6	5.41	144.82	128.60
6	2G	45	GLU	N-CA-C	-5.34	106.73	113.20
5	2F	21	ALA	CA-C-N	5.23	131.11	121.70
5	2F	21	ALA	C-N-CA	5.23	131.11	121.70
1	1A	2689	U	C2'-C3'-O3'	5.17	117.26	109.50
1	2A	1992	G	P-O3'-C3'	5.01	127.71	120.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	2b	8	LYS	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	61852	0	31195	427	0
1	2A	60322	0	30426	496	0
2	1B	2577	0	1305	13	0
2	2B	2575	0	1303	30	0
3	1D	2136	0	2218	28	0
3	2D	2136	0	2218	28	0
4	1E	1559	0	1618	17	0
4	2E	1559	0	1618	26	0
5	1F	1584	0	1625	24	0
5	2F	1580	0	1619	37	0
6	1G	1423	0	1436	31	0
6	2G	1428	0	1438	48	0
7	1H	1330	0	1407	22	0
7	2H	1330	0	1407	25	0
8	1I	1097	0	1140	29	0
8	2I	1064	0	1082	76	0
9	1N	1117	0	1184	10	0
9	2N	1117	0	1184	19	0
10	1O	933	0	996	11	0
10	2O	933	0	996	11	0
11	1P	1135	0	1212	20	0
11	2P	1135	0	1212	28	0
12	1Q	1122	0	1179	11	0
12	2Q	1122	0	1179	15	0
13	1R	968	0	1033	11	0
13	2R	968	0	1033	13	0
14	1S	873	0	927	8	0
14	2S	870	0	923	32	0
15	1T	1091	0	1151	7	0
15	2T	1083	0	1136	26	0
16	1U	959	0	1019	7	0
16	2U	959	0	1019	20	0
17	1V	771	0	830	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	2V	771	0	830	12	0
18	1W	886	0	940	11	0
18	2W	886	0	940	8	0
19	1X	750	0	814	10	0
19	2X	750	0	814	17	0
20	1Y	806	0	881	17	0
20	2Y	806	0	881	18	0
21	1Z	1240	0	1240	26	0
21	2Z	1271	0	1273	47	0
22	10	653	0	674	6	0
22	20	653	0	674	12	0
23	11	755	0	826	7	0
23	21	755	0	826	16	0
24	12	588	0	643	5	0
24	22	588	0	643	9	0
25	13	469	0	518	7	0
25	23	464	0	514	11	0
26	14	552	0	533	27	0
26	24	532	0	503	26	0
27	15	455	0	465	3	0
27	25	455	0	465	4	0
28	16	453	0	473	12	0
28	26	449	0	469	12	0
29	17	418	0	467	5	0
29	27	418	0	467	6	0
30	18	517	0	582	7	0
30	28	517	0	582	9	0
31	19	307	0	335	3	0
31	29	307	0	335	6	0
32	1a	32246	0	16295	284	0
32	2a	32327	0	16338	354	0
33	1b	1846	0	1867	68	0
33	2b	1825	0	1828	77	0
34	1c	1548	0	1535	38	0
34	2c	1542	0	1517	48	0
35	1d	1655	0	1672	36	0
35	2d	1674	0	1714	52	0
36	1e	1129	0	1185	30	0
36	2e	1133	0	1191	37	0
37	1f	810	0	804	23	0
37	2f	816	0	808	15	0
38	1g	1231	0	1238	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	2g	1235	0	1249	24	0
39	1h	1088	0	1126	24	0
39	2h	1088	0	1126	16	0
40	1i	983	0	986	25	0
40	2i	978	0	966	31	0
41	1j	709	0	650	21	0
41	2j	714	0	672	25	0
42	1k	829	0	825	12	0
42	2k	833	0	836	18	0
43	1l	932	0	981	8	0
43	2l	932	0	981	13	0
44	1m	958	0	1002	21	0
44	2m	950	0	988	25	0
45	1n	492	0	529	6	0
45	2n	492	0	529	13	0
46	1o	728	0	760	15	0
46	2o	728	0	760	13	0
47	1p	681	0	697	10	0
47	2p	677	0	686	15	0
48	1q	823	0	891	15	0
48	2q	823	0	891	14	0
49	1r	555	0	618	9	0
49	2r	555	0	618	22	0
50	1s	652	0	662	13	0
50	2s	646	0	644	28	0
51	1t	728	0	798	16	0
51	2t	727	0	796	12	0
52	1u	199	0	208	3	0
52	2u	199	0	208	6	0
53	1v	277	0	140	1	0
53	2v	277	0	140	1	0
54	1w	1592	0	817	16	0
54	2w	1544	0	786	24	0
55	1x	1646	0	838	10	0
55	2x	1646	0	838	8	0
56	1y	1585	0	803	33	0
56	2y	1565	0	794	30	0
57	10	9	0	0	0	0
57	11	4	0	0	0	0
57	12	2	0	0	0	0
57	13	4	0	0	0	0
57	14	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	15	8	0	0	0	0
57	16	3	0	0	0	0
57	17	4	0	0	0	0
57	18	3	0	0	0	0
57	19	2	0	0	0	0
57	1A	1108	0	0	0	0
57	1B	36	0	0	0	0
57	1D	13	0	0	0	0
57	1E	14	0	0	0	0
57	1F	13	0	0	0	0
57	1G	5	0	0	0	0
57	1I	1	0	0	0	0
57	1N	7	0	0	0	0
57	1O	5	0	0	0	0
57	1P	6	0	0	0	0
57	1Q	6	0	0	0	0
57	1R	5	0	0	0	0
57	1S	3	0	0	0	0
57	1T	2	0	0	0	0
57	1U	7	0	0	0	0
57	1V	8	0	0	0	0
57	1W	6	0	0	0	0
57	1X	8	0	0	0	0
57	1Y	2	0	0	0	0
57	1Z	3	0	0	0	0
57	1a	217	0	0	0	0
57	1b	1	0	0	0	0
57	1d	1	0	0	0	0
57	1e	2	0	0	0	0
57	1f	2	0	0	0	0
57	1h	1	0	0	0	0
57	1l	2	0	0	0	0
57	1m	2	0	0	0	0
57	1n	2	0	0	0	0
57	1q	1	0	0	0	0
57	1t	1	0	0	0	0
57	1v	1	0	0	0	0
57	1w	8	0	0	0	0
57	1x	14	0	0	0	0
57	1y	1	0	0	0	0
57	20	2	0	0	0	0
57	21	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	23	2	0	0	0	0
57	25	7	0	0	0	0
57	26	1	0	0	0	0
57	27	2	0	0	0	0
57	28	3	0	0	0	0
57	29	1	0	0	0	0
57	2A	861	0	0	0	0
57	2B	19	0	0	0	0
57	2D	6	0	0	0	0
57	2E	7	0	0	0	0
57	2F	8	0	0	0	0
57	2G	1	0	0	0	0
57	2O	2	0	0	0	0
57	2P	2	0	0	0	0
57	2Q	2	0	0	0	0
57	2R	2	0	0	0	0
57	2S	1	0	0	0	0
57	2T	4	0	0	0	0
57	2U	2	0	0	0	0
57	2V	2	0	0	0	0
57	2W	2	0	0	0	0
57	2X	2	0	0	0	0
57	2Y	1	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	238	0	0	0	0
57	2d	2	0	0	0	0
57	2e	1	0	0	0	0
57	2f	2	0	0	0	0
57	2g	1	0	0	0	0
57	2j	1	0	0	0	0
57	2l	3	0	0	0	0
57	2p	1	0	0	0	0
57	2q	2	0	0	0	0
57	2r	1	0	0	0	0
57	2t	1	0	0	0	0
57	2v	2	0	0	0	0
57	2w	7	0	0	0	0
57	2x	6	0	0	0	0
57	2y	4	0	0	0	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	1A	72	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	2A	72	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
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	1	0
61	2d	8	0	0	0	0
62	1w	11	0	8	1	0
62	2w	11	0	8	1	0
63	1x	10	0	10	0	0
63	2x	10	0	10	0	0
64	10	11	0	0	0	0
64	11	12	0	0	0	0
64	12	4	0	0	0	0
64	13	5	0	0	0	0
64	14	1	0	0	0	0
64	15	6	0	0	0	0
64	16	3	0	0	0	0
64	17	7	0	0	1	0
64	18	12	0	0	1	0
64	1A	2019	0	0	71	0
64	1B	62	0	0	2	0
64	1D	27	0	0	0	0
64	1E	25	0	0	1	0
64	1F	18	0	0	3	0
64	1G	2	0	0	0	0
64	1H	2	0	0	0	0
64	1N	5	0	0	0	0
64	1O	6	0	0	1	0
64	1P	21	0	0	2	0
64	1Q	9	0	0	0	0
64	1R	11	0	0	0	0
64	1S	3	0	0	0	0
64	1T	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	1U	11	0	0	0	0
64	1V	7	0	0	0	0
64	1W	8	0	0	0	0
64	1X	4	0	0	0	0
64	1Y	3	0	0	1	0
64	1Z	1	0	0	0	0
64	1a	391	0	0	25	0
64	1b	1	0	0	0	0
64	1d	1	0	0	0	0
64	1e	1	0	0	0	0
64	1f	1	0	0	0	0
64	1g	1	0	0	0	0
64	1j	1	0	0	0	0
64	1l	5	0	0	0	0
64	1m	1	0	0	0	0
64	1n	1	0	0	0	0
64	1o	1	0	0	0	0
64	1p	1	0	0	0	0
64	1q	2	0	0	0	0
64	1t	1	0	0	0	0
64	1u	1	0	0	1	0
64	1v	5	0	0	0	0
64	1w	13	0	0	0	0
64	1x	12	0	0	0	0
64	1y	1	0	0	0	0
64	20	1	0	0	0	0
64	21	11	0	0	0	0
64	22	1	0	0	0	0
64	23	3	0	0	1	0
64	25	2	0	0	1	0
64	27	4	0	0	0	0
64	28	3	0	0	0	0
64	29	1	0	0	0	0
64	2A	1149	0	0	63	0
64	2B	20	0	0	2	0
64	2D	20	0	0	0	0
64	2E	14	0	0	0	0
64	2F	12	0	0	0	0
64	2I	1	0	0	1	0
64	2O	1	0	0	0	0
64	2P	12	0	0	0	0
64	2Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	2R	4	0	0	0	0
64	2T	5	0	0	0	0
64	2U	3	0	0	0	0
64	2W	3	0	0	0	0
64	2X	1	0	0	0	0
64	2Y	1	0	0	0	0
64	2a	288	0	0	20	0
64	2c	1	0	0	0	0
64	2d	3	0	0	0	0
64	2e	2	0	0	0	0
64	2j	1	0	0	0	0
64	2l	6	0	0	0	0
64	2n	1	0	0	0	0
64	2p	2	0	0	0	0
64	2q	1	0	0	0	0
64	2r	1	0	0	0	0
64	2t	2	0	0	0	0
64	2v	2	0	0	0	0
64	2w	3	0	0	0	0
64	2x	9	0	0	2	0
64	2y	5	0	0	0	0
All	All	300368	0	196742	3230	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 (3230) 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	1.28	1.32
1:1A:1082:U:O4	1:1A:1086:A:N1	1.97	0.98
56:2y:18:G:H22	56:2y:55:PSU:HN3	1.09	0.98
1:1A:1054:A:H61	1:1A:1105:U:H3	1.06	0.98
29:17:24:THR:HG22	29:17:27:GLY:H	1.30	0.94
1:2A:2136:C:N4	1:2A:2155:G:H1	1.66	0.93
1:2A:2298:A:H62	1:2A:2318:G:H8	1.10	0.92
32:1a:376:G:H5"	47:1p:5:ARG:HG2	1.51	0.91
32:1a:664:G:H22	32:1a:741:G:H1	1.19	0.90
56:2y:18:G:N2	56:2y:55:PSU:HN3	1.70	0.90
5:1F:53:THR:HG22	5:1F:55:GLY:H	1.38	0.89
1:1A:1082:U:N3	1:1A:1086:A:N6	2.12	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2427:C:OP1	64:1A:4203:HOH:O	1.92	0.86
54:2w:4:C:H42	54:2w:69:G:H1	1.21	0.86
1:2A:1689:A:H62	1:2A:1698:A:H2	1.23	0.85
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.20	0.85
54:2w:27:G:H1	54:2w:43:C:H42	1.24	0.85
33:1b:95:GLN:HE22	33:1b:147:LYS:HG2	1.39	0.85
34:2c:58:GLU:HB3	41:2j:92:THR:HG21	1.58	0.85
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.58	0.84
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.59	0.84
56:1y:26:A:H61	56:1y:44:G:H1	1.26	0.84
1:2A:2137:C:N4	1:2A:2154:G:H1	1.76	0.83
44:1m:3:ARG:HD2	44:1m:9:ILE:HG12	1.59	0.83
21:2Z:124:ILE:HD11	21:2Z:165:VAL:HG21	1.61	0.83
5:1F:155:LEU:HD11	5:1F:176:LEU:HD12	1.59	0.83
1:2A:2135:A:H61	1:2A:2156:G:H21	1.25	0.83
1:2A:880:G:H2'	1:2A:881:G:H8	1.41	0.82
27:15:40:LYS:NZ	27:15:44:THR:O	2.12	0.82
26:24:24:THR:OG1	26:24:25:TYR:N	2.11	0.82
1:2A:981:A:OP1	64:2A:3901:HOH:O	1.97	0.82
32:2a:1271:G:N2	32:2a:1272:G:N7	2.28	0.82
38:2g:68:ASN:HD22	38:2g:128:ALA:HA	1.45	0.82
32:2a:1029:C:C4	32:2a:1032:G:N1	2.48	0.82
1:1A:2822:G:OP2	64:1A:4204:HOH:O	1.98	0.81
1:2A:1031:G:H5"	31:29:8:LYS:HE3	1.63	0.81
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.13	0.81
1:1A:2100:G:H1	1:1A:2189:U:H3	1.25	0.81
32:1a:1505:G:OP2	64:1a:1905:HOH:O	1.98	0.81
32:1a:1027:C:C2	32:1a:1034:G:N2	2.49	0.81
1:2A:1204:A:H2	1:2A:1241:A:H62	1.28	0.80
21:2Z:154:ASP:N	21:2Z:154:ASP:OD1	2.15	0.80
32:1a:1009:G:O6	32:1a:1020:U:O2	1.98	0.80
1:2A:1693:U:O2'	3:2D:14:ARG:NH2	2.14	0.79
26:24:53:GLU:HG2	26:24:55:ARG:H	1.46	0.79
1:1A:2431:U:OP2	64:1A:4205:HOH:O	2.00	0.79
34:2c:52:LEU:HD13	34:2c:68:VAL:HG13	1.62	0.79
1:1A:1054:A:N6	1:1A:1105:U:H3	1.78	0.79
1:1A:2533:A:OP2	64:1A:4206:HOH:O	2.01	0.79
33:2b:8:LYS:HD2	33:2b:9:GLU:H	1.48	0.79
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.57	0.78
8:2I:73:GLU:HG3	8:2I:138:ILE:HG23	1.66	0.78
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.66	0.78
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.64	0.78
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.17	0.78
33:1b:15:VAL:HG13	33:1b:209:ARG:HG3	1.65	0.77
32:1a:224:C:OP1	51:1t:74:LYS:NZ	2.16	0.77
32:2a:1352:C:OP1	52:2u:3:LYS:NZ	2.17	0.77
1:1A:2428:G:OP1	64:1A:4203:HOH:O	2.02	0.77
32:2a:664:G:H22	32:2a:741:G:H1	1.31	0.77
1:1A:1014:U:OP2	64:1A:4207:HOH:O	2.01	0.77
1:1A:2277:G:OP2	22:10:10:THR:HG21	1.84	0.77
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.67	0.77
32:2a:975:A:H4'	32:2a:976:G:H5"	1.66	0.77
45:2n:9:LYS:HG3	45:2n:12:ARG:HH21	1.48	0.77
52:1u:5:ASP:OD2	64:1u:101:HOH:O	2.01	0.77
21:2Z:93:ASP:HA	21:2Z:131:ARG:HH12	1.48	0.77
32:2a:266:G:H5"	32:2a:268:C:H41	1.49	0.77
37:2f:97:PHE:HD2	49:2r:31:LEU:HD11	1.47	0.77
1:1A:1332:G:OP1	64:1A:4208:HOH:O	2.01	0.76
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	1.66	0.76
41:1j:50:ILE:HA	41:1j:60:ARG:HG2	1.66	0.76
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.50	0.76
1:2A:397:G:N7	64:2A:3941:HOH:O	2.19	0.76
14:2S:48:LEU:HD23	14:2S:82:ILE:HD11	1.65	0.76
44:2m:3:ARG:HH22	44:2m:11:ARG:HG3	1.48	0.76
1:2A:2136:C:N3	1:2A:2155:G:N2	2.31	0.76
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.49	0.76
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.19	0.76
1:2A:2319:G:H22	14:2S:3:ARG:HH11	1.31	0.76
33:1b:33:TYR:HB2	33:1b:43:ASP:HB2	1.67	0.75
32:2a:770:C:OP1	64:2a:3302:HOH:O	2.03	0.75
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.22	0.75
1:1A:2575:C:OP2	64:1A:4209:HOH:O	2.04	0.75
47:1p:53:VAL:HG13	47:1p:79:VAL:HG22	1.68	0.75
1:1A:1058:G:H1	1:1A:1080:C:H42	1.32	0.75
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.34	0.75
8:2I:52:ARG:O	8:2I:56:LYS:N	2.17	0.75
1:1A:741:G:OP2	64:1A:4210:HOH:O	2.04	0.75
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.69	0.75
1:1A:2099:U:H3	1:1A:2190:G:H1	1.32	0.74
32:2a:117:G:OP2	64:2a:3303:HOH:O	2.04	0.74
1:1A:668:G:N7	64:1A:4239:HOH:O	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2677:G:N3	64:2A:3948:HOH:O	2.21	0.74
56:2y:18:G:N2	56:2y:55:PSU:N3	2.33	0.74
1:2A:973:A:OP2	64:2A:3904:HOH:O	2.06	0.74
1:2A:1271:G:OP2	64:2A:3902:HOH:O	2.04	0.74
32:1a:975:A:H4'	32:1a:976:G:H5"	1.68	0.74
32:2a:742:G:OP2	46:2o:35:ARG:NH2	2.20	0.74
44:2m:23:TYR:HB3	44:2m:67:GLU:HA	1.68	0.74
56:2y:18:G:N7	56:2y:56:C:N4	2.35	0.74
41:1j:8:LEU:HD22	41:1j:96:ILE:HG12	1.70	0.74
50:2s:28:LYS:HB3	50:2s:29:ARG:HA	1.69	0.74
1:2A:2063:C:OP1	64:2A:3906:HOH:O	2.06	0.74
1:1A:2131:G:N2	1:1A:2158:A:N1	2.34	0.73
32:1a:1499:A:OP2	64:1a:1905:HOH:O	2.05	0.73
1:2A:792:G:O6	64:2A:3903:HOH:O	2.04	0.73
32:2a:1086:U:H3	32:2a:1099:G:H22	1.35	0.73
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.69	0.73
32:1a:576:G:OP1	64:1a:1906:HOH:O	2.07	0.73
34:1c:57:ILE:HG12	34:1c:66:VAL:HG12	1.71	0.73
8:2I:84:GLY:N	8:2I:87:LYS:O	2.21	0.73
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.69	0.73
1:2A:1670:C:OP1	64:2A:3905:HOH:O	2.06	0.73
42:1k:99:GLN:HG2	42:1k:105:VAL:HG11	1.70	0.72
1:2A:2136:C:N4	1:2A:2155:G:N1	2.37	0.72
46:2o:16:ALA:HB1	46:2o:21:ASP:HB3	1.70	0.72
1:2A:1648:C:OP1	64:2A:3902:HOH:O	2.06	0.72
1:2A:2110:G:OP1	1:2A:2118:U:N3	2.21	0.72
1:2A:2319:G:H22	14:2S:3:ARG:HD2	1.54	0.72
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.72	0.72
1:1A:1013:C:OP2	64:1A:4207:HOH:O	2.07	0.72
1:2A:963:U:OP2	64:2A:3907:HOH:O	2.06	0.72
54:2w:4:C:N4	54:2w:69:G:H1	1.86	0.72
1:1A:582:G:OP2	64:1A:4211:HOH:O	2.06	0.72
56:1y:3:C:H42	56:1y:70:G:H1	1.37	0.72
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.72	0.72
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.23	0.72
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.71	0.71
32:2a:446:G:O6	64:2a:3304:HOH:O	2.07	0.71
1:2A:570:G:O6	64:2A:3909:HOH:O	2.08	0.71
1:2A:2137:C:H42	1:2A:2154:G:H1	1.38	0.71
1:1A:826:U:OP1	64:1A:4203:HOH:O	2.09	0.71
32:1a:1086:U:H3	32:1a:1099:G:H22	1.35	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:816:C:OP2	64:2A:3912:HOH:O	2.08	0.71
32:2a:1272:G:N2	32:2a:1273:G:N7	2.38	0.71
1:2A:2407:G:OP1	64:2A:3910:HOH:O	2.08	0.71
2:2B:9:G:H1	2:2B:112:U:H3	1.36	0.71
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.24	0.71
1:1A:2821:A:OP2	64:1A:4204:HOH:O	2.09	0.71
32:1a:544:G:OP1	35:1d:59:ARG:NH2	2.21	0.71
33:1b:12:GLU:HB2	33:1b:213:LEU:HD21	1.73	0.71
1:2A:2151:G:H2'	1:2A:2152:G:H8	1.56	0.71
64:1A:4204:HOH:O	13:1R:3:HIS:NE2	2.23	0.71
33:1b:158:LEU:HD13	33:1b:182:ILE:HD11	1.73	0.71
8:2I:45:LYS:O	8:2I:49:ALA:N	2.20	0.71
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.24	0.70
1:2A:509:C:OP1	64:2A:3908:HOH:O	2.07	0.70
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.72	0.70
21:2Z:138:GLU:H	21:2Z:156:LYS:HE2	1.56	0.70
54:2w:18:G:HO2'	54:2w:57:G:H22	1.38	0.70
1:2A:2140:C:H42	1:2A:2151:G:H1	1.39	0.70
23:21:50:ARG:HG2	23:21:59:THR:HG22	1.72	0.70
54:2w:18:G:O2'	54:2w:57:G:N2	2.17	0.70
26:14:55:ARG:N	26:14:56:VAL:HA	2.06	0.70
56:1y:8:4SU:H4'	56:1y:48:C:H4'	1.73	0.70
1:2A:1830:C:OP2	64:2A:3911:HOH:O	2.08	0.70
1:2A:2619:C:OP1	4:2E:152:LYS:NZ	2.24	0.70
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.74	0.70
2:2B:56:G:H5'	6:2G:27:ASN:HD21	1.56	0.70
1:1A:1938:A:OP2	64:1A:4212:HOH:O	2.08	0.70
32:2a:390:C:O3'	47:2p:28:ARG:NH2	2.24	0.70
2:1B:23:G:O6	64:1B:301:HOH:O	2.07	0.70
17:1V:98:GLU:OE2	17:1V:100:ARG:NH1	2.24	0.70
32:2a:331:G:OP2	64:2a:3305:HOH:O	2.08	0.70
1:1A:1023:U:OP2	64:1A:4213:HOH:O	2.08	0.70
26:14:55:ARG:H	26:14:56:VAL:HA	1.57	0.70
33:2b:178:ARG:HH22	39:2h:68:ARG:HH12	1.39	0.70
62:2w:108:PHE:N	55:2x:76:8AN:HO2'	1.88	0.70
33:2b:189:ASP:N	33:2b:189:ASP:OD1	2.25	0.70
1:1A:642:G:OP1	64:1A:4215:HOH:O	2.09	0.70
5:1F:185:ASP:OD1	5:1F:188:ARG:NH1	2.23	0.70
1:1A:1993:U:OP2	64:1A:4217:HOH:O	2.10	0.70
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.74	0.70
10:1O:48:PRO:HB3	32:1a:1422:G:H5"	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:2o:4:THR:N	46:2o:7:GLU:OE1	2.24	0.69
1:1A:2790:A:H5'	1:1A:2893:G:H21	1.57	0.69
32:1a:176:C:OP1	51:1t:29:LYS:NZ	2.24	0.69
1:1A:1452:A:OP2	64:1A:4214:HOH:O	2.09	0.69
32:1a:574:A:OP2	64:1a:1907:HOH:O	2.10	0.69
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.74	0.69
32:2a:437:U:OP2	64:2a:3306:HOH:O	2.09	0.69
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	1.74	0.69
35:2d:154:ASN:O	35:2d:159:ARG:NH2	2.26	0.69
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.25	0.69
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.56	0.69
12:2Q:56:ARG:HH22	12:2Q:59:ARG:HH21	1.39	0.69
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.26	0.69
14:2S:84:GLN:H	14:2S:111:GLU:HB2	1.58	0.69
5:1F:165:ARG:HA	5:1F:168:ARG:HD2	1.74	0.69
32:2a:1272:G:N2	32:2a:1273:G:C5	2.61	0.69
40:1i:110:GLU:OE2	40:1i:113:LYS:NZ	2.25	0.69
1:2A:2495:G:H5"	12:2Q:82:ARG:HG2	1.74	0.69
1:1A:1315:C:OP2	64:1A:4208:HOH:O	2.11	0.69
32:1a:677:U:H3	32:1a:713:G:H22	1.40	0.69
33:1b:82:ARG:NH1	33:1b:86:GLU:OE2	2.26	0.69
8:2I:75:LEU:HB2	8:2I:140:LEU:HD11	1.75	0.69
5:1F:61:GLY:O	64:1F:401:HOH:O	2.11	0.68
19:2X:35:THR:HG22	19:2X:37:THR:H	1.57	0.68
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.24	0.68
1:2A:1604:C:OP2	64:2A:3916:HOH:O	2.12	0.68
46:2o:7:GLU:OE2	46:2o:38:ARG:NH2	2.26	0.68
32:1a:1316:G:H22	32:1a:1319:A:H5"	1.58	0.68
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.75	0.68
32:2a:1417:G:O6	64:2a:3307:HOH:O	2.11	0.68
41:2j:15:THR:HB	41:2j:94:VAL:HG22	1.75	0.68
47:2p:53:VAL:HG13	47:2p:79:VAL:HG22	1.75	0.68
32:1a:557:G:OP1	64:1a:1910:HOH:O	2.12	0.68
1:2A:1324:G:N7	64:2A:3969:HOH:O	2.26	0.68
8:2I:87:LYS:HB2	8:2I:121:LYS:HZ3	1.57	0.68
11:2P:39:LYS:HB2	11:2P:45:LEU:HD13	1.74	0.68
1:2A:1812:A:OP2	64:2A:3915:HOH:O	2.12	0.68
35:1d:15:GLU:OE2	35:1d:66:ARG:NH1	2.27	0.68
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.27	0.68
33:2b:104:ASN:OD1	33:2b:107:THR:OG1	2.12	0.68
1:1A:2573:C:OP1	64:1A:4209:HOH:O	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:69:LEU:HB3	33:1b:162:ILE:HG22	1.76	0.68
54:1w:68:C:H2'	54:1w:69:G:C8	2.28	0.68
1:2A:1840:G:OP2	64:2A:3914:HOH:O	2.11	0.68
38:2g:78:ARG:HH21	38:2g:79:ARG:HE	1.39	0.68
12:1Q:1:MET:HE3	12:1Q:45:GLN:HG3	1.76	0.68
43:1l:39:VAL:HG11	43:1l:41:ARG:HH11	1.58	0.68
1:1A:1669:A:OP2	64:1A:4219:HOH:O	2.11	0.67
1:2A:1203:G:O6	64:2A:3913:HOH:O	2.09	0.67
1:2A:1721:G:H8	1:2A:1741:A:H62	1.41	0.67
1:1A:2472:G:OP2	64:1A:4220:HOH:O	2.11	0.67
32:1a:1136:U:H5"	32:1a:1137:C:C4	2.30	0.67
32:2a:1244:C:H42	32:2a:1293:G:H1	1.41	0.67
1:1A:1041:C:H42	1:1A:1114:G:H1	1.43	0.67
33:1b:195:ASP:O	39:1h:68:ARG:NH2	2.28	0.67
35:1d:187:ARG:NH2	35:1d:193:ASP:OD2	2.27	0.67
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.29	0.67
34:2c:20:SER:HB3	34:2c:22:TRP:HE1	1.60	0.67
1:1A:271(V):G:O6	64:1A:4223:HOH:O	2.12	0.67
1:1A:338:G:OP2	64:1A:4221:HOH:O	2.12	0.67
1:1A:1948:G:O6	64:1A:4218:HOH:O	2.11	0.67
32:1a:1521:G:N3	64:1a:1931:HOH:O	2.27	0.67
1:2A:2049:G:N7	64:2A:3977:HOH:O	2.27	0.67
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.29	0.67
32:2a:953:G:H5'	32:2a:965:A:H61	1.60	0.67
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.12	0.67
32:1a:405:U:OP2	35:1d:3:ARG:NH1	2.27	0.67
26:24:16:CYS:HA	26:24:33:VAL:HG12	1.76	0.67
35:2d:18:LYS:HG3	35:2d:33:MET:HG2	1.76	0.67
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.28	0.67
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.77	0.67
1:1A:1062:G:H1	1:1A:1077:A:H61	1.42	0.67
1:2A:1647:G:OP1	64:2A:3902:HOH:O	2.12	0.67
1:2A:2431:U:OP2	64:2A:3918:HOH:O	2.13	0.67
1:1A:739:G:OP1	64:1A:4222:HOH:O	2.12	0.67
28:16:12:GLU:OE1	28:16:19:ARG:NH1	2.28	0.67
1:1A:1314:C:OP1	64:1A:4208:HOH:O	2.13	0.67
40:1i:53:VAL:O	40:1i:55:ALA:N	2.28	0.67
33:1b:60:ASP:HA	33:1b:63:MET:HE3	1.77	0.66
39:1h:34:GLU:OE1	39:1h:37:ARG:NH1	2.28	0.66
39:1h:98:LYS:HD3	39:1h:98:LYS:H	1.59	0.66
56:1y:26:A:N6	56:1y:44:G:H1	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2100:G:H1	1:2A:2189:U:H3	1.41	0.66
1:2A:2316:C:O2'	6:2G:128:ARG:NH2	2.28	0.66
9:1N:128:HIS:O	9:1N:131:GLN:NE2	2.27	0.66
25:13:26:LEU:O	25:13:35:ARG:NE	2.28	0.66
32:1a:116:A:OP1	64:1a:1909:HOH:O	2.11	0.66
1:2A:2849:U:O4	15:2T:23:ARG:NH2	2.28	0.66
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.76	0.66
1:2A:271(L):U:H5'	8:2I:50:ARG:HH11	1.59	0.66
1:2A:948:G:OP1	64:2A:3907:HOH:O	2.13	0.66
1:2A:1187:G:OP2	64:2A:3917:HOH:O	2.13	0.66
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.11	0.66
35:2d:157:LEU:O	35:2d:161:ASN:ND2	2.28	0.66
1:1A:2127:G:H21	1:1A:2173:A:H1'	1.60	0.66
1:2A:198:C:OP2	64:2A:3924:HOH:O	2.14	0.66
10:2O:66:LYS:NZ	10:2O:80:ASP:O	2.27	0.66
32:2a:588:G:OP2	64:2a:3308:HOH:O	2.12	0.66
42:2k:48:ILE:O	42:2k:50:TYR:N	2.25	0.66
54:2w:27:G:H1	54:2w:43:C:N4	1.93	0.66
35:1d:65:ARG:HG3	35:1d:70:ILE:HG22	1.77	0.66
1:1A:192:C:OP1	64:1A:4224:HOH:O	2.13	0.66
32:1a:1470:G:N7	64:1a:1932:HOH:O	2.27	0.66
1:2A:1225:G:H4'	17:2V:84:LYS:HG2	1.76	0.66
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.28	0.66
32:2a:1521:G:N3	64:2a:3324:HOH:O	2.28	0.66
35:1d:7:PRO:HB2	35:1d:10:ARG:HD2	1.76	0.66
32:2a:1030(A):G:N1	32:2a:1030(D):A:OP2	2.29	0.66
32:1a:1467:G:O6	64:1a:1908:HOH:O	2.11	0.66
1:2A:775:G:O3'	64:2A:3923:HOH:O	2.14	0.66
14:2S:67:ARG:NH1	14:2S:107:GLU:OE2	2.29	0.66
35:2d:8:VAL:HG22	35:2d:21:LEU:HD13	1.78	0.66
50:2s:53:ASN:OD1	50:2s:54:GLY:N	2.28	0.66
1:1A:84:A:H5"	20:1Y:8:LYS:HE3	1.78	0.65
4:1E:77:ILE:HD12	4:1E:195:LEU:HD13	1.78	0.65
35:1d:111:ALA:HB2	35:1d:120:LEU:HD12	1.79	0.65
27:25:40:LYS:NZ	27:25:44:THR:O	2.30	0.65
44:2m:33:ALA:HA	44:2m:59:TYR:HE2	1.62	0.65
1:1A:1466:G:O2'	1:1A:1546:C:O2'	2.13	0.65
1:1A:1498:C:OP1	64:1A:4225:HOH:O	2.13	0.65
2:1B:18:G:N7	64:1B:302:HOH:O	2.29	0.65
1:2A:749:C:OP2	64:2A:3920:HOH:O	2.13	0.65
1:2A:2135:A:H2'	1:2A:2136:C:C5	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1439:A:OP1	64:1A:4227:HOH:O	2.14	0.65
32:1a:892:A:OP2	64:1a:1912:HOH:O	2.14	0.65
32:2a:484:G:N3	64:2a:3326:HOH:O	2.29	0.65
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.28	0.65
33:2b:185:ILE:HG22	33:2b:199:TYR:HB2	1.78	0.65
6:2G:63:ILE:HD11	6:2G:144:ILE:HG13	1.78	0.65
11:1P:42:SER:O	64:1P:301:HOH:O	2.13	0.65
32:1a:1337:G:OP2	64:1a:1911:HOH:O	2.13	0.65
15:2T:16:ARG:NH2	15:2T:18:ASP:OD2	2.29	0.65
32:1a:505:G:N7	64:1a:1935:HOH:O	2.28	0.65
42:1k:48:ILE:O	42:1k:50:TYR:N	2.29	0.65
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.61	0.65
1:2A:1632:A:OP2	64:2A:3926:HOH:O	2.15	0.65
8:2I:78:THR:HA	8:2I:143:SER:HB2	1.77	0.65
21:2Z:156:LYS:HE3	21:2Z:158:PRO:HD3	1.77	0.65
28:26:11:LEU:HB2	28:26:21:TYR:HB2	1.78	0.65
32:2a:504:C:OP1	64:2a:3310:HOH:O	2.14	0.65
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.29	0.65
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.79	0.65
1:1A:1058:G:H1	1:1A:1080:C:N4	1.94	0.65
33:1b:95:GLN:NE2	33:1b:147:LYS:O	2.30	0.65
40:2i:85:LEU:HB3	40:2i:92:TYR:HD2	1.60	0.65
1:1A:847:U:OP2	64:1A:4228:HOH:O	2.15	0.65
37:1f:8:ILE:HD11	37:1f:79:LEU:HD13	1.79	0.64
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.30	0.64
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.78	0.64
1:2A:817:C:OP2	64:2A:3928:HOH:O	2.15	0.64
1:2A:1025:G:O2'	64:2A:3930:HOH:O	2.15	0.64
1:2A:2238:G:OP2	64:2A:3921:HOH:O	2.14	0.64
32:2a:596:C:OP2	64:2a:3309:HOH:O	2.13	0.64
34:2c:78:GLY:HA3	34:2c:83:ARG:H	1.61	0.64
36:2e:8:GLU:HG2	36:2e:34:VAL:HG23	1.79	0.64
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.29	0.64
9:2N:12:ARG:HH21	9:2N:38:HIS:HE2	1.45	0.64
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.70	0.64
32:2a:273:A:N7	64:2a:3327:HOH:O	2.30	0.64
1:2A:1975:G:OP2	64:2A:3922:HOH:O	2.14	0.64
1:2A:2168:G:H8	1:2A:2170:A:N7	1.96	0.64
1:2A:2319:G:N2	14:2S:3:ARG:HD2	2.12	0.64
11:2P:126:VAL:HG12	11:2P:148:LEU:HD22	1.79	0.64
8:1I:87:LYS:O	8:1I:87:LYS:NZ	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1224:G:OP1	64:1a:1914:HOH:O	2.14	0.64
25:23:40:THR:HG22	25:23:42:ALA:H	1.62	0.64
32:2a:1345:U:OP2	64:2a:3311:HOH:O	2.15	0.64
1:1A:11:G:H2'	1:1A:12:U:H5'	1.80	0.64
1:2A:975:C:OP1	64:2A:3925:HOH:O	2.14	0.64
1:2A:1675:C:OP2	64:2A:3932:HOH:O	2.15	0.64
32:2a:401:C:OP2	35:2d:73:ARG:NH2	2.30	0.64
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.79	0.64
1:2A:1254:A:OP2	64:2A:3929:HOH:O	2.15	0.64
1:2A:2637:U:OP1	4:2E:82:ARG:NH1	2.31	0.64
32:2a:1133:G:H1	32:2a:1141:C:H42	1.46	0.64
44:2m:58:GLU:O	44:2m:62:ASN:ND2	2.30	0.64
8:1I:3:VAL:HG12	8:1I:38:LEU:HA	1.79	0.64
32:1a:560:U:O2'	32:1a:561:U:OP2	2.13	0.64
2:2B:54:G:OP2	64:2B:301:HOH:O	2.15	0.64
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.63	0.64
6:2G:114:ILE:HA	6:2G:140:ILE:HD11	1.78	0.64
11:2P:121:LYS:O	11:2P:123:LEU:N	2.31	0.64
41:2j:6:ILE:HB	41:2j:72:VAL:HG13	1.77	0.64
1:1A:1647:G:OP1	64:1A:4226:HOH:O	2.14	0.64
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.31	0.64
15:2T:109:GLU:HG2	15:2T:112:ARG:HH22	1.61	0.64
20:2Y:86:ARG:HB2	20:2Y:98:VAL:HG23	1.80	0.64
32:2a:64:G:H4'	32:2a:65:U:H3'	1.80	0.64
33:2b:101:MET:HA	33:2b:108:ILE:HD12	1.80	0.64
9:1N:46:VAL:HG23	9:1N:48:MET:HG2	1.80	0.63
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.80	0.63
2:2B:106:G:H5'	21:2Z:31:ARG:HB3	1.80	0.63
1:1A:880:G:H1	1:1A:898:C:H42	1.47	0.63
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.80	0.63
8:2I:130:TYR:HB3	8:2I:132:PRO:HD3	1.80	0.63
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	1.80	0.63
1:1A:2849:U:OP2	15:1T:95:ARG:NH1	2.32	0.63
32:1a:627:G:O6	64:1a:1913:HOH:O	2.14	0.63
1:2A:2849:U:OP2	15:2T:95:ARG:NH1	2.31	0.63
32:2a:435:C:H2'	32:2a:436:C:H6	1.64	0.63
32:2a:673:G:H2'	32:2a:674:G:C8	2.34	0.63
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.34	0.63
1:1A:1163:G:OP1	17:1V:24:LYS:NZ	2.31	0.63
1:1A:2067:G:N7	64:1A:4294:HOH:O	2.30	0.63
1:2A:1970:A:OP1	64:2A:3933:HOH:O	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:65:LYS:HE3	15:1T:67:SER:HB2	1.80	0.63
1:2A:1824:G:N7	64:2A:3983:HOH:O	2.30	0.63
1:1A:2550:G:OP1	64:1A:4219:HOH:O	2.15	0.63
56:1y:5:G:H1'	56:1y:69:G:N2	2.13	0.63
1:1A:392:C:OP1	64:1A:4229:HOH:O	2.15	0.63
32:1a:1505:G:OP1	64:1a:1916:HOH:O	2.16	0.63
34:2c:37:GLN:NE2	45:2n:52:GLN:OE1	2.31	0.63
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.32	0.63
32:1a:509:A:OP2	64:1a:1917:HOH:O	2.16	0.63
37:1f:6:VAL:HG22	37:1f:90:VAL:HG22	1.79	0.63
51:2t:57:ARG:HH12	51:2t:100:ILE:HD12	1.63	0.63
32:2a:972:C:O2'	41:2j:55:LYS:O	2.17	0.62
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.31	0.62
44:1m:121:LYS:H	44:1m:121:LYS:HE3	1.64	0.62
32:2a:1301:U:O2'	32:2a:1302:U:H5'	1.98	0.62
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.33	0.62
1:2A:106:C:H1'	20:2Y:1:MET:HE2	1.81	0.62
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.34	0.62
56:2y:14:A:O2'	56:2y:15:G:OP1	2.17	0.62
1:1A:1062:G:H22	1:1A:1077:A:H61	1.46	0.62
54:1w:26:A:H61	54:1w:44:G:H1	1.46	0.62
32:2a:662:G:O2'	32:2a:836:G:OP1	2.18	0.62
50:2s:32:LYS:HA	50:2s:50:ALA:HB3	1.81	0.62
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.15	0.62
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.81	0.62
42:2k:34:ASP:HB3	42:2k:40:ILE:HD11	1.81	0.62
1:1A:1851:U:H4'	56:1y:71:G:H4'	1.81	0.62
1:2A:20:C:OP1	16:2U:22:LYS:NZ	2.28	0.62
1:2A:531:C:OP1	1:2A:561:G:N1	2.32	0.62
33:2b:9:GLU:O	33:2b:11:LEU:N	2.31	0.62
1:1A:2276:G:N7	64:1A:4297:HOH:O	2.31	0.62
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.18	0.62
21:2Z:77:ASP:OD2	21:2Z:80:ARG:NH1	2.26	0.62
33:2b:188:ALA:HB1	33:2b:192:SER:HB2	1.80	0.62
32:1a:1006:C:H42	32:1a:1023:G:H1	1.48	0.62
37:1f:42:GLU:OE2	37:1f:59:TYR:OH	2.15	0.62
1:2A:195:A:N7	64:2A:3924:HOH:O	2.31	0.62
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.31	0.62
35:2d:20:TYR:HD1	35:2d:26:CYS:HB3	1.65	0.62
37:2f:68:PRO:HB2	37:2f:71:ARG:HG3	1.81	0.62
37:1f:2:ARG:HD2	37:1f:69:GLU:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:121:LYS:HB3	11:2P:123:LEU:HD13	1.80	0.62
26:14:46:GLN:O	26:14:48:ARG:N	2.32	0.62
32:1a:1030(A):G:H1'	32:1a:1031:G:H22	1.65	0.62
32:1a:684:A:N6	64:1a:1944:HOH:O	2.33	0.61
1:2A:1021:A:H62	1:2A:1141:U:H3	1.46	0.61
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.34	0.61
11:1P:126:VAL:HG12	11:1P:148:LEU:HD22	1.82	0.61
1:2A:993:G:OP1	16:2U:50:ARG:NH2	2.33	0.61
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.82	0.61
8:2I:88:ILE:H	8:2I:121:LYS:HE2	1.64	0.61
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.83	0.61
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.33	0.61
34:1c:152:ILE:HG23	34:1c:167:TRP:HB3	1.82	0.61
41:1j:81:THR:C	41:1j:83:GLU:H	2.09	0.61
32:2a:947:G:H1	32:2a:1234:C:H42	1.47	0.61
44:2m:82:MET:HE3	44:2m:92:HIS:HB3	1.82	0.61
8:1I:126:TYR:HB2	8:1I:142:VAL:HG23	1.83	0.61
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.36	0.61
32:2a:1002:G:C2	32:2a:1003:G:H1'	2.36	0.61
32:2a:1312:G:H5'	50:2s:5:LEU:HD11	1.82	0.61
54:2w:47:U:H5"	54:2w:48:C:H5"	1.83	0.61
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.36	0.61
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.83	0.61
32:1a:559:A:OP1	36:1e:126:ARG:NH2	2.28	0.61
32:1a:742:G:OP2	46:1o:35:ARG:NH2	2.33	0.61
33:1b:77:ALA:HB2	33:1b:211:ILE:HD13	1.82	0.61
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.33	0.61
56:2y:9:A:O2'	56:2y:11:C:N4	2.25	0.61
1:1A:1356:G:OP2	64:1A:4232:HOH:O	2.16	0.61
1:1A:1890:A:OP2	64:1A:4231:HOH:O	2.16	0.61
32:1a:757:U:H2'	32:1a:758:G:O4'	2.01	0.61
32:1a:937:A:OP2	64:1a:1915:HOH:O	2.16	0.61
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.00	0.61
32:2a:8:A:H5'	36:2e:101:ILE:HG22	1.82	0.61
1:1A:1670:C:OP2	64:1A:4219:HOH:O	2.16	0.61
37:1f:36:ARG:H	37:1f:65:VAL:HG13	1.66	0.61
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.01	0.61
28:26:34:LEU:HB2	28:26:51:GLU:HB2	1.83	0.61
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.35	0.61
1:2A:1490:A:O2'	3:2D:99:ASP:OD1	2.19	0.61
1:2A:2690:C:OP1	13:2R:17:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1130:A:H5”	40:2i:18:PHE:CE2	2.36	0.61
35:2d:111:ALA:HB2	35:2d:120:LEU:HD12	1.81	0.61
39:2h:17:THR:O	39:2h:78:GLN:NE2	2.34	0.61
32:1a:36:C:OP1	43:1l:123:LYS:NZ	2.34	0.60
33:1b:101:MET:HA	33:1b:108:ILE:HD12	1.83	0.60
6:2G:124:SER:O	6:2G:124:SER:OG	2.18	0.60
8:2I:122:GLU:O	8:2I:126:TYR:OH	2.19	0.60
10:2O:48:PRO:HB3	32:2a:1422:G:H5”	1.83	0.60
21:2Z:102:LEU:HD23	21:2Z:139:VAL:HG21	1.82	0.60
33:2b:88:ALA:HB2	33:2b:219:VAL:HG23	1.83	0.60
51:2t:50:GLU:HG3	51:2t:100:ILE:HD13	1.83	0.60
5:1F:117:ARG:NH2	5:1F:189:THR:O	2.34	0.60
32:1a:700:G:N7	64:1a:1940:HOH:O	2.31	0.60
56:1y:37:MIA:H2’	56:1y:38:A:H8	1.66	0.60
1:2A:1452:A:OP2	64:2A:3931:HOH:O	2.15	0.60
6:1G:170:ARG:NH2	6:1G:182:LYS:O	2.32	0.60
9:1N:123:TYR:OH	9:1N:130:HIS:NE2	2.34	0.60
35:1d:119:GLN:HG2	35:1d:123:HIS:CD2	2.37	0.60
1:2A:1300:U:H4’	1:2A:1301:A:H5”	1.83	0.60
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.35	0.60
17:2V:72:VAL:HB	17:2V:85:LYS:HB3	1.82	0.60
3:1D:147:LEU:HD13	3:1D:155:LEU:HD21	1.81	0.60
7:1H:7:LEU:HD12	7:1H:8:PRO:HD2	1.84	0.60
32:1a:953:G:H5’	32:1a:965:A:H61	1.66	0.60
1:2A:411:G:OP1	64:2A:3935:HOH:O	2.16	0.60
1:2A:1507:A:O2’	1:2A:1508:A:O5’	2.20	0.60
1:2A:2117:A:N6	1:2A:2171:A:N1	2.49	0.60
32:2a:1119:C:H2’	32:2a:1120:G:H8	1.65	0.60
56:2y:18:G:N1	56:2y:55:PSU:C4	2.69	0.60
1:1A:1075:C:H2’	1:1A:1076:C:H2’	1.83	0.60
32:1a:78:G:C6	32:1a:91:C:N4	2.68	0.60
32:1a:108:G:C6	51:1t:15:ARG:HD2	2.37	0.60
35:1d:107:ARG:HH21	35:1d:194:LEU:HD21	1.66	0.60
3:2D:125:ILE:HB	37:2f:81:ILE:HD11	1.83	0.60
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.66	0.60
32:2a:1271:G:C2	32:2a:1272:G:N7	2.70	0.60
1:1A:1048:A:N1	1:1A:1112:G:O2’	2.31	0.60
1:1A:1176:G:N2	1:1A:1178:C:OP2	2.34	0.60
1:2A:943:U:OP2	64:2A:3936:HOH:O	2.17	0.60
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.34	0.60
22:20:46:LYS:HE3	22:20:76:GLY:HA3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2f:95:GLU:O	49:2r:32:ARG:NH1	2.34	0.60
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.19	0.60
43:2l:82:VAL:HG13	43:2l:105:TYR:HB3	1.82	0.60
25:13:55:ARG:HH22	25:13:57:GLU:HB2	1.67	0.60
41:1j:38:ILE:HD11	41:1j:71:LEU:HD23	1.84	0.60
8:2I:48:GLU:HA	8:2I:51:ILE:HG22	1.83	0.60
10:2O:80:ASP:OD1	15:2T:64:ARG:NH2	2.35	0.60
34:2c:47:LEU:O	34:2c:51:GLY:N	2.34	0.60
38:2g:50:ILE:HD11	38:2g:58:PRO:HA	1.82	0.60
41:2j:8:LEU:HD11	41:2j:20:ALA:HB2	1.84	0.60
1:1A:2096:U:H3	1:1A:2193:G:H1	1.49	0.60
1:2A:2306:C:N4	6:2G:42:GLY:O	2.29	0.60
8:2I:112:LYS:O	8:2I:114:LEU:N	2.34	0.60
27:25:2:ALA:N	64:25:201:HOH:O	2.34	0.60
1:1A:2439:A:N6	55:1x:76:8AN:O1P	2.35	0.60
2:1B:103:G:H21	21:1Z:73:GLN:HE22	1.49	0.60
21:2Z:45:ASP:OD1	21:2Z:49:ARG:NE	2.35	0.60
28:26:14:THR:OG1	28:26:48:VAL:O	2.18	0.60
1:1A:1300:U:H4'	1:1A:1301:A:H5"	1.84	0.59
21:1Z:79:ARG:HD2	21:1Z:80:ARG:HH12	1.67	0.59
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.84	0.59
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.35	0.59
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.84	0.59
44:2m:84:ILE:HB	50:2s:66:MET:HE2	1.84	0.59
1:1A:2102:U:H3	1:1A:2187:G:H1	1.50	0.59
1:2A:2135:A:H61	1:2A:2156:G:N2	1.99	0.59
6:2G:73:ALA:HB3	6:2G:85:GLY:H	1.65	0.59
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.83	0.59
32:2a:921:U:O2	36:2e:19:MET:HB2	2.01	0.59
50:2s:53:ASN:HD21	50:2s:56:GLN:HB2	1.67	0.59
8:1I:107:VAL:HG12	8:1I:109:ILE:HG12	1.84	0.59
56:1y:19:G:N2	56:1y:56:C:N3	2.51	0.59
21:2Z:53:ILE:HG22	21:2Z:71:VAL:HG23	1.84	0.59
24:22:29:LYS:HG2	24:22:57:ILE:HD13	1.83	0.59
32:2a:646:U:H2'	32:2a:647:C:C6	2.38	0.59
42:2k:27:ASN:OD1	42:2k:28:THR:N	2.34	0.59
1:2A:2137:C:N3	1:2A:2154:G:N2	2.48	0.59
32:1a:1040:U:H2'	32:1a:1041:A:C8	2.38	0.59
39:1h:21:LYS:O	39:1h:65:TYR:OH	2.16	0.59
4:2E:119:ARG:HD2	4:2E:160:TYR:HB2	1.84	0.59
32:2a:1006:C:H42	32:2a:1023:G:H1	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:946:A:H2'	32:1a:947:G:C8	2.37	0.59
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.84	0.59
1:2A:2183:C:H2'	1:2A:2184:G:C8	2.37	0.59
32:2a:410:G:OP1	35:2d:30:LYS:NZ	2.32	0.59
32:2a:1089:G:H1	32:2a:1096:C:H42	1.50	0.59
1:1A:1071:G:H1'	1:1A:1089:G:H2'	1.83	0.59
32:2a:573:A:N3	32:2a:883:C:O2'	2.35	0.59
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.17	0.59
8:1I:116:LEU:HD21	8:1I:119:PRO:HA	1.84	0.59
62:1w:109:PHE:N	55:1x:76:8AN:HO2'	2.00	0.59
1:2A:304:G:O6	64:2A:3919:HOH:O	2.13	0.59
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.38	0.59
1:2A:880:G:H2'	1:2A:881:G:C8	2.32	0.59
1:2A:2469:A:H5'	1:2A:2470:G:OP2	2.03	0.59
14:2S:15:ARG:O	14:2S:19:LYS:HG2	2.02	0.59
14:2S:28:VAL:HG11	14:2S:98:VAL:HG13	1.85	0.59
19:2X:11:PRO:HB3	19:2X:92:LEU:HD11	1.85	0.59
21:2Z:126:VAL:HB	21:2Z:161:VAL:HG23	1.84	0.59
1:1A:1693:U:O2'	3:1D:14:ARG:NH2	2.35	0.59
18:1W:68:ARG:HH12	18:1W:112:GLY:H	1.50	0.59
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.21	0.59
1:2A:668:G:H5'	1:2A:669:G:OP2	2.02	0.59
2:2B:11:C:OP2	22:20:72:ARG:NH2	2.36	0.59
7:2H:80:SER:OG	7:2H:81:GLU:OE1	2.18	0.59
8:2I:114:LEU:HA	8:2I:130:TYR:HA	1.84	0.59
50:2s:49:ILE:HG22	50:2s:62:ILE:HD11	1.85	0.59
32:1a:532:A:N6	32:1a:1206:G:O2'	2.36	0.58
1:2A:276:A:H5"	1:2A:277:C:H5'	1.83	0.58
1:2A:468:G:N7	29:27:39:ARG:NH2	2.50	0.58
1:2A:2303:G:O2'	6:2G:132:ASN:ND2	2.36	0.58
56:2y:65:G:H2'	56:2y:66:U:C6	2.38	0.58
1:1A:2127:G:N2	1:1A:2173:A:H1'	2.17	0.58
1:1A:2136:C:N3	1:1A:2155:G:C2	2.71	0.58
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.03	0.58
32:1a:1039:C:H2'	32:1a:1040:U:C6	2.39	0.58
40:1i:21:PRO:HA	40:1i:59:PHE:HA	1.85	0.58
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.03	0.58
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.03	0.58
8:2I:45:LYS:HD3	8:2I:48:GLU:HB3	1.85	0.58
17:2V:16:PRO:HD3	17:2V:99:ILE:HD11	1.86	0.58
32:2a:187:C:O2'	51:2t:89:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1191:A:OP1	34:1c:4:LYS:NZ	2.27	0.58
18:1W:12:ILE:HD13	18:1W:17:VAL:HG13	1.85	0.58
1:2A:962:G:OP1	64:2A:3907:HOH:O	2.16	0.58
1:2A:2278:A:OP2	22:20:12:ASN:ND2	2.37	0.58
1:2A:2483:C:N3	12:2Q:124:LYS:NZ	2.51	0.58
15:2T:127:ALA:C	15:2T:129:ARG:H	2.11	0.58
16:2U:49:HIS:HA	16:2U:52:ARG:HB2	1.85	0.58
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.31	0.58
1:1A:2331:G:O2'	22:10:43:THR:HG22	2.03	0.58
4:1E:12:THR:HG22	4:1E:13:ARG:H	1.67	0.58
1:2A:307:G:N1	1:2A:310:A:OP2	2.32	0.58
21:2Z:105:VAL:N	21:2Z:139:VAL:O	2.36	0.58
33:2b:7:VAL:O	33:2b:217:ARG:NE	2.21	0.58
51:2t:43:LEU:O	51:2t:47:GLY:N	2.26	0.58
20:1Y:14:LEU:HB2	20:1Y:75:ILE:HD11	1.85	0.58
26:14:15:ILE:HG13	26:14:21:VAL:HG22	1.86	0.58
1:2A:2743:C:OP1	31:29:33:LYS:NZ	2.36	0.58
32:2a:148:G:H2'	32:2a:149:A:H8	1.68	0.58
35:2d:187:ARG:NH1	35:2d:190:ASP:OD1	2.37	0.58
47:2p:22:THR:HA	47:2p:33:ILE:HG13	1.85	0.58
32:1a:507:C:OP2	32:1a:508:C:O2'	2.18	0.58
40:1i:16:ARG:HB2	40:1i:64:THR:HB	1.86	0.58
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.49	0.58
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.39	0.58
33:2b:197:VAL:HB	33:2b:200:ILE:HG13	1.86	0.58
37:2f:82:ARG:HB2	37:2f:85:VAL:HG23	1.85	0.58
44:2m:3:ARG:NH2	44:2m:9:ILE:O	2.35	0.58
1:1A:2108:C:H2'	1:1A:2109:U:C6	2.39	0.58
21:1Z:132:ASN:HD22	21:1Z:160:GLY:HA3	1.69	0.58
34:1c:157:ILE:HD12	34:1c:164:ARG:HB3	1.86	0.58
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.52	0.58
21:2Z:157:LEU:HD21	21:2Z:163:LEU:HG	1.86	0.58
25:23:13:ILE:O	64:23:201:HOH:O	2.17	0.58
32:1a:1157:A:H5'	32:1a:1158:C:C6	2.39	0.58
32:1a:1183:A:O2'	32:1a:1184:G:OP1	2.22	0.58
36:1e:77:PRO:HD2	36:1e:142:LEU:HD13	1.85	0.58
1:2A:568:U:H5'	1:2A:945:A:N1	2.18	0.58
2:2B:75:G:H22	21:2Z:73:GLN:HE21	1.52	0.58
46:2o:87:ILE:HG22	46:2o:88:ARG:H	1.68	0.58
50:1s:80:TYR:CZ	50:1s:82:GLY:HA2	2.40	0.57
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:253:C:O2'	64:2A:3938:HOH:O	2.17	0.57
1:2A:2659:G:P	7:2H:158:HIS:HE2	2.27	0.57
4:2E:7:VAL:HG13	4:2E:27:LEU:HB3	1.86	0.57
8:2I:127:VAL:HG21	8:2I:139:GLN:HB3	1.85	0.57
36:2e:60:TYR:OH	36:2e:64:ARG:NH1	2.37	0.57
41:2j:47:PHE:N	41:2j:63:PHE:O	2.33	0.57
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.39	0.57
32:1a:110:C:O2'	47:1p:25:ARG:O	2.19	0.57
35:1d:30:LYS:HA	35:1d:35:ARG:HH11	1.70	0.57
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.39	0.57
16:2U:50:ARG:HH22	17:2V:72:VAL:HG22	1.69	0.57
32:2a:624:C:H2'	32:2a:625:G:H8	1.70	0.57
7:1H:11:VAL:HG13	7:1H:15:VAL:HG23	1.84	0.57
1:2A:855:G:O2'	22:20:27:GLU:OE2	2.22	0.57
1:2A:1629:U:OP1	64:2A:3939:HOH:O	2.18	0.57
12:2Q:11:LYS:NZ	12:2Q:88:GLY:O	2.34	0.57
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.69	0.57
56:1y:51:U:H2'	56:1y:52:G:H8	1.70	0.57
8:2I:79:ILE:HD11	8:2I:97:ILE:HG23	1.86	0.57
64:1A:4230:HOH:O	6:1G:45:GLU:OE2	2.17	0.57
34:1c:40:ARG:NH2	34:1c:55:VAL:O	2.38	0.57
6:2G:9:ARG:NE	6:2G:13:GLU:OE2	2.28	0.57
32:2a:137:C:H2'	32:2a:138:G:C8	2.40	0.57
33:2b:74:LYS:HG2	33:2b:75:LYS:H	1.69	0.57
33:2b:212:GLN:HE21	33:2b:235:SER:HA	1.69	0.57
1:1A:2334:G:O6	22:10:74:ARG:NH2	2.38	0.57
35:1d:173:TRP:CZ3	35:1d:174:LEU:HG	2.40	0.57
1:2A:881:G:C2	1:2A:882:G:H1'	2.39	0.57
23:21:83:GLU:OE1	23:21:83:GLU:N	2.37	0.57
34:2c:112:SER:HB3	34:2c:115:LEU:HD22	1.87	0.57
39:2h:41:ARG:NH2	39:2h:123:GLU:OE2	2.38	0.57
49:2r:52:PRO:HB2	49:2r:54:ARG:HG3	1.86	0.57
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	1.86	0.57
32:1a:486:U:H2'	32:1a:487:A:H8	1.70	0.57
32:1a:501:C:H2'	32:1a:502:G:C8	2.40	0.57
1:2A:922:U:H2'	1:2A:923:C:C6	2.40	0.57
1:2A:1653:G:H3'	13:2R:2:ARG:HD3	1.87	0.57
1:2A:1973:G:OP1	64:2A:3937:HOH:O	2.17	0.57
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.86	0.57
11:2P:118:GLY:O	11:2P:137:LYS:NZ	2.29	0.57
38:2g:89:MET:SD	38:2g:155:ARG:HB2	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1e:85:GLY:O	36:1e:87:SER:N	2.38	0.57
23:21:8:SER:HB3	23:21:66:HIS:CD2	2.40	0.57
32:1a:1035:A:H2'	32:1a:1036:G:H21	1.70	0.57
33:1b:114:ARG:NH1	33:1b:117:GLU:OE1	2.36	0.57
33:1b:122:PHE:HZ	33:1b:135:GLN:HG3	1.68	0.57
39:1h:35:ILE:HD11	39:1h:134:ILE:HG21	1.86	0.57
32:2a:1181:G:O2'	32:2a:1182:G:N7	2.36	0.57
32:2a:1330:U:H4'	44:2m:23:TYR:CE1	2.40	0.57
36:2e:83:GLU:HA	36:2e:88:LYS:HA	1.86	0.57
40:2i:79:LEU:HG	40:2i:83:ARG:HD2	1.87	0.57
44:2m:37:THR:O	44:2m:55:ARG:NH1	2.36	0.57
50:1s:12:ASP:OD2	50:1s:35:SER:OG	2.11	0.56
21:2Z:51:ALA:O	21:2Z:52:SER:HB3	2.04	0.56
26:24:44:THR:O	26:24:46:GLN:N	2.36	0.56
32:2a:136:C:H42	32:2a:227:G:H1	1.52	0.56
1:1A:897:C:H5'	54:1w:56:C:OP1	2.05	0.56
32:2a:448:A:P	32:2a:485:G:H22	2.27	0.56
32:2a:1272:G:N2	32:2a:1273:G:C8	2.73	0.56
51:2t:9:ASN:O	51:2t:10:LEU:HB2	2.06	0.56
1:1A:1119:C:N4	64:1A:4234:HOH:O	2.34	0.56
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.88	0.56
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.06	0.56
12:1Q:89:ASN:HB2	55:1x:1:C:C4	2.40	0.56
32:1a:1035:A:N3	32:1a:1036:G:N2	2.54	0.56
39:1h:87:SER:HB2	39:1h:93:VAL:H	1.69	0.56
1:2A:1019:U:H2'	1:2A:1020:A:H8	1.69	0.56
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.22	0.56
1:2A:2805:G:H2'	1:2A:2807:G:H8	1.71	0.56
32:2a:137:C:H2'	32:2a:138:G:H8	1.70	0.56
41:2j:33:GLN:HG2	41:2j:34:VAL:H	1.70	0.56
1:1A:2376:A:H2'	1:1A:2377:A:O4'	2.04	0.56
32:1a:1007:C:H2'	32:1a:1008:C:C6	2.41	0.56
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.41	0.56
32:1a:1414:U:H3	32:1a:1486:G:H1	1.53	0.56
50:1s:27:GLU:OE1	50:1s:27:GLU:N	2.33	0.56
1:2A:2206:G:H5"	1:2A:2207:G:C5	2.40	0.56
32:2a:1286:A:H8	32:2a:1287:A:H4'	1.69	0.56
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.21	0.56
36:2e:20:GLN:NE2	36:2e:21:ALA:O	2.38	0.56
32:1a:51:A:OP2	64:1a:1919:HOH:O	2.18	0.56
36:1e:95:ALA:HB1	36:1e:96:PRO:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:5:LEU:O	21:2Z:59:LEU:HA	2.04	0.56
33:2b:120:ALA:O	33:2b:125:PRO:HD2	2.04	0.56
1:1A:271(O):C:H2'	1:1A:271(P):C:C6	2.41	0.56
32:1a:1032:G:H2'	32:1a:1033:G:O4'	2.05	0.56
1:2A:900:A:O2'	1:2A:901:A:OP1	2.23	0.56
23:21:56:GLN:HE21	23:21:87:PRO:HG3	1.69	0.56
1:1A:143:G:H4'	19:1X:35:THR:HG21	1.87	0.56
11:1P:39:LYS:HB2	11:1P:45:LEU:HD13	1.88	0.56
1:2A:2447:G:N2	1:2A:2450:A:OP2	2.38	0.56
32:2a:677:U:H3	32:2a:713:G:H22	1.53	0.56
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.73	0.56
6:1G:126:ASP:HB3	6:1G:128:ARG:H	1.71	0.56
56:1y:37:MIA:H2'	56:1y:38:A:C8	2.41	0.56
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.39	0.56
13:2R:36:THR:HG22	13:2R:37:THR:H	1.71	0.56
26:24:46:GLN:C	26:24:48:ARG:H	2.14	0.56
32:2a:973:G:H3'	32:2a:974:A:H5"	1.88	0.56
32:2a:1263:C:N3	32:2a:1272:G:O6	2.39	0.56
51:2t:72:LEU:HD23	51:2t:77:ALA:HB2	1.87	0.56
1:2A:2448:A:OP1	64:2A:3909:HOH:O	2.18	0.56
9:2N:38:HIS:NE2	9:2N:50:ASP:OD2	2.38	0.56
32:2a:1202:G:O4'	45:2n:29:ARG:NH1	2.39	0.56
28:16:13:CYS:SG	28:16:47:THR:HG21	2.46	0.56
32:1a:975:A:H5'	32:1a:975:A:H8	1.71	0.56
48:1q:12:SER:HB3	48:1q:20:THR:HB	1.88	0.56
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.20	0.56
32:2a:376:G:H5"	47:2p:5:ARG:HB2	1.88	0.56
33:2b:17:PHE:HA	33:2b:44:LEU:HD21	1.87	0.56
34:2c:6:HIS:HD2	34:2c:8:ILE:H	1.54	0.56
35:1d:15:GLU:OE2	35:1d:59:ARG:NH1	2.39	0.55
1:2A:1325:G:OP1	1:2A:1647:G:O2'	2.20	0.55
8:2I:80:PRO:HA	8:2I:145:VAL:HG13	1.88	0.55
33:2b:218:ALA:O	33:2b:222:ILE:HG23	2.07	0.55
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.21	0.55
9:1N:62:VAL:HG22	9:1N:66:LYS:HD2	1.88	0.55
25:13:3:ARG:NE	25:13:60:GLU:OE1	2.38	0.55
54:1w:23:A:H3'	54:1w:24:G:H8	1.71	0.55
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.28	0.55
1:2A:2099:U:H3	1:2A:2190:G:H1	1.54	0.55
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.40	0.55
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1226:C:H4'	50:2s:80:TYR:CZ	2.41	0.55
35:2d:149:ALA:HB3	35:2d:152:SER:HB2	1.88	0.55
40:2i:9:ARG:HG2	40:2i:14:VAL:HA	1.87	0.55
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.69	0.55
2:1B:33:G:H5'	6:1G:2:PRO:HD3	1.88	0.55
32:1a:204:U:H4'	32:1a:216:G:H5"	1.88	0.55
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.41	0.55
1:2A:2141:G:H2'	1:2A:2142:C:O4'	2.06	0.55
7:2H:3:ARG:NH1	7:2H:4:ILE:H	2.05	0.55
8:2I:83:ALA:HB2	8:2I:123:LEU:HD22	1.88	0.55
8:2I:129:THR:OG1	8:2I:130:TYR:N	2.39	0.55
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.88	0.55
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.89	0.55
32:1a:78:G:N1	32:1a:91:C:N4	2.55	0.55
32:1a:1531:A:H8	32:1a:1531:A:O5'	1.88	0.55
42:1k:48:ILE:O	42:1k:48:ILE:HG12	2.06	0.55
43:1l:117:ARG:HB3	43:1l:122:THR:HB	1.88	0.55
5:2F:116:ASP:OD2	11:2P:1:MET:N	2.30	0.55
8:2I:130:TYR:HD1	8:2I:132:PRO:HG3	1.70	0.55
32:2a:1016:A:H2'	32:2a:1017:G:O4'	2.05	0.55
1:1A:916:G:OP1	64:1A:4236:HOH:O	2.18	0.55
1:1A:1039:G:H1	1:1A:1116:C:H42	1.55	0.55
1:1A:1062:G:H2'	1:1A:1063:G:C8	2.41	0.55
1:1A:1937:A:H1'	1:1A:1939:5MU:H72	1.89	0.55
1:1A:2182:G:H2'	1:1A:2183:C:C6	2.41	0.55
9:2N:123:TYR:OH	9:2N:130:HIS:NE2	2.36	0.55
32:2a:1316:G:H22	32:2a:1319:A:H5"	1.71	0.55
1:1A:1192:G:OP2	64:1A:4233:HOH:O	2.18	0.55
8:1I:77:LEU:HD13	8:1I:79:ILE:HD11	1.88	0.55
26:14:13:ARG:NH1	26:14:23:GLU:OE2	2.35	0.55
2:2B:24:G:H4'	2:2B:25:A:C8	2.42	0.55
18:2W:4:LYS:HD3	18:2W:6:ILE:HD11	1.87	0.55
33:2b:134:GLU:O	33:2b:138:LEU:HG	2.06	0.55
1:1A:528:A:O2'	1:1A:529:A:H5'	2.07	0.55
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.42	0.55
13:1R:118:GLU:H	13:1R:118:GLU:CD	2.14	0.55
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.32	0.55
32:2a:17:U:H2'	32:2a:18:C:C6	2.41	0.55
32:2a:1029:C:C2	32:2a:1032:G:N2	2.73	0.55
39:1h:112:LEU:HA	39:1h:134:ILE:HG12	1.88	0.55
44:1m:3:ARG:HG2	44:1m:8:GLU:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1651:G:OP1	13:2R:40:LYS:NZ	2.40	0.55
21:2Z:55:HIS:HE1	21:2Z:135:GLU:HB2	1.72	0.55
26:24:45:GLY:O	26:24:47:GLN:N	2.34	0.55
32:2a:435:C:H2'	32:2a:436:C:C6	2.42	0.55
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.22	0.55
1:1A:588:U:H2'	1:1A:589:C:C6	2.41	0.55
32:1a:70:G:H1	32:1a:99:U:H3	1.54	0.55
1:2A:94(A):G:O3'	24:22:45:SER:OG	2.24	0.55
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.07	0.55
14:2S:10:ARG:NE	14:2S:91:PRO:O	2.36	0.55
35:2d:119:GLN:HG3	35:2d:123:HIS:CD2	2.42	0.55
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.40	0.55
1:1A:2572:A:C8	4:1E:144:ARG:HD3	2.42	0.55
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.89	0.55
21:1Z:4:ARG:HH21	21:1Z:60:GLU:HG2	1.72	0.55
34:1c:52:LEU:HD13	34:1c:68:VAL:HG13	1.89	0.55
56:1y:51:U:H2'	56:1y:52:G:C8	2.42	0.55
1:2A:1178:C:H2'	1:2A:1179:C:C6	2.42	0.55
1:2A:2165:G:H22	1:2A:2172:U:H5	1.53	0.55
26:24:9:LEU:HD12	26:24:27:THR:HG23	1.88	0.55
32:2a:1305:G:H22	32:2a:1331:G:H1'	1.73	0.55
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.90	0.54
48:1q:9:VAL:HG22	48:1q:56:VAL:HG22	1.88	0.54
8:2I:48:GLU:HG3	8:2I:52:ARG:HH11	1.72	0.54
32:2a:1002:G:N3	32:2a:1003:G:H1'	2.22	0.54
32:2a:1239:A:H62	32:2a:1299:A:N6	2.05	0.54
33:2b:15:VAL:HG12	33:2b:209:ARG:HB3	1.90	0.54
41:2j:61:GLU:OE2	45:2n:58:LYS:NZ	2.37	0.54
18:1W:68:ARG:NH1	18:1W:112:GLY:H	2.04	0.54
33:1b:15:VAL:HG21	33:1b:213:LEU:HD22	1.87	0.54
33:1b:84:GLU:OE1	33:1b:87:ARG:NH1	2.40	0.54
40:1i:48:GLU:HA	40:1i:51:ARG:HD3	1.89	0.54
1:2A:307:G:H21	1:2A:330:A:H62	1.56	0.54
1:2A:332:A:O2'	1:2A:334:C:OP2	2.22	0.54
32:2a:7:G:O2'	36:2e:120:THR:O	2.24	0.54
32:2a:1051:C:H2'	32:2a:1052:U:C6	2.42	0.54
39:2h:21:LYS:O	39:2h:65:TYR:OH	2.26	0.54
1:1A:1036:G:O6	64:1A:4234:HOH:O	2.18	0.54
15:1T:15:VAL:HG13	15:1T:79:HIS:CE1	2.43	0.54
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.15	0.54
32:1a:165:C:H2'	32:1a:166:G:H8	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.71	0.54
32:2a:67:C:H2'	32:2a:68:G:C8	2.42	0.54
35:2d:158:ILE:HG23	35:2d:162:LEU:HD12	1.88	0.54
1:1A:1864:U:OP1	1:1A:2410:G:O2'	2.24	0.54
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.22	0.54
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.40	0.54
36:1e:78:HIS:HE1	36:1e:143:ARG:H	1.55	0.54
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.24	0.54
1:2A:700:G:O2'	1:2A:1632:A:N3	2.30	0.54
1:2A:2164:C:C4	1:2A:2165:G:H1'	2.42	0.54
33:2b:231:GLU:H	33:2b:232:PRO:CD	2.20	0.54
36:2e:89:ILE:HG12	36:2e:135:THR:HG22	1.89	0.54
1:1A:2134:A:O2'	1:1A:2135:A:OP1	2.18	0.54
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	1.90	0.54
9:1N:67:LEU:O	9:1N:88:GLU:HG3	2.07	0.54
9:1N:123:TYR:HH	9:1N:130:HIS:HE2	1.51	0.54
22:10:23:VAL:HG22	22:10:38:VAL:HG22	1.90	0.54
33:1b:95:GLN:NE2	33:1b:147:LYS:HG2	2.17	0.54
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.42	0.54
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	1.90	0.54
11:2P:91:PHE:O	11:2P:121:LYS:NZ	2.38	0.54
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.20	0.54
32:2a:1054:C:C4	54:2w:34:G:H1'	2.43	0.54
42:2k:79:SER:HB2	42:2k:106:LYS:HE3	1.88	0.54
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.08	0.54
32:1a:266:G:H5"	32:1a:268:C:H41	1.71	0.54
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.22	0.54
46:1o:87:ILE:HG22	46:1o:88:ARG:H	1.73	0.54
5:2F:102:PRO:HB2	5:2F:105:VAL:HG23	1.88	0.54
8:2I:50:ARG:HA	8:2I:53:ALA:HB3	1.88	0.54
12:2Q:111:GLU:OE2	12:2Q:133:ARG:NH2	2.41	0.54
32:2a:976:G:H5'	32:2a:1358:U:O2'	2.07	0.54
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.43	0.54
32:2a:710:G:O6	64:2a:3313:HOH:O	2.18	0.54
32:2a:1129:C:H2'	32:2a:1139:G:N7	2.22	0.54
39:2h:119:LEU:HB3	39:2h:123:GLU:HB2	1.90	0.54
48:2q:53:LEU:HD23	48:2q:82:MET:HE1	1.90	0.54
6:1G:67:LYS:HD3	26:14:5:ILE:HD12	1.89	0.54
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.54	0.54
32:1a:78:G:N2	32:1a:91:C:N3	2.55	0.54
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.38	0.54
32:2a:544:G:OP1	35:2d:62:GLN:NE2	2.36	0.54
35:2d:191:ARG:NH1	35:2d:191:ARG:O	2.40	0.54
1:1A:1058:G:N2	1:1A:1080:C:N3	2.49	0.54
5:1F:89:VAL:O	64:1F:402:HOH:O	2.18	0.54
32:1a:1347:G:O2'	32:1a:1373:G:O6	2.24	0.54
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.43	0.54
1:2A:392:C:H5"	1:2A:409:C:H5"	1.90	0.54
1:2A:752:A:H3'	29:27:1:MET:HE1	1.88	0.54
1:2A:1015:G:H2'	1:2A:1016:G:C8	2.40	0.54
1:2A:2140:C:N4	1:2A:2151:G:H1	2.06	0.54
8:2I:52:ARG:HA	8:2I:55:ALA:HB3	1.90	0.54
8:2I:57:ARG:O	8:2I:62:LYS:NZ	2.41	0.54
8:2I:87:LYS:HG2	8:2I:88:ILE:N	2.22	0.54
33:2b:16:HIS:CB	33:2b:210:SER:HB2	2.37	0.54
33:2b:60:ASP:O	33:2b:64:ARG:HG2	2.08	0.54
32:1a:584:G:H2'	32:1a:585:G:C8	2.42	0.54
32:1a:1023:G:H3'	32:1a:1024:G:H8	1.73	0.54
40:1i:85:LEU:O	40:1i:88:TYR:HB3	2.07	0.54
5:2F:53:THR:HG22	5:2F:56:GLU:HG3	1.89	0.54
1:1A:106:C:H1'	20:1Y:1:MET:HE2	1.89	0.53
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.88	0.53
32:1a:1123:A:O2'	41:1j:37:PRO:O	2.26	0.53
56:1y:3:C:N4	56:1y:70:G:H1	2.04	0.53
1:2A:2218:U:O2	23:21:52:ARG:NH1	2.41	0.53
6:2G:179:PRO:HG3	26:24:43:TYR:CZ	2.43	0.53
19:2X:2:LYS:NZ	19:2X:38:GLU:OE2	2.30	0.53
26:24:40:HIS:HD1	26:24:43:TYR:HD2	1.56	0.53
1:1A:1082:U:H3	1:1A:1086:A:H61	0.59	0.53
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.41	0.53
39:1h:81:HIS:N	39:1h:138:TRP:O	2.42	0.53
6:2G:113:ARG:NH2	6:2G:139:LEU:O	2.42	0.53
32:2a:134:A:H61	47:2p:25:ARG:NH1	2.07	0.53
32:2a:979:C:N4	64:2a:3342:HOH:O	2.42	0.53
32:2a:1194:U:H4'	36:2e:22:GLY:HA2	1.89	0.53
32:2a:1305:G:O2'	32:2a:1331:G:N2	2.40	0.53
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.23	0.53
35:2d:140:VAL:HG11	35:2d:146:ILE:HD11	1.91	0.53
49:2r:53:ARG:HH21	49:2r:59:SER:HA	1.74	0.53
1:1A:1800:C:OP1	3:1D:260:ARG:NH2	2.41	0.53
8:1I:109:ILE:HG23	8:1I:130:TYR:CZ	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:110:THR:OG1	12:1Q:113:GLN:NE2	2.41	0.53
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.23	0.53
32:1a:1036:G:H5"	32:1a:1037:C:C5	2.44	0.53
32:1a:1381:U:H1'	38:1g:79:ARG:HG2	1.90	0.53
1:2A:652(T):C:H2'	1:2A:652(U):G:C8	2.44	0.53
11:2P:38:GLN:O	11:2P:39:LYS:HB3	2.09	0.53
32:2a:21:G:H2'	32:2a:22:G:C8	2.42	0.53
32:2a:165:C:H2'	32:2a:166:G:C8	2.43	0.53
32:2a:445:G:H1	32:2a:489:C:H42	1.56	0.53
36:1e:81:GLU:HG2	36:1e:90:VAL:HG22	1.90	0.53
38:1g:106:GLN:O	38:1g:110:GLN:HG2	2.08	0.53
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.41	0.53
2:2B:8:U:O3'	14:2S:25:ARG:NH2	2.40	0.53
4:2E:77:ILE:HD13	4:2E:195:LEU:HD22	1.91	0.53
8:2I:81:VAL:HG23	8:2I:82:ARG:H	1.74	0.53
26:24:61:ARG:NH1	26:24:62:ARG:O	2.42	0.53
32:2a:148:G:H2'	32:2a:149:A:C8	2.44	0.53
43:2l:71:PRO:O	43:2l:102:ARG:NH1	2.40	0.53
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.90	0.53
1:1A:1455:G:O2'	1:1A:2853:C:OP1	2.20	0.53
56:1y:20:U:O2	56:1y:21:A:O2'	2.23	0.53
1:2A:1639:U:H2'	1:2A:1640:C:H5"	1.91	0.53
50:2s:28:LYS:HB3	50:2s:29:ARG:CA	2.37	0.53
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.43	0.53
1:1A:2171:A:O2'	1:1A:2172:U:H5"	2.09	0.53
37:1f:33:TYR:CD2	37:1f:75:LEU:HD23	2.43	0.53
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.44	0.53
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.36	0.53
6:2G:27:ASN:HB3	6:2G:30:GLU:HB2	1.89	0.53
19:2X:46:ALA:HB1	24:22:33:MET:HE1	1.90	0.53
21:2Z:55:HIS:CE1	21:2Z:135:GLU:HB2	2.43	0.53
21:2Z:150:LEU:H	21:2Z:171:ILE:HD11	1.72	0.53
32:2a:165:C:H2'	32:2a:166:G:H8	1.73	0.53
33:2b:112:VAL:HG23	33:2b:149:LEU:HD13	1.89	0.53
37:2f:2:ARG:NE	37:2f:69:GLU:HG2	2.23	0.53
1:1A:2218:U:O4'	23:11:52:ARG:NH2	2.42	0.53
7:1H:40:GLU:OE1	7:1H:61:HIS:NE2	2.42	0.53
34:1c:15:THR:HG21	34:1c:181:ASN:HA	1.89	0.53
36:1e:85:GLY:C	36:1e:87:SER:H	2.17	0.53
44:1m:23:TYR:HB3	44:1m:67:GLU:HA	1.91	0.53
6:2G:67:LYS:HD3	26:24:5:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2Y:8:LYS:HD3	20:2Y:97:ARG:NH1	2.24	0.53
32:2a:1099:G:OP2	33:2b:144:ARG:NH2	2.42	0.53
37:2f:97:PHE:CD2	49:2r:31:LEU:HD11	2.38	0.53
33:1b:139:LYS:O	33:1b:143:GLU:HG3	2.09	0.53
38:1g:78:ARG:NH1	38:1g:154:TYR:O	2.41	0.53
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.44	0.53
1:2A:981:A:N1	1:2A:2027:G:O2'	2.42	0.53
34:2c:40:ARG:HE	34:2c:55:VAL:HG13	1.74	0.53
55:2x:74:C:OP2	64:2x:201:HOH:O	2.18	0.53
1:1A:1602:U:O4	64:1A:4216:HOH:O	2.10	0.53
1:1A:2319:G:H22	14:1S:3:ARG:HD3	1.74	0.53
8:2I:69:LYS:HG2	8:2I:138:ILE:HG12	1.91	0.53
15:2T:83:ILE:HD13	15:2T:86:ILE:HD11	1.90	0.53
32:2a:995:C:N3	32:2a:1046:A:O2'	2.39	0.53
32:2a:1031:G:H2'	32:2a:1032:G:C8	2.43	0.53
41:2j:78:ASN:O	41:2j:80:LYS:N	2.42	0.53
1:1A:1453:U:O2'	1:1A:1455:G:N7	2.41	0.53
26:14:59:PHE:CE2	50:1s:64:GLU:HB3	2.44	0.53
32:1a:67:C:H2'	32:1a:68:G:C8	2.44	0.53
32:1a:92:C:H2'	32:1a:93:G:C8	2.44	0.53
32:1a:382:A:H2'	32:1a:383:A:C8	2.43	0.53
32:1a:976:G:OP2	32:1a:1358:U:O2'	2.23	0.53
46:1o:16:ALA:HB1	46:1o:21:ASP:HB3	1.90	0.53
48:1q:26:GLN:HG2	48:1q:37:LYS:HG2	1.89	0.53
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	1.91	0.53
15:2T:109:GLU:HG2	15:2T:112:ARG:NH2	2.24	0.53
32:2a:200:G:H1	32:2a:217:C:H42	1.57	0.53
33:2b:73:THR:OG1	33:2b:170:GLU:OE2	2.20	0.53
33:2b:77:ALA:HB2	33:2b:211:ILE:HD13	1.91	0.53
40:2i:18:PHE:O	40:2i:61:ALA:HA	2.09	0.53
44:2m:10:PRO:HB2	44:2m:13:LYS:HD2	1.91	0.53
1:1A:120:U:OP2	64:1A:4237:HOH:O	2.19	0.52
8:1I:77:LEU:HB3	8:1I:142:VAL:HG12	1.91	0.52
11:1P:38:GLN:O	11:1P:40:SER:N	2.36	0.52
14:1S:106:ARG:NE	14:1S:112:PHE:OXT	2.35	0.52
1:2A:141:A:H8	1:2A:1408:C:HO2'	1.57	0.52
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.44	0.52
5:2F:101:LEU:O	5:2F:106:ARG:NH1	2.42	0.52
6:2G:44:GLY:HA2	6:2G:88:ILE:HG22	1.90	0.52
7:2H:88:LEU:HD11	7:2H:165:ALA:HA	1.90	0.52
8:2I:91:SER:OG	8:2I:92:VAL:N	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:43:HIS:HB3	35:2d:46:LYS:HD2	1.90	0.52
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.90	0.52
32:1a:1529:G:H4'	32:1a:1530:G:OP2	2.09	0.52
33:1b:125:PRO:O	33:1b:127:ILE:N	2.41	0.52
5:2F:109:GLY:HA2	5:2F:112:MET:HE3	1.91	0.52
32:2a:134:A:H61	47:2p:25:ARG:HH12	1.55	0.52
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.91	0.52
38:2g:113:GLU:HB2	38:2g:119:ARG:HG2	1.91	0.52
1:1A:1062:G:H5"	1:1A:1070:A:H4'	1.92	0.52
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.37	0.52
5:1F:31:HIS:NE2	5:1F:35:GLU:OE2	2.42	0.52
18:1W:86:LEU:HD22	18:1W:96:ILE:HD11	1.91	0.52
32:1a:1040:U:H2'	32:1a:1041:A:H8	1.73	0.52
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	1.90	0.52
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.45	0.52
26:24:41:PRO:HG3	26:24:49:PHE:CE1	2.44	0.52
32:2a:56:U:H2'	32:2a:57:G:C8	2.45	0.52
32:2a:203:U:H2'	32:2a:203:U:OP2	2.09	0.52
56:2y:10:G:H1	56:2y:25:C:H42	1.56	0.52
56:2y:21:A:H61	56:2y:46:G7M:H1'	1.74	0.52
1:1A:897:C:N3	1:1A:898:C:N4	2.57	0.52
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.40	0.52
36:1e:43:LEU:HD21	36:1e:132:ALA:HB1	1.91	0.52
1:2A:1847:A:H3'	1:2A:1848:A:H5'	1.90	0.52
11:2P:87:ASP:O	11:2P:90:ARG:NH1	2.43	0.52
32:2a:45:U:H2'	32:2a:46:G:C8	2.45	0.52
48:2q:9:VAL:HG23	48:2q:56:VAL:HG22	1.91	0.52
1:1A:2165:G:H1	1:1A:2171:A:H2'	1.74	0.52
4:1E:176:ILE:HB	4:1E:181:LEU:HB2	1.91	0.52
10:1O:68:GLU:HB3	10:1O:78:ARG:HB2	1.89	0.52
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.74	0.52
20:1Y:6:HIS:H	20:1Y:6:HIS:CD2	2.27	0.52
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.24	0.52
1:2A:146:G:O6	64:2A:3934:HOH:O	2.16	0.52
1:2A:644:A:H4'	1:2A:645:C:C4	2.45	0.52
8:2I:69:LYS:O	8:2I:73:GLU:HB2	2.10	0.52
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.10	0.52
32:2a:157:G:H2'	32:2a:158:G:H8	1.75	0.52
32:2a:401:C:P	35:2d:73:ARG:HH21	2.32	0.52
32:2a:1274:G:N2	32:2a:1275:A:N7	2.56	0.52
34:2c:127:ARG:NH2	34:2c:192:THR:OG1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:155:GLY:HA3	34:2c:196:LEU:HD22	1.91	0.52
33:1b:163:PHE:CD1	33:1b:185:ILE:HG13	2.44	0.52
1:2A:910:A:N3	1:2A:2264:C:O2'	2.40	0.52
5:2F:120:GLU:HG3	5:2F:122:LYS:HG2	1.91	0.52
8:2I:55:ALA:HA	8:2I:58:LEU:HD12	1.92	0.52
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.45	0.52
32:2a:406:G:H21	35:2d:119:GLN:HE22	1.58	0.52
1:1A:1058:G:N2	1:1A:1081:U:O2	2.43	0.52
10:1O:110:GLY:HA2	10:1O:112:MET:HE2	1.91	0.52
34:1c:71:ALA:HA	34:1c:106:VAL:HG21	1.92	0.52
1:2A:2298:A:N6	1:2A:2318:G:H8	1.93	0.52
32:2a:1265:G:C4	32:2a:1271:G:N2	2.78	0.52
47:2p:15:PRO:O	47:2p:16:HIS:ND1	2.43	0.52
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.44	0.52
1:1A:1543:C:H5"	64:1A:5495:HOH:O	2.09	0.52
1:1A:2611:U:H5'	1:1A:2611:U:H6	1.75	0.52
1:1A:2713:A:OP1	13:1R:14:SER:OG	2.20	0.52
32:1a:1316:G:N1	32:1a:1319:A:OP2	2.42	0.52
35:1d:99:SER:OG	35:1d:140:VAL:O	2.27	0.52
1:2A:288:C:H2'	1:2A:289:A:C8	2.44	0.52
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.43	0.52
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.45	0.52
32:2a:662:G:H2'	32:2a:663:A:C8	2.45	0.52
35:2d:96:LEU:HD12	35:2d:139:ARG:CZ	2.39	0.52
35:2d:199:ASN:HB3	35:2d:202:LEU:HD12	1.92	0.52
36:2e:43:LEU:O	36:2e:65:ASN:ND2	2.42	0.52
1:1A:1060:U:H3	1:1A:1088:A:H8	1.57	0.52
7:1H:56:SER:OG	7:1H:57:ASP:N	2.42	0.52
8:1I:72:LEU:HD21	8:1I:107:VAL:HG11	1.92	0.52
34:1c:150:LYS:HG3	34:1c:169:ALA:HB2	1.92	0.52
1:2A:38:A:H2'	1:2A:39:C:C6	2.44	0.52
1:2A:375:C:H2'	1:2A:376:C:C6	2.45	0.52
1:2A:881:G:H3'	1:2A:882:G:C8	2.45	0.52
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.45	0.52
8:2I:128:LEU:HD12	8:2I:142:VAL:HG21	1.92	0.52
32:2a:1244:C:N4	32:2a:1293:G:H1	2.05	0.52
1:1A:11:G:C2'	1:1A:12:U:H5'	2.40	0.52
1:1A:2820:A:O2'	1:1A:2821:A:OP1	2.27	0.52
46:1o:6:GLU:OE1	46:1o:6:GLU:N	2.40	0.52
49:1r:47:THR:O	49:1r:83:GLU:N	2.40	0.52
1:2A:893:C:H5'	1:2A:894:C:C5	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2802:G:H2'	1:2A:2803:C:O4'	2.10	0.52
6:2G:109:VAL:HG11	26:24:14:ILE:HG21	1.92	0.52
8:2I:113:ARG:CB	8:2I:132:PRO:HB3	2.40	0.52
34:2c:20:SER:HB3	34:2c:22:TRP:NE1	2.24	0.52
1:1A:1798:U:H5'	3:1D:259:THR:CG2	2.37	0.51
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	1.91	0.51
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.93	0.51
1:2A:483:A:O2'	20:2Y:49:VAL:O	2.20	0.51
1:2A:900:A:H2'	1:2A:901:A:H8	1.74	0.51
9:2N:15:LEU:HB2	9:2N:135:PRO:HB2	1.92	0.51
14:2S:36:TYR:HD1	14:2S:52:SER:HB3	1.74	0.51
37:2f:99:ALA:HB1	49:2r:23:LYS:NZ	2.25	0.51
6:1G:60:LEU:HB3	6:1G:68:PRO:HG3	1.92	0.51
39:1h:121:ASP:HB2	39:1h:125:ARG:NH2	2.25	0.51
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.75	0.51
1:2A:2065:C:H4'	1:2A:2251:OMG:HM22	1.91	0.51
9:2N:96:GLU:CD	9:2N:96:GLU:H	2.18	0.51
14:2S:105:ALA:HB1	14:2S:110:LEU:HD23	1.93	0.51
15:2T:24:PRO:HA	15:2T:49:VAL:HG12	1.91	0.51
32:2a:457:C:H2'	32:2a:458:C:H6	1.73	0.51
32:2a:942:G:N2	40:2i:124:GLN:OE1	2.34	0.51
32:2a:1138:G:O2'	32:2a:1140:C:H5'	2.10	0.51
40:2i:15:ALA:HB2	40:2i:65:VAL:HG23	1.90	0.51
1:1A:1991:U:H2'	1:1A:1992:G:H5"	1.91	0.51
1:1A:2156:G:H2'	1:1A:2157:G:C2	2.45	0.51
33:1b:97:TRP:HZ2	33:1b:102:LEU:HD13	1.75	0.51
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.25	0.51
32:2a:1104:G:O3'	33:2b:111:ARG:NH2	2.42	0.51
50:2s:30:LEU:HD11	50:2s:50:ALA:HB2	1.92	0.51
1:1A:800:A:H8	1:1A:800:A:OP1	1.93	0.51
1:1A:1745(A):C:H5'	1:1A:1746:G:OP2	2.10	0.51
21:1Z:42:VAL:HG13	21:1Z:46:LYS:HE2	1.93	0.51
26:14:61:ARG:NH1	50:1s:42:PRO:HD3	2.25	0.51
32:1a:1112:C:H1'	34:1c:179:ARG:NH1	2.26	0.51
33:1b:174:VAL:O	33:1b:178:ARG:HG2	2.10	0.51
36:1e:147:ASP:O	36:1e:151:LEU:HD12	2.10	0.51
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.44	0.51
1:2A:2079:U:OP1	23:21:21:ARG:NH2	2.34	0.51
32:2a:1292:U:H5'	40:2i:38:GLN:HE21	1.75	0.51
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.09	0.51
32:1a:1101:A:H4'	32:1a:1102:A:O5'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:208:ILE:HD13	33:1b:208:ILE:H	1.76	0.51
32:2a:157:G:H2'	32:2a:158:G:C8	2.46	0.51
32:2a:985:C:H2'	32:2a:986:A:C8	2.45	0.51
32:2a:1134:G:H1	32:2a:1140:C:H42	1.57	0.51
50:2s:15:LEU:HD12	50:2s:18:LYS:HD2	1.92	0.51
54:2w:39:PSU:H2'	54:2w:40:C:H6	1.74	0.51
56:2y:51:U:H3	56:2y:63:G:H1	1.57	0.51
1:1A:1506:C:H2'	1:1A:1507:A:H8	1.75	0.51
3:1D:180:GLY:HA3	3:1D:275:LYS:HG2	1.93	0.51
4:2E:128:SER:OG	4:2E:129:HIS:N	2.41	0.51
21:2Z:29:TYR:HB3	21:2Z:34:ASN:HD22	1.76	0.51
55:2x:50:U:H2'	55:2x:51:C:C6	2.46	0.51
1:1A:548:A:H1'	1:1A:549:G:OP1	2.11	0.51
3:1D:20:ASP:OD2	3:1D:22:SER:OG	2.29	0.51
32:1a:1025:U:O2	32:1a:1036:G:O6	2.29	0.51
1:2A:2155:G:C5	1:2A:2156:G:H1'	2.45	0.51
26:24:40:HIS:CD2	26:24:41:PRO:HD2	2.46	0.51
45:2n:48:ALA:HB2	45:2n:53:LEU:HD12	1.93	0.51
8:1I:93:THR:HG22	8:1I:119:PRO:HB3	1.92	0.51
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.93	0.51
31:19:17:ILE:HD13	31:19:26:ILE:HD13	1.93	0.51
32:1a:309:G:O2'	32:1a:607:A:N1	2.43	0.51
32:1a:1129:C:O2'	32:1a:1139:G:N7	2.38	0.51
1:2A:646:A:H2'	1:2A:647:G:O4'	2.11	0.51
7:2H:15:VAL:HG12	7:2H:28:GLY:HA3	1.92	0.51
32:2a:1194:U:H2'	32:2a:1195:C:C6	2.46	0.51
33:2b:171:ALA:O	33:2b:175:ARG:N	2.42	0.51
33:2b:185:ILE:HG22	33:2b:199:TYR:CD2	2.46	0.51
47:2p:57:ARG:NH2	47:2p:79:VAL:O	2.42	0.51
1:1A:1062:G:H1	1:1A:1077:A:N6	2.08	0.51
1:1A:1420:U:O2'	1:1A:1421:G:OP1	2.28	0.51
1:1A:2155:G:H2'	1:1A:2155:G:N3	2.26	0.51
1:2A:1237:A:OP1	64:2A:3942:HOH:O	2.19	0.51
1:2A:1345:C:OP2	64:2A:3940:HOH:O	2.18	0.51
32:2a:447:G:O6	32:2a:485:G:O2'	2.28	0.51
37:2f:50:TYR:CE2	49:2r:77:GLY:HA2	2.46	0.51
43:2l:53:ARG:HG3	43:2l:93:LEU:HD21	1.93	0.51
43:2l:56:ALA:HB2	43:2l:70:ILE:HD11	1.93	0.51
1:1A:652(D):C:H42	1:1A:652(U):G:H1	1.57	0.51
1:1A:1041:C:N4	1:1A:1114:G:H1	2.08	0.51
1:1A:1371:G:N7	64:1A:4313:HOH:O	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1W:19:LEU:HB3	27:15:25:LEU:HD11	1.93	0.51
42:1k:16:SER:O	42:1k:35:PRO:HD3	2.10	0.51
2:2B:3:C:H2'	2:2B:4:C:C6	2.46	0.51
2:2B:87:G:N1	64:2B:302:HOH:O	2.34	0.51
5:2F:133:ASN:N	5:2F:138:GLU:OE1	2.44	0.51
26:24:16:CYS:SG	26:24:17:GLY:N	2.84	0.51
32:2a:7:G:H5'	32:2a:298:A:O4'	2.11	0.51
32:2a:141:A:H1'	32:2a:182:U:O2	2.11	0.51
32:2a:1004:A:C6	32:2a:1037:C:H1'	2.46	0.51
33:2b:170:GLU:HB3	33:2b:173:ALA:HB3	1.92	0.51
1:1A:2612:C:OP2	27:15:2:ALA:N	2.44	0.50
32:1a:841:U:OP2	32:1a:841:U:H6	1.94	0.50
39:1h:14:ARG:O	39:1h:18:ARG:HD2	2.10	0.50
1:2A:1385:G:O2'	1:2A:1396:U:O2	2.26	0.50
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.12	0.50
8:2I:84:GLY:C	8:2I:86:THR:H	2.18	0.50
8:2I:86:THR:O	8:2I:123:LEU:HB2	2.11	0.50
32:2a:841:U:C5	32:2a:848:C:H1'	2.47	0.50
32:2a:1273:G:C6	32:2a:1274:G:C4	3.00	0.50
50:2s:38:SER:HB2	50:2s:71:LEU:HD22	1.91	0.50
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.27	0.50
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.47	0.50
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.26	0.50
16:1U:78:THR:HG22	16:1U:117:GLN:HE22	1.76	0.50
32:1a:222:U:H2'	32:1a:223:U:C6	2.46	0.50
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.11	0.50
32:1a:1198:G:N7	64:1a:1948:HOH:O	2.35	0.50
33:1b:47:THR:HA	33:1b:202:PRO:HG2	1.93	0.50
40:1i:17:VAL:HG21	40:1i:81:ILE:HG12	1.92	0.50
1:2A:2506:U:O2'	54:2w:76:8AN:H4'	2.11	0.50
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.44	0.50
32:2a:974:A:H8	32:2a:974:A:OP1	1.94	0.50
1:1A:639:U:H2'	1:1A:640:C:C6	2.47	0.50
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.46	0.50
32:1a:192:U:O2'	51:1t:60:GLU:OE1	2.19	0.50
1:2A:597:U:H2'	1:2A:598:G:C8	2.46	0.50
1:2A:2064:C:H2'	1:2A:2065:C:C6	2.47	0.50
1:2A:2125:G:H1'	1:2A:2173:A:H61	1.76	0.50
8:2I:38:LEU:HB2	8:2I:40:THR:HG23	1.92	0.50
26:24:64:GLY:C	26:24:66:SER:H	2.20	0.50
32:2a:444:C:H2'	32:2a:445:G:H8	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:43:C:H2'	54:2w:44:G:C8	2.46	0.50
1:1A:536:A:H2'	1:1A:537:C:C6	2.46	0.50
1:1A:910:A:N1	1:1A:2277:G:H1'	2.26	0.50
44:1m:2:ALA:N	44:1m:8:GLU:OE1	2.44	0.50
44:1m:40:ASN:O	44:1m:43:THR:OG1	2.29	0.50
55:1x:17:C:OP2	55:1x:17(A):U:O2'	2.29	0.50
1:2A:1340:U:OP1	19:2X:16:LYS:NZ	2.43	0.50
32:2a:160:A:H1'	32:2a:344:A:C5	2.47	0.50
32:2a:779:C:H2'	32:2a:780:A:O4'	2.12	0.50
33:2b:87:ARG:NH2	33:2b:220:ASP:OD1	2.44	0.50
39:2h:6:ILE:O	39:2h:10:LEU:HG	2.12	0.50
39:2h:19:VAL:HG23	39:2h:21:LYS:HG3	1.92	0.50
1:1A:534:U:H2'	1:1A:535:C:C6	2.46	0.50
1:1A:1278:A:OP1	13:1R:36:THR:HG23	2.12	0.50
8:1I:116:LEU:HD11	8:1I:120:ILE:HG13	1.92	0.50
21:1Z:103:ARG:O	21:1Z:139:VAL:N	2.43	0.50
32:1a:1226:C:H4'	50:1s:80:TYR:OH	2.12	0.50
1:2A:2148:G:H2'	1:2A:2149:G:C8	2.46	0.50
4:2E:34:VAL:HG21	4:2E:78:LEU:HD11	1.93	0.50
4:2E:50:GLY:HA3	4:2E:75:VAL:HG21	1.93	0.50
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	1.93	0.50
32:2a:1010:G:C2	32:2a:1020:U:H1'	2.47	0.50
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.47	0.50
37:2f:99:ALA:HB1	49:2r:23:LYS:HZ3	1.76	0.50
48:2q:45:HIS:HB2	48:2q:65:ILE:HD13	1.93	0.50
1:1A:518:G:H2'	1:1A:519:U:C6	2.46	0.50
1:1A:884:C:H42	1:1A:892:G:H1	1.58	0.50
1:1A:2291:U:OP1	1:1A:2380:C:O2'	2.27	0.50
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.26	0.50
19:1X:35:THR:HG22	19:1X:38:GLU:H	1.75	0.50
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.46	0.50
51:1t:83:ARG:HA	51:1t:86:ARG:HH11	1.77	0.50
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.11	0.50
1:2A:2151:G:H2'	1:2A:2152:G:C8	2.43	0.50
14:2S:30:ARG:HB2	14:2S:35:ILE:HD12	1.93	0.50
21:2Z:126:VAL:HG12	21:2Z:163:LEU:HD23	1.92	0.50
24:22:63:VAL:O	24:22:67:LYS:HG2	2.11	0.50
32:2a:603:U:H2'	32:2a:604:G:H8	1.76	0.50
1:1A:1508:A:H4'	1:1A:1509:C:OP1	2.12	0.50
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.77	0.50
1:1A:2136:C:N3	1:1A:2155:G:N2	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:14:ILE:HB	26:14:22:ILE:HB	1.93	0.50
1:2A:271(D):G:H1	1:2A:271(T):C:H42	1.60	0.50
36:2e:110:LEU:HD13	36:2e:118:ILE:HG21	1.92	0.50
37:2f:91:VAL:HG11	49:2r:72:ARG:NH1	2.26	0.50
38:2g:15:ASP:OD1	38:2g:19:GLY:N	2.45	0.50
38:2g:78:ARG:HG3	38:2g:156:TRP:HZ3	1.77	0.50
39:2h:51:VAL:HG21	39:2h:60:ARG:HB2	1.94	0.50
48:2q:27:PHE:CE1	48:2q:36:ILE:HD11	2.46	0.50
1:1A:621:A:OP2	11:1P:108:LYS:NZ	2.44	0.50
1:1A:1069:A:H1'	1:1A:1096:A:H4'	1.94	0.50
1:1A:1800:C:OP2	3:1D:183:ARG:NH2	2.45	0.50
10:1O:98:VAL:HG22	10:1O:118:ALA:HA	1.94	0.50
1:2A:580:C:H2'	1:2A:581:C:H6	1.76	0.50
1:2A:1169:G:N1	1:2A:1170:G:N7	2.59	0.50
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.11	0.50
8:2I:5:LEU:HD11	8:2I:19:VAL:HG13	1.94	0.50
21:2Z:145:GLU:HB3	21:2Z:148:ASP:HB2	1.93	0.50
26:24:45:GLY:C	26:24:47:GLN:H	2.17	0.50
32:2a:1224:G:OP1	64:2a:3314:HOH:O	2.20	0.50
40:2i:99:LEU:HB3	40:2i:101:PHE:CE2	2.46	0.50
1:1A:732:C:OP1	64:1A:4238:HOH:O	2.19	0.50
12:1Q:37:LEU:HD21	12:1Q:130:LYS:HE2	1.93	0.50
21:1Z:28:MET:HE2	21:1Z:35:ARG:HB2	1.94	0.50
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.11	0.50
36:1e:74:GLY:HA3	36:1e:116:THR:HG22	1.94	0.50
37:1f:89:MET:HE1	49:1r:72:ARG:HB3	1.93	0.50
41:1j:78:ASN:O	41:1j:80:LYS:N	2.45	0.50
1:2A:893:C:H2'	1:2A:894:C:C4	2.47	0.50
36:2e:81:GLU:HG2	36:2e:90:VAL:HG22	1.93	0.50
9:1N:35:ARG:HD3	9:1N:37:LYS:HD2	1.93	0.49
28:16:5:VAL:HG21	28:16:28:ARG:HE	1.76	0.49
32:1a:100:C:H2'	32:1a:101:A:C8	2.47	0.49
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.93	0.49
32:1a:1302:U:C5	44:1m:17:VAL:HG21	2.48	0.49
1:2A:1537:G:H2'	1:2A:1538:G:H8	1.77	0.49
1:2A:1568:G:N7	64:2A:4000:HOH:O	2.33	0.49
32:2a:995:C:O2	45:2n:4:LYS:NZ	2.29	0.49
32:2a:1148:U:H2'	32:2a:1149:C:O4'	2.12	0.49
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.47	0.49
34:2c:148:GLY:HA3	34:2c:172:ARG:O	2.11	0.49
40:2i:8:GLY:O	40:2i:15:ALA:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:2r:52:PRO:O	49:2r:56:THR:HG23	2.11	0.49
1:1A:1062:G:H22	1:1A:1077:A:N6	2.11	0.49
1:1A:1394:U:H2'	1:1A:1395:A:O4'	2.12	0.49
5:1F:72:ARG:NH2	64:1F:404:HOH:O	2.45	0.49
6:1G:66:GLN:HG3	26:14:1:MET:HE1	1.93	0.49
8:1I:31:LEU:HD21	8:1I:38:LEU:HD22	1.93	0.49
15:1T:127:ALA:C	15:1T:129:ARG:H	2.21	0.49
32:1a:1149:C:P	40:1i:9:ARG:HH21	2.35	0.49
32:1a:1530:G:H2'	32:1a:1531:A:C8	2.47	0.49
40:1i:4:TYR:CD1	40:1i:88:TYR:HA	2.47	0.49
1:2A:2755:C:OP1	64:2A:3944:HOH:O	2.19	0.49
8:2I:101:LEU:HD21	8:2I:107:VAL:HB	1.94	0.49
32:2a:1055:A:N7	32:2a:1200:C:N4	2.60	0.49
32:2a:1320:C:N3	50:2s:36:ARG:NH2	2.58	0.49
32:2a:1329:A:OP2	52:2u:7:ARG:NH2	2.44	0.49
33:2b:82:ARG:HB3	33:2b:94:ASN:OD1	2.12	0.49
35:2d:150:GLU:H	35:2d:150:GLU:CD	2.18	0.49
1:1A:1038:C:H42	1:1A:1117:G:H1	1.60	0.49
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.47	0.49
18:1W:4:LYS:HD3	18:1W:6:ILE:HD11	1.94	0.49
28:16:12:GLU:OE2	28:16:17:LYS:NZ	2.38	0.49
35:1d:8:VAL:HG22	35:1d:21:LEU:HD13	1.94	0.49
46:1o:62:GLN:HA	46:1o:62:GLN:HE21	1.77	0.49
1:2A:288:C:H2'	1:2A:289:A:H8	1.78	0.49
6:2G:111:LEU:HD21	6:2G:120:LEU:HD21	1.93	0.49
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	1.93	0.49
32:2a:79:G:H1	32:2a:90:U:H3	1.61	0.49
32:2a:109:A:C6	32:2a:326:G:C6	3.00	0.49
32:2a:406:G:H21	35:2d:119:GLN:NE2	2.10	0.49
32:2a:920:U:H2'	32:2a:921:U:C6	2.47	0.49
32:2a:1469:G:H2'	32:2a:1470:G:C8	2.47	0.49
1:1A:84:A:OP2	20:1Y:8:LYS:NZ	2.32	0.49
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.12	0.49
6:1G:126:ASP:HB2	6:1G:130:ASN:H	1.77	0.49
34:1c:36:ASP:O	34:1c:40:ARG:HG3	2.13	0.49
1:2A:34:C:N4	1:2A:454:A:O2'	2.45	0.49
16:2U:97:ASP:OD1	16:2U:101:ARG:NH1	2.43	0.49
32:2a:818:G:O2'	32:2a:819:A:H5'	2.12	0.49
42:2k:81:ASP:OD1	42:2k:107:SER:OG	2.16	0.49
1:1A:39:C:O2	5:1F:46:ARG:NH2	2.43	0.49
20:1Y:98:VAL:HG12	20:1Y:105:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1843:C:H5'	3:2D:253:GLN:OE1	2.13	0.49
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.74	0.49
23:21:82:LEU:HA	23:21:85:LEU:HD12	1.94	0.49
30:28:62:LEU:HB3	30:28:65:GLU:HG2	1.94	0.49
32:2a:1314:C:OP2	50:2s:4:SER:OG	2.11	0.49
33:2b:98:LEU:HB2	33:2b:101:MET:HE3	1.93	0.49
33:2b:230:VAL:HG22	33:2b:231:GLU:H	1.77	0.49
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.77	0.49
34:1c:43:LEU:HD21	34:1c:91:LEU:HD11	1.95	0.49
35:1d:112:VAL:HG23	35:1d:116:GLN:HE22	1.77	0.49
46:1o:84:LYS:O	46:1o:84:LYS:HD3	2.11	0.49
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.13	0.49
1:2A:2134:A:H3'	1:2A:2135:A:C8	2.48	0.49
6:2G:106:LEU:O	6:2G:110:ALA:HB3	2.13	0.49
8:2I:51:ILE:HA	8:2I:54:GLN:HB2	1.94	0.49
32:2a:570:G:H1'	32:2a:820:U:C4	2.47	0.49
32:2a:1299:A:H2'	32:2a:1299:A:N3	2.27	0.49
33:2b:18:GLY:HA2	33:2b:42:ILE:HG13	1.95	0.49
33:2b:139:LYS:NZ	33:2b:143:GLU:OE2	2.45	0.49
56:2y:61:C:H2'	56:2y:62:C:C6	2.48	0.49
1:1A:1062:G:C5'	1:1A:1070:A:HO2'	2.26	0.49
1:1A:1588:C:H2'	1:1A:1589:C:C6	2.48	0.49
1:1A:1800:C:OP1	3:1D:264:LYS:NZ	2.39	0.49
3:1D:164:GLN:OE1	3:1D:176:ARG:NH1	2.37	0.49
32:1a:92:C:H2'	32:1a:93:G:H8	1.78	0.49
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.48	0.49
32:1a:216:G:H2'	32:1a:217:C:C6	2.47	0.49
32:1a:974:A:H8	32:1a:974:A:OP1	1.95	0.49
34:1c:35:GLU:CD	34:1c:59:ARG:HH22	2.21	0.49
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.48	0.49
14:2S:78:LEU:HD11	14:2S:109:GLY:HA3	1.95	0.49
32:2a:157:G:H1	32:2a:164:U:H3	1.61	0.49
32:2a:1095:U:H5"	32:2a:1109:C:O2	2.12	0.49
34:2c:152:ILE:HG13	34:2c:199:LYS:HB2	1.94	0.49
36:2e:5:ASP:CG	36:2e:6:PHE:H	2.20	0.49
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.12	0.49
20:1Y:83:THR:HG21	20:1Y:99:CYS:HB2	1.95	0.49
23:11:85:LEU:HD13	23:11:89:GLU:HB3	1.93	0.49
32:1a:1035:A:C4	32:1a:1036:G:N2	2.80	0.49
33:1b:37:ASN:HB2	33:1b:39:ILE:HD12	1.94	0.49
1:2A:1023:U:OP2	64:2A:3930:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:32:LEU:HD22	5:2F:112:MET:HE1	1.93	0.49
10:2O:49:ARG:NH1	32:2a:1422:G:O3'	2.34	0.49
32:2a:1004:A:N6	32:2a:1037:C:H1'	2.28	0.49
32:2a:1273:G:H3'	32:2a:1274:G:H8	1.78	0.49
32:2a:1427:U:H2'	32:2a:1428:A:C8	2.47	0.49
41:2j:35:SER:HB3	41:2j:73:ASP:H	1.78	0.49
50:2s:36:ARG:HG2	50:2s:51:VAL:HG12	1.94	0.49
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.46	0.49
1:1A:2165:G:N1	1:1A:2171:A:H8	2.11	0.49
5:1F:123:LEU:HD13	5:1F:192:LEU:HD13	1.95	0.49
32:1a:501:C:H2'	32:1a:502:G:H8	1.78	0.49
1:2A:1399:C:OP1	19:2X:25:LYS:NZ	2.45	0.49
1:2A:2127:G:H1	1:2A:2161:C:H42	1.60	0.49
23:21:3:LYS:HB2	23:21:61:ARG:HH22	1.77	0.49
32:2a:532:A:N6	32:2a:1206:G:O2'	2.46	0.49
32:2a:1053:G:N7	32:2a:1200:C:H5"	2.28	0.49
32:2a:1239:A:H62	32:2a:1299:A:H62	1.59	0.49
46:2o:3:ILE:HG23	46:2o:38:ARG:HH21	1.78	0.49
1:1A:247:G:H4'	1:1A:386:G:C5	2.47	0.49
1:1A:615:G:OP1	5:1F:40:GLN:NE2	2.42	0.49
1:1A:2105:C:H2'	1:1A:2106:G:C8	2.47	0.49
1:1A:2108:C:H2'	1:1A:2109:U:H6	1.77	0.49
1:1A:2285:C:OP2	28:16:6:ARG:NH1	2.46	0.49
6:1G:133:LEU:HD11	6:1G:157:ILE:HD12	1.95	0.49
20:1Y:6:HIS:HE1	20:1Y:72:VAL:O	1.96	0.49
26:14:26:SER:OG	26:14:27:THR:N	2.46	0.49
32:1a:1269:A:H2	32:1a:1312:G:N3	2.11	0.49
32:1a:1503:A:N1	53:1v:12:A:H2	2.10	0.49
41:1j:13:HIS:HB3	41:1j:68:HIS:CD2	2.48	0.49
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.13	0.49
1:2A:839:U:H2'	1:2A:840:C:C6	2.48	0.49
1:2A:882:G:H22	1:2A:894:C:H42	1.60	0.49
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.46	0.49
34:2c:52:LEU:HA	34:2c:70:VAL:HG12	1.95	0.49
1:1A:286:C:H2'	1:1A:287:C:C6	2.48	0.48
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.95	0.48
32:1a:96:U:H2'	32:1a:97:G:C8	2.48	0.48
32:1a:719:C:H1'	49:1r:49:LYS:HB3	1.95	0.48
32:1a:741:G:H2'	32:1a:742:G:O4'	2.13	0.48
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.30	0.48
33:1b:114:ARG:CZ	33:1b:118:LEU:HD21	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:53:ASP:N	35:1d:53:ASP:OD1	2.45	0.48
35:1d:173:TRP:CD2	35:1d:189:PRO:HG3	2.48	0.48
1:2A:848:G:H2'	1:2A:849:A:C8	2.48	0.48
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.12	0.48
8:2I:71:ILE:O	8:2I:75:LEU:HG	2.13	0.48
15:2T:91:ARG:HB2	15:2T:121:ILE:HG13	1.94	0.48
1:1A:185:U:H4'	1:1A:218:A:H4'	1.95	0.48
1:1A:278:A:O2'	1:1A:279:C:OP1	2.25	0.48
1:1A:668:G:OP2	64:1A:4240:HOH:O	2.20	0.48
1:1A:887:A:H1'	1:1A:889:C:OP2	2.14	0.48
1:1A:2136:C:N4	1:1A:2155:G:N1	2.62	0.48
1:1A:2422:A:O4'	56:1y:76:A:N6	2.45	0.48
32:1a:939:G:H5'	38:1g:102:ARG:NH1	2.27	0.48
36:1e:144:THR:H	36:1e:147:ASP:HB2	1.77	0.48
1:2A:30:G:H2'	1:2A:31:C:C6	2.48	0.48
1:2A:892:G:H3'	1:2A:893:C:C5'	2.43	0.48
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.12	0.48
32:2a:407:G:H5"	35:2d:115:ARG:HB3	1.95	0.48
32:2a:1095:U:H2'	32:2a:1096:C:C6	2.47	0.48
54:2w:4:C:N3	54:2w:69:G:N2	2.55	0.48
1:1A:796:C:H2'	1:1A:797:C:C6	2.48	0.48
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	1.94	0.48
21:1Z:52:SER:O	21:1Z:52:SER:OG	2.26	0.48
21:1Z:137:ILE:HA	21:1Z:156:LYS:HZ3	1.78	0.48
32:1a:948:C:OP1	44:1m:109:THR:OG1	2.31	0.48
34:1c:124:ILE:HG22	34:1c:130:VAL:HG22	1.95	0.48
1:2A:2821:A:H2'	1:2A:2822:G:C8	2.48	0.48
2:2B:7:G:H21	14:2S:38:GLN:NE2	2.00	0.48
2:2B:45:A:OP2	6:2G:96:ARG:NH2	2.33	0.48
5:2F:178:PRO:HB3	5:2F:198:ALA:HA	1.96	0.48
32:2a:328:C:H4'	32:2a:329:A:H5'	1.94	0.48
39:2h:82:HIS:N	39:2h:138:TRP:O	2.46	0.48
40:2i:8:GLY:HA2	40:2i:79:LEU:HD23	1.95	0.48
54:2w:18:G:H4'	54:2w:60:U:C5	2.48	0.48
55:2x:61:C:H2'	55:2x:62:C:H6	1.77	0.48
1:1A:881:G:N2	1:1A:897:C:O2	2.46	0.48
1:1A:2375:G:N7	64:1A:4315:HOH:O	2.35	0.48
6:1G:179:PRO:HG3	26:14:43:TYR:CZ	2.48	0.48
10:1O:24:VAL:HG13	10:1O:33:ALA:HB2	1.95	0.48
21:1Z:8:TYR:HB2	21:1Z:38:TYR:CE2	2.49	0.48
32:1a:200:G:H1	32:1a:217:C:H42	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1347:G:H5"	40:1i:107:ARG:HB3	1.95	0.48
45:1n:48:ALA:HB2	45:1n:53:LEU:HD12	1.94	0.48
1:2A:774:A:H2'	1:2A:774:A:N3	2.28	0.48
1:2A:1192:G:OP2	11:2P:17:LYS:NZ	2.36	0.48
6:2G:170:ARG:NH2	6:2G:182:LYS:O	2.47	0.48
8:2I:140:LEU:HD12	64:2I:201:HOH:O	2.14	0.48
32:2a:1030(A):G:N2	32:2a:1030(C):G:H3'	2.29	0.48
35:2d:127:THR:HG23	35:2d:147:ALA:HB3	1.94	0.48
45:2n:24:CYS:HB2	45:2n:40:CYS:HB3	1.95	0.48
54:2w:10:G:H2'	54:2w:11:C:H6	1.79	0.48
1:1A:1448:G:H4'	1:1A:1542:A:OP1	2.14	0.48
42:1k:34:ASP:HB2	42:1k:35:PRO:HD2	1.96	0.48
56:1y:40:C:H2'	56:1y:41:C:C6	2.48	0.48
1:2A:2118:U:OP1	1:2A:2148:G:H4'	2.13	0.48
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.48	0.48
20:2Y:11:ASP:OD2	20:2Y:97:ARG:NH2	2.35	0.48
32:2a:1360:A:H2'	32:2a:1361:G:O4'	2.13	0.48
49:2r:53:ARG:HG2	49:2r:63:GLN:HE21	1.79	0.48
30:18:42:ARG:HD2	64:18:202:HOH:O	2.13	0.48
33:1b:162:ILE:O	33:1b:185:ILE:HG12	2.13	0.48
36:1e:90:VAL:O	36:1e:120:THR:HA	2.14	0.48
1:2A:1657:C:H2'	1:2A:1658:C:H6	1.78	0.48
1:2A:1815:A:P	3:2D:54:ARG:HH22	2.36	0.48
32:2a:457:C:H2'	32:2a:458:C:C6	2.48	0.48
32:2a:757:U:H2'	32:2a:758:G:O4'	2.14	0.48
32:2a:985:C:H2'	32:2a:986:A:H8	1.78	0.48
35:2d:165:MET:HG2	35:2d:168:ARG:HH11	1.78	0.48
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.49	0.48
5:1F:144:LYS:HB3	5:1F:144:LYS:HE3	1.58	0.48
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.94	0.48
32:1a:148:G:H2'	32:1a:149:A:C8	2.48	0.48
32:1a:1011:G:H1	32:1a:1018:C:H42	1.61	0.48
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.95	0.48
1:2A:580:C:H2'	1:2A:581:C:C6	2.49	0.48
4:2E:34:VAL:HB	4:2E:48:GLN:HE21	1.77	0.48
8:2I:92:VAL:HG23	8:2I:96:ASP:HB2	1.95	0.48
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.95	0.48
32:2a:109:A:H5'	32:2a:110:C:C5	2.48	0.48
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.14	0.48
32:2a:772:U:H2'	32:2a:773:G:O4'	2.13	0.48
33:2b:91:PRO:HA	33:2b:151:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:2t:79:ARG:HD2	51:2t:83:ARG:HH21	1.77	0.48
1:1A:2131:G:H5'	1:1A:2133:G:C8	2.48	0.48
32:1a:78:G:N1	32:1a:91:C:C4	2.81	0.48
32:1a:627:G:H2'	32:1a:628:G:H8	1.78	0.48
37:1f:99:ALA:HB1	49:1r:23:LYS:NZ	2.29	0.48
47:1p:15:PRO:O	47:1p:16:HIS:ND1	2.47	0.48
1:2A:2131:G:N7	1:2A:2133:G:N2	2.61	0.48
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.76	0.48
1:2A:2611:U:H6	1:2A:2611:U:H5'	1.79	0.48
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.49	0.48
12:2Q:82:ARG:NH2	22:20:4:LYS:HG3	2.29	0.48
21:2Z:144:LEU:HG	21:2Z:145:GLU:H	1.79	0.48
32:2a:241:C:H42	32:2a:285:G:H1	1.62	0.48
32:2a:434:U:H2'	32:2a:435:C:C6	2.48	0.48
34:2c:120:VAL:HA	34:2c:123:GLN:HB2	1.94	0.48
32:1a:17:U:H2'	32:1a:18:C:C6	2.49	0.48
33:1b:13:ALA:HB2	33:1b:44:LEU:HD13	1.95	0.48
1:2A:886:C:H2'	1:2A:887:A:O4'	2.13	0.48
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.44	0.48
1:2A:2816:C:O3'	13:2R:99:LYS:NZ	2.46	0.48
30:28:26:LYS:HG2	30:28:46:ARG:O	2.14	0.48
32:2a:179:A:H2'	32:2a:180:U:C6	2.49	0.48
32:2a:967:5MC:H2'	32:2a:968:A:C8	2.49	0.48
32:2a:1029:C:N4	32:2a:1032:G:C6	2.82	0.48
32:2a:1077:G:N2	32:2a:1080:A:OP2	2.46	0.48
32:2a:1305:G:H5'	52:2u:4:GLY:HA3	1.95	0.48
39:2h:49:GLU:OE2	39:2h:62:TYR:OH	2.20	0.48
44:2m:13:LYS:O	44:2m:45:VAL:N	2.45	0.48
50:2s:64:GLU:CD	50:2s:64:GLU:H	2.21	0.48
1:1A:127:A:H5"	1:1A:128:C:C6	2.49	0.48
1:1A:668:G:H5'	1:1A:669:G:OP2	2.13	0.48
1:1A:884:C:C4	1:1A:885:C:H1'	2.49	0.48
1:1A:1762:A:N1	64:1A:4314:HOH:O	2.35	0.48
1:1A:2014:A:OP1	64:1A:4242:HOH:O	2.20	0.48
8:1I:109:ILE:HD12	8:1I:130:TYR:CE2	2.49	0.48
32:1a:110:C:H2'	32:1a:111:G:O4'	2.14	0.48
32:1a:1239:A:H62	32:1a:1299:A:N6	2.12	0.48
32:1a:1353:G:OP1	52:1u:10:ARG:NH1	2.47	0.48
34:1c:65:ALA:O	34:1c:66:VAL:HG13	2.14	0.48
35:1d:182:LYS:HG2	35:1d:183:GLY:N	2.29	0.48
2:2B:13:A:N1	2:2B:69:G:O2'	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:86:THR:HG22	8:2I:123:LEU:H	1.79	0.48
11:2P:81:GLN:NE2	11:2P:106:LEU:HA	2.29	0.48
21:2Z:163:LEU:HD22	21:2Z:165:VAL:HG22	1.96	0.48
32:2a:862:C:H1'	32:2a:874:G:H5"	1.96	0.48
35:2d:86:LYS:H	35:2d:86:LYS:HD2	1.79	0.48
54:2w:23:A:H2'	54:2w:24:G:C8	2.49	0.48
1:1A:264:C:O2'	1:1A:265:A:H2'	2.14	0.47
1:1A:1173:G:OP2	1:1A:1173:G:H2'	2.14	0.47
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.47	0.47
21:1Z:105:VAL:N	21:1Z:139:VAL:O	2.26	0.47
32:1a:326:G:O6	64:1a:1921:HOH:O	2.20	0.47
32:1a:1149:C:H2'	32:1a:1150:U:C6	2.49	0.47
32:1a:1323:G:H2'	32:1a:1324:A:C8	2.49	0.47
37:1f:68:PRO:HG2	37:1f:71:ARG:HD2	1.96	0.47
1:2A:2060:A:N3	64:2A:4017:HOH:O	2.35	0.47
1:2A:2127:G:H1	1:2A:2161:C:N4	2.11	0.47
7:2H:97:ARG:O	7:2H:103:LEU:HD12	2.14	0.47
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	1.95	0.47
40:2i:7:THR:HB	40:2i:83:ARG:NH1	2.28	0.47
1:1A:242:G:C8	30:18:5:LYS:HG2	2.48	0.47
1:1A:251:A:C5	1:1A:252:G:H1'	2.48	0.47
1:1A:2105:C:H2'	1:1A:2106:G:H8	1.79	0.47
22:10:24:LYS:O	22:10:25:ARG:NH1	2.42	0.47
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.12	0.47
32:1a:165:C:H2'	32:1a:166:G:C8	2.49	0.47
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.49	0.47
56:1y:57:G:H2'	56:1y:58:A:H5'	1.97	0.47
1:2A:1783:A:OP2	64:2A:3945:HOH:O	2.20	0.47
1:2A:2025:C:H2'	1:2A:2026:C:C6	2.48	0.47
19:2X:92:LEU:O	19:2X:94:GLY:N	2.46	0.47
32:2a:792:A:H4'	32:2a:793:U:H5"	1.96	0.47
1:1A:603:A:O2'	11:1P:90:ARG:NH2	2.46	0.47
7:1H:97:ARG:NE	7:1H:104:GLU:OE1	2.47	0.47
28:16:26:ASN:HD21	28:16:28:ARG:NH2	2.13	0.47
32:1a:1136:U:H5"	32:1a:1137:C:N3	2.28	0.47
1:2A:1359:A:H2	1:2A:1372:U:O4	1.96	0.47
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.96	0.47
1:2A:2138:C:H42	1:2A:2153:G:H1	1.63	0.47
8:2I:82:ARG:HB2	8:2I:82:ARG:CZ	2.44	0.47
8:2I:115:ALA:O	8:2I:128:LEU:HB3	2.14	0.47
33:2b:16:HIS:HB2	33:2b:204:ASN:CB	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:16:LEU:HD22	41:2j:94:VAL:HG13	1.97	0.47
54:2w:51:U:H2'	54:2w:52:G:C8	2.49	0.47
1:1A:272(G):C:H42	1:1A:363(C):G:H1	1.62	0.47
1:1A:882:G:H4'	54:1w:19:G:C6	2.50	0.47
1:1A:1055:G:H1	1:1A:1104:C:H42	1.62	0.47
10:1O:87:ILE:HD12	10:1O:91:LEU:HA	1.95	0.47
32:1a:679:C:H2'	32:1a:680:C:H6	1.80	0.47
1:2A:271(P):C:O3'	8:2I:42:SER:HB2	2.15	0.47
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.24	0.47
6:2G:43:LEU:HD13	6:2G:43:LEU:HA	1.79	0.47
21:2Z:95:PRO:HA	21:2Z:129:SER:HA	1.95	0.47
32:2a:180:U:O4	64:2a:3312:HOH:O	2.18	0.47
32:2a:1469:G:H2'	32:2a:1470:G:H8	1.80	0.47
54:2w:19:G:H1	54:2w:56:C:H42	1.63	0.47
1:1A:882:G:H4'	54:1w:19:G:O6	2.14	0.47
1:1A:1509(A):A:H3'	1:1A:1509(B):A:H8	1.80	0.47
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.14	0.47
1:1A:2162:G:H5'	1:1A:2163:C:OP2	2.15	0.47
6:1G:32:PRO:HB3	6:1G:163:ALA:HB2	1.95	0.47
9:1N:96:GLU:H	9:1N:96:GLU:CD	2.22	0.47
10:1O:17:ARG:HB2	10:1O:45:GLU:HG2	1.95	0.47
1:2A:748:G:C8	18:2W:89:ALA:HB1	2.50	0.47
1:2A:956:G:H2'	1:2A:957:A:H2'	1.96	0.47
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.14	0.47
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.13	0.47
1:2A:2150:U:H2'	1:2A:2151:G:C8	2.48	0.47
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.49	0.47
32:2a:109:A:H5'	32:2a:110:C:H5	1.80	0.47
56:2y:49:C:H2'	56:2y:50:U:C6	2.49	0.47
1:1A:284:U:H2'	1:1A:285:C:C6	2.50	0.47
1:1A:880:G:N2	1:1A:898:C:N3	2.60	0.47
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.15	0.47
1:1A:2361:A:OP2	30:18:26:LYS:NZ	2.42	0.47
4:1E:29:GLY:HA3	64:1E:401:HOH:O	2.14	0.47
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.13	0.47
32:1a:731:G:H5'	32:1a:766:A:H4'	1.96	0.47
32:1a:1152:A:OP1	41:1j:68:HIS:ND1	2.47	0.47
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.48	0.47
36:1e:41:VAL:O	36:1e:66:MET:HA	2.14	0.47
38:1g:28:ASN:HD21	38:1g:36:LYS:NZ	2.12	0.47
51:1t:100:ILE:H	51:1t:100:ILE:HG12	1.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:570:G:H2'	1:2A:2030:A:C5	2.49	0.47
1:2A:1216:G:P	16:2U:12:ARG:HH21	2.36	0.47
1:2A:1791:A:H5'	3:2D:206:LEU:HD12	1.96	0.47
1:2A:2119:A:C2	1:2A:2170:A:H2'	2.50	0.47
1:2A:2165:G:N2	1:2A:2172:U:H5	2.12	0.47
8:2I:93:THR:C	8:2I:95:LYS:H	2.23	0.47
14:2S:77:ALA:HB1	14:2S:82:ILE:HB	1.96	0.47
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.33	0.47
21:2Z:98:MET:O	21:2Z:125:LEU:HA	2.14	0.47
32:2a:838:G:H1	32:2a:848:C:H42	1.62	0.47
32:2a:1085:U:H3'	32:2a:1086:U:C6	2.50	0.47
32:2a:1178:G:N2	32:2a:1181:G:OP2	2.47	0.47
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.14	0.47
1:1A:400:G:N7	64:1A:4311:HOH:O	2.34	0.47
1:1A:602:G:O2'	1:1A:655:A:N6	2.47	0.47
1:1A:1607:C:H4'	1:1A:1608:A:O5'	2.14	0.47
1:1A:2306:C:O2	64:1A:4230:HOH:O	2.15	0.47
7:1H:106:THR:HG22	7:1H:112:PRO:HB3	1.95	0.47
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.15	0.47
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.50	0.47
25:13:7:LYS:HE3	25:13:32:GLN:NE2	2.30	0.47
32:1a:627:G:H2'	32:1a:628:G:C8	2.50	0.47
32:1a:945:G:OP2	64:1a:1923:HOH:O	2.20	0.47
32:1a:955:U:O2'	50:1s:83:HIS:HD2	1.98	0.47
35:1d:157:LEU:HD22	35:1d:161:ASN:HD21	1.79	0.47
54:1w:18:G:H4'	54:1w:60:U:C5	2.50	0.47
1:2A:886:C:O2'	1:2A:889:C:N4	2.47	0.47
1:2A:1417:C:H2'	1:2A:1418:G:O4'	2.14	0.47
1:2A:1639:U:OP1	64:2A:3947:HOH:O	2.20	0.47
1:2A:1754:C:H5	15:2T:96:ARG:NH2	2.12	0.47
1:2A:2144:U:O2'	1:2A:2147:G:O6	2.28	0.47
1:2A:2154:G:H2'	1:2A:2155:G:H8	1.79	0.47
1:2A:2438:U:O2'	1:2A:2440:C:OP1	2.27	0.47
1:2A:2507:C:H5"	1:2A:2573:C:N4	2.30	0.47
1:2A:2811:G:N2	1:2A:2891:G:H1'	2.30	0.47
2:2B:22:U:H3	2:2B:61:G:H1	1.62	0.47
8:2I:73:GLU:OE2	8:2I:138:ILE:HA	2.15	0.47
21:2Z:146:ILE:HG12	21:2Z:174:VAL:HG13	1.95	0.47
32:2a:921:U:O2'	36:2e:19:MET:O	2.26	0.47
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.50	0.47
34:2c:60:ALA:HB3	34:2c:63:ASN:HD21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:181:ASN:HD21	34:2c:204:LEU:HD12	1.80	0.47
38:2g:15:ASP:OD2	38:2g:44:TYR:OH	2.29	0.47
39:2h:112:LEU:HA	39:2h:134:ILE:HG12	1.96	0.47
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.97	0.47
1:1A:1065:U:H5"	1:1A:1066:U:OP2	2.13	0.47
1:1A:1266:G:O2'	1:1A:2012:G:O6	2.31	0.47
6:1G:122:PRO:HG3	6:1G:182:LYS:H	1.78	0.47
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.15	0.47
32:1a:21:G:H2'	32:1a:22:G:C8	2.50	0.47
32:1a:44:G:O6	64:1a:1924:HOH:O	2.21	0.47
32:1a:711:G:OP1	37:1f:54:LYS:NZ	2.43	0.47
33:1b:122:PHE:HE2	33:1b:139:LYS:HB2	1.79	0.47
56:1y:20:U:H1'	56:1y:21:A:H4'	1.97	0.47
1:2A:184:C:H2'	1:2A:185:U:C6	2.49	0.47
1:2A:645:C:H5"	1:2A:646:A:OP2	2.15	0.47
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.96	0.47
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.49	0.47
2:2B:4:C:H42	2:2B:117:G:H1	1.62	0.47
2:2B:17:C:H2'	2:2B:18:G:O4'	2.15	0.47
4:2E:104:VAL:HG22	4:2E:198:VAL:HG22	1.96	0.47
11:2P:99:LEU:HD12	11:2P:102:ARG:HH21	1.79	0.47
21:2Z:159:PRO:HA	21:2Z:161:VAL:H	1.78	0.47
32:2a:1006:C:N4	32:2a:1023:G:H1	2.13	0.47
32:2a:1051:C:H2'	32:2a:1052:U:H6	1.80	0.47
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.49	0.47
34:2c:155:GLY:O	34:2c:157:ILE:N	2.48	0.47
49:2r:53:ARG:HA	49:2r:56:THR:HG1	1.79	0.47
56:2y:9:A:H5'	56:2y:46:G7M:N3	2.30	0.47
1:1A:479:A:N3	1:1A:481:G:H5"	2.30	0.47
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.15	0.47
1:1A:2153:G:H2'	1:1A:2154:G:C8	2.50	0.47
1:1A:2181:G:O2'	1:1A:2182:G:OP1	2.30	0.47
50:1s:11:VAL:HG11	50:1s:16:LEU:HB2	1.96	0.47
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.50	0.47
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.49	0.47
14:2S:3:ARG:NH2	14:2S:4:LEU:O	2.48	0.47
24:22:32:LEU:HD13	24:22:53:LEU:HB3	1.96	0.47
32:2a:381:C:H2'	32:2a:382:A:O4'	2.15	0.47
32:2a:645:C:OP2	64:2a:3316:HOH:O	2.20	0.47
32:2a:1081:G:OP1	36:2e:18:ARG:HG2	2.15	0.47
33:2b:219:VAL:HA	33:2b:222:ILE:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1580:A:OP2	1:1A:1580:A:H8	1.97	0.47
2:1B:48:A:H2'	2:1B:49:C:C6	2.50	0.47
37:1f:82:ARG:HB2	37:1f:85:VAL:HG23	1.97	0.47
45:1n:4:LYS:HA	45:1n:7:ILE:HB	1.97	0.47
51:1t:10:LEU:HD22	51:1t:10:LEU:HA	1.79	0.47
1:2A:93:G:H2'	1:2A:94:C:C6	2.50	0.47
8:2I:97:ILE:H	8:2I:97:ILE:HD12	1.79	0.47
8:2I:114:LEU:HD12	8:2I:130:TYR:CE2	2.50	0.47
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.15	0.47
25:23:59:VAL:HG12	25:23:60:GLU:H	1.80	0.47
32:2a:523:A:H61	43:2l:92:0TD:CG	2.28	0.47
32:2a:978:A:O2'	32:2a:1322:C:N3	2.42	0.47
36:2e:24:ARG:NH1	53:2v:24:A:OP2	2.48	0.47
48:2q:45:HIS:NE2	48:2q:47:PRO:HG3	2.29	0.47
7:1H:3:ARG:HH11	7:1H:4:ILE:H	1.62	0.46
8:1I:38:LEU:HD23	8:1I:38:LEU:H	1.79	0.46
18:1W:58:ALA:HB1	18:1W:64:MET:HB2	1.97	0.46
56:1y:7:A:O2'	56:1y:49:C:OP2	2.23	0.46
1:2A:709:U:H2'	1:2A:710:G:C8	2.51	0.46
1:2A:1163:G:OP1	17:2V:24:LYS:NZ	2.38	0.46
1:2A:1364:G:P	23:21:3:LYS:HG3	2.55	0.46
1:2A:2037:G:H2'	1:2A:2038:G:C8	2.51	0.46
21:2Z:70:LEU:HD22	21:2Z:71:VAL:N	2.29	0.46
32:2a:1106:G:H5"	34:2c:172:ARG:HG2	1.97	0.46
32:2a:1133:G:H1	32:2a:1141:C:N4	2.10	0.46
32:2a:1168:A:C6	32:2a:1169:A:C6	3.03	0.46
32:2a:1251:A:H2'	32:2a:1252:A:C8	2.50	0.46
35:2d:104:VAL:HG21	35:2d:140:VAL:HG21	1.97	0.46
1:1A:286:C:H2'	1:1A:287:C:H6	1.80	0.46
1:1A:2759:G:N7	64:1A:4317:HOH:O	2.35	0.46
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.50	0.46
32:1a:118:U:H3'	32:1a:288:A:H61	1.79	0.46
32:1a:254:G:OP1	48:1q:66:SER:OG	2.28	0.46
33:1b:134:GLU:HA	33:1b:137:ARG:HE	1.81	0.46
54:1w:37:MIA:H162	54:1w:37:MIA:H121	1.72	0.46
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.15	0.46
1:2A:764:A:H5"	3:2D:210:GLY:HA2	1.97	0.46
1:2A:897:C:H5'	54:2w:56:C:OP1	2.15	0.46
1:2A:1580:A:H3'	1:2A:1581:G:H8	1.80	0.46
1:2A:1636:C:OP2	64:2A:3946:HOH:O	2.20	0.46
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:54:G:H21	6:2G:29:TRP:HE1	1.62	0.46
4:2E:48:GLN:HA	4:2E:80:GLU:HA	1.98	0.46
5:2F:137:LYS:HE2	5:2F:137:LYS:HB3	1.50	0.46
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.97	0.46
16:2U:5:LYS:HG2	16:2U:6:THR:N	2.29	0.46
16:2U:105:VAL:HG22	17:2V:45:THR:HG23	1.97	0.46
32:2a:266:G:H2'	32:2a:266:G:N3	2.30	0.46
32:2a:458:C:H2'	32:2a:460:G:O4'	2.15	0.46
32:2a:975:A:N1	41:2j:48:THR:HB	2.30	0.46
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.81	0.46
33:2b:91:PRO:HG3	33:2b:154:LEU:HB2	1.96	0.46
39:2h:10:LEU:HD22	39:2h:83:ILE:HD11	1.96	0.46
1:1A:191:A:H2'	1:1A:192:C:C6	2.49	0.46
1:1A:829:A:N7	1:1A:2248:C:H5'	2.31	0.46
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.29	0.46
1:1A:2136:C:N4	1:1A:2155:G:C6	2.84	0.46
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.50	0.46
1:1A:2722:G:H2'	1:1A:2723:C:C6	2.50	0.46
32:1a:236:G:H5"	48:1q:42:TYR:OH	2.14	0.46
32:1a:691:G:H2'	32:1a:692:U:C6	2.51	0.46
32:1a:1343:G:H1'	40:1i:121:ARG:NH1	2.29	0.46
32:1a:1458:G:OP1	51:1t:35:THR:OG1	2.19	0.46
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.51	0.46
1:2A:883:G:N1	1:2A:894:C:O2	2.46	0.46
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.97	0.46
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.29	0.46
8:2I:96:ASP:O	8:2I:100:ALA:N	2.49	0.46
19:2X:35:THR:HG22	19:2X:37:THR:N	2.29	0.46
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.97	0.46
32:2a:859:A:H2'	32:2a:860:A:O4'	2.14	0.46
33:2b:24:TRP:CH2	33:2b:26:PRO:HA	2.50	0.46
33:2b:158:LEU:HD12	33:2b:158:LEU:H	1.80	0.46
34:2c:181:ASN:ND2	34:2c:204:LEU:HD12	2.30	0.46
35:2d:52:SER:O	35:2d:56:VAL:HG23	2.15	0.46
44:2m:40:ASN:HB3	44:2m:43:THR:HG23	1.96	0.46
45:2n:33:VAL:HA	45:2n:40:CYS:HA	1.97	0.46
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.15	0.46
1:1A:2464:C:H1'	64:1A:4463:HOH:O	2.16	0.46
2:1B:66:A:H61	2:1B:108:U:H2'	1.80	0.46
3:1D:6:PHE:HE2	3:1D:18:VAL:HG13	1.81	0.46
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1Y:34:LYS:NZ	64:1Y:301:HOH:O	2.48	0.46
32:1a:736:C:H2'	32:1a:737:A:C8	2.50	0.46
32:1a:1148:U:H2'	32:1a:1149:C:O4'	2.14	0.46
32:1a:1255:G:N7	41:1j:43:ARG:NH2	2.64	0.46
32:1a:1262:C:H2'	32:1a:1263:C:C6	2.51	0.46
33:1b:16:HIS:CD2	33:1b:17:PHE:N	2.84	0.46
33:1b:134:GLU:HA	33:1b:137:ARG:NE	2.31	0.46
1:2A:795:C:H2'	1:2A:796:C:C6	2.50	0.46
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.51	0.46
1:2A:2112:G:C6	1:2A:2113:U:H1'	2.50	0.46
8:2I:87:LYS:HA	8:2I:121:LYS:O	2.15	0.46
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.15	0.46
21:2Z:70:LEU:HD22	21:2Z:71:VAL:H	1.81	0.46
32:2a:560:U:H5'	32:2a:566:G:N2	2.30	0.46
32:2a:1089:G:H1	32:2a:1096:C:N4	2.12	0.46
32:2a:1180:A:OP1	40:2i:103:THR:OG1	2.32	0.46
40:2i:5:TYR:OH	40:2i:16:ARG:HG2	2.15	0.46
42:2k:98:LEU:O	42:2k:101:SER:OG	2.30	0.46
49:2r:33:ASP:OD2	49:2r:36:ASN:HB2	2.16	0.46
8:1I:75:LEU:O	8:1I:141:LYS:NZ	2.43	0.46
11:1P:135:LEU:HD23	11:1P:135:LEU:HA	1.77	0.46
32:1a:509:A:HO2'	32:1a:510:A:P	2.37	0.46
32:1a:691:G:OP2	42:1k:26:ASN:ND2	2.41	0.46
41:1j:38:ILE:HG13	41:1j:71:LEU:HB3	1.98	0.46
56:1y:6:G:C6	56:1y:7:A:C6	3.04	0.46
1:2A:1580:A:H8	1:2A:1580:A:OP2	1.97	0.46
1:2A:2112:G:N1	1:2A:2113:U:H1'	2.31	0.46
16:2U:86:ALA:HB2	16:2U:116:ALA:HB2	1.97	0.46
28:26:12:GLU:OE1	28:26:19:ARG:NH1	2.49	0.46
32:2a:444:C:H2'	32:2a:445:G:C8	2.51	0.46
32:2a:1518:MA6:H93	32:2a:1519:MA6:H92	1.98	0.46
33:2b:124:SER:HB3	33:2b:125:PRO:HD3	1.97	0.46
34:2c:32:LEU:O	34:2c:36:ASP:HB2	2.15	0.46
38:2g:26:PHE:CD2	38:2g:62:PHE:HE1	2.33	0.46
47:2p:15:PRO:HD2	47:2p:42:ARG:HD2	1.97	0.46
1:1A:880:G:H1	1:1A:898:C:N4	2.11	0.46
1:1A:1187:G:H5"	17:1V:81:TYR:CE1	2.51	0.46
6:1G:7:LEU:N	6:1G:104:GLU:OE1	2.45	0.46
8:1I:38:LEU:HG	8:1I:40:THR:HG23	1.98	0.46
18:1W:1:MET:HE3	18:1W:2:GLU:H	1.81	0.46
26:14:63:TYR:N	26:14:63:TYR:CD1	2.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:353:A:H5'	32:1a:353:A:H8	1.81	0.46
38:1g:69:VAL:HG12	38:1g:100:ALA:HA	1.97	0.46
1:2A:234:C:H2'	1:2A:235:U:H6	1.81	0.46
1:2A:247:G:H4'	1:2A:386:G:C5	2.51	0.46
1:2A:2114:A:N7	1:2A:2170:A:N6	2.64	0.46
6:2G:43:LEU:HD11	6:2G:153:ARG:HG2	1.97	0.46
8:2I:45:LYS:HD3	8:2I:45:LYS:HA	1.71	0.46
11:2P:81:GLN:HE22	11:2P:106:LEU:HA	1.81	0.46
16:2U:104:GLN:NE2	16:2U:105:VAL:HG23	2.29	0.46
30:28:6:THR:HG21	30:28:11:LYS:HD2	1.97	0.46
32:2a:603:U:H2'	32:2a:604:G:C8	2.51	0.46
33:2b:107:THR:O	33:2b:110:GLN:HB3	2.16	0.46
33:2b:212:GLN:NE2	33:2b:235:SER:HA	2.30	0.46
40:2i:37:PHE:HB3	40:2i:43:ALA:HB2	1.97	0.46
54:2w:25:C:H2'	54:2w:26:A:C8	2.51	0.46
56:2y:2:C:H2'	56:2y:3:C:C6	2.50	0.46
1:1A:1021:A:H3'	1:1A:1021:A:N3	2.31	0.46
1:1A:1184:G:H5'	25:13:29:ARG:HH12	1.81	0.46
11:1P:1:MET:HB2	11:1P:1:MET:HE3	1.65	0.46
21:1Z:72:ARG:NH2	21:1Z:97:GLU:O	2.48	0.46
32:1a:973:G:H3'	32:1a:974:A:H5"	1.98	0.46
35:1d:172:PRO:C	35:1d:174:LEU:H	2.23	0.46
44:1m:3:ARG:HG3	44:1m:4:ILE:N	2.31	0.46
56:1y:67:C:H2'	56:1y:68:C:C6	2.49	0.46
1:2A:321:G:OP1	5:2F:135:LYS:NZ	2.49	0.46
1:2A:500:G:N1	1:2A:503:A:OP2	2.48	0.46
1:2A:1866:C:H2'	1:2A:1876:A:O4'	2.15	0.46
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.34	0.46
5:2F:18:ARG:HB3	5:2F:19:GLU:H	1.52	0.46
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.41	0.46
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.98	0.46
25:23:6:VAL:HA	25:23:56:VAL:HG22	1.97	0.46
32:2a:352:C:O2'	32:2a:354:G:OP1	2.30	0.46
32:2a:1190:G:H5'	34:2c:176:HIS:CE1	2.51	0.46
32:2a:1255:G:OP1	41:2j:45:ARG:NH2	2.49	0.46
33:2b:223:ILE:HA	33:2b:226:ARG:HG2	1.98	0.46
1:1A:821:A:H2'	1:1A:946:G:H5"	1.96	0.46
1:1A:1506:C:H2'	1:1A:1507:A:C8	2.51	0.46
21:1Z:52:SER:O	21:1Z:54:HIS:N	2.47	0.46
21:1Z:151:HIS:CE1	21:1Z:170:THR:HG22	2.50	0.46
35:1d:30:LYS:HA	35:1d:35:ARG:NH1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1e:10:MET:H	36:1e:10:MET:HG2	1.62	0.46
36:1e:78:HIS:CE1	36:1e:143:ARG:H	2.32	0.46
37:1f:38:GLU:HB2	37:1f:64:GLN:HG2	1.97	0.46
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.34	0.46
8:2I:127:VAL:CG2	8:2I:139:GLN:HB3	2.46	0.46
15:2T:55:ASN:HB3	15:2T:58:ASN:HB2	1.96	0.46
21:2Z:73:GLN:O	21:2Z:87:ASP:N	2.46	0.46
33:2b:149:LEU:HD22	33:2b:152:PHE:CD2	2.51	0.46
35:2d:191:ARG:HA	35:2d:191:ARG:HD2	1.80	0.46
36:2e:146:ALA:O	36:2e:150:ARG:HG2	2.16	0.46
42:2k:67:ASP:OD1	42:2k:71:LYS:HE3	2.15	0.46
1:1A:858:U:O2	1:1A:2268:A:H2'	2.15	0.46
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.51	0.46
2:1B:103:G:N2	21:1Z:73:GLN:HE22	2.14	0.46
12:1Q:10:ARG:HH11	12:1Q:11:LYS:HE2	1.81	0.46
24:12:51:ARG:O	24:12:55:ARG:HG3	2.16	0.46
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.51	0.46
32:1a:148:G:H2'	32:1a:149:A:H8	1.81	0.46
32:1a:1212:U:H4'	32:1a:1213:A:C8	2.51	0.46
35:1d:178:VAL:C	35:1d:180:GLY:H	2.23	0.46
56:1y:28:G:H2'	56:1y:29:G:C8	2.51	0.46
56:1y:69:G:C2	56:1y:70:G:H1'	2.50	0.46
1:2A:340:A:H2'	1:2A:341:G:O4'	2.16	0.46
1:2A:796:C:H2'	1:2A:797:C:C6	2.51	0.46
1:2A:1503:U:H2'	1:2A:1504:C:C6	2.50	0.46
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.31	0.46
21:2Z:91:LEU:HD12	21:2Z:96:VAL:HG11	1.98	0.46
33:2b:74:LYS:O	33:2b:78:GLN:HG3	2.16	0.46
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.51	0.46
54:2w:10:G:H2'	54:2w:11:C:C6	2.51	0.46
22:10:82:ARG:HE	22:10:82:ARG:HB2	1.45	0.46
32:1a:445:G:H2'	32:1a:446:G:O4'	2.16	0.46
32:1a:453:A:C5	32:1a:454:C:C4	3.03	0.46
32:1a:1107:C:OP1	34:1c:172:ARG:HG3	2.16	0.46
33:1b:59:GLU:HB2	33:1b:221:LEU:HD11	1.97	0.46
36:1e:105:VAL:HB	36:1e:106:PRO:HD3	1.96	0.46
40:1i:14:VAL:HG23	40:1i:66:ARG:O	2.16	0.46
41:1j:85:LEU:C	41:1j:87:THR:H	2.23	0.46
1:2A:265:A:H1'	1:2A:266:G:O4'	2.15	0.46
1:2A:515:A:H1'	1:2A:581:C:H1'	1.98	0.46
1:2A:1453:U:O2'	1:2A:1455:G:N7	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2131:G:H4'	1:2A:2132:U:H3'	1.96	0.46
1:2A:2572:A:C8	4:2E:144:ARG:HD3	2.50	0.46
18:2W:86:LEU:HD22	18:2W:96:ILE:HD11	1.97	0.46
33:2b:111:ARG:HA	33:2b:111:ARG:HD3	1.70	0.46
34:2c:156:ARG:HB3	34:2c:160:ALA:O	2.16	0.46
35:2d:72:GLU:OE2	35:2d:207:TYR:OH	2.34	0.46
43:2l:8:ASN:O	43:2l:12:ARG:HG3	2.16	0.46
43:2l:27:LEU:HD23	43:2l:33:ARG:HB2	1.97	0.46
1:1A:305:U:H2'	1:1A:306:U:C6	2.51	0.45
1:1A:657:U:H2'	1:1A:658:C:C6	2.51	0.45
1:1A:1079:C:H2'	1:1A:1080:C:O4'	2.16	0.45
1:1A:2130:U:H2'	1:1A:2158:A:H61	1.81	0.45
11:1P:85:LEU:HG	11:1P:115:LEU:O	2.16	0.45
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.16	0.45
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.98	0.45
41:1j:27:ALA:HA	41:1j:81:THR:HG21	1.98	0.45
56:1y:66:U:H2'	56:1y:67:C:C6	2.51	0.45
7:2H:140:LYS:HE3	7:2H:140:LYS:HB2	1.74	0.45
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.97	0.45
20:2Y:5:MET:HE1	20:2Y:32:PRO:HA	1.97	0.45
33:2b:187:LEU:HD23	33:2b:188:ALA:N	2.32	0.45
35:2d:121:VAL:O	35:2d:134:ASP:HA	2.16	0.45
36:2e:95:ALA:O	36:2e:97:GLY:N	2.49	0.45
41:2j:23:ILE:HD13	41:2j:23:ILE:HA	1.80	0.45
42:2k:98:LEU:HA	42:2k:101:SER:HB3	1.98	0.45
42:2k:99:GLN:HG2	42:2k:105:VAL:HG21	1.98	0.45
1:1A:710:G:H2'	1:1A:711:G:C8	2.51	0.45
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.99	0.45
21:1Z:31:ARG:H	21:1Z:31:ARG:HG3	1.47	0.45
32:1a:119:A:H4'	32:1a:120:A:C8	2.51	0.45
32:1a:250:A:H4'	32:1a:251:G:O5'	2.14	0.45
32:1a:1278:U:H5"	32:1a:1279:A:O4'	2.17	0.45
32:1a:1293:G:H2'	32:1a:1294:G:C8	2.52	0.45
38:1g:12:LEU:HD12	38:1g:12:LEU:H	1.81	0.45
1:2A:1142(A):A:O2'	1:2A:1143:A:H3'	2.17	0.45
1:2A:1219:G:H1	1:2A:1230:C:H42	1.64	0.45
1:2A:2010:G:H5"	18:2W:42:ARG:HB2	1.98	0.45
9:2N:73:THR:HB	9:2N:82:LEU:HD11	1.98	0.45
29:27:24:THR:HG22	29:27:26:GLY:N	2.32	0.45
33:2b:163:PHE:CD1	33:2b:185:ILE:HG13	2.51	0.45
1:1A:880:G:H8	1:1A:880:G:OP2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1164:G:H2'	1:1A:1165:U:C6	2.52	0.45
1:1A:2123:G:H2'	1:1A:2124:G:C8	2.51	0.45
1:1A:2139:C:H2'	1:1A:2140:C:O4'	2.16	0.45
25:13:23:LEU:HD13	25:13:50:VAL:HG11	1.97	0.45
44:1m:3:ARG:HG3	44:1m:4:ILE:H	1.81	0.45
1:2A:14:A:N6	1:2A:15:G:C2	2.85	0.45
1:2A:861:A:N3	2:2B:79:C:O2'	2.49	0.45
1:2A:931:G:O2'	25:23:24:LYS:HE2	2.16	0.45
1:2A:994:C:H3'	16:2U:54:LYS:HE3	1.98	0.45
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.31	0.45
1:2A:2150:U:H2'	1:2A:2151:G:H8	1.81	0.45
1:2A:2819:G:N7	64:2A:4020:HOH:O	2.36	0.45
28:26:9:LEU:HD21	28:26:25:LYS:HB3	1.99	0.45
28:26:10:LEU:HB2	28:26:52:VAL:HG12	1.97	0.45
32:2a:1119:C:OP2	40:2i:9:ARG:NH2	2.49	0.45
41:2j:8:LEU:HG	41:2j:70:ARG:HB2	1.99	0.45
47:2p:28:ARG:HG2	47:2p:29:ASP:OD1	2.17	0.45
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.52	0.45
6:1G:3:LEU:O	6:1G:8:LYS:NZ	2.35	0.45
12:1Q:56:ARG:HH22	12:1Q:59:ARG:NH2	2.14	0.45
13:1R:28:LEU:HD23	13:1R:48:VAL:HG21	1.97	0.45
19:1X:88:LYS:NZ	19:1X:90:GLU:OE1	2.33	0.45
35:1d:31:CYS:HB2	61:1d:302:SF4:S3	2.56	0.45
39:1h:124:ALA:O	39:1h:128:GLY:N	2.49	0.45
1:2A:1782:C:H1'	1:2A:2609:U:H5"	1.98	0.45
1:2A:2166:G:N7	1:2A:2167:U:H2'	2.31	0.45
10:2O:29:ASN:N	10:2O:29:ASN:OD1	2.50	0.45
32:2a:22:G:H4'	32:2a:885:G:C8	2.52	0.45
32:2a:1226:C:OP2	44:2m:91:ARG:NH1	2.50	0.45
32:2a:1280:A:O2'	32:2a:1281:U:H5'	2.17	0.45
37:2f:100:ASN:C	49:2r:28:GLU:HG3	2.41	0.45
44:2m:3:ARG:O	44:2m:57:ARG:NH2	2.42	0.45
32:1a:73:G:H1	32:1a:96:U:H3	1.64	0.45
34:1c:69:HIS:CD2	34:1c:104:GLN:HG2	2.52	0.45
36:1e:142:LEU:O	36:1e:143:ARG:NH1	2.47	0.45
37:1f:60:PHE:O	37:1f:61:LEU:HD12	2.17	0.45
51:1t:77:ALA:O	51:1t:81:LYS:HG3	2.16	0.45
1:2A:657:U:H2'	1:2A:658:C:C6	2.51	0.45
1:2A:731:C:OP1	64:2A:3950:HOH:O	2.21	0.45
1:2A:907:U:HO2'	12:2Q:101:ARG:HH22	1.61	0.45
1:2A:1425:G:C6	1:2A:1426:G:C6	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1639:U:C2'	1:2A:1640:C:H5"	2.46	0.45
1:2A:1837:C:OP1	32:2a:784:C:H4'	2.17	0.45
1:2A:2741:A:H2'	1:2A:2742:C:O4'	2.16	0.45
3:2D:2:ALA:N	3:2D:200:ASP:OD2	2.50	0.45
4:2E:119:ARG:HG2	4:2E:120:TRP:NE1	2.31	0.45
12:2Q:32:TYR:OH	12:2Q:111:GLU:OE2	2.34	0.45
12:2Q:63:LYS:HG2	12:2Q:65:PHE:CE2	2.51	0.45
32:2a:1020:U:H2'	32:2a:1021:G:C8	2.52	0.45
34:2c:18:TRP:HE3	34:2c:18:TRP:H	1.63	0.45
34:2c:37:GLN:O	34:2c:40:ARG:N	2.49	0.45
34:2c:138:VAL:HG13	34:2c:149:ALA:HB3	1.99	0.45
44:2m:23:TYR:HE2	44:2m:70:LEU:HD22	1.81	0.45
56:2y:74:C:H2'	56:2y:75:C:C6	2.51	0.45
1:1A:234:C:H2'	1:1A:235:U:H6	1.82	0.45
1:1A:671:C:N4	64:1A:4444:HOH:O	2.49	0.45
1:1A:998:C:OP1	64:1A:4243:HOH:O	2.21	0.45
1:1A:2176:A:H2'	1:1A:2177:C:C6	2.51	0.45
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.51	0.45
21:1Z:1:MET:HA	21:1Z:2:GLU:HA	1.68	0.45
32:1a:78:G:C2	32:1a:91:C:N3	2.84	0.45
32:1a:276:G:O3'	48:1q:68:ARG:NH1	2.49	0.45
32:1a:690:G:C6	32:1a:691:G:C6	3.05	0.45
32:1a:872:A:C8	32:1a:874:G:C8	3.05	0.45
32:1a:1145:C:H4'	32:1a:1146:A:H5'	1.98	0.45
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.98	0.45
6:2G:145:THR:O	6:2G:148:MET:HG2	2.17	0.45
7:2H:11:VAL:HG21	7:2H:50:VAL:HG23	1.98	0.45
19:2X:44:GLU:HG3	19:2X:51:VAL:HG23	1.99	0.45
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.99	0.45
32:2a:405:U:O4	35:2d:2:GLY:N	2.50	0.45
32:2a:1152:A:H5'	41:2j:13:HIS:CD2	2.52	0.45
34:2c:119:ARG:HE	34:2c:140:ARG:NH2	2.14	0.45
35:2d:101:LEU:O	35:2d:104:VAL:HG22	2.17	0.45
51:2t:92:LEU:HD23	51:2t:92:LEU:HA	1.87	0.45
56:2y:36:A:H2'	56:2y:37:MIA:O4'	2.16	0.45
1:1A:7:G:H2'	1:1A:8:A:O4'	2.16	0.45
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.52	0.45
8:1I:78:THR:O	8:1I:104:GLN:NE2	2.41	0.45
32:1a:679:C:H2'	32:1a:680:C:C6	2.52	0.45
33:1b:178:ARG:NH2	39:1h:74:PRO:HB3	2.31	0.45
36:1e:18:ARG:HH11	36:1e:27:ARG:HH12	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1e:84:PHE:CE2	36:1e:133:TYR:HD2	2.35	0.45
51:1t:10:LEU:HD12	51:1t:12:ALA:HB2	1.99	0.45
1:2A:212:G:H2'	1:2A:213:A:O4'	2.17	0.45
1:2A:579:G:H2'	1:2A:580:C:C6	2.51	0.45
1:2A:631:A:H2'	1:2A:632:A:O4'	2.15	0.45
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.52	0.45
1:2A:2161:C:H2'	1:2A:2162:G:O4'	2.17	0.45
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.51	0.45
8:2I:85:GLU:O	8:2I:86:THR:OG1	2.33	0.45
10:2O:2:ILE:HD12	10:2O:6:THR:HG21	1.99	0.45
15:2T:16:ARG:HB3	15:2T:18:ASP:OD1	2.17	0.45
20:2Y:28:LYS:HD2	20:2Y:40:GLU:HG2	1.98	0.45
29:27:24:THR:HG22	29:27:26:GLY:H	1.81	0.45
32:2a:1005:A:H3'	32:2a:1006:C:C6	2.51	0.45
34:2c:104:GLN:HG3	34:2c:105:GLU:N	2.31	0.45
34:2c:131:ARG:HE	34:2c:135:LYS:NZ	2.14	0.45
35:2d:173:TRP:CD2	35:2d:189:PRO:HB3	2.52	0.45
36:2e:41:VAL:O	36:2e:66:MET:HA	2.17	0.45
17:1V:24:LYS:HE2	17:1V:24:LYS:HB3	1.68	0.45
20:1Y:87:LYS:HD2	20:1Y:95:LYS:HD3	1.99	0.45
21:1Z:121:HIS:NE2	21:1Z:169:GLU:OE2	2.46	0.45
32:1a:263:A:OP1	51:1t:79:ARG:NH1	2.50	0.45
32:1a:1343:G:H2'	32:1a:1344:C:C6	2.52	0.45
37:1f:100:ASN:HB2	49:1r:28:GLU:HA	1.98	0.45
42:1k:59:TYR:CZ	42:1k:63:LEU:HD11	2.52	0.45
55:1x:8:4SU:O2	55:1x:21:A:H2	2.00	0.45
1:2A:2853:C:H2'	1:2A:2854:G:C8	2.52	0.45
9:2N:73:THR:HG22	9:2N:84:LYS:HG2	1.99	0.45
32:2a:1056:U:H5'	34:2c:163:ALA:HB2	1.97	0.45
32:2a:1318:A:H1'	50:2s:37:ARG:HE	1.81	0.45
1:1A:39:C:H2'	1:1A:40:C:C6	2.51	0.45
1:1A:784:A:N6	3:1D:229:VAL:HG11	2.32	0.45
1:1A:1052:C:H2'	1:1A:1053:C:H6	1.82	0.45
1:1A:2319:G:H1	14:1S:3:ARG:HA	1.82	0.45
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.98	0.45
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.99	0.45
6:1G:115:ARG:HG2	6:1G:136:ARG:HH22	1.81	0.45
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.97	0.45
32:1a:486:U:H2'	32:1a:487:A:C8	2.50	0.45
32:1a:509:A:O2'	32:1a:510:A:OP1	2.23	0.45
33:1b:21:ARG:HB3	33:1b:39:ILE:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:119:GLU:OE2	33:1b:153:ARG:NH1	2.45	0.45
40:1i:19:LEU:HD11	40:1i:85:LEU:HG	1.99	0.45
43:1l:110:VAL:O	43:1l:122:THR:OG1	2.35	0.45
51:1t:60:GLU:HG3	51:1t:81:LYS:HD2	1.98	0.45
1:2A:1283:G:O2'	1:2A:1285:G:N7	2.43	0.45
1:2A:2651:C:H42	1:2A:2669:G:H1	1.64	0.45
5:2F:10:PRO:HB3	5:2F:17:ARG:NH1	2.32	0.45
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.99	0.45
26:24:48:ARG:HA	26:24:48:ARG:HD2	1.81	0.45
55:2x:50:U:H3	55:2x:64:G:H1	1.65	0.45
28:16:47:THR:HG22	28:16:48:VAL:O	2.16	0.45
32:1a:189(D):C:H2'	32:1a:189(E):U:O4'	2.17	0.45
56:1y:36:A:H2'	56:1y:37:MIA:O4'	2.17	0.45
1:2A:407:G:H2'	1:2A:408:G:C8	2.52	0.45
1:2A:868:U:C4	1:2A:869:G:N7	2.85	0.45
1:2A:1341:U:OP2	1:2A:1394:U:O2'	2.29	0.45
1:2A:2116:G:N7	1:2A:2166:G:N2	2.64	0.45
5:2F:180:GLY:O	5:2F:182:ASN:ND2	2.43	0.45
7:2H:70:THR:HG22	7:2H:74:ASN:HD21	1.81	0.45
20:2Y:5:MET:HB2	20:2Y:5:MET:HE2	1.65	0.45
21:2Z:23:LYS:HD3	21:2Z:23:LYS:HA	1.72	0.45
32:2a:1032:G:H2'	32:2a:1033:G:C8	2.52	0.45
48:2q:45:HIS:CD2	48:2q:47:PRO:HG3	2.52	0.45
48:2q:45:HIS:HB3	48:2q:72:ARG:HG2	2.00	0.45
54:2w:9:A:H5'	54:2w:46:G7M:N3	2.32	0.45
1:1A:579:G:H2'	1:1A:580:C:C6	2.52	0.44
1:1A:881:G:H3'	1:1A:882:G:H8	1.82	0.44
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.51	0.44
1:1A:1116:C:H5'	1:1A:1117:G:OP2	2.16	0.44
5:1F:39:TRP:CZ2	5:1F:43:LYS:HE2	2.53	0.44
26:14:16:CYS:SG	26:14:17:GLY:N	2.90	0.44
29:17:24:THR:HG23	64:17:202:HOH:O	2.17	0.44
32:1a:767:A:H2'	32:1a:768:A:O4'	2.17	0.44
32:1a:977:A:H1'	32:1a:982:U:O4	2.16	0.44
36:1e:12:LEU:HB3	36:1e:31:LEU:HB2	2.00	0.44
39:1h:119:LEU:HB3	39:1h:123:GLU:HB2	1.99	0.44
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.52	0.44
1:2A:2102:U:H2'	1:2A:2103:C:C6	2.51	0.44
1:2A:2484:G:C2	1:2A:2485:G:C8	3.04	0.44
5:2F:28:ILE:HD11	5:2F:115:ALA:HB3	1.99	0.44
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:187:VAL:HG11	11:2P:6:LEU:HD11	2.00	0.44
15:2T:51:ARG:HG3	15:2T:98:LYS:HD2	1.98	0.44
32:2a:429:U:OP2	35:2d:36:ARG:NH2	2.45	0.44
32:2a:1058:G:H2'	32:2a:1059:C:C6	2.52	0.44
32:2a:1228:C:H2'	32:2a:1229:A:H8	1.83	0.44
33:2b:162:ILE:HD11	33:2b:177:ALA:HB2	1.99	0.44
35:2d:133:VAL:HG12	35:2d:135:LEU:H	1.82	0.44
38:2g:71:PRO:HG3	38:2g:103:TRP:CH2	2.52	0.44
40:2i:85:LEU:HB3	40:2i:92:TYR:CD2	2.47	0.44
49:2r:56:THR:HG21	49:2r:63:GLN:HE22	1.81	0.44
1:1A:1059:G:H2'	1:1A:1060:U:C5	2.52	0.44
1:1A:2029:G:H2'	1:1A:2031:A:OP1	2.17	0.44
7:1H:37:VAL:HG22	7:1H:68:THR:HG23	2.00	0.44
11:1P:38:GLN:O	11:1P:39:LYS:HB3	2.17	0.44
17:1V:72:VAL:HB	17:1V:85:LYS:HG2	1.99	0.44
26:14:56:VAL:HB	26:14:60:GLN:HG3	1.99	0.44
32:1a:269:C:H2'	32:1a:270:A:C8	2.53	0.44
32:1a:1126:U:O2	32:1a:1280:A:H2'	2.17	0.44
37:1f:100:ASN:C	49:1r:28:GLU:HG3	2.43	0.44
46:1o:74:ASP:HB3	46:1o:77:ARG:HB2	1.98	0.44
51:1t:25:ARG:O	51:1t:29:LYS:HG3	2.16	0.44
1:2A:330:A:H2	1:2A:1210:A:O2'	1.99	0.44
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.47	0.44
1:2A:2393:A:H5"	11:2P:63:PRO:HB3	1.99	0.44
10:2O:98:VAL:HG22	10:2O:118:ALA:HA	1.99	0.44
32:2a:1146:A:H2'	32:2a:1147:C:O4'	2.17	0.44
32:2a:1517:G:N7	32:2a:1518:MA6:H103	2.32	0.44
34:2c:23:TYR:HB2	41:2j:10:GLY:HA2	1.99	0.44
34:2c:149:ALA:HA	34:2c:201:TYR:O	2.16	0.44
38:2g:26:PHE:HE2	38:2g:124:LEU:HD11	1.82	0.44
1:1A:184:C:H2'	1:1A:185:U:C6	2.51	0.44
1:1A:429:A:OP2	64:1A:4245:HOH:O	2.21	0.44
1:1A:862:G:H2'	1:1A:863:A:O4'	2.18	0.44
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.82	0.44
1:1A:2074:U:H2'	1:1A:2075:U:C6	2.52	0.44
1:1A:2251:OMG:HM23	1:1A:2251:OMG:H1'	1.84	0.44
8:1I:81:VAL:O	8:1I:146:ALA:HA	2.18	0.44
13:1R:103:ARG:HD2	13:1R:108:GLY:O	2.17	0.44
29:17:24:THR:HG22	29:17:27:GLY:N	2.13	0.44
35:1d:59:ARG:HH12	35:1d:62:GLN:HB2	1.83	0.44
39:1h:49:GLU:HG2	39:1h:62:TYR:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:1y:19:G:N1	56:1y:56:C:N4	2.64	0.44
1:2A:1022:G:N2	1:2A:1023:U:O4	2.48	0.44
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.52	0.44
11:2P:98:GLU:O	11:2P:102:ARG:HG3	2.17	0.44
12:2Q:17:LEU:HB3	12:2Q:39:PRO:HB2	1.97	0.44
32:2a:947:G:H1	32:2a:1234:C:N4	2.13	0.44
32:2a:952:U:H2'	32:2a:953:G:H8	1.82	0.44
50:2s:27:GLU:H	50:2s:27:GLU:HG2	1.51	0.44
4:1E:54:GLN:NE2	4:1E:76:ARG:HG2	2.33	0.44
5:1F:122:LYS:HD2	5:1F:191:ARG:HG2	2.00	0.44
32:1a:439:A:C5	32:1a:441:A:H1'	2.52	0.44
37:1f:61:LEU:HD23	37:1f:63:TYR:CE2	2.52	0.44
50:1s:27:GLU:HG2	50:1s:28:LYS:HG2	1.99	0.44
54:1w:26:A:N6	54:1w:44:G:H1	2.12	0.44
1:2A:2125:G:H2'	1:2A:2126:A:C8	2.52	0.44
1:2A:2206:G:H8	1:2A:2207:G:N7	2.15	0.44
1:2A:2626:C:H2'	1:2A:2627:G:O4'	2.18	0.44
26:24:1:MET:HE2	26:24:6:HIS:CD2	2.53	0.44
1:1A:81:G:H21	20:1Y:1:MET:HE1	1.82	0.44
1:1A:637:A:H2'	11:1P:117:GLU:OE1	2.18	0.44
1:1A:2158:A:H1'	1:1A:2159:G:O4'	2.18	0.44
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.52	0.44
5:1F:14:PRO:HD2	5:1F:127:GLU:OE1	2.17	0.44
26:14:53:GLU:H	26:14:53:GLU:HG3	1.50	0.44
32:1a:96:U:H2'	32:1a:97:G:H8	1.83	0.44
32:1a:555:C:H2'	32:1a:556:C:C6	2.52	0.44
1:2A:882:G:H2'	1:2A:883:G:C8	2.53	0.44
1:2A:1125:G:H5'	31:29:37:GLY:HA2	1.99	0.44
1:2A:2097:C:H2'	1:2A:2098:U:O4'	2.17	0.44
1:2A:2120:G:H2'	1:2A:2121:G:C8	2.53	0.44
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.52	0.44
1:2A:2649:U:H2'	1:2A:2650:U:C6	2.53	0.44
6:2G:116:ASP:OD2	44:2m:68:GLY:HA3	2.17	0.44
32:2a:297:G:N2	32:2a:300:A:OP2	2.50	0.44
32:2a:529:G:O6	43:2l:49:ASN:HA	2.18	0.44
48:2q:95:TYR:HA	48:2q:98:LEU:HD12	1.98	0.44
1:1A:886:C:H3'	1:1A:887:A:H5"	1.98	0.44
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.99	0.44
43:1l:77:LEU:HD21	43:1l:107:ALA:HA	2.00	0.44
1:2A:711:G:H1	1:2A:720:C:H42	1.66	0.44
1:2A:1123:C:H1'	31:29:18:ARG:HH21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.33	0.44
11:2P:75:ILE:H	11:2P:75:ILE:HD12	1.83	0.44
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.18	0.44
32:2a:1352:C:H2'	32:2a:1353:G:C8	2.52	0.44
56:2y:19:G:O6	56:2y:56:C:N3	2.51	0.44
1:1A:548:A:H3'	1:1A:548:A:OP2	2.17	0.44
6:1G:99:MET:HE2	6:1G:99:MET:HB3	1.89	0.44
23:11:2:SER:HB3	23:11:46:LEU:HD12	1.99	0.44
32:1a:62:U:OP1	32:1a:385:C:O2'	2.33	0.44
32:1a:584:G:H5'	48:1q:91:ARG:NH2	2.32	0.44
33:1b:16:HIS:C	33:1b:18:GLY:H	2.26	0.44
33:1b:122:PHE:CZ	33:1b:135:GLN:HG3	2.50	0.44
36:1e:24:ARG:H	36:1e:24:ARG:HG2	1.45	0.44
54:1w:9:A:O2'	54:1w:10:G:N7	2.51	0.44
1:2A:141:A:H8	1:2A:1408:C:O2'	2.00	0.44
1:2A:1012:U:C5	9:2N:28:THR:HG21	2.53	0.44
1:2A:1371:G:H2'	1:2A:1372:U:H5	1.82	0.44
5:2F:64:ILE:HD11	5:2F:75:HIS:HB2	1.99	0.44
20:2Y:43:ASN:CG	20:2Y:65:ALA:HB3	2.42	0.44
32:2a:1010:G:H2'	32:2a:1011:G:H8	1.83	0.44
33:2b:219:VAL:O	33:2b:223:ILE:HG13	2.18	0.44
36:2e:83:GLU:HB3	36:2e:88:LYS:HB2	2.00	0.44
41:2j:38:ILE:HG13	41:2j:71:LEU:HD23	2.00	0.44
1:1A:1371:G:H2'	1:1A:1372:U:H5	1.83	0.44
1:1A:1740:G:H2'	1:1A:1741:A:C8	2.53	0.44
7:1H:3:ARG:HD2	7:1H:3:ARG:HA	1.79	0.44
8:1I:4:ILE:HD13	8:1I:47:LEU:HG	1.99	0.44
10:1O:49:ARG:HH12	32:1a:1423:G:P	2.41	0.44
32:1a:78:G:O2'	32:1a:79:G:O5'	2.32	0.44
32:1a:629:G:H2'	32:1a:630:G:C8	2.53	0.44
32:1a:1006:C:N4	32:1a:1023:G:H1	2.14	0.44
33:1b:20:GLU:HG2	33:1b:23:ARG:HH11	1.83	0.44
34:1c:122:GLU:O	34:1c:126:ARG:HD2	2.18	0.44
1:2A:900:A:H2'	1:2A:901:A:C8	2.51	0.44
1:2A:1257:C:H4'	5:2F:83:PHE:CD1	2.53	0.44
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.32	0.44
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.53	0.44
1:2A:2131:G:C8	1:2A:2133:G:C2	3.06	0.44
8:2I:72:LEU:HB2	8:2I:138:ILE:HG21	2.00	0.44
8:2I:137:PRO:O	8:2I:139:GLN:NE2	2.51	0.44
32:2a:153:C:H2'	32:2a:154:C:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:76:GLN:NE2	33:2b:206:ASP:O	2.51	0.44
33:2b:167:PRO:HD3	33:2b:187:LEU:O	2.18	0.44
52:2u:5:ASP:O	52:2u:11:GLY:HA3	2.18	0.44
56:2y:42:C:H2'	56:2y:43:C:H6	1.81	0.44
1:1A:218:A:C2	1:1A:235:U:H4'	2.52	0.44
1:1A:292:C:H2'	1:1A:293:U:C6	2.53	0.44
1:1A:396:G:H1'	23:11:42:GLN:HB3	2.00	0.44
1:1A:1676:A:N7	64:1A:4321:HOH:O	2.36	0.44
1:1A:2576:G:H1'	64:1A:5012:HOH:O	2.18	0.44
2:1B:86:G:H1	2:1B:91:C:H42	1.66	0.44
4:1E:79:ARG:HD3	4:1E:79:ARG:HA	1.79	0.44
32:1a:60:A:H4'	32:1a:61:G:H5'	1.99	0.44
32:1a:562:C:O2	43:1l:16:GLU:N	2.45	0.44
32:1a:828:A:H2'	32:1a:829:G:O4'	2.18	0.44
32:1a:875:C:O2'	39:1h:14:ARG:HD2	2.18	0.44
32:1a:890:G:O2'	32:1a:906:G:O6	2.34	0.44
32:1a:1064:G:O2'	32:1a:1190:G:N2	2.51	0.44
32:1a:1402:4OC:O5'	32:1a:1402:4OC:H6	2.18	0.44
32:1a:1427:U:H2'	32:1a:1428:A:C8	2.53	0.44
34:1c:6:HIS:CD2	34:1c:8:ILE:H	2.24	0.44
34:1c:130:VAL:HG21	34:1c:157:ILE:HG23	1.99	0.44
36:1e:131:ILE:HD13	36:1e:131:ILE:HA	1.87	0.44
44:1m:11:ARG:C	44:1m:13:LYS:H	2.25	0.44
46:1o:82:ILE:O	46:1o:86:GLY:N	2.48	0.44
54:1w:23:A:H3'	54:1w:24:G:C8	2.51	0.44
1:2A:191:A:H2'	1:2A:192:C:C6	2.53	0.44
1:2A:2119:A:N1	1:2A:2170:A:H2'	2.33	0.44
1:2A:2756:U:H1'	1:2A:2757:A:H5"	2.00	0.44
32:2a:130:A:O2'	32:2a:131:C:O5'	2.35	0.44
32:2a:829:G:N7	64:2a:3335:HOH:O	2.36	0.44
32:2a:838:G:H1	32:2a:848:C:N4	2.16	0.44
33:2b:98:LEU:HD13	33:2b:101:MET:HE3	2.00	0.44
36:2e:57:LYS:HE3	36:2e:57:LYS:HB2	1.84	0.44
38:2g:132:GLY:O	38:2g:135:VAL:HG12	2.18	0.44
44:2m:30:ALA:O	44:2m:34:LEU:HG	2.17	0.44
56:2y:34:G:H2'	56:2y:35:A:C8	2.53	0.44
1:1A:154:G:H1	1:1A:172:C:H42	1.66	0.43
1:1A:1065:U:H1'	1:1A:1074:G:N1	2.33	0.43
1:1A:1936:A:OP1	1:1A:1937:A:H5'	2.18	0.43
1:1A:2123:G:H2'	1:1A:2124:G:H8	1.83	0.43
6:1G:72:ARG:HH12	6:1G:87:PRO:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:12:31:GLU:HG2	24:12:53:LEU:HD11	1.99	0.43
32:1a:266:G:H2'	32:1a:266:G:N3	2.33	0.43
32:1a:418:C:H1'	32:1a:540:G:O2'	2.18	0.43
32:1a:1066:C:O2'	32:1a:1067:A:H5'	2.17	0.43
33:1b:87:ARG:CZ	33:1b:233:SER:HB2	2.48	0.43
33:1b:121:LEU:HD21	33:1b:130:ARG:HH21	1.83	0.43
1:2A:1247:A:OP1	5:2F:95:ARG:NH2	2.31	0.43
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.17	0.43
2:2B:54:G:H21	6:2G:29:TRP:NE1	2.15	0.43
7:2H:3:ARG:HH21	7:2H:65:HIS:HB3	1.83	0.43
23:21:89:GLU:O	23:21:93:GLU:HG2	2.18	0.43
32:2a:524:G:H2'	32:2a:525:C:C6	2.53	0.43
32:2a:920:U:H2'	32:2a:921:U:H6	1.83	0.43
32:2a:1025:U:H1'	32:2a:1026:G:C6	2.53	0.43
33:2b:96:ARG:HG2	33:2b:98:LEU:HD12	1.98	0.43
33:2b:167:PRO:HG2	33:2b:192:SER:HB3	1.99	0.43
54:2w:39:PSU:H2'	54:2w:40:C:C6	2.53	0.43
1:1A:583:G:OP2	16:1U:10:ARG:HD2	2.18	0.43
1:1A:899:A:H2'	1:1A:899:A:N3	2.32	0.43
1:1A:1805:U:O2	3:1D:50:THR:HB	2.18	0.43
1:1A:2492:U:H2'	1:1A:2493:U:C6	2.54	0.43
8:1I:117:GLU:HG3	8:1I:118:LYS:H	1.84	0.43
10:1O:20:MET:HE3	64:1O:302:HOH:O	2.18	0.43
32:1a:811:C:O2'	32:1a:901:A:N1	2.47	0.43
32:1a:1108:G:O6	64:1a:1920:HOH:O	2.20	0.43
32:1a:1127:G:H1'	32:1a:1280:A:C6	2.53	0.43
32:1a:1319:A:OP1	50:1s:3:ARG:HD2	2.18	0.43
39:1h:17:THR:O	39:1h:78:GLN:NE2	2.38	0.43
41:1j:75:ILE:O	41:1j:77:PRO:HD3	2.17	0.43
1:2A:122:G:O6	64:2A:3949:HOH:O	2.21	0.43
6:2G:59:GLU:O	6:2G:63:ILE:HG12	2.18	0.43
6:2G:91:ARG:CZ	6:2G:91:ARG:HB3	2.48	0.43
8:2I:47:LEU:O	8:2I:51:ILE:N	2.35	0.43
14:2S:84:GLN:HG3	14:2S:111:GLU:OE1	2.18	0.43
26:24:57:GLU:HA	26:24:58:ARG:HA	1.60	0.43
32:2a:955:U:O2'	50:2s:83:HIS:HD2	2.01	0.43
33:2b:122:PHE:O	33:2b:127:ILE:HB	2.18	0.43
35:2d:20:TYR:CD1	35:2d:26:CYS:HB3	2.49	0.43
48:2q:26:GLN:HG2	48:2q:37:LYS:HG2	1.99	0.43
56:2y:63:G:H2'	56:2y:64:A:C8	2.54	0.43
1:1A:530:G:N1	1:1A:2023:G:OP1	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:548:A:N6	17:1V:19:LYS:H	2.16	0.43
1:1A:710:G:H2'	1:1A:711:G:H8	1.82	0.43
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.18	0.43
1:1A:1062:G:O5'	1:1A:1070:A:O2'	2.35	0.43
1:1A:1069:A:O4'	1:1A:1096:A:O2'	2.36	0.43
1:1A:1641:A:H2'	1:1A:1642:G:O4'	2.17	0.43
21:1Z:72:ARG:HA	21:1Z:72:ARG:HD3	1.71	0.43
23:11:52:ARG:HA	23:11:56:GLN:O	2.19	0.43
32:1a:300:A:H1'	32:1a:565:U:O2	2.18	0.43
32:1a:911:U:H2'	32:1a:912:C:C6	2.53	0.43
32:1a:975:A:H5'	32:1a:975:A:C8	2.51	0.43
32:1a:1302:U:H5	44:1m:17:VAL:HG21	1.82	0.43
33:1b:103:THR:HA	33:1b:180:LEU:HD11	1.99	0.43
34:1c:8:ILE:HG13	34:1c:16:ARG:NE	2.33	0.43
46:1o:8:LYS:HE3	46:1o:31:LEU:HD22	1.99	0.43
56:1y:6:G:O6	56:1y:7:A:N6	2.51	0.43
56:1y:50:U:H2'	56:1y:51:U:C6	2.53	0.43
1:2A:154(A):C:H42	1:2A:171:G:H1	1.66	0.43
1:2A:1311:G:H2'	29:27:47:ARG:NH2	2.33	0.43
1:2A:2292:C:H2'	1:2A:2293:C:C6	2.53	0.43
3:2D:168:ARG:HG2	3:2D:173:VAL:HG12	1.99	0.43
15:2T:91:ARG:HD2	15:2T:120:ARG:NH1	2.33	0.43
15:2T:127:ALA:C	15:2T:129:ARG:N	2.75	0.43
26:24:61:ARG:HD2	26:24:61:ARG:HA	1.79	0.43
33:2b:19:HIS:CE1	33:2b:206:ASP:HB2	2.53	0.43
33:2b:219:VAL:HG22	33:2b:223:ILE:HD11	2.00	0.43
44:2m:20:THR:C	44:2m:22:ILE:H	2.25	0.43
48:2q:76:LEU:HD12	48:2q:77:VAL:H	1.82	0.43
56:2y:52:G:H1	56:2y:62:C:N4	2.15	0.43
1:1A:436:C:H2'	1:1A:437:G:H8	1.84	0.43
1:1A:987:G:O2'	1:1A:1000:A:N3	2.46	0.43
1:1A:2124:G:H1	1:1A:2174:C:H42	1.64	0.43
1:1A:2649:U:H2'	1:1A:2650:U:C6	2.53	0.43
2:1B:52:A:OP2	2:1B:52:A:H8	2.01	0.43
21:1Z:48:PHE:CE1	21:1Z:52:SER:HA	2.53	0.43
32:1a:994:A:N1	32:1a:1047:G:H4'	2.33	0.43
33:1b:109:SER:HA	33:1b:112:VAL:HG13	2.00	0.43
40:1i:50:LEU:HD13	40:1i:56:LEU:HA	1.99	0.43
1:2A:234:C:H2'	1:2A:235:U:C6	2.53	0.43
1:2A:597:U:H2'	1:2A:598:G:H8	1.84	0.43
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2096:U:H2'	1:2A:2097:C:C6	2.54	0.43
1:2A:2318:G:H21	14:2S:3:ARG:HD3	1.83	0.43
22:20:33:ALA:N	22:20:64:ASP:OD1	2.39	0.43
32:2a:340:U:H2'	32:2a:341:C:C6	2.53	0.43
32:2a:1133:G:H2'	32:2a:1134:G:O4'	2.18	0.43
32:2a:1202:G:N2	45:2n:46:GLU:OE2	2.48	0.43
32:2a:1305:G:C2	32:2a:1331:G:N3	2.87	0.43
34:2c:119:ARG:HE	34:2c:140:ARG:CZ	2.31	0.43
35:2d:61:LYS:HG3	35:2d:203:VAL:HG13	2.00	0.43
35:2d:70:ILE:HD11	35:2d:74:GLN:HB3	2.00	0.43
44:2m:67:GLU:HG3	44:2m:71:ARG:NH2	2.32	0.43
1:1A:181:A:H5"	29:17:36:GLN:NE2	2.33	0.43
1:1A:2765:A:OP2	64:1A:4244:HOH:O	2.21	0.43
6:1G:45:GLU:H	6:1G:45:GLU:CD	2.27	0.43
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.54	0.43
38:1g:72:ARG:HD3	38:1g:142:GLU:OE2	2.19	0.43
46:1o:43:LEU:HD12	46:1o:56:LEU:HD22	2.01	0.43
56:1y:68:C:N3	56:1y:69:G:C8	2.86	0.43
56:1y:71:G:H2'	56:1y:72:C:C6	2.53	0.43
1:2A:811:U:H2'	11:2P:21:ARG:HA	2.01	0.43
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.37	0.43
6:2G:26:GLN:N	6:2G:26:GLN:OE1	2.51	0.43
7:2H:86:GLU:OE2	7:2H:130:ARG:NH1	2.51	0.43
8:2I:87:LYS:HB2	8:2I:121:LYS:NZ	2.30	0.43
9:2N:1:MET:HE1	16:2U:94:ASN:ND2	2.34	0.43
9:2N:42:TRP:CH2	9:2N:44:PRO:HB3	2.53	0.43
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.54	0.43
21:2Z:146:ILE:HG23	21:2Z:174:VAL:O	2.19	0.43
26:24:46:GLN:HG2	26:24:48:ARG:H	1.84	0.43
32:2a:120:A:C6	32:2a:122:G:C2	3.07	0.43
32:2a:957:U:O2'	32:2a:959:A:N7	2.43	0.43
32:2a:991:U:C4	32:2a:1212:U:H1'	2.54	0.43
32:2a:1149:C:H2'	32:2a:1150:U:C6	2.54	0.43
36:2e:42:GLY:HA2	36:2e:65:ASN:O	2.18	0.43
50:2s:52:TYR:HB2	50:2s:57:HIS:CE1	2.54	0.43
1:1A:444:C:H5"	64:1A:4487:HOH:O	2.19	0.43
1:1A:839:U:H2'	1:1A:840:C:C6	2.53	0.43
1:1A:1827:C:O2'	1:1A:1970:A:N3	2.47	0.43
1:1A:2817:G:OP1	13:1R:99:LYS:NZ	2.52	0.43
26:14:53:GLU:HB2	26:14:55:ARG:O	2.18	0.43
32:1a:1112:C:H1'	34:1c:179:ARG:HH12	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:108:ASN:ND2	34:1c:144:SER:HB3	2.34	0.43
38:1g:74:GLU:HG2	38:1g:91:VAL:HG22	2.01	0.43
41:1j:57:LYS:HE2	41:1j:60:ARG:NH2	2.34	0.43
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.18	0.43
1:2A:851:U:H5'	25:23:49:LYS:HD2	1.99	0.43
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.19	0.43
1:2A:2387:U:H1'	22:20:41:ARG:HE	1.83	0.43
5:2F:178:PRO:HG2	5:2F:179:GLU:OE2	2.19	0.43
6:2G:111:LEU:HD23	6:2G:117:PHE:CE1	2.54	0.43
7:2H:56:SER:OG	7:2H:57:ASP:N	2.50	0.43
8:2I:56:LYS:O	8:2I:60:GLU:N	2.51	0.43
8:2I:126:TYR:CD2	8:2I:126:TYR:N	2.86	0.43
11:2P:59:LEU:HD11	30:28:10:ALA:HA	2.00	0.43
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	1.99	0.43
29:27:1:MET:HE3	29:27:3:ARG:NH2	2.33	0.43
32:2a:1291:G:C6	32:2a:1292:U:C4	3.06	0.43
35:2d:94:LEU:HD12	35:2d:94:LEU:HA	1.79	0.43
40:2i:16:ARG:HB2	40:2i:64:THR:HG22	2.01	0.43
40:2i:86:VAL:HG13	40:2i:90:PRO:HA	2.00	0.43
41:2j:38:ILE:H	41:2j:38:ILE:HG12	1.59	0.43
1:1A:864:G:O2'	1:1A:865:C:H5'	2.19	0.43
1:1A:1434:A:H2'	1:1A:1435:G:C8	2.53	0.43
1:1A:2756:U:H1'	1:1A:2757:A:H5"	2.00	0.43
3:1D:147:LEU:HD22	3:1D:155:LEU:HD11	2.00	0.43
4:1E:181:LEU:HD23	4:1E:181:LEU:HA	1.79	0.43
11:1P:91:PHE:CD1	11:1P:99:LEU:HD21	2.54	0.43
26:14:63:TYR:HD1	26:14:63:TYR:H	1.65	0.43
32:1a:163:C:H2'	32:1a:164:U:C6	2.54	0.43
32:1a:438:G:H4'	35:1d:123:HIS:ND1	2.34	0.43
32:1a:1315:U:H2'	32:1a:1316:G:O4'	2.19	0.43
33:1b:87:ARG:NH2	33:1b:220:ASP:OD1	2.45	0.43
33:1b:204:ASN:OD1	33:1b:205:ASP:N	2.52	0.43
47:1p:74:LEU:HG	47:1p:79:VAL:HG21	2.01	0.43
1:2A:31:C:H5"	1:2A:1239:G:OP1	2.18	0.43
1:2A:639:U:H2'	1:2A:640:C:C6	2.53	0.43
1:2A:1015:G:O2'	1:2A:1016:G:H5'	2.19	0.43
1:2A:2031:A:N3	1:2A:2455:G:O2'	2.35	0.43
7:2H:8:PRO:O	7:2H:10:PRO:HD3	2.18	0.43
9:2N:35:ARG:O	9:2N:42:TRP:NE1	2.44	0.43
13:2R:103:ARG:HD3	13:2R:108:GLY:O	2.18	0.43
21:2Z:23:LYS:HD3	21:2Z:40:ASP:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:53:GLU:HG2	26:24:55:ARG:N	2.22	0.43
32:2a:109:A:H2'	32:2a:326:G:N2	2.33	0.43
32:2a:502:G:H2'	32:2a:503:C:O4'	2.18	0.43
32:2a:736:C:H2'	32:2a:737:A:C8	2.54	0.43
32:2a:909:A:H2'	32:2a:910:C:O4'	2.19	0.43
32:2a:984:C:H2'	32:2a:985:C:C6	2.53	0.43
32:2a:1236:A:O2'	32:2a:1304:G:H4'	2.19	0.43
32:2a:1260:C:O5'	32:2a:1284:C:H4'	2.19	0.43
34:2c:23:TYR:CG	34:2c:24:ALA:N	2.86	0.43
34:2c:179:ARG:HH12	34:2c:206:GLU:CD	2.24	0.43
42:2k:102:GLY:C	42:2k:103:LEU:HD12	2.43	0.43
1:1A:2143:C:H2'	1:1A:2144:U:O4'	2.19	0.43
2:1B:103:G:H21	21:1Z:73:GLN:NE2	2.15	0.43
3:1D:72:LYS:NZ	3:1D:99:ASP:OD2	2.31	0.43
32:1a:1054:C:C5	54:1w:34:G:H1'	2.53	0.43
33:1b:127:ILE:HD12	33:1b:130:ARG:HD3	2.00	0.43
42:1k:15:ALA:HA	42:1k:76:GLY:O	2.18	0.43
56:1y:55:PSU:C4	56:1y:57:G:H5'	2.53	0.43
1:2A:884:C:H3'	1:2A:885:C:C6	2.53	0.43
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.53	0.43
1:2A:1641:A:H2'	1:2A:1642:G:O4'	2.19	0.43
1:2A:2474:C:H5"	1:2A:2475:C:OP2	2.18	0.43
8:2I:5:LEU:H	8:2I:5:LEU:HD12	1.83	0.43
32:2a:960:U:H1'	32:2a:1222:G:O2'	2.18	0.43
32:2a:1080:A:H5"	32:2a:1081:G:OP2	2.18	0.43
32:2a:1157:A:H5'	32:2a:1158:C:C6	2.54	0.43
35:2d:63:LYS:HB2	35:2d:63:LYS:HE3	1.72	0.43
36:2e:53:LEU:HD12	36:2e:53:LEU:H	1.84	0.43
38:2g:78:ARG:NH2	38:2g:79:ARG:HE	2.13	0.43
42:2k:18:ARG:NH2	42:2k:35:PRO:O	2.50	0.43
52:2u:6:ARG:C	52:2u:8:THR:H	2.27	0.43
1:1A:884:C:N3	1:1A:885:C:O2'	2.47	0.43
1:1A:1843:C:H5'	3:1D:253:GLN:OE1	2.18	0.43
1:1A:2849:U:P	15:1T:95:ARG:HH12	2.41	0.43
2:1B:88:C:H2'	2:1B:89:G:O4'	2.19	0.43
32:1a:1239:A:C4	32:1a:1298:C:N4	2.87	0.43
33:1b:16:HIS:O	33:1b:18:GLY:N	2.52	0.43
33:1b:21:ARG:HH22	33:1b:23:ARG:HD2	1.82	0.43
33:1b:151:GLY:HA2	33:1b:154:LEU:HD13	2.01	0.43
34:1c:65:ALA:HA	34:1c:100:ALA:HB3	2.01	0.43
1:2A:832:G:H5'	11:2P:45:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:912:C:OP1	12:2Q:8:LYS:NZ	2.37	0.43
1:2A:1341:U:O2	19:2X:80:ILE:HD12	2.18	0.43
4:2E:6:GLY:O	4:2E:195:LEU:HD12	2.18	0.43
8:2I:123:LEU:HG	8:2I:144:VAL:O	2.19	0.43
32:2a:256:U:H2'	32:2a:257:G:C8	2.54	0.43
32:2a:1316:G:N2	32:2a:1318:A:H3'	2.33	0.43
33:2b:16:HIS:HB2	33:2b:204:ASN:HB2	2.00	0.43
33:2b:52:GLU:O	33:2b:56:ARG:NH1	2.51	0.43
39:2h:121:ASP:N	39:2h:121:ASP:OD1	2.51	0.43
42:2k:51:LYS:HD2	42:2k:51:LYS:HA	1.80	0.43
47:2p:73:LEU:HD12	47:2p:73:LEU:HA	1.77	0.43
55:2x:76:8AN:H1'	64:2x:205:HOH:O	2.19	0.43
56:2y:9:A:H4'	56:2y:46:G7M:H5'	2.01	0.43
1:1A:234:C:H2'	1:1A:235:U:C6	2.54	0.43
3:1D:71:ASP:CB	3:1D:103:ARG:HH12	2.32	0.43
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.62	0.43
11:1P:27:HIS:HB2	64:1P:305:HOH:O	2.18	0.43
12:1Q:57:HIS:HD2	12:1Q:117:ALA:HB2	1.82	0.43
25:13:8:LEU:HG	25:13:31:LEU:HD23	2.00	0.43
32:1a:664:G:N2	32:1a:741:G:H1	2.01	0.43
32:1a:721:G:H4'	32:1a:722:A:O4'	2.19	0.43
32:1a:1136:U:H5"	32:1a:1137:C:N4	2.34	0.43
36:1e:92:LYS:HB3	36:1e:119:LEU:HB2	2.00	0.43
40:1i:50:LEU:HB3	40:1i:85:LEU:HD11	2.01	0.43
42:1k:20:TYR:CE1	42:1k:83:ILE:HD12	2.54	0.43
45:1n:9:LYS:HG3	45:1n:12:ARG:NH2	2.33	0.43
48:1q:62:SER:OG	48:1q:72:ARG:NE	2.49	0.43
1:2A:1665:A:H2'	1:2A:1666:G:O4'	2.18	0.43
1:2A:2228:G:OP1	3:2D:261:LYS:NZ	2.43	0.43
1:2A:2317:C:H2'	1:2A:2318:G:H5'	2.01	0.43
2:2B:80:U:H2'	2:2B:81:G:C8	2.54	0.43
6:2G:123:ASN:O	6:2G:125:PHE:N	2.47	0.43
10:2O:2:ILE:HB	10:2O:33:ALA:HB3	2.00	0.43
15:2T:27:THR:C	15:2T:89:VAL:HG23	2.44	0.43
22:20:23:VAL:HG22	22:20:38:VAL:HG22	2.01	0.43
32:2a:9:G:H2'	32:2a:10:A:C8	2.54	0.43
32:2a:114:U:H1'	32:2a:353:A:H1'	2.01	0.43
32:2a:522:C:OP2	43:2l:69:TYR:OH	2.28	0.43
32:2a:936:C:H2'	32:2a:937:A:O4'	2.19	0.43
32:2a:1040:U:H2'	32:2a:1041:A:C8	2.53	0.43
32:2a:1368:G:H5"	40:2i:112:LYS:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:63:PHE:HE2	45:2n:45:ARG:HA	1.84	0.43
56:2y:19:G:N1	56:2y:56:C:O2	2.49	0.43
1:1A:340:A:H2'	1:1A:341:G:O4'	2.19	0.42
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.19	0.42
1:1A:1359:A:H2'	1:1A:1360:A:H5'	2.01	0.42
1:1A:1815:A:P	3:1D:54:ARG:HH22	2.42	0.42
1:1A:2478:A:H5'	31:19:31:LYS:HE2	2.00	0.42
16:1U:16:LYS:HB3	16:1U:16:LYS:HE2	1.78	0.42
32:1a:277:C:P	48:1q:68:ARG:HH12	2.41	0.42
32:1a:1003:G:C4	32:1a:1004:A:H2	2.37	0.42
33:1b:8:LYS:H	33:1b:8:LYS:HD3	1.84	0.42
33:1b:155:LEU:HD12	33:1b:155:LEU:HA	1.88	0.42
35:1d:178:VAL:HG12	35:1d:179:GLU:H	1.84	0.42
50:1s:18:LYS:O	50:1s:22:LEU:HG	2.19	0.42
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.55	0.42
1:2A:1512:U:H2'	1:2A:1513:C:C6	2.54	0.42
2:2B:3:C:H2'	2:2B:4:C:H6	1.84	0.42
7:2H:8:PRO:HA	7:2H:51:ARG:HB3	2.01	0.42
32:2a:157:G:C2	32:2a:165:C:C2	3.07	0.42
32:2a:1201:A:H4'	32:2a:1202:G:O5'	2.19	0.42
32:2a:1264:C:N3	32:2a:1272:G:O6	2.52	0.42
33:2b:178:ARG:NH1	33:2b:196:LEU:O	2.49	0.42
34:2c:7:PRO:HG2	34:2c:184:TYR:HB2	2.01	0.42
36:2e:147:ASP:OD1	36:2e:147:ASP:N	2.50	0.42
49:2r:74:ARG:HB3	49:2r:81:PHE:CE1	2.54	0.42
1:1A:816:C:H4'	64:1A:4496:HOH:O	2.18	0.42
1:1A:1093:G:H3'	1:1A:1094:U:H5"	2.02	0.42
1:1A:1503:U:H2'	1:1A:1504:C:C6	2.53	0.42
1:1A:1951:U:H2'	1:1A:1953:A:OP2	2.18	0.42
1:1A:2316:C:O2'	6:1G:128:ARG:NH2	2.52	0.42
9:1N:15:LEU:HB2	9:1N:135:PRO:HB2	2.01	0.42
28:16:12:GLU:OE1	28:16:52:VAL:HG11	2.20	0.42
32:1a:673:G:H2'	32:1a:674:G:C8	2.53	0.42
32:1a:682:G:H2'	32:1a:683:G:O4'	2.18	0.42
32:1a:1060:C:C5	34:1c:2:GLY:HA3	2.54	0.42
32:1a:1262:C:H2'	32:1a:1263:C:H6	1.84	0.42
34:1c:59:ARG:HG2	34:1c:64:VAL:HB	2.00	0.42
35:1d:64:LEU:HB2	35:1d:198:VAL:HG11	2.01	0.42
48:1q:45:HIS:NE2	48:1q:47:PRO:HG3	2.34	0.42
1:2A:567:A:H4'	1:2A:808:G:OP1	2.19	0.42
1:2A:1356:G:OP1	64:2A:3951:HOH:O	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.19	0.42
1:2A:2128:C:H6	1:2A:2128:C:O5'	2.02	0.42
1:2A:2747:G:O2'	7:2H:67:LEU:HD12	2.19	0.42
10:2O:113:LYS:HD2	10:2O:113:LYS:HA	1.86	0.42
25:23:2:PRO:HB2	25:23:3:ARG:H	1.73	0.42
32:2a:1434:A:H2'	32:2a:1435:G:O4'	2.19	0.42
35:2d:109:GLY:HA3	35:2d:165:MET:HG3	2.00	0.42
36:2e:71:LEU:C	36:2e:72:GLN:HE21	2.26	0.42
44:2m:86:CYS:HB2	50:2s:73:GLU:HG2	2.01	0.42
46:2o:87:ILE:HG22	46:2o:88:ARG:N	2.34	0.42
55:2x:21:A:N6	55:2x:46:G:H2'	2.35	0.42
1:1A:657:U:H2'	1:1A:658:C:H6	1.84	0.42
1:1A:1062:G:N2	1:1A:1077:A:H61	2.14	0.42
1:1A:2344:U:OP1	28:16:37:ARG:NH1	2.53	0.42
10:1O:97:ARG:NH1	32:1a:339:C:OP2	2.47	0.42
32:1a:1241:G:H2'	32:1a:1242:C:H6	1.84	0.42
35:1d:107:ARG:HH22	35:1d:194:LEU:HD11	1.84	0.42
42:1k:33:THR:OG1	42:1k:34:ASP:N	2.50	0.42
44:1m:15:VAL:HG11	44:1m:48:LEU:HD21	2.00	0.42
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	2.02	0.42
1:2A:902:C:H2'	1:2A:903:C:C6	2.55	0.42
1:2A:1116:C:H2'	1:2A:1117:G:H8	1.82	0.42
1:2A:1815:A:H8	1:2A:1815:A:OP1	2.03	0.42
3:2D:8:PRO:HB3	3:2D:14:ARG:HG2	2.02	0.42
8:2I:3:VAL:O	8:2I:18:VAL:HA	2.19	0.42
14:2S:87:PHE:CE1	14:2S:102:ALA:HB2	2.54	0.42
21:2Z:165:VAL:HB	21:2Z:166:SER:H	1.68	0.42
23:21:98:LEU:HD23	23:21:98:LEU:HA	1.89	0.42
32:2a:540:G:C6	32:2a:541:G:C5	3.07	0.42
32:2a:1092:A:H2'	32:2a:1093:A:C8	2.54	0.42
32:2a:1271:G:N2	32:2a:1272:G:C8	2.87	0.42
32:2a:1518:MA6:H93	32:2a:1519:MA6:C9	2.50	0.42
33:2b:76:GLN:HB2	33:2b:208:ILE:CG1	2.49	0.42
34:2c:134:ILE:HG23	34:2c:151:VAL:HB	2.01	0.42
37:2f:82:ARG:HE	37:2f:82:ARG:HB3	1.74	0.42
41:2j:42:THR:HG22	41:2j:68:HIS:HA	2.00	0.42
47:2p:8:ARG:HB3	47:2p:28:ARG:NH1	2.35	0.42
1:1A:26:G:C6	1:1A:27:G:N1	2.87	0.42
1:1A:250:G:C6	1:1A:251:A:C6	3.08	0.42
1:1A:620:G:N3	1:1A:620:G:H5'	2.33	0.42
1:1A:2094:G:OP1	8:1I:22:LYS:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2136:C:C2	1:1A:2155:G:N2	2.87	0.42
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	2.00	0.42
8:1I:134:PRO:C	8:1I:136:VAL:H	2.27	0.42
26:14:49:PHE:HD1	26:14:49:PHE:HA	1.72	0.42
30:18:15:LYS:HB3	30:18:23:VAL:HG23	2.02	0.42
32:1a:568:G:O2'	32:1a:574:A:N1	2.48	0.42
32:1a:1263:C:H2'	32:1a:1264:C:C6	2.55	0.42
32:1a:1329:A:H5"	44:1m:26:GLY:H	1.84	0.42
33:1b:115:LEU:HD13	33:1b:145:LEU:HB3	2.01	0.42
34:1c:134:ILE:HG22	34:1c:168:ALA:HB3	2.02	0.42
54:1w:68:C:H2'	54:1w:69:G:H8	1.79	0.42
1:2A:1405:U:H2'	1:2A:1406:U:H6	1.79	0.42
6:2G:45:GLU:H	6:2G:45:GLU:HG2	1.55	0.42
8:2I:64:GLU:C	8:2I:66:GLU:H	2.27	0.42
9:2N:61:ARG:HD3	9:2N:61:ARG:HA	1.76	0.42
23:21:32:LYS:HE3	23:21:32:LYS:HB3	1.89	0.42
32:2a:841:U:H6	32:2a:841:U:P	2.42	0.42
32:2a:946:A:H2'	32:2a:947:G:C8	2.54	0.42
32:2a:1139:G:N2	32:2a:1142:G:O6	2.42	0.42
32:2a:1402:4OC:H6	32:2a:1402:4OC:O5'	2.19	0.42
33:2b:52:GLU:HG2	33:2b:56:ARG:HH12	1.84	0.42
33:2b:185:ILE:O	33:2b:185:ILE:HG12	2.18	0.42
33:2b:215:LEU:HD23	33:2b:215:LEU:HA	1.78	0.42
34:2c:40:ARG:O	34:2c:44:GLU:HB2	2.19	0.42
42:2k:14:VAL:HG11	42:2k:34:ASP:HB2	2.01	0.42
1:1A:1420:U:O5'	1:1A:1420:U:H6	2.03	0.42
1:1A:2110:G:C2	1:1A:2120:G:H1'	2.55	0.42
1:1A:2319:G:H22	14:1S:3:ARG:CD	2.32	0.42
1:1A:2712:U:OP1	1:1A:2714:G:H4'	2.19	0.42
7:1H:89:ILE:O	7:1H:129:THR:HG22	2.20	0.42
17:1V:28:GLU:HG3	17:1V:29:PRO:HD2	2.00	0.42
26:14:62:ARG:HB3	26:14:63:TYR:H	1.60	0.42
32:1a:1241:G:H2'	32:1a:1242:C:C6	2.54	0.42
33:1b:22:LYS:HE2	33:1b:35:GLU:OE2	2.19	0.42
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.52	0.42
37:1f:1:MET:HA	37:1f:68:PRO:HA	2.00	0.42
48:1q:22:LEU:HD11	48:1q:39:SER:HB2	2.01	0.42
1:2A:403:U:H4'	1:2A:404:C:H5'	2.02	0.42
1:2A:1263:U:C4	1:2A:1264:G:C6	3.07	0.42
8:2I:83:ALA:HB2	8:2I:146:ALA:HA	2.02	0.42
12:2Q:15:GLY:H	12:2Q:41:TRP:HZ2	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1442:G:O2'	32:2a:1442(A):G:H5'	2.19	0.42
34:2c:125:GLU:HB3	34:2c:190:ARG:HH21	1.84	0.42
38:2g:111:ARG:NH2	38:2g:126:ASP:OD2	2.52	0.42
40:2i:18:PHE:CD2	40:2i:62:TYR:HD2	2.37	0.42
51:2t:67:ALA:HA	51:2t:72:LEU:O	2.20	0.42
56:2y:15:G:N2	56:2y:21:A:H1'	2.35	0.42
1:1A:1489:U:HO2'	1:1A:1490:A:H8	1.67	0.42
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.20	0.42
6:1G:34:LEU:HD23	6:1G:161:THR:HG22	2.00	0.42
7:1H:6:ARG:NH2	7:1H:54:ARG:HH22	2.18	0.42
18:1W:46:PHE:O	18:1W:50:VAL:HG23	2.19	0.42
32:1a:176:C:H2'	32:1a:177:C:H6	1.85	0.42
33:1b:83:MET:HB3	33:1b:234:PRO:HG3	2.01	0.42
35:1d:157:LEU:HD22	35:1d:161:ASN:ND2	2.35	0.42
37:1f:91:VAL:HG11	49:1r:72:ARG:NH1	2.35	0.42
1:2A:286:C:H2'	1:2A:287:C:C6	2.55	0.42
1:2A:800:A:H8	1:2A:800:A:OP1	2.03	0.42
1:2A:1529:G:C6	1:2A:1530:C:N4	2.88	0.42
1:2A:2103:C:H2'	1:2A:2104:G:C8	2.55	0.42
1:2A:2125:G:H1'	1:2A:2173:A:N6	2.34	0.42
3:2D:70:TRP:CE2	3:2D:150:LYS:HD3	2.55	0.42
15:2T:119:LYS:O	15:2T:123:GLN:HG3	2.20	0.42
16:2U:78:THR:O	16:2U:117:GLN:NE2	2.53	0.42
21:2Z:163:LEU:HD23	21:2Z:163:LEU:HA	1.76	0.42
23:21:64:ALA:HA	23:21:67:ILE:HG13	2.01	0.42
25:23:18:ASP:N	25:23:18:ASP:OD1	2.52	0.42
32:2a:66:G:H8	32:2a:66:G:OP1	2.03	0.42
32:2a:966:M2G:HM23	32:2a:967:5MC:H1'	2.02	0.42
32:2a:1151:A:O2'	32:2a:1152:A:O5'	2.36	0.42
36:2e:7:GLU:OE1	36:2e:37:ARG:NH2	2.46	0.42
39:2h:121:ASP:HB2	39:2h:125:ARG:HH21	1.83	0.42
41:2j:47:PHE:HB2	41:2j:63:PHE:HB2	2.02	0.42
1:1A:2100:G:H2'	1:1A:2101:G:C8	2.54	0.42
1:1A:2130:U:O5'	1:1A:2130:U:H6	2.02	0.42
1:1A:2836:U:H2'	1:1A:2837:G:C8	2.55	0.42
20:1Y:5:MET:HE2	20:1Y:5:MET:HB2	1.95	0.42
21:1Z:52:SER:C	21:1Z:54:HIS:N	2.77	0.42
26:14:61:ARG:O	26:14:62:ARG:C	2.62	0.42
32:1a:620:C:H2'	32:1a:621:A:O4'	2.19	0.42
32:1a:836:G:OP1	49:1r:61:LYS:NZ	2.38	0.42
35:1d:173:TRP:CE2	35:1d:189:PRO:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1g:115:ARG:HG3	38:1g:118:VAL:CG2	2.49	0.42
40:1i:3:GLN:HG2	40:1i:20:ARG:NE	2.35	0.42
42:1k:82:VAL:HB	42:1k:107:SER:O	2.20	0.42
44:1m:78:ILE:O	44:1m:82:MET:HG3	2.20	0.42
44:1m:108:ARG:HA	44:1m:108:ARG:HD3	1.56	0.42
1:2A:1022:G:N7	9:2N:66:LYS:HE2	2.35	0.42
1:2A:2114:A:H2'	1:2A:2114:A:N3	2.34	0.42
2:2B:13:A:O2'	2:2B:14:U:H3'	2.19	0.42
2:2B:42:C:O2'	6:2G:66:GLN:HG2	2.20	0.42
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.55	0.42
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	2.01	0.42
8:2I:55:ALA:O	8:2I:58:LEU:HB2	2.20	0.42
8:2I:97:ILE:O	8:2I:100:ALA:HB3	2.20	0.42
15:2T:125:ARG:HE	15:2T:125:ARG:HB3	1.70	0.42
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	2.02	0.42
32:2a:1221:G:H4'	50:2s:53:ASN:O	2.19	0.42
33:2b:163:PHE:HA	33:2b:185:ILE:O	2.20	0.42
34:2c:3:ASN:OD1	34:2c:4:LYS:NZ	2.45	0.42
34:2c:57:ILE:HD13	34:2c:66:VAL:HG22	2.01	0.42
40:2i:55:ALA:HA	40:2i:58:HIS:CD2	2.54	0.42
43:2l:117:ARG:HB3	43:2l:122:THR:O	2.20	0.42
1:1A:747:U:O2	1:1A:2014:A:H1'	2.19	0.42
1:1A:1082:U:C4	1:1A:1086:A:N1	2.82	0.42
11:1P:101:VAL:HG21	11:1P:108:LYS:HG2	2.01	0.42
12:1Q:109:VAL:HG13	12:1Q:110:THR:O	2.19	0.42
32:1a:551:U:H2'	32:1a:552:U:C6	2.55	0.42
34:1c:71:ALA:HA	34:1c:106:VAL:CG2	2.50	0.42
47:1p:43:LYS:HG2	47:1p:48:TRP:CE2	2.55	0.42
1:2A:71:A:H5"	1:2A:73:A:C8	2.55	0.42
1:2A:299:A:N1	1:2A:322:A:O2'	2.44	0.42
1:2A:2471:C:N4	1:2A:2476:A:O2'	2.46	0.42
8:2I:126:TYR:O	8:2I:142:VAL:HG22	2.19	0.42
11:2P:94:GLU:OE2	11:2P:124:LYS:NZ	2.36	0.42
14:2S:62:LYS:HA	14:2S:65:VAL:HG22	2.02	0.42
36:2e:67:VAL:HG22	36:2e:68:GLU:H	1.85	0.42
38:2g:65:ALA:O	38:2g:69:VAL:HG23	2.19	0.42
50:2s:16:LEU:HG	50:2s:20:LEU:HD22	2.02	0.42
1:1A:118:A:C8	1:1A:119:A:C8	3.08	0.42
1:1A:1359:A:C2	1:1A:1372:U:O4	2.73	0.42
1:1A:2206:G:H3'	1:1A:2207:G:N7	2.35	0.42
4:1E:13:ARG:HD2	4:1E:20:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1X:44:GLU:HG2	19:1X:49:VAL:O	2.19	0.42
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.84	0.42
36:1e:68:GLU:OE1	36:1e:70:PRO:HG3	2.20	0.42
36:1e:99:GLY:N	36:1e:117:ASP:OD1	2.46	0.42
51:1t:65:LYS:HA	51:1t:68:LYS:HD3	2.00	0.42
54:1w:70:G:H2'	54:1w:71:G:O4'	2.19	0.42
56:1y:35:A:OP2	56:1y:35:A:H8	2.03	0.42
1:2A:271(P):C:H4'	8:2I:42:SER:O	2.19	0.42
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.55	0.42
1:2A:2318:G:N2	14:2S:3:ARG:HD3	2.35	0.42
5:2F:89:VAL:HG12	5:2F:90:PHE:CD2	2.55	0.42
6:2G:11:TYR:OH	6:2G:16:ARG:HD3	2.20	0.42
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.48	0.42
17:2V:60:GLU:HB2	17:2V:97:LYS:HE2	2.02	0.42
32:2a:624:C:H2'	32:2a:625:G:C8	2.53	0.42
32:2a:1456:G:O2'	51:2t:39:LYS:HE3	2.20	0.42
1:1A:945:A:C4	1:1A:2448:A:C2	3.08	0.42
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.35	0.42
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.18	0.42
32:1a:116:A:H61	32:1a:313:A:H1'	1.84	0.42
32:1a:382:A:H2'	32:1a:383:A:H8	1.84	0.42
32:1a:692:U:O2'	32:1a:694:A:N7	2.40	0.42
41:1j:81:THR:C	41:1j:83:GLU:N	2.76	0.42
44:1m:70:LEU:HD23	44:1m:70:LEU:HA	1.89	0.42
48:1q:82:MET:O	48:1q:86:GLU:HG2	2.20	0.42
1:2A:141:A:C8	1:2A:1408:C:O2'	2.71	0.42
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.44	0.42
1:2A:2052:G:H4'	4:2E:143:ASN:O	2.20	0.42
17:2V:24:LYS:HE2	17:2V:24:LYS:HB3	1.86	0.42
19:2X:2:LYS:HD2	19:2X:2:LYS:HA	1.71	0.42
32:2a:108:G:C6	51:2t:15:ARG:HG2	2.54	0.42
35:2d:176:LEU:HD12	35:2d:182:LYS:O	2.19	0.42
37:2f:76:ALA:O	37:2f:80:ARG:HG3	2.20	0.42
38:2g:29:LYS:HB2	38:2g:105:VAL:HG21	2.02	0.42
38:2g:77:SER:HA	38:2g:85:TYR:O	2.20	0.42
39:2h:23:SER:OG	39:2h:24:THR:N	2.53	0.42
45:2n:42:ILE:O	45:2n:46:GLU:HG3	2.20	0.42
48:2q:10:VAL:HA	48:2q:20:THR:O	2.20	0.42
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	2.01	0.42
56:2y:55:PSU:N1	56:2y:57:G:H5'	2.34	0.42
1:1A:2406:U:H6	1:1A:2406:U:H2'	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2747:G:O6	1:1A:2755:C:H5”	2.19	0.41
1:1A:2839:G:H5’	13:1R:46:GLY:HA2	2.02	0.41
6:1G:101:ILE:HD13	26:14:25:TYR:HB2	2.02	0.41
6:1G:115:ARG:HG2	6:1G:136:ARG:NH2	2.35	0.41
8:1I:132:PRO:HD2	8:1I:136:VAL:O	2.19	0.41
12:1Q:110:THR:OG1	12:1Q:113:GLN:HB2	2.20	0.41
31:19:25:VAL:HB	31:19:34:GLN:HB2	2.02	0.41
32:1a:473:G:OP2	47:1p:75:ARG:NH1	2.53	0.41
32:1a:674:G:H2’	32:1a:675:A:H8	1.83	0.41
34:1c:8:ILE:HD13	34:1c:184:TYR:HB3	2.01	0.41
47:1p:49:LEU:HD12	47:1p:50:LYS:N	2.34	0.41
50:1s:28:LYS:HB3	50:1s:47:HIS:HD2	1.85	0.41
1:2A:196:A:N3	1:2A:196:A:H2’	2.35	0.41
1:2A:890:A:H2’	1:2A:892:G:C8	2.55	0.41
1:2A:1024:G:OP2	64:2A:3930:HOH:O	2.21	0.41
1:2A:1179:C:H2’	1:2A:1180:C:C6	2.55	0.41
3:2D:123:ALA:HB3	3:2D:131:LEU:HG	2.02	0.41
3:2D:132:PRO:HD3	3:2D:190:TYR:CZ	2.55	0.41
8:2I:101:LEU:HD11	8:2I:107:VAL:HG23	2.02	0.41
9:2N:55:VAL:HB	9:2N:125:GLY:O	2.20	0.41
14:2S:35:ILE:HG12	14:2S:101:LEU:HD12	2.01	0.41
32:2a:9:G:H2’	32:2a:10:A:H8	1.84	0.41
32:2a:23:C:H5	32:2a:561:U:O4	2.03	0.41
32:2a:460:G:N2	32:2a:471:G:N7	2.68	0.41
32:2a:1070:U:H2’	32:2a:1071:C:H6	1.85	0.41
32:2a:1130:A:H5”	40:2i:18:PHE:CZ	2.55	0.41
32:2a:1151:A:O2’	32:2a:1152:A:H8	2.03	0.41
32:2a:1318:A:H5”	50:2s:3:ARG:NH2	2.35	0.41
33:2b:171:ALA:O	33:2b:175:ARG:HB2	2.20	0.41
34:2c:136:GLN:O	34:2c:140:ARG:HG3	2.20	0.41
35:2d:128:VAL:N	35:2d:131:ARG:O	2.43	0.41
36:2e:69:VAL:HG12	36:2e:71:LEU:HD21	2.02	0.41
38:2g:111:ARG:NH1	38:2g:113:GLU:OE2	2.52	0.41
40:2i:97:LYS:HA	40:2i:102:LEU:HG	2.01	0.41
1:1A:819:A:C4	1:1A:1189:A:C2	3.08	0.41
1:1A:2557:G:H2’	1:1A:2558:C:C6	2.55	0.41
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	2.03	0.41
7:1H:22:GLY:C	7:1H:23:ARG:HG3	2.45	0.41
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.54	0.41
24:12:1:MET:HE3	24:12:1:MET:HB2	1.93	0.41
24:12:38:GLN:HG3	24:12:43:GLN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1127:G:H5'	32:1a:1280:A:O2'	2.20	0.41
33:1b:8:LYS:O	33:1b:217:ARG:NH1	2.52	0.41
34:1c:12:LEU:HD23	34:1c:12:LEU:HA	1.87	0.41
35:1d:60:GLU:HG3	35:1d:202:LEU:HD12	2.01	0.41
46:1o:85:LEU:HD23	46:1o:85:LEU:HA	1.76	0.41
51:1t:56:MET:HE3	51:1t:85:MET:HE2	2.02	0.41
54:1w:11:C:H2'	54:1w:12:U:C6	2.56	0.41
1:2A:2166:G:H3'	1:2A:2167:U:H5"	2.02	0.41
2:2B:31:C:H4'	6:2G:29:TRP:CH2	2.54	0.41
20:2Y:86:ARG:HE	20:2Y:100:ALA:HA	1.85	0.41
21:2Z:152:ALA:HB2	21:2Z:169:GLU:HB3	2.02	0.41
32:2a:197:A:N6	32:2a:221:C:H5'	2.35	0.41
32:2a:1085:U:H3'	32:2a:1086:U:H6	1.85	0.41
40:2i:99:LEU:HB3	40:2i:101:PHE:HE2	1.84	0.41
41:2j:32:ALA:HA	41:2j:33:GLN:HA	1.91	0.41
48:2q:48:GLU:OE2	48:2q:50:LYS:HD3	2.20	0.41
50:2s:27:GLU:HB3	50:2s:47:HIS:NE2	2.35	0.41
1:1A:1094:U:H1'	1:1A:1097:U:C4	2.56	0.41
1:1A:1779:U:H2'	64:1A:4548:HOH:O	2.20	0.41
1:1A:2031:A:C6	1:1A:2498:C:H1'	2.56	0.41
8:1I:93:THR:H	8:1I:96:ASP:HB2	1.86	0.41
19:1X:54:VAL:HG22	19:1X:81:VAL:HG12	2.02	0.41
26:14:57:GLU:HA	26:14:58:ARG:HA	1.75	0.41
34:1c:22:TRP:CZ2	45:1n:54:PRO:HG2	2.55	0.41
37:1f:89:MET:HG2	37:1f:91:VAL:HG23	2.02	0.41
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.51	0.41
1:2A:265:A:C8	1:2A:266:G:H1'	2.56	0.41
1:2A:1359:A:C2	1:2A:1372:U:O4	2.73	0.41
1:2A:2112:G:H2'	1:2A:2112:G:N3	2.35	0.41
1:2A:2815:C:H2'	1:2A:2816:C:C6	2.55	0.41
5:2F:196:LEU:HD23	5:2F:196:LEU:HA	1.84	0.41
6:2G:20:ILE:HA	6:2G:25:TYR:HD2	1.85	0.41
7:2H:3:ARG:HA	7:2H:3:ARG:HD2	1.92	0.41
7:2H:102:ALA:HA	7:2H:117:PRO:HD3	2.02	0.41
14:2S:87:PHE:HB2	14:2S:112:PHE:CE1	2.56	0.41
21:2Z:43:GLU:O	21:2Z:47:VAL:HG12	2.20	0.41
22:20:53:MET:HG3	22:20:59:LEU:HD23	2.01	0.41
25:23:7:LYS:NZ	25:23:32:GLN:O	2.52	0.41
28:26:38:LYS:HE3	28:26:38:LYS:HB3	1.68	0.41
32:2a:509:A:N3	32:2a:543:C:O2'	2.49	0.41
32:2a:991:U:C5	32:2a:1212:U:H1'	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1029:C:C4	32:2a:1032:G:C6	3.08	0.41
36:2e:105:VAL:HB	36:2e:106:PRO:HD3	2.01	0.41
47:2p:28:ARG:HG2	47:2p:28:ARG:HH11	1.85	0.41
1:1A:288:C:H2'	1:1A:289:A:H8	1.85	0.41
1:1A:436:C:H2'	1:1A:437:G:C8	2.56	0.41
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.21	0.41
1:1A:898:C:N4	1:1A:899:A:H62	2.18	0.41
3:1D:38:LYS:C	3:1D:38:LYS:HD3	2.46	0.41
19:1X:92:LEU:O	19:1X:94:GLY:N	2.53	0.41
32:1a:632:A:H2'	32:1a:633:G:O4'	2.20	0.41
32:1a:841:U:C4	32:1a:848:C:H1'	2.55	0.41
32:1a:1441:G:H21	32:1a:1460:A:H62	1.67	0.41
35:1d:108:LEU:HD23	35:1d:110:PHE:CZ	2.55	0.41
41:1j:49:VAL:HG21	45:1n:44:LEU:HD22	2.03	0.41
48:1q:88:TYR:HD2	48:1q:89:LEU:HD12	1.85	0.41
1:2A:34:C:H2'	1:2A:35:G:H5'	2.02	0.41
1:2A:674:G:H1'	5:2F:74:ARG:HD3	2.02	0.41
1:2A:1198:U:H2'	1:2A:1199:U:C6	2.56	0.41
1:2A:2330:G:O2'	22:20:41:ARG:O	2.29	0.41
1:2A:2557:G:H2'	1:2A:2558:C:C6	2.55	0.41
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.55	0.41
1:2A:2723:C:OP2	4:2E:109:LYS:NZ	2.52	0.41
7:2H:116:GLU:HG3	7:2H:117:PRO:HD2	2.03	0.41
21:2Z:125:LEU:HB3	21:2Z:165:VAL:HG13	2.02	0.41
32:2a:429:U:H1'	32:2a:430:A:H5"	2.03	0.41
32:2a:1149:C:H2'	32:2a:1150:U:H6	1.85	0.41
32:2a:1245:A:H2'	32:2a:1246:C:O4'	2.19	0.41
38:2g:120:ILE:HG22	38:2g:124:LEU:HD12	2.01	0.41
43:2l:34:ARG:HE	43:2l:34:ARG:HB3	1.67	0.41
1:1A:526:A:H5"	1:1A:527:C:OP1	2.20	0.41
1:1A:1062:G:H5"	1:1A:1070:A:C4'	2.51	0.41
1:1A:1096:A:C5	1:1A:1097:U:H1'	2.55	0.41
7:1H:72:ILE:O	7:1H:76:VAL:HG23	2.20	0.41
9:1N:4:TYR:HB2	16:1U:101:ARG:NH1	2.35	0.41
32:1a:674:G:H2'	32:1a:675:A:C8	2.56	0.41
33:1b:121:LEU:HD21	33:1b:130:ARG:NH2	2.35	0.41
34:1c:120:VAL:O	34:1c:124:ILE:HG12	2.20	0.41
39:1h:9:MET:HG3	39:1h:26:VAL:HG21	2.02	0.41
1:2A:244:A:C2	1:2A:255:A:C4	3.08	0.41
1:2A:250:G:H2'	1:2A:251:A:C8	2.56	0.41
13:2R:36:THR:HG22	13:2R:37:THR:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:25:ARG:NH1	14:2S:42:ASP:OD1	2.54	0.41
20:2Y:55:TYR:N	20:2Y:56:PRO:HD3	2.36	0.41
24:22:51:ARG:HE	24:22:51:ARG:HB2	1.65	0.41
32:2a:1033:G:H2'	32:2a:1034:G:C8	2.56	0.41
32:2a:1102:A:O3'	33:2b:96:ARG:NH2	2.54	0.41
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.55	0.41
40:2i:4:TYR:CE1	40:2i:88:TYR:HA	2.56	0.41
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	2.02	0.41
42:2k:54:ARG:NH2	56:2y:39:PSU:O2'	2.53	0.41
42:2k:110:ASP:HB3	49:2r:85:LEU:HB3	2.02	0.41
48:2q:78:GLU:OE2	48:2q:81:ARG:NH1	2.40	0.41
56:2y:58:A:H4'	56:2y:59:U:OP1	2.20	0.41
1:1A:2721:A:H2'	1:1A:2722:G:O4'	2.20	0.41
5:1F:7:TYR:CD2	5:1F:24:LEU:HB2	2.56	0.41
5:1F:18:ARG:NH2	5:1F:127:GLU:OE2	2.52	0.41
11:1P:126:VAL:HG12	11:1P:148:LEU:CD2	2.48	0.41
26:14:34:GLU:H	26:14:34:GLU:CD	2.28	0.41
29:17:48:LYS:HE2	29:17:48:LYS:HB2	1.78	0.41
33:1b:162:ILE:HD11	33:1b:184:VAL:HG22	2.02	0.41
35:1d:112:VAL:HG23	35:1d:116:GLN:NE2	2.36	0.41
40:1i:17:VAL:HG11	40:1i:80:GLY:C	2.46	0.41
41:1j:78:ASN:C	41:1j:80:LYS:H	2.28	0.41
46:1o:6:GLU:O	46:1o:10:LYS:HG3	2.20	0.41
1:2A:223:A:N1	1:2A:407:G:O2'	2.49	0.41
1:2A:536:A:H2'	1:2A:537:C:C6	2.56	0.41
1:2A:2078:C:C4	1:2A:2079:U:C4	3.09	0.41
9:2N:99:LEU:O	9:2N:103:VAL:HG23	2.21	0.41
15:2T:105:LEU:HB2	15:2T:110:ILE:HG13	2.01	0.41
21:2Z:40:ASP:OD2	21:2Z:43:GLU:HG3	2.20	0.41
28:26:23:THR:OG1	28:26:24:GLU:N	2.53	0.41
28:26:40:CYS:O	28:26:44:ARG:N	2.50	0.41
32:2a:60:A:H4'	32:2a:61:G:O5'	2.21	0.41
32:2a:580:U:H2'	32:2a:581:G:O4'	2.20	0.41
32:2a:608:A:H2'	32:2a:609:A:O4'	2.20	0.41
32:2a:1003:G:H2'	32:2a:1004:A:O4'	2.21	0.41
32:2a:1313:U:OP1	50:2s:5:LEU:HB2	2.20	0.41
34:2c:72:LYS:HD3	34:2c:72:LYS:HA	1.86	0.41
35:2d:25:ARG:HA	35:2d:28:SER:HB3	2.03	0.41
50:2s:51:VAL:O	50:2s:58:VAL:N	2.54	0.41
1:1A:754:C:H2'	1:1A:755:C:C6	2.56	0.41
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	2.01	0.41
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.56	0.41
6:1G:67:LYS:H	26:14:6:HIS:CE1	2.38	0.41
28:16:38:LYS:HE3	28:16:38:LYS:HB3	1.90	0.41
32:1a:186:C:H2'	32:1a:187:C:C6	2.55	0.41
32:1a:621:A:H2'	32:1a:622:A:C8	2.56	0.41
32:1a:953:G:H5'	32:1a:965:A:N6	2.33	0.41
43:1l:42:THR:HA	43:1l:53:ARG:O	2.21	0.41
1:2A:116:C:H2'	1:2A:117:G:O4'	2.21	0.41
1:2A:298:G:H5"	1:2A:299:A:OP1	2.20	0.41
1:2A:1151:G:H4'	16:2U:81:HIS:ND1	2.35	0.41
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.55	0.41
1:2A:2184:G:O2'	1:2A:2185:C:H5'	2.21	0.41
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.55	0.41
2:2B:33:G:C2	2:2B:50:G:C2	3.08	0.41
22:20:32:ARG:H	22:20:35:ASN:ND2	2.19	0.41
32:2a:615:C:H2'	32:2a:616:G:O4'	2.21	0.41
32:2a:954:G:H5"	44:2m:120:LYS:HZ2	1.86	0.41
32:2a:1251:A:N1	32:2a:1354:C:O2'	2.49	0.41
32:2a:1314:C:H2'	32:2a:1315:U:C6	2.56	0.41
32:2a:1530:G:OP1	32:2a:1530:G:H4'	2.20	0.41
34:2c:131:ARG:HE	34:2c:135:LYS:HZ2	1.67	0.41
34:2c:179:ARG:NH1	34:2c:206:GLU:HB2	2.36	0.41
40:2i:17:VAL:HG11	40:2i:81:ILE:HG12	2.01	0.41
42:2k:51:LYS:HZ3	42:2k:55:LYS:HD3	1.84	0.41
43:2l:10:LEU:HD23	43:2l:10:LEU:HA	1.89	0.41
54:2w:10:G:H8	54:2w:10:G:OP1	2.03	0.41
1:1A:1047:G:H2'	1:1A:1110:G:N2	2.34	0.41
1:1A:1153:C:H2'	1:1A:1154:G:O4'	2.21	0.41
1:1A:2846:G:H2'	1:1A:2847:U:O4'	2.21	0.41
32:1a:401:C:H2'	32:1a:402:G:C8	2.55	0.41
33:1b:21:ARG:NH2	33:1b:23:ARG:HD2	2.36	0.41
36:1e:37:ARG:NH1	36:1e:112:LEU:HD23	2.35	0.41
39:1h:98:LYS:HG2	39:1h:99:GLU:HG3	2.03	0.41
41:1j:31:GLY:HA3	41:1j:32:ALA:HA	1.68	0.41
42:1k:18:ARG:HG3	42:1k:33:THR:OG1	2.21	0.41
46:1o:56:LEU:O	46:1o:60:VAL:HG23	2.20	0.41
3:2D:182:LEU:HD23	3:2D:182:LEU:HA	1.88	0.41
6:2G:129:GLY:O	6:2G:161:THR:HB	2.21	0.41
9:2N:73:THR:HA	9:2N:83:LYS:O	2.20	0.41
25:23:35:ARG:HE	25:23:37:LEU:HD21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:377:G:OP1	47:2p:3:LYS:HE2	2.20	0.41
32:2a:1466:C:H2'	32:2a:1467:G:O4'	2.20	0.41
36:2e:36:ASP:C	36:2e:38:GLN:H	2.28	0.41
36:2e:68:GLU:OE2	36:2e:70:PRO:HG3	2.21	0.41
1:1A:226:G:H21	1:1A:228:A:H62	1.69	0.41
1:1A:226:G:N2	1:1A:228:A:H62	2.19	0.41
1:1A:744:G:OP1	64:1A:4246:HOH:O	2.22	0.41
1:1A:848:G:O6	1:1A:928:G:H2'	2.20	0.41
1:1A:1082:U:O4	1:1A:1086:A:C6	2.70	0.41
1:1A:1216:G:P	16:1U:11:ARG:HH21	2.42	0.41
1:1A:1876:A:H2'	1:1A:1877:A:C8	2.56	0.41
1:1A:2051:A:H5'	1:1A:2578:G:O4'	2.20	0.41
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.54	0.41
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.56	0.41
1:1A:2771:C:H2'	1:1A:2772:C:C6	2.55	0.41
8:1I:101:LEU:HD12	8:1I:107:VAL:HB	2.02	0.41
13:1R:1:MET:HE3	13:1R:1:MET:HB2	1.95	0.41
13:1R:92:GLY:HA2	13:1R:94:TYR:CZ	2.56	0.41
14:1S:27:SER:HA	14:1S:88:ASP:HB3	2.02	0.41
17:1V:62:LEU:HD12	17:1V:93:GLU:HG2	2.03	0.41
18:1W:13:SER:HB3	18:1W:16:LYS:HD2	2.03	0.41
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.60	0.41
21:1Z:137:ILE:HG23	21:1Z:156:LYS:HB3	2.02	0.41
32:1a:109:A:C6	32:1a:326:G:C6	3.08	0.41
32:1a:243:A:C2	32:1a:246:A:C8	3.09	0.41
32:1a:865:A:H2	32:1a:918:A:H4'	1.86	0.41
32:1a:1073:U:O2'	33:1b:104:ASN:OD1	2.39	0.41
33:1b:115:LEU:HD11	33:1b:146:GLN:HG3	2.03	0.41
36:1e:84:PHE:HB2	36:1e:134:ALA:HB2	2.03	0.41
36:1e:91:LEU:HB3	36:1e:118:ILE:HD11	2.03	0.41
40:1i:128:ARG:NH1	55:1x:35:A:OP2	2.54	0.41
45:1n:46:GLU:O	45:1n:50:LYS:HG3	2.21	0.41
48:1q:64:PRO:HA	48:1q:70:ARG:HD3	2.02	0.41
56:1y:9:A:H4'	56:1y:46:G7M:OP2	2.21	0.41
56:1y:23:A:H2'	56:1y:24:G:C8	2.55	0.41
1:2A:26:G:C6	1:2A:27:G:N1	2.89	0.41
1:2A:625:G:O6	11:2P:107:LYS:NZ	2.49	0.41
1:2A:656:G:H2'	1:2A:657:U:O4'	2.21	0.41
1:2A:882:G:H22	1:2A:894:C:N4	2.18	0.41
1:2A:1786:A:C4	1:2A:1938:A:C6	3.09	0.41
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2506:U:C2	1:2A:2585:U:O4	2.74	0.41
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.21	0.41
2:2B:2:C:H2'	2:2B:3:C:C6	2.56	0.41
2:2B:78:A:C2	2:2B:100:A:C4	3.09	0.41
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	2.02	0.41
6:2G:170:ARG:O	6:2G:174:GLU:HB2	2.20	0.41
7:2H:127:GLU:C	7:2H:129:THR:H	2.29	0.41
8:2I:101:LEU:HG	8:2I:107:VAL:O	2.21	0.41
10:2O:48:PRO:CB	32:2a:1422:G:H5"	2.49	0.41
14:2S:64:GLU:H	14:2S:64:GLU:HG3	1.48	0.41
18:2W:14:PRO:O	18:2W:18:ARG:HG3	2.21	0.41
19:2X:5:TYR:CZ	24:22:30:ARG:HB2	2.56	0.41
20:2Y:2:ARG:NH2	20:2Y:4:LYS:HD3	2.35	0.41
21:2Z:151:HIS:HD2	21:2Z:168:GLU:O	2.04	0.41
26:24:64:GLY:O	26:24:66:SER:N	2.54	0.41
28:26:9:LEU:HD11	28:26:34:LEU:HD12	2.02	0.41
32:2a:406:G:N2	35:2d:119:GLN:HE22	2.18	0.41
32:2a:620:C:C2	35:2d:135:LEU:HG	2.56	0.41
32:2a:737:A:H2'	32:2a:738:C:C6	2.56	0.41
32:2a:1004:A:C8	32:2a:1025:U:O4	2.74	0.41
32:2a:1010:G:N2	32:2a:1020:U:O2'	2.54	0.41
32:2a:1216:G:H5"	45:2n:5:ALA:HB2	2.01	0.41
32:2a:1310:G:H5'	44:2m:77:ASN:ND2	2.36	0.41
33:2b:155:LEU:HD21	33:2b:159:PRO:HD3	2.01	0.41
35:2d:112:VAL:HG13	35:2d:161:ASN:OD1	2.20	0.41
36:2e:33:VAL:HG13	36:2e:112:LEU:HD12	2.03	0.41
36:2e:99:GLY:O	36:2e:117:ASP:HA	2.20	0.41
40:2i:26:VAL:HG22	40:2i:61:ALA:HB3	2.03	0.41
44:2m:43:THR:HB	44:2m:48:LEU:HD21	2.02	0.41
48:2q:40:LYS:HD3	48:2q:42:TYR:CZ	2.56	0.41
49:2r:35:ARG:O	49:2r:37:VAL:N	2.54	0.41
1:1A:271(K):U:O2	8:1I:50:ARG:NE	2.54	0.41
1:1A:484:C:H2'	1:1A:485:C:C6	2.56	0.41
1:1A:548:A:H61	17:1V:18:LEU:HA	1.85	0.41
1:1A:1924:C:H4'	55:1x:13:C:O2'	2.21	0.41
1:1A:2573:C:H3'	64:1A:4656:HOH:O	2.20	0.41
1:1A:2693:A:H2'	1:1A:2694:G:C8	2.56	0.41
2:1B:66:A:H61	2:1B:109:C:H5'	1.86	0.41
3:1D:71:ASP:HB2	3:1D:103:ARG:HH12	1.86	0.41
7:1H:7:LEU:HD12	7:1H:8:PRO:CD	2.49	0.41
30:18:62:LEU:HB3	30:18:65:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:405:U:O4	35:1d:2:GLY:N	2.54	0.41
32:1a:838:G:H2'	32:1a:839:U:H2'	2.03	0.41
32:1a:958:A:C6	32:1a:959:A:N1	2.89	0.41
32:1a:1090:U:H2'	32:1a:1091:U:C6	2.56	0.41
32:1a:1137:C:H4'	32:1a:1138:G:C2	2.56	0.41
33:1b:131:PRO:C	33:1b:133:LYS:H	2.29	0.41
35:1d:108:LEU:HD12	35:1d:174:LEU:HD13	2.02	0.41
37:1f:76:ALA:O	37:1f:80:ARG:HG3	2.20	0.41
40:1i:115:GLY:O	40:1i:116:LYS:HD3	2.21	0.41
44:1m:34:LEU:HD13	44:1m:41:PRO:HA	2.03	0.41
1:2A:643:A:N1	1:2A:2369:A:O2'	2.51	0.41
1:2A:807:U:OP2	11:2P:41:ARG:NH2	2.54	0.41
1:2A:819:A:OP2	1:2A:1187:G:N2	2.41	0.41
1:2A:900:A:HO2'	1:2A:901:A:P	2.41	0.41
1:2A:1790:C:H5"	1:2A:1791:A:OP1	2.20	0.41
1:2A:2405:G:O2'	1:2A:2406:U:OP1	2.36	0.41
3:2D:118:VAL:HG22	3:2D:119:ALA:H	1.86	0.41
4:2E:5:LEU:HD11	4:2E:79:ARG:HB2	2.03	0.41
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	2.03	0.41
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.21	0.41
7:2H:15:VAL:HG12	7:2H:28:GLY:CA	2.51	0.41
8:2I:126:TYR:HD2	8:2I:142:VAL:HG23	1.86	0.41
18:2W:82:LEU:HD22	18:2W:84:ARG:NH2	2.35	0.41
32:2a:118:U:H3'	32:2a:288:A:H61	1.85	0.41
32:2a:189(D):C:H2'	32:2a:189(E):U:O4'	2.20	0.41
32:2a:232:G:H1'	32:2a:262:A:N1	2.36	0.41
32:2a:316:G:OP2	32:2a:351:G:O2'	2.35	0.41
32:2a:674:G:N2	32:2a:717:C:O2	2.54	0.41
34:2c:113:ALA:N	34:2c:114:PRO:HD2	2.36	0.41
34:2c:124:ILE:HD12	34:2c:127:ARG:HA	2.01	0.41
37:2f:46:ARG:HH22	49:2r:37:VAL:HG11	1.85	0.41
38:2g:60:LYS:HA	38:2g:63:LYS:CD	2.51	0.41
38:2g:149:ARG:O	38:2g:149:ARG:HG3	2.21	0.41
42:2k:79:SER:HB3	42:2k:104:GLN:HE21	1.86	0.41
56:2y:26:A:N1	56:2y:44:G:C6	2.88	0.41
1:1A:1584:C:O2'	1:1A:1586:A:H5'	2.20	0.40
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.56	0.40
1:1A:1796:U:H2'	1:1A:1797:C:H6	1.85	0.40
1:1A:2506:U:C2	1:1A:2585:U:O4	2.75	0.40
1:1A:2615:U:H2'	1:1A:2616:C:H6	1.86	0.40
1:1A:2889:C:H2'	1:1A:2891:G:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:390:C:H2'	32:1a:391:G:C8	2.55	0.40
32:1a:582:U:C2	32:1a:583:A:C8	3.09	0.40
32:1a:1044:A:C5	32:1a:1045:C:H1'	2.56	0.40
36:1e:144:THR:O	36:1e:148:VAL:HG13	2.21	0.40
1:2A:883:G:O6	1:2A:893:C:O2'	2.39	0.40
1:2A:921:G:H2'	1:2A:922:U:C6	2.57	0.40
1:2A:2564:A:C2	1:2A:2647:U:H4'	2.55	0.40
4:2E:178:GLU:H	4:2E:178:GLU:CD	2.28	0.40
12:2Q:89:ASN:HB2	55:2x:1:C:C4	2.55	0.40
13:2R:72:ASP:O	13:2R:76:VAL:HG23	2.21	0.40
14:2S:27:SER:HA	14:2S:88:ASP:HB3	2.03	0.40
15:2T:27:THR:O	15:2T:89:VAL:HG23	2.21	0.40
15:2T:77:PRO:HB2	15:2T:80:SER:HB2	2.02	0.40
16:2U:106:PHE:O	16:2U:110:VAL:HG23	2.21	0.40
16:2U:109:LEU:HD23	16:2U:109:LEU:HA	1.94	0.40
18:2W:64:MET:HE2	18:2W:109:GLU:HG3	2.04	0.40
19:2X:5:TYR:HD1	24:22:33:MET:HE2	1.86	0.40
20:2Y:52:SER:OG	20:2Y:55:TYR:HB2	2.21	0.40
23:21:50:ARG:HG2	23:21:59:THR:CG2	2.48	0.40
32:2a:509:A:H5"	35:2d:55:ALA:HB2	2.03	0.40
32:2a:651:C:N4	32:2a:753:A:OP2	2.50	0.40
32:2a:1502:A:C8	32:2a:1505:G:N2	2.89	0.40
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.56	0.40
36:2e:7:GLU:CD	36:2e:37:ARG:HH21	2.27	0.40
38:2g:70:LYS:HG2	38:2g:96:GLN:HB3	2.02	0.40
1:1A:749:C:H4'	1:1A:1271:G:N3	2.36	0.40
1:1A:1803:A:H4'	3:1D:259:THR:HG23	2.02	0.40
30:18:26:LYS:HG2	30:18:46:ARG:O	2.21	0.40
32:1a:114:U:O2'	32:1a:115:G:H5'	2.21	0.40
33:1b:158:LEU:HD23	33:1b:158:LEU:HA	1.83	0.40
54:1w:18:G:N2	54:1w:57:G:H2'	2.36	0.40
55:1x:19:G:H4'	55:1x:20:U:OP2	2.20	0.40
1:2A:477:A:H2'	1:2A:478:A:C8	2.56	0.40
1:2A:1255:U:O5'	1:2A:1256:G:H5"	2.20	0.40
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.21	0.40
1:2A:1714:G:H1	1:2A:1745(A):C:H42	1.69	0.40
1:2A:2507:C:H2'	1:2A:2508:G:O4'	2.21	0.40
1:2A:2748:A:H2'	1:2A:2749:A:O4'	2.21	0.40
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	2.03	0.40
4:2E:59:VAL:O	4:2E:64:LYS:HE3	2.22	0.40
32:2a:114:U:O2'	32:2a:115:G:H5'	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:229:U:H5”	47:2p:33:ILE:HD13	2.03	0.40
32:2a:448:A:OP2	32:2a:485:G:N2	2.40	0.40
32:2a:554:C:O2’	64:2a:3317:HOH:O	2.22	0.40
32:2a:755:G:OP2	46:2o:65:ARG:HD2	2.21	0.40
32:2a:952:U:H2’	32:2a:953:G:C8	2.56	0.40
32:2a:1101:A:H4’	32:2a:1102:A:O5’	2.22	0.40
33:2b:54:THR:HG23	33:2b:199:TYR:HB3	2.03	0.40
40:2i:28:VAL:HG22	40:2i:63:ILE:HD12	2.02	0.40
49:2r:22:VAL:HB	49:2r:56:THR:HA	2.03	0.40
56:2y:57:G:N3	56:2y:57:G:H2’	2.35	0.40
1:1A:1762:A:H2’	64:1A:6013:HOH:O	2.20	0.40
1:1A:1790:C:H2’	1:1A:1791:A:C5	2.56	0.40
1:1A:1816:G:O2’	1:1A:1817:G:OP2	2.30	0.40
1:1A:2064:C:H2’	1:1A:2065:C:C6	2.56	0.40
4:1E:12:THR:HG22	4:1E:13:ARG:N	2.32	0.40
6:1G:18:GLU:OE2	6:1G:22:ARG:HD2	2.22	0.40
11:1P:85:LEU:HA	11:1P:88:LEU:HD12	2.03	0.40
32:1a:684:A:N6	32:1a:685:G:C6	2.90	0.40
32:1a:1169:A:H2’	32:1a:1170:A:C8	2.56	0.40
32:1a:1292:U:H5’	40:1i:38:GLN:OE1	2.20	0.40
33:1b:21:ARG:H	33:1b:21:ARG:HG3	1.59	0.40
37:1f:21:LEU:O	37:1f:25:ILE:HG13	2.21	0.40
37:1f:35:ALA:HB1	37:1f:65:VAL:HG11	2.03	0.40
38:1g:115:ARG:H	38:1g:115:ARG:HG2	1.52	0.40
39:1h:4:ASP:OD2	39:1h:85:ARG:NE	2.41	0.40
1:2A:887:A:H4’	1:2A:888:C:H5	1.86	0.40
1:2A:1159:U:H2’	1:2A:1160:G:H8	1.87	0.40
1:2A:1429:G:H2’	1:2A:1430:C:C6	2.56	0.40
1:2A:1448:G:H2’	1:2A:1449:A:C8	2.56	0.40
1:2A:1686:C:H2’	1:2A:1687:G:O4’	2.21	0.40
5:2F:64:ILE:HD12	5:2F:65:TRP:CZ3	2.56	0.40
6:2G:14:GLU:O	6:2G:17:PRO:HD2	2.21	0.40
8:2I:60:GLU:CB	8:2I:61:ARG:HH21	2.34	0.40
8:2I:100:ALA:O	8:2I:104:GLN:N	2.55	0.40
14:2S:41:ASP:OD1	14:2S:44:LYS:N	2.55	0.40
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.57	0.40
26:24:16:CYS:HB2	26:24:36:CYS:HB3	2.04	0.40
35:2d:4:TYR:O	35:2d:6:GLY:N	2.54	0.40
35:2d:165:MET:HE2	35:2d:168:ARG:CZ	2.51	0.40
38:2g:68:ASN:O	38:2g:135:VAL:HG23	2.20	0.40
38:2g:111:ARG:HB3	38:2g:113:GLU:OE1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:23:TYR:CD2	44:2m:70:LEU:HD13	2.56	0.40
52:2u:9:ARG:O	52:2u:13:ILE:HG13	2.22	0.40
1:1A:207:A:H2'	1:1A:208:C:O4'	2.20	0.40
1:1A:601:C:O2'	1:1A:605:C:H5"	2.22	0.40
1:1A:784:A:C8	1:1A:792:G:C5	3.09	0.40
1:1A:1055:G:H3'	1:1A:1056:G:H8	1.86	0.40
1:1A:1071:G:OP1	1:1A:1071:G:H3'	2.21	0.40
1:1A:1080:C:H5'	1:1A:1081:U:OP2	2.21	0.40
1:1A:2693:A:H2'	1:1A:2694:G:H8	1.85	0.40
1:1A:2751:G:C5	7:1H:2:SER:N	2.90	0.40
6:1G:159:VAL:HG21	6:1G:173:LEU:HD21	2.04	0.40
24:12:24:LEU:O	24:12:28:LYS:HG3	2.22	0.40
32:1a:1429:C:H2'	32:1a:1430:C:C6	2.57	0.40
33:1b:112:VAL:HG12	33:1b:149:LEU:HD13	2.03	0.40
34:1c:83:ARG:O	34:1c:87:LEU:HG	2.21	0.40
34:1c:130:VAL:O	34:1c:134:ILE:HG13	2.22	0.40
37:1f:61:LEU:HD23	37:1f:63:TYR:HE2	1.87	0.40
40:1i:5:TYR:CG	40:1i:6:GLY:N	2.90	0.40
44:1m:82:MET:O	44:1m:93:ARG:NH2	2.46	0.40
1:2A:2061:G:H5"	1:2A:2503:2MA:C2	2.52	0.40
1:2A:2156:G:H2'	1:2A:2157:G:C4	2.57	0.40
1:2A:2169:A:H2'	1:2A:2170:A:C8	2.57	0.40
1:2A:2792:G:H2'	1:2A:2792:G:N3	2.36	0.40
3:2D:77:ALA:HB2	3:2D:97:TYR:CD1	2.57	0.40
6:2G:122:PRO:O	6:2G:125:PHE:HD2	2.04	0.40
13:2R:78:LYS:HE2	13:2R:83:ILE:HD11	2.03	0.40
23:21:67:ILE:N	23:21:68:PRO:HD2	2.36	0.40
25:23:4:LEU:O	25:23:36:VAL:HA	2.22	0.40
31:29:10:ILE:HD12	31:29:32:HIS:HA	2.04	0.40
46:2o:71:GLN:HB2	46:2o:78:TYR:CD1	2.56	0.40
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.46	0.40
54:2w:48:C:C2	54:2w:59:U:H1'	2.57	0.40
1:1A:1052:C:H2'	1:1A:1053:C:C6	2.56	0.40
3:1D:206:LEU:HA	3:1D:211:ARG:NH1	2.36	0.40
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.20	0.40
32:1a:45:U:H2'	32:1a:46:G:C8	2.57	0.40
32:1a:420:U:H2'	32:1a:422:C:C5	2.57	0.40
32:1a:598:U:H2'	32:1a:599:C:C6	2.56	0.40
32:1a:1006:C:H2'	32:1a:1007:C:C6	2.57	0.40
32:1a:1021:G:O2'	32:1a:1022:G:O4'	2.36	0.40
32:1a:1025:U:C2	32:1a:1036:G:O6	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1072:G:C6	32:1a:1073:U:C4	3.10	0.40
32:1a:1342:C:O2'	40:1i:124:GLN:HG3	2.21	0.40
32:1a:1518:MA6:H93	32:1a:1519:MA6:C9	2.51	0.40
33:1b:55:PHE:CD1	33:1b:221:LEU:HD22	2.56	0.40
34:1c:124:ILE:HG12	34:1c:124:ILE:H	1.57	0.40
39:1h:4:ASP:CG	39:1h:85:ARG:HH21	2.29	0.40
39:1h:17:THR:HB	39:1h:78:GLN:OE1	2.22	0.40
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.48	0.40
47:1p:50:LYS:HD2	47:1p:50:LYS:HA	1.90	0.40
1:2A:455:C:N3	1:2A:472:A:H2'	2.36	0.40
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.57	0.40
6:2G:49:ASP:O	6:2G:50:ALA:C	2.64	0.40
6:2G:167:GLU:OE1	6:2G:167:GLU:N	2.52	0.40
30:28:32:LEU:O	30:28:36:LYS:HE3	2.22	0.40
32:2a:1309:G:OP1	44:2m:88:ARG:NH2	2.52	0.40
32:2a:1511:G:H2'	32:2a:1512:U:O4'	2.21	0.40
33:2b:28:PHE:CD2	33:2b:190:THR:HA	2.57	0.40
33:2b:219:VAL:O	33:2b:222:ILE:HG12	2.21	0.40
40:2i:5:TYR:CE1	40:2i:18:PHE:HE1	2.40	0.40
41:2j:54:PHE:CD2	41:2j:55:LYS:HB3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	256 (94%)	17 (6%)	0	100	100
3	2D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	25	34
4	2E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	25	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	1F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	25 34
5	2F	201/210 (96%)	191 (95%)	7 (4%)	3 (2%)	8 11
6	1G	179/182 (98%)	168 (94%)	11 (6%)	0	100 100
6	2G	179/182 (98%)	156 (87%)	19 (11%)	4 (2%)	5 5
7	1H	172/180 (96%)	164 (95%)	8 (5%)	0	100 100
7	2H	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	22 29
8	1I	144/148 (97%)	129 (90%)	14 (10%)	1 (1%)	19 26
8	2I	144/148 (97%)	97 (67%)	36 (25%)	11 (8%)	1 0
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100 100
9	2N	138/140 (99%)	131 (95%)	7 (5%)	0	100 100
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100 100
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16 23
11	1P	147/150 (98%)	132 (90%)	11 (8%)	4 (3%)	4 3
11	2P	147/150 (98%)	131 (89%)	10 (7%)	6 (4%)	2 1
12	1Q	139/141 (99%)	130 (94%)	9 (6%)	0	100 100
12	2Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	19 26
13	1R	116/118 (98%)	114 (98%)	2 (2%)	0	100 100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100 100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100 100
14	2S	108/112 (96%)	97 (90%)	9 (8%)	2 (2%)	6 7
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100 100
15	2T	129/146 (88%)	117 (91%)	12 (9%)	0	100 100
16	1U	114/118 (97%)	114 (100%)	0	0	100 100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100 100
17	1V	99/101 (98%)	92 (93%)	4 (4%)	3 (3%)	3 2
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	13 18
18	1W	110/113 (97%)	110 (100%)	0	0	100 100
18	2W	110/113 (97%)	106 (96%)	4 (4%)	0	100 100
19	1X	93/96 (97%)	88 (95%)	3 (3%)	2 (2%)	5 5
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	12 15
20	1Y	105/110 (96%)	96 (91%)	7 (7%)	2 (2%)	6 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
20	2Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	13 18
21	1Z	148/206 (72%)	131 (88%)	14 (10%)	3 (2%)	6 6
21	2Z	156/206 (76%)	134 (86%)	17 (11%)	5 (3%)	3 2
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100 100
22	20	81/85 (95%)	76 (94%)	5 (6%)	0	100 100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	12 15
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	12 15
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
25	13	57/60 (95%)	57 (100%)	0	0	100 100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
26	14	67/71 (94%)	56 (84%)	6 (9%)	5 (8%)	1 0
26	24	67/71 (94%)	54 (81%)	10 (15%)	3 (4%)	2 1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
27	25	57/60 (95%)	55 (96%)	2 (4%)	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%)	62 (100%)	0	0	100 100
30	28	62/65 (95%)	62 (100%)	0	0	100 100
31	19	35/37 (95%)	35 (100%)	0	0	100 100
31	29	35/37 (95%)	35 (100%)	0	0	100 100
33	1b	229/256 (90%)	198 (86%)	24 (10%)	7 (3%)	3 2
33	2b	229/256 (90%)	189 (82%)	32 (14%)	8 (4%)	3 1
34	1c	204/239 (85%)	187 (92%)	14 (7%)	3 (2%)	8 11
34	2c	204/239 (85%)	172 (84%)	28 (14%)	4 (2%)	6 6
35	1d	206/209 (99%)	191 (93%)	14 (7%)	1 (0%)	25 34
35	2d	206/209 (99%)	194 (94%)	10 (5%)	2 (1%)	13 18
36	1e	146/162 (90%)	131 (90%)	9 (6%)	6 (4%)	2 1
36	2e	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	19 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
37	1f	98/101 (97%)	93 (95%)	4 (4%)	1 (1%)	13 18
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100 100
38	1g	153/156 (98%)	141 (92%)	11 (7%)	1 (1%)	19 26
38	2g	153/156 (98%)	141 (92%)	10 (6%)	2 (1%)	10 13
39	1h	135/138 (98%)	127 (94%)	7 (5%)	1 (1%)	19 26
39	2h	135/138 (98%)	129 (96%)	6 (4%)	0	100 100
40	1i	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	16 23
40	2i	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	16 23
41	1j	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	2 1
41	2j	94/105 (90%)	80 (85%)	10 (11%)	4 (4%)	2 1
42	1k	112/129 (87%)	104 (93%)	7 (6%)	1 (1%)	14 21
42	2k	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	7 8
43	1l	119/132 (90%)	112 (94%)	7 (6%)	0	100 100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100 100
44	1m	121/126 (96%)	114 (94%)	6 (5%)	1 (1%)	16 23
44	2m	120/126 (95%)	107 (89%)	10 (8%)	3 (2%)	4 4
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100 100
45	2n	58/61 (95%)	50 (86%)	8 (14%)	0	100 100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100 100
46	2o	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	11 14
47	1p	80/88 (91%)	72 (90%)	8 (10%)	0	100 100
47	2p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	10 13
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100 100
48	2q	97/105 (92%)	92 (95%)	5 (5%)	0	100 100
49	1r	66/88 (75%)	63 (96%)	3 (4%)	0	100 100
49	2r	66/88 (75%)	61 (92%)	5 (8%)	0	100 100
50	1s	81/93 (87%)	73 (90%)	8 (10%)	0	100 100
50	2s	81/93 (87%)	69 (85%)	11 (14%)	1 (1%)	11 14
51	1t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2 1
51	2t	94/106 (89%)	85 (90%)	7 (7%)	2 (2%)	5 6
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
52	2u	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2 1
All	All	11370/12128 (94%)	10516 (92%)	725 (6%)	129 (1%)	12 15

All (129) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	1P	44	GLY
21	1Z	53	ILE
23	11	3	LYS
26	14	47	GLN
26	14	62	ARG
33	1b	17	PHE
33	1b	126	GLU
34	1c	66	VAL
40	1i	54	ASP
44	1m	67	GLU
5	2F	130	ALA
6	2G	126	ASP
8	2I	113	ARG
21	2Z	52	SER
33	2b	17	PHE
33	2b	231	GLU
34	2c	43	LEU
35	2d	5	ILE
38	2g	80	VAL
44	2m	67	GLU
44	2m	106	ASN
11	1P	38	GLN
17	1V	79	VAL
20	1Y	102	CYS
33	1b	132	LYS
34	1c	107	GLN
35	1d	173	TRP
41	1j	29	ARG
41	1j	79	ARG
42	1k	49	GLY
51	1t	47	GLY
51	1t	100	ILE
5	2F	18	ARG
6	2G	43	LEU
8	2I	40	THR
8	2I	58	LEU

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Mol	Chain	Res	Type
8	2I	81	VAL
11	2P	29	LYS
11	2P	44	GLY
11	2P	45	LEU
17	2V	79	VAL
26	24	45	GLY
34	2c	156	ARG
38	2g	55	GLY
40	2i	88	TYR
41	2j	79	ARG
42	2k	49	GLY
51	2t	10	LEU
8	1I	40	THR
17	1V	43	GLU
17	1V	100	ARG
19	1X	93	GLU
26	14	49	PHE
26	14	63	TYR
34	1c	65	ALA
36	1e	6	PHE
36	1e	86	ALA
38	1g	52	GLU
41	1j	78	ASN
51	1t	95	ALA
5	2F	21	ALA
8	2I	86	THR
8	2I	100	ALA
11	2P	36	LYS
12	2Q	16	ARG
14	2S	84	GLN
19	2X	93	GLU
20	2Y	103	GLY
26	24	49	PHE
33	2b	20	GLU
33	2b	74	LYS
33	2b	126	GLU
33	2b	155	LEU
35	2d	3	ARG
41	2j	78	ASN
47	2p	52	ASP
4	1E	52	LEU
5	1F	130	ALA

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Mol	Chain	Res	Type
11	1P	45	LEU
21	1Z	156	LYS
33	1b	20	GLU
33	1b	124	SER
33	1b	125	PRO
33	1b	231	GLU
36	1e	27	ARG
39	1h	133	LEU
4	2E	52	LEU
6	2G	47	LYS
6	2G	124	SER
8	2I	117	GLU
8	2I	121	LYS
8	2I	131	LYS
26	24	65	ASP
33	2b	10	LEU
41	2j	51	ARG
44	2m	21	TYR
11	1P	29	LYS
19	1X	2	LYS
36	1e	21	ALA
36	1e	69	VAL
36	1e	85	GLY
10	2O	26	LYS
11	2P	122	PRO
21	2Z	171	ILE
34	2c	91	LEU
42	2k	90	GLY
46	2o	88	ARG
51	2t	47	GLY
52	2u	7	ARG
21	2Z	144	LEU
23	21	3	LYS
33	2b	123	ALA
34	2c	107	GLN
36	2e	96	PRO
37	1f	40	VAL
8	2I	88	ILE
20	1Y	103	GLY
41	1j	82	ILE
51	1t	102	GLY
11	2P	93	GLY

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Mol	Chain	Res	Type
14	2S	109	GLY
50	2s	54	GLY
21	2Z	146	ILE
21	1Z	157	LEU
26	14	56	VAL
8	2I	106	GLY
21	2Z	165	VAL
41	2j	77	PRO
7	2H	21	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%)	201 (94%)	14 (6%)	14 18
3	2D	215/218 (99%)	197 (92%)	18 (8%)	9 11
4	1E	164/166 (99%)	158 (96%)	6 (4%)	29 42
4	2E	164/166 (99%)	151 (92%)	13 (8%)	10 13
5	1F	160/166 (96%)	144 (90%)	16 (10%)	6 7
5	2F	159/166 (96%)	149 (94%)	10 (6%)	15 19
6	1G	143/156 (92%)	128 (90%)	15 (10%)	5 6
6	2G	143/156 (92%)	122 (85%)	21 (15%)	2 2
7	1H	144/148 (97%)	134 (93%)	10 (7%)	13 16
7	2H	144/148 (97%)	130 (90%)	14 (10%)	6 7
8	1I	113/124 (91%)	97 (86%)	16 (14%)	2 2
8	2I	105/124 (85%)	83 (79%)	22 (21%)	1 0
9	1N	118/119 (99%)	109 (92%)	9 (8%)	11 14
9	2N	118/119 (99%)	107 (91%)	11 (9%)	7 8
10	1O	100/100 (100%)	96 (96%)	4 (4%)	27 40
10	2O	100/100 (100%)	96 (96%)	4 (4%)	27 40
11	1P	115/116 (99%)	106 (92%)	9 (8%)	10 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	2P	115/116 (99%)	108 (94%)	7 (6%)	15 20
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	9 12
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	23 34
13	1R	101/101 (100%)	95 (94%)	6 (6%)	16 21
13	2R	101/101 (100%)	99 (98%)	2 (2%)	50 69
14	1S	86/88 (98%)	82 (95%)	4 (5%)	22 32
14	2S	85/88 (97%)	74 (87%)	11 (13%)	3 3
15	1T	115/127 (91%)	109 (95%)	6 (5%)	19 27
15	2T	113/127 (89%)	105 (93%)	8 (7%)	12 16
16	1U	93/94 (99%)	88 (95%)	5 (5%)	18 25
16	2U	93/94 (99%)	88 (95%)	5 (5%)	18 25
17	1V	80/82 (98%)	74 (92%)	6 (8%)	11 15
17	2V	80/82 (98%)	74 (92%)	6 (8%)	11 15
18	1W	90/92 (98%)	87 (97%)	3 (3%)	33 48
18	2W	90/92 (98%)	85 (94%)	5 (6%)	17 24
19	1X	77/78 (99%)	74 (96%)	3 (4%)	27 41
19	2X	77/78 (99%)	74 (96%)	3 (4%)	27 41
20	1Y	85/91 (93%)	75 (88%)	10 (12%)	4 4
20	2Y	85/91 (93%)	78 (92%)	7 (8%)	9 12
21	1Z	135/179 (75%)	123 (91%)	12 (9%)	8 9
21	2Z	137/179 (76%)	118 (86%)	19 (14%)	3 2
22	10	65/67 (97%)	64 (98%)	1 (2%)	60 76
22	20	65/67 (97%)	63 (97%)	2 (3%)	35 50
23	11	80/83 (96%)	79 (99%)	1 (1%)	65 79
23	21	80/83 (96%)	75 (94%)	5 (6%)	15 19
24	12	65/67 (97%)	64 (98%)	1 (2%)	60 76
24	22	65/67 (97%)	63 (97%)	2 (3%)	35 50
25	13	51/52 (98%)	47 (92%)	4 (8%)	10 13
25	23	50/52 (96%)	47 (94%)	3 (6%)	16 21
26	14	59/63 (94%)	50 (85%)	9 (15%)	2 2
26	24	53/63 (84%)	42 (79%)	11 (21%)	1 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	15	50/52 (96%)	47 (94%)	3 (6%)	16 21
27	25	50/52 (96%)	46 (92%)	4 (8%)	10 12
28	16	51/52 (98%)	48 (94%)	3 (6%)	16 21
28	26	50/52 (96%)	45 (90%)	5 (10%)	6 7
29	17	41/42 (98%)	36 (88%)	5 (12%)	4 3
29	27	41/42 (98%)	38 (93%)	3 (7%)	11 15
30	18	54/55 (98%)	50 (93%)	4 (7%)	11 15
30	28	54/55 (98%)	49 (91%)	5 (9%)	7 8
31	19	34/34 (100%)	34 (100%)	0	100 100
31	29	34/34 (100%)	31 (91%)	3 (9%)	8 10
33	1b	192/220 (87%)	168 (88%)	24 (12%)	3 3
33	2b	187/220 (85%)	168 (90%)	19 (10%)	6 6
34	1c	142/188 (76%)	130 (92%)	12 (8%)	8 11
34	2c	140/188 (74%)	130 (93%)	10 (7%)	12 16
35	1d	169/181 (93%)	150 (89%)	19 (11%)	5 5
35	2d	173/181 (96%)	154 (89%)	19 (11%)	5 5
36	1e	113/123 (92%)	103 (91%)	10 (9%)	8 10
36	2e	114/123 (93%)	101 (89%)	13 (11%)	4 4
37	1f	84/90 (93%)	75 (89%)	9 (11%)	5 6
37	2f	85/90 (94%)	79 (93%)	6 (7%)	12 16
38	1g	119/127 (94%)	109 (92%)	10 (8%)	9 11
38	2g	120/127 (94%)	111 (92%)	9 (8%)	11 15
39	1h	114/119 (96%)	104 (91%)	10 (9%)	8 10
39	2h	114/119 (96%)	104 (91%)	10 (9%)	8 10
40	1i	90/99 (91%)	75 (83%)	15 (17%)	2 1
40	2i	89/99 (90%)	81 (91%)	8 (9%)	8 9
41	1j	66/92 (72%)	54 (82%)	12 (18%)	1 1
41	2j	69/92 (75%)	58 (84%)	11 (16%)	2 1
42	1k	82/99 (83%)	73 (89%)	9 (11%)	5 5
42	2k	83/99 (84%)	76 (92%)	7 (8%)	9 11
43	1l	96/108 (89%)	90 (94%)	6 (6%)	15 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
43	2l	96/108 (89%)	93 (97%)	3 (3%)	35 50
44	1m	93/101 (92%)	84 (90%)	9 (10%)	6 7
44	2m	92/101 (91%)	76 (83%)	16 (17%)	1 1
45	1n	49/50 (98%)	44 (90%)	5 (10%)	6 6
45	2n	49/50 (98%)	46 (94%)	3 (6%)	15 20
46	1o	78/80 (98%)	75 (96%)	3 (4%)	28 41
46	2o	78/80 (98%)	75 (96%)	3 (4%)	28 41
47	1p	69/74 (93%)	62 (90%)	7 (10%)	6 7
47	2p	68/74 (92%)	60 (88%)	8 (12%)	4 4
48	1q	94/97 (97%)	87 (93%)	7 (7%)	11 15
48	2q	94/97 (97%)	90 (96%)	4 (4%)	25 36
49	1r	59/77 (77%)	51 (86%)	8 (14%)	3 2
49	2r	59/77 (77%)	54 (92%)	5 (8%)	8 11
50	1s	69/80 (86%)	63 (91%)	6 (9%)	8 10
50	2s	67/80 (84%)	60 (90%)	7 (10%)	5 6
51	1t	70/82 (85%)	66 (94%)	4 (6%)	17 23
51	2t	70/82 (85%)	68 (97%)	2 (3%)	37 54
52	1u	18/22 (82%)	18 (100%)	0	100 100
52	2u	18/22 (82%)	18 (100%)	0	100 100
All	All	9303/10064 (92%)	8527 (92%)	776 (8%)	9 12

All (776) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	14	ARG
3	1D	22	SER
3	1D	32	SER
3	1D	37	LEU
3	1D	38	LYS
3	1D	106	ILE
3	1D	142	VAL
3	1D	155	LEU
3	1D	229	VAL
3	1D	242	ARG

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Mol	Chain	Res	Type
3	1D	259	THR
3	1D	273	ARG
3	1D	275	LYS
4	1E	9	VAL
4	1E	47	VAL
4	1E	78	LEU
4	1E	81	ILE
4	1E	92	THR
4	1E	116	VAL
5	1F	24	LEU
5	1F	28	ILE
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	132	VAL
5	1F	140	LEU
5	1F	162	LEU
5	1F	168	ARG
5	1F	175	THR
5	1F	183	VAL
5	1F	192	LEU
5	1F	195	ASP
5	1F	201	VAL
6	1G	5	VAL
6	1G	7	LEU
6	1G	22	ARG
6	1G	31	VAL
6	1G	33	ARG
6	1G	43	LEU
6	1G	60	LEU
6	1G	82	LEU
6	1G	126	ASP
6	1G	139	LEU
6	1G	140	ILE
6	1G	148	MET
6	1G	149	VAL
6	1G	152	LEU
6	1G	159	VAL
7	1H	2	SER
7	1H	23	ARG

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Mol	Chain	Res	Type
7	1H	33	LEU
7	1H	37	VAL
7	1H	56	SER
7	1H	76	VAL
7	1H	98	LEU
7	1H	125	VAL
7	1H	129	THR
7	1H	149	ARG
8	1I	10	GLU
8	1I	12	LEU
8	1I	47	LEU
8	1I	61	ARG
8	1I	68	LEU
8	1I	77	LEU
8	1I	87	LYS
8	1I	92	VAL
8	1I	101	LEU
8	1I	108	THR
8	1I	110	ASP
8	1I	123	LEU
8	1I	127	VAL
8	1I	129	THR
8	1I	133	HIS
8	1I	144	VAL
9	1N	1	MET
9	1N	9	VAL
9	1N	10	GLU
9	1N	14	VAL
9	1N	28	THR
9	1N	48	MET
9	1N	62	VAL
9	1N	67	LEU
9	1N	96	GLU
10	1O	20	MET
10	1O	66	LYS
10	1O	91	LEU
10	1O	98	VAL
11	1P	1	MET
11	1P	45	LEU
11	1P	75	ILE
11	1P	86	LYS
11	1P	95	VAL

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Mol	Chain	Res	Type
11	1P	125	VAL
11	1P	126	VAL
11	1P	147	LEU
11	1P	149	GLU
12	1Q	8	LYS
12	1Q	56	ARG
12	1Q	59	ARG
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	110	THR
12	1Q	112	GLU
12	1Q	113	GLN
12	1Q	133	ARG
13	1R	6	SER
13	1R	14	SER
13	1R	15	SER
13	1R	36	THR
13	1R	111	LEU
13	1R	114	VAL
14	1S	46	VAL
14	1S	69	VAL
14	1S	85	VAL
14	1S	110	LEU
15	1T	23	ARG
15	1T	28	VAL
15	1T	34	VAL
15	1T	36	GLU
15	1T	51	ARG
15	1T	128	GLU
16	1U	8	VAL
16	1U	9	VAL
16	1U	27	LEU
16	1U	31	SER
16	1U	74	LEU
17	1V	45	THR
17	1V	56	SER
17	1V	61	VAL
17	1V	79	VAL
17	1V	85	LYS
17	1V	100	ARG
18	1W	11	ARG
18	1W	17	VAL

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Mol	Chain	Res	Type
18	1W	19	LEU
19	1X	35	THR
19	1X	52	VAL
19	1X	92	LEU
20	1Y	1	MET
20	1Y	7	VAL
20	1Y	8	LYS
20	1Y	31	LEU
20	1Y	43	ASN
20	1Y	72	VAL
20	1Y	85	VAL
20	1Y	91	GLU
20	1Y	99	CYS
20	1Y	107	ASP
21	1Z	31	ARG
21	1Z	53	ILE
21	1Z	72	ARG
21	1Z	84	GLU
21	1Z	123	ASP
21	1Z	124	ILE
21	1Z	129	SER
21	1Z	135	GLU
21	1Z	150	LEU
21	1Z	153	SER
21	1Z	154	ASP
21	1Z	171	ILE
22	10	10	THR
23	11	40	ARG
24	12	53	LEU
25	13	23	LEU
25	13	29	ARG
25	13	37	LEU
25	13	54	VAL
26	14	1	MET
26	14	49	PHE
26	14	50	VAL
26	14	52	THR
26	14	53	GLU
26	14	59	PHE
26	14	61	ARG
26	14	63	TYR
26	14	66	SER

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Mol	Chain	Res	Type
27	15	6	VAL
27	15	57	VAL
27	15	58	LEU
28	16	4	GLU
28	16	17	LYS
28	16	19	ARG
29	17	24	THR
29	17	29	LYS
29	17	43	THR
29	17	46	VAL
29	17	48	LYS
30	18	14	VAL
30	18	34	TRP
30	18	46	ARG
30	18	50	LEU
33	1b	7	VAL
33	1b	8	LYS
33	1b	12	GLU
33	1b	21	ARG
33	1b	35	GLU
33	1b	43	ASP
33	1b	54	THR
33	1b	80	ILE
33	1b	93	VAL
33	1b	95	GLN
33	1b	112	VAL
33	1b	127	ILE
33	1b	156	LYS
33	1b	158	LEU
33	1b	170	GLU
33	1b	185	ILE
33	1b	197	VAL
33	1b	208	ILE
33	1b	213	LEU
33	1b	215	LEU
33	1b	219	VAL
33	1b	222	ILE
33	1b	231	GLU
33	1b	233	SER
34	1c	3	ASN
34	1c	8	ILE
34	1c	17	ASP

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Mol	Chain	Res	Type
34	1c	49	SER
34	1c	64	VAL
34	1c	77	ILE
34	1c	85	ARG
34	1c	103	VAL
34	1c	112	SER
34	1c	124	ILE
34	1c	195	VAL
34	1c	207	VAL
35	1d	3	ARG
35	1d	19	LEU
35	1d	31	CYS
35	1d	53	ASP
35	1d	59	ARG
35	1d	70	ILE
35	1d	76	ARG
35	1d	83	SER
35	1d	88	VAL
35	1d	112	VAL
35	1d	119	GLN
35	1d	127	THR
35	1d	135	LEU
35	1d	140	VAL
35	1d	157	LEU
35	1d	170	VAL
35	1d	175	SER
35	1d	194	LEU
35	1d	200	GLU
36	1e	5	ASP
36	1e	9	LYS
36	1e	24	ARG
36	1e	31	LEU
36	1e	41	VAL
36	1e	47	LYS
36	1e	51	VAL
36	1e	126	ARG
36	1e	131	ILE
36	1e	151	LEU
37	1f	1	MET
37	1f	40	VAL
37	1f	57	GLN
37	1f	64	GLN

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Mol	Chain	Res	Type
37	1f	72	VAL
37	1f	73	ASN
37	1f	75	LEU
37	1f	78	GLU
37	1f	92	LYS
38	1g	12	LEU
38	1g	16	LEU
38	1g	50	ILE
38	1g	57	GLU
38	1g	59	LEU
38	1g	61	VAL
38	1g	66	VAL
38	1g	97	GLN
38	1g	113	GLU
38	1g	115	ARG
39	1h	2	LEU
39	1h	35	ILE
39	1h	38	ILE
39	1h	51	VAL
39	1h	52	ASP
39	1h	54	ASP
39	1h	77	GLU
39	1h	82	HIS
39	1h	112	LEU
39	1h	133	LEU
40	1i	14	VAL
40	1i	23	ASN
40	1i	27	THR
40	1i	42	ARG
40	1i	53	VAL
40	1i	64	THR
40	1i	75	ASP
40	1i	83	ARG
40	1i	89	ASN
40	1i	92	TYR
40	1i	96	LEU
40	1i	103	THR
40	1i	108	VAL
40	1i	111	ARG
40	1i	128	ARG
41	1j	8	LEU
41	1j	23	ILE

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Mol	Chain	Res	Type
41	1j	38	ILE
41	1j	42	THR
41	1j	44	VAL
41	1j	46	ARG
41	1j	49	VAL
41	1j	55	LYS
41	1j	81	THR
41	1j	92	THR
41	1j	94	VAL
41	1j	98	ILE
42	1k	14	VAL
42	1k	18	ARG
42	1k	31	THR
42	1k	33	THR
42	1k	48	ILE
42	1k	105	VAL
42	1k	109	VAL
42	1k	114	VAL
42	1k	117	ASN
43	1l	18	VAL
43	1l	33	ARG
43	1l	57	LYS
43	1l	62	SER
43	1l	89	ARG
43	1l	90	VAL
44	1m	4	ILE
44	1m	43	THR
44	1m	49	THR
44	1m	64	TRP
44	1m	67	GLU
44	1m	70	LEU
44	1m	102	ARG
44	1m	109	THR
44	1m	121	LYS
45	1n	7	ILE
45	1n	17	LYS
45	1n	18	VAL
45	1n	33	VAL
45	1n	47	LEU
46	1o	24	SER
46	1o	62	GLN
46	1o	87	ILE

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Mol	Chain	Res	Type
47	1p	11	SER
47	1p	20	VAL
47	1p	27	LYS
47	1p	45	THR
47	1p	49	LEU
47	1p	62	VAL
47	1p	67	THR
48	1q	14	LYS
48	1q	34	LYS
48	1q	52	LYS
48	1q	79	SER
48	1q	85	VAL
48	1q	96	GLU
48	1q	97	SER
49	1r	31	LEU
49	1r	37	VAL
49	1r	46	GLU
49	1r	47	THR
49	1r	76	LEU
49	1r	84	LYS
49	1r	86	VAL
49	1r	87	ARG
50	1s	5	LEU
50	1s	12	ASP
50	1s	28	LYS
50	1s	30	LEU
50	1s	40	ILE
50	1s	41	VAL
51	1t	10	LEU
51	1t	24	LEU
51	1t	62	LEU
51	1t	100	ILE
3	2D	3	VAL
3	2D	14	ARG
3	2D	32	SER
3	2D	37	LEU
3	2D	38	LYS
3	2D	71	ASP
3	2D	99	ASP
3	2D	105	ILE
3	2D	106	ILE
3	2D	111	LEU

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Mol	Chain	Res	Type
3	2D	116	GLN
3	2D	142	VAL
3	2D	155	LEU
3	2D	183	ARG
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	275	LYS
4	2E	7	VAL
4	2E	12	THR
4	2E	33	VAL
4	2E	38	THR
4	2E	69	LYS
4	2E	78	LEU
4	2E	82	ARG
4	2E	90	THR
4	2E	103	ASP
4	2E	116	VAL
4	2E	119	ARG
4	2E	128	SER
4	2E	145	LYS
5	2F	20	LEU
5	2F	53	THR
5	2F	74	ARG
5	2F	124	LEU
5	2F	126	VAL
5	2F	137	LYS
5	2F	157	VAL
5	2F	158	THR
5	2F	161	GLU
5	2F	195	ASP
6	2G	5	VAL
6	2G	18	GLU
6	2G	28	VAL
6	2G	43	LEU
6	2G	45	GLU
6	2G	49	ASP
6	2G	51	ARG
6	2G	53	LEU
6	2G	58	GLN
6	2G	60	LEU
6	2G	70	VAL

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Mol	Chain	Res	Type
6	2G	91	ARG
6	2G	111	LEU
6	2G	124	SER
6	2G	133	LEU
6	2G	137	GLU
6	2G	139	LEU
6	2G	140	ILE
6	2G	145	THR
6	2G	159	VAL
6	2G	165	THR
7	2H	23	ARG
7	2H	37	VAL
7	2H	45	VAL
7	2H	52	VAL
7	2H	57	ASP
7	2H	67	LEU
7	2H	71	LEU
7	2H	90	LYS
7	2H	95	ARG
7	2H	114	VAL
7	2H	115	VAL
7	2H	127	GLU
7	2H	129	THR
7	2H	136	ILE
8	2I	31	LEU
8	2I	38	LEU
8	2I	52	ARG
8	2I	61	ARG
8	2I	62	LYS
8	2I	68	LEU
8	2I	81	VAL
8	2I	82	ARG
8	2I	87	LYS
8	2I	88	ILE
8	2I	89	TYR
8	2I	93	THR
8	2I	96	ASP
8	2I	107	VAL
8	2I	116	LEU
8	2I	121	LYS
8	2I	123	LEU
8	2I	126	TYR

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Mol	Chain	Res	Type
8	2I	127	VAL
8	2I	129	THR
8	2I	130	TYR
8	2I	145	VAL
9	2N	1	MET
9	2N	5	VAL
9	2N	9	VAL
9	2N	15	LEU
9	2N	28	THR
9	2N	38	HIS
9	2N	48	MET
9	2N	58	ASP
9	2N	61	ARG
9	2N	62	VAL
9	2N	138	LEU
10	2O	35	VAL
10	2O	96	THR
10	2O	98	VAL
10	2O	116	SER
11	2P	35	HIS
11	2P	75	ILE
11	2P	95	VAL
11	2P	119	GLU
11	2P	133	SER
11	2P	135	LEU
11	2P	149	GLU
12	2Q	22	LYS
12	2Q	66	ILE
12	2Q	75	THR
12	2Q	110	THR
12	2Q	139	GLU
13	2R	73	VAL
13	2R	114	VAL
14	2S	21	THR
14	2S	35	ILE
14	2S	52	SER
14	2S	53	SER
14	2S	58	LEU
14	2S	63	THR
14	2S	64	GLU
14	2S	68	GLN
14	2S	85	VAL

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Mol	Chain	Res	Type
14	2S	110	LEU
14	2S	112	PHE
15	2T	40	THR
15	2T	64	ARG
15	2T	67	SER
15	2T	72	VAL
15	2T	89	VAL
15	2T	96	ARG
15	2T	102	ILE
15	2T	115	ARG
16	2U	5	LYS
16	2U	8	VAL
16	2U	17	ILE
16	2U	74	LEU
16	2U	100	VAL
17	2V	38	LEU
17	2V	45	THR
17	2V	46	VAL
17	2V	56	SER
17	2V	61	VAL
17	2V	79	VAL
18	2W	11	ARG
18	2W	17	VAL
18	2W	19	LEU
18	2W	67	ASP
18	2W	78	GLU
19	2X	81	VAL
19	2X	88	LYS
19	2X	92	LEU
20	2Y	1	MET
20	2Y	5	MET
20	2Y	9	LYS
20	2Y	39	VAL
20	2Y	40	GLU
20	2Y	72	VAL
20	2Y	99	CYS
21	2Z	6	LYS
21	2Z	27	VAL
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	58	VAL
21	2Z	70	LEU

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Mol	Chain	Res	Type
21	2Z	74	VAL
21	2Z	91	LEU
21	2Z	94	GLU
21	2Z	123	ASP
21	2Z	129	SER
21	2Z	144	LEU
21	2Z	148	ASP
21	2Z	149	SER
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	161	VAL
21	2Z	171	ILE
21	2Z	174	VAL
22	20	10	THR
22	20	36	ILE
23	21	35	THR
23	21	40	ARG
23	21	69	LYS
23	21	80	LEU
23	21	92	LYS
24	22	2	LYS
24	22	59	ARG
25	23	31	LEU
25	23	37	LEU
25	23	59	VAL
26	24	9	LEU
26	24	13	ARG
26	24	24	THR
26	24	27	THR
26	24	33	VAL
26	24	34	GLU
26	24	49	PHE
26	24	50	VAL
26	24	59	PHE
26	24	63	TYR
26	24	67	TYR
27	25	6	VAL
27	25	21	SER
27	25	40	LYS
27	25	58	LEU
28	26	5	VAL
28	26	9	LEU

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Mol	Chain	Res	Type
28	26	19	ARG
28	26	20	ASN
28	26	32	ASN
29	27	32	LYS
29	27	43	THR
29	27	46	VAL
30	28	14	VAL
30	28	34	TRP
30	28	37	SER
30	28	48	PHE
30	28	50	LEU
31	29	26	ILE
31	29	28	GLU
31	29	33	LYS
33	2b	7	VAL
33	2b	8	LYS
33	2b	9	GLU
33	2b	16	HIS
33	2b	53	ARG
33	2b	71	VAL
33	2b	76	GLN
33	2b	94	ASN
33	2b	102	LEU
33	2b	107	THR
33	2b	108	ILE
33	2b	112	VAL
33	2b	115	LEU
33	2b	117	GLU
33	2b	136	VAL
33	2b	185	ILE
33	2b	189	ASP
33	2b	213	LEU
33	2b	224	GLN
34	2c	15	THR
34	2c	43	LEU
34	2c	44	GLU
34	2c	55	VAL
34	2c	77	ILE
34	2c	140	ARG
34	2c	182	ILE
34	2c	190	ARG
34	2c	198	VAL

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Mol	Chain	Res	Type
34	2c	202	ILE
35	2d	5	ILE
35	2d	8	VAL
35	2d	17	VAL
35	2d	19	LEU
35	2d	34	GLU
35	2d	45	GLN
35	2d	47	ARG
35	2d	53	ASP
35	2d	76	ARG
35	2d	78	LEU
35	2d	94	LEU
35	2d	113	SER
35	2d	135	LEU
35	2d	150	GLU
35	2d	158	ILE
35	2d	162	LEU
35	2d	175	SER
35	2d	187	ARG
35	2d	193	ASP
36	2e	13	ILE
36	2e	18	ARG
36	2e	24	ARG
36	2e	25	ARG
36	2e	34	VAL
36	2e	51	VAL
36	2e	55	VAL
36	2e	75	THR
36	2e	83	GLU
36	2e	91	LEU
36	2e	112	LEU
36	2e	120	THR
36	2e	151	LEU
37	2f	65	VAL
37	2f	69	GLU
37	2f	70	ASP
37	2f	71	ARG
37	2f	81	ILE
37	2f	92	LYS
38	2g	24	THR
38	2g	51	GLN
38	2g	75	VAL

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Mol	Chain	Res	Type
38	2g	77	SER
38	2g	78	ARG
38	2g	79	ARG
38	2g	85	TYR
38	2g	97	GLN
38	2g	144	MET
39	2h	2	LEU
39	2h	23	SER
39	2h	52	ASP
39	2h	56	LYS
39	2h	98	LYS
39	2h	99	GLU
39	2h	109	ILE
39	2h	112	LEU
39	2h	133	LEU
39	2h	136	GLU
40	2i	17	VAL
40	2i	54	ASP
40	2i	63	ILE
40	2i	65	VAL
40	2i	88	TYR
40	2i	89	ASN
40	2i	102	LEU
40	2i	128	ARG
41	2j	16	LEU
41	2j	23	ILE
41	2j	30	SER
41	2j	38	ILE
41	2j	45	ARG
41	2j	46	ARG
41	2j	67	THR
41	2j	72	VAL
41	2j	81	THR
41	2j	89	ASP
41	2j	94	VAL
42	2k	14	VAL
42	2k	51	LYS
42	2k	53	SER
42	2k	54	ARG
42	2k	82	VAL
42	2k	109	VAL
42	2k	114	VAL

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Mol	Chain	Res	Type
43	2l	18	VAL
43	2l	24	VAL
43	2l	65	GLU
44	2m	4	ILE
44	2m	15	VAL
44	2m	17	VAL
44	2m	32	GLU
44	2m	39	ILE
44	2m	45	VAL
44	2m	49	THR
44	2m	50	GLU
44	2m	62	ASN
44	2m	67	GLU
44	2m	69	GLU
44	2m	92	HIS
44	2m	98	VAL
44	2m	102	ARG
44	2m	103	THR
44	2m	106	ASN
45	2n	18	VAL
45	2n	32	SER
45	2n	33	VAL
46	2o	3	ILE
46	2o	83	GLU
46	2o	84	LYS
47	2p	2	VAL
47	2p	5	ARG
47	2p	12	LYS
47	2p	20	VAL
47	2p	45	THR
47	2p	60	LEU
47	2p	72	ARG
47	2p	73	LEU
48	2q	9	VAL
48	2q	14	LYS
48	2q	53	LEU
48	2q	63	ARG
49	2r	25	THR
49	2r	31	LEU
49	2r	37	VAL
49	2r	54	ARG
49	2r	82	THR

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Mol	Chain	Res	Type
50	2s	22	LEU
50	2s	27	GLU
50	2s	31	ILE
50	2s	37	ARG
50	2s	41	VAL
50	2s	51	VAL
50	2s	77	THR
51	2t	46	GLU
51	2t	72	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	126	GLN
4	1E	143	ASN
5	1F	8	GLN
5	1F	69	HIS
5	1F	169	ASN
6	1G	26	GLN
11	1P	81	GLN
12	1Q	12	GLN
12	1Q	57	HIS
12	1Q	113	GLN
13	1R	31	HIS
13	1R	50	HIS
14	1S	68	GLN
16	1U	81	HIS
16	1U	94	ASN
16	1U	117	GLN
19	1X	31	HIS
19	1X	82	GLN
21	1Z	54	HIS
21	1Z	73	GLN
21	1Z	151	HIS
22	10	3	HIS
23	11	56	GLN
25	13	32	GLN
26	14	40	HIS
26	14	46	GLN
31	19	34	GLN
33	1b	16	HIS
33	1b	19	HIS

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Mol	Chain	Res	Type
33	1b	94	ASN
34	1c	6	HIS
34	1c	69	HIS
34	1c	162	GLN
35	1d	77	ASN
35	1d	116	GLN
35	1d	161	ASN
36	1e	78	HIS
37	1f	73	ASN
37	1f	100	ASN
38	1g	28	ASN
38	1g	106	GLN
38	1g	148	ASN
38	1g	153	HIS
40	1i	31	GLN
40	1i	34	ASN
40	1i	58	HIS
40	1i	124	GLN
41	1j	56	HIS
43	1l	8	ASN
43	1l	80	HIS
43	1l	99	HIS
46	1o	9	GLN
46	1o	62	GLN
48	1q	94	ASN
49	1r	63	GLN
50	1s	47	HIS
50	1s	57	HIS
50	1s	83	HIS
3	2D	87	ASN
3	2D	126	GLN
4	2E	48	GLN
4	2E	121	ASN
5	2F	69	HIS
6	2G	27	ASN
6	2G	41	GLN
6	2G	132	ASN
7	2H	74	ASN
8	2I	43	ASN
8	2I	133	HIS
9	2N	101	HIS
9	2N	131	GLN

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Mol	Chain	Res	Type
10	2O	3	GLN
10	2O	5	GLN
12	2Q	12	GLN
12	2Q	57	HIS
13	2R	13	HIS
13	2R	31	HIS
13	2R	50	HIS
13	2R	71	GLN
14	2S	38	GLN
15	2T	43	GLN
16	2U	94	ASN
19	2X	31	HIS
19	2X	82	GLN
20	2Y	43	ASN
21	2Z	32	HIS
21	2Z	34	ASN
21	2Z	55	HIS
21	2Z	73	GLN
21	2Z	151	HIS
23	21	56	GLN
25	23	32	GLN
30	28	43	GLN
33	2b	37	ASN
33	2b	135	GLN
33	2b	140	HIS
33	2b	212	GLN
34	2c	6	HIS
34	2c	63	ASN
34	2c	69	HIS
34	2c	162	GLN
34	2c	181	ASN
35	2d	62	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
36	2e	72	GLN
36	2e	73	ASN
37	2f	13	ASN
37	2f	100	ASN
38	2g	28	ASN

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Mol	Chain	Res	Type
38	2g	51	GLN
38	2g	68	ASN
38	2g	110	GLN
40	2i	3	GLN
40	2i	31	GLN
40	2i	58	HIS
40	2i	117	HIS
41	2j	13	HIS
41	2j	21	GLN
41	2j	33	GLN
41	2j	62	HIS
41	2j	84	GLN
42	2k	99	GLN
42	2k	104	GLN
43	2l	99	HIS
44	2m	62	ASN
46	2o	9	GLN
48	2q	26	GLN
49	2r	63	GLN
50	2s	69	HIS
50	2s	83	HIS
51	2t	26	ASN
51	2t	75	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	427 (14%)	26 (0%)
1	2A	2791/2915 (95%)	443 (15%)	28 (1%)
2	1B	119/121 (98%)	13 (10%)	0
2	2B	118/121 (97%)	19 (16%)	0
32	1a	1497/1521 (98%)	231 (15%)	0
32	2a	1501/1521 (98%)	267 (17%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	12/24 (50%)	4 (33%)	0
54	1w	71/76 (93%)	21 (29%)	0
54	2w	68/76 (89%)	25 (36%)	0
55	1x	75/77 (97%)	6 (8%)	0
55	2x	75/77 (97%)	7 (9%)	0
56	1y	72/76 (94%)	32 (44%)	0
56	2y	70/76 (92%)	27 (38%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	9345/9620 (97%)	1525 (16%)	54 (0%)

All (1525) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	G
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	61	G
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	181	A
1	1A	196	A
1	1A	197	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(H)	C
1	1A	272(I)	U
1	1A	275	G
1	1A	279	C

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Mol	Chain	Res	Type
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	357	A
1	1A	363	G
1	1A	363(B)	G
1	1A	386	G
1	1A	405	U
1	1A	411	G
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	456	C
1	1A	457	A
1	1A	481	G
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	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	652(D)	C
1	1A	652(E)	G
1	1A	652(F)	G
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	762	U
1	1A	764	A
1	1A	774	A
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	783	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	811	U
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	889	C
1	1A	890	A
1	1A	893	C
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	899	A
1	1A	910	A
1	1A	932	G

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Mol	Chain	Res	Type
1	1A	938	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1005	C
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	1039	G
1	1A	1040	C
1	1A	1044	G
1	1A	1046	A
1	1A	1047	G
1	1A	1053	C
1	1A	1054	A
1	1A	1055	G
1	1A	1057	A
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G
1	1A	1066	U
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	1081	U
1	1A	1083	U
1	1A	1087	G
1	1A	1088	A

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Mol	Chain	Res	Type
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1096	A
1	1A	1100	C
1	1A	1110	G
1	1A	1112	G
1	1A	1115	G
1	1A	1116	C
1	1A	1128	A
1	1A	1135	C
1	1A	1136	G
1	1A	1170	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1244	G
1	1A	1248	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1320	C
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1370	C
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G

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Mol	Chain	Res	Type
1	1A	1395	A
1	1A	1396	U
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
1	1A	1461	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1542	A
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1577	C
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1648	C
1	1A	1674	G
1	1A	1693	U
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1746	G
1	1A	1756	G

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Mol	Chain	Res	Type
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1817	G
1	1A	1829	A
1	1A	1839	G
1	1A	1847	A
1	1A	1848	A
1	1A	1858	G
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G

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Mol	Chain	Res	Type
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2098	U
1	1A	2102	U
1	1A	2107	C
1	1A	2108	C
1	1A	2110	G
1	1A	2113	U
1	1A	2116	G
1	1A	2118	U
1	1A	2121	G
1	1A	2127	G
1	1A	2129	C
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2145	C
1	1A	2146	C
1	1A	2147	G
1	1A	2149	G
1	1A	2150	U
1	1A	2151	G
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2161	C
1	1A	2162	G
1	1A	2165	G
1	1A	2166	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A

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Mol	Chain	Res	Type
1	1A	2181	G
1	1A	2182	G
1	1A	2183	C
1	1A	2184	G
1	1A	2189	U
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2219	G
1	1A	2225	A
1	1A	2234	G
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2280	G
1	1A	2283	C
1	1A	2287	A
1	1A	2305	A
1	1A	2307	G
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2354	G
1	1A	2361	A
1	1A	2372	G
1	1A	2379	G
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2407	G
1	1A	2414	G
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A

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Mol	Chain	Res	Type
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2447	G
1	1A	2448	A
1	1A	2468	G
1	1A	2476	A
1	1A	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	2574	G
1	1A	2602	A
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2663	G
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	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	2769	C
1	1A	2778	A
1	1A	2790	A

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Mol	Chain	Res	Type
1	1A	2791	C
1	1A	2794	C
1	1A	2802	G
1	1A	2804	C
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2872	G
1	1A	2880	C
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	12	C
2	1B	24	G
2	1B	32	C
2	1B	45	A
2	1B	52	A
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	91	C
2	1B	92	C
2	1B	110	G
2	1B	120	A
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	52	G
32	1a	61	G
32	1a	65	U
32	1a	72	C
32	1a	77	G
32	1a	79	G
32	1a	98	G
32	1a	101	A
32	1a	115	G
32	1a	116	A

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Mol	Chain	Res	Type
32	1a	121	C
32	1a	131	C
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(A)	C
32	1a	189(H)	G
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	217	C
32	1a	243	A
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	328	C
32	1a	332	G
32	1a	342	C
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	388	G
32	1a	392	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	423	G
32	1a	424	G
32	1a	429	U

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Mol	Chain	Res	Type
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	457	C
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	524	G
32	1a	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
32	1a	577	G
32	1a	592	G
32	1a	607	A
32	1a	630	G
32	1a	653	A
32	1a	657	G
32	1a	665	A
32	1a	666	G
32	1a	672	U
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	695	A
32	1a	723	U
32	1a	731	G
32	1a	749	C

Continued on next page...

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Mol	Chain	Res	Type
32	1a	755	G
32	1a	774	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	870	U
32	1a	874	G
32	1a	884	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	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	996	A
32	1a	1000	U
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1008	C
32	1a	1010	G
32	1a	1011	G
32	1a	1020	U

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Mol	Chain	Res	Type
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1030(D)	A
32	1a	1031	G
32	1a	1034	G
32	1a	1037	C
32	1a	1039	C
32	1a	1044	A
32	1a	1046	A
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1134	G
32	1a	1135	U
32	1a	1136	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1157	A
32	1a	1158	C
32	1a	1159	U
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1213	A

Continued on next page...

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Mol	Chain	Res	Type
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	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1312	G
32	1a	1319	A
32	1a	1320	C
32	1a	1338	G
32	1a	1340	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1364	U
32	1a	1370	G
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1458	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G

Continued on next page...

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Mol	Chain	Res	Type
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	14	A
53	1v	24	A
54	1w	2	C
54	1w	6	G
54	1w	9	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	45	U
54	1w	46	G7M
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	62	C
54	1w	66	U
54	1w	68	C
54	1w	69	G
54	1w	70	G
54	1w	71	G
54	1w	73	A
54	1w	74	C
55	1x	9	G
55	1x	19	G
55	1x	30	G
55	1x	47	U
55	1x	49	G
55	1x	61	C
56	1y	5	G
56	1y	8	4SU
56	1y	9	A
56	1y	11	C
56	1y	13	C
56	1y	14	A
56	1y	19	G
56	1y	20	U

Continued on next page...

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Mol	Chain	Res	Type
56	1y	21	A
56	1y	22	G
56	1y	23	A
56	1y	27	G
56	1y	37	MIA
56	1y	40	C
56	1y	44	G
56	1y	45	U
56	1y	46	G7M
56	1y	47	U
56	1y	48	C
56	1y	56	C
56	1y	57	G
56	1y	58	A
56	1y	59	U
56	1y	60	U
56	1y	61	C
56	1y	62	C
56	1y	66	U
56	1y	69	G
56	1y	70	G
56	1y	71	G
56	1y	72	C
56	1y	76	A
1	2A	8	A
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	64	A
1	2A	71	A
1	2A	72	U
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	141	A

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Mol	Chain	Res	Type
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	266	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272	G
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	352	G
1	2A	363	G
1	2A	386	G
1	2A	396	G
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	443	A
1	2A	444	C

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Mol	Chain	Res	Type
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	494	G
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	551	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	603	A
1	2A	604	G
1	2A	606	U
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	775	G
1	2A	776	G

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Mol	Chain	Res	Type
1	2A	782	A
1	2A	783	A
1	2A	784	A
1	2A	785	G
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	829	A
1	2A	859	G
1	2A	867	C
1	2A	874	G
1	2A	875	G
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	904	C
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	959	A
1	2A	961	C
1	2A	974	G

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Mol	Chain	Res	Type
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	999	U
1	2A	1012	U
1	2A	1013	C
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	1043	C
1	2A	1116	C
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1144	G
1	2A	1167	U
1	2A	1169	G
1	2A	1171	G
1	2A	1188	U
1	2A	1195	G
1	2A	1206	G
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1244	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1284	A
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1345	C

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Mol	Chain	Res	Type
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1416	G
1	2A	1417	C
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1435	G
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1495	A
1	2A	1496	A
1	2A	1497	U
1	2A	1505	C
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1540	U
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A

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Mol	Chain	Res	Type
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1639	U
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	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1861	G
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A

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Mol	Chain	Res	Type
1	2A	1914	C
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
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1992	G
1	2A	1993	U
1	2A	1996	C
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2070	G
1	2A	2099	U
1	2A	2101	G
1	2A	2111	C
1	2A	2116	G
1	2A	2120	G
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A

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Mol	Chain	Res	Type
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C
1	2A	2141	G
1	2A	2142	C
1	2A	2145	C
1	2A	2146	C
1	2A	2148	G
1	2A	2150	U
1	2A	2151	G
1	2A	2156	G
1	2A	2157	G
1	2A	2160	G
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2176	A
1	2A	2178	C
1	2A	2183	C
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2275	C
1	2A	2278	A
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U

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Mol	Chain	Res	Type
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2396	G
1	2A	2403	C
1	2A	2406	U
1	2A	2422	A
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2460	U
1	2A	2465	C
1	2A	2474	C
1	2A	2476	A
1	2A	2478	A
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	2525	G
1	2A	2529	G
1	2A	2549	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G

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Mol	Chain	Res	Type
1	2A	2573	C
1	2A	2578	G
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2646	C
1	2A	2654	A
1	2A	2663	G
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2748	A
1	2A	2751	G
1	2A	2757	A
1	2A	2758	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2769	C
1	2A	2778	A
1	2A	2783	G
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	2803	C
1	2A	2808	U
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G

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Mol	Chain	Res	Type
1	2A	2873	A
1	2A	2879	C
1	2A	2880	C
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	13	A
2	2B	17	C
2	2B	34	U
2	2B	41	U
2	2B	42	C
2	2B	44	G
2	2B	53	A
2	2B	56	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	84	C
2	2B	88	C
2	2B	105	A
2	2B	108	U
2	2B	110	G
2	2B	120	A
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	52	G
32	2a	66	G
32	2a	73	G
32	2a	79	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	97	G
32	2a	98	G

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Mol	Chain	Res	Type
32	2a	101	A
32	2a	115	G
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	142	G
32	2a	159	G
32	2a	160	A
32	2a	163	C
32	2a	189(F)	U
32	2a	189(J)	G
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	346	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	406	G
32	2a	412	A

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Mol	Chain	Res	Type
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	470	C
32	2a	477	A
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	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	550	G
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	653	A
32	2a	665	A
32	2a	666	G
32	2a	671	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	723	U
32	2a	724	G

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Mol	Chain	Res	Type
32	2a	731	G
32	2a	733	A
32	2a	749	C
32	2a	755	G
32	2a	773	G
32	2a	774	G
32	2a	777	A
32	2a	787	A
32	2a	792	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	834	C
32	2a	840	C
32	2a	841	U
32	2a	850	U
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	874	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	935	A
32	2a	942	G
32	2a	952	U
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	963	G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G

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Mol	Chain	Res	Type
32	2a	977	A
32	2a	982	U
32	2a	990	C
32	2a	992	U
32	2a	993	G
32	2a	997	U
32	2a	999	C
32	2a	1002	G
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	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	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1033	G
32	2a	1035	A
32	2a	1036	G
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1042	G
32	2a	1043	C
32	2a	1045	C
32	2a	1053	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G

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Mol	Chain	Res	Type
32	2a	1077	G
32	2a	1081	G
32	2a	1086	U
32	2a	1091	U
32	2a	1092	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1108	G
32	2a	1125	U
32	2a	1127	G
32	2a	1128	C
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1143	G
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1172	C
32	2a	1174	G
32	2a	1182	G
32	2a	1184	G
32	2a	1187	G
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1211	U
32	2a	1213	A
32	2a	1214	C
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A

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Mol	Chain	Res	Type
32	2a	1249	C
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1273	G
32	2a	1276	G
32	2a	1277	C
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1319	A
32	2a	1338	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1358	U
32	2a	1363	C
32	2a	1381	U
32	2a	1397	C
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	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	15	A

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Mol	Chain	Res	Type
53	2v	24	A
54	2w	3	C
54	2w	4	C
54	2w	5	G
54	2w	6	G
54	2w	8	4SU
54	2w	11	C
54	2w	12	U
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	29	G
54	2w	30	G
54	2w	46	G7M
54	2w	47	U
54	2w	48	C
54	2w	64	A
54	2w	65	G
54	2w	66	U
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	72	C
54	2w	73	A
54	2w	74	C
55	2x	7	G
55	2x	9	G
55	2x	19	G
55	2x	30	G
55	2x	47	U
55	2x	53	G
55	2x	61	C
56	2y	7	A
56	2y	15	G
56	2y	19	G
56	2y	24	G
56	2y	25	C
56	2y	27	G
56	2y	34	G
56	2y	38	A
56	2y	40	C

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Mol	Chain	Res	Type
56	2y	45	U
56	2y	48	C
56	2y	49	C
56	2y	50	U
56	2y	52	G
56	2y	53	G
56	2y	54	5MU
56	2y	55	PSU
56	2y	56	C
56	2y	57	G
56	2y	58	A
56	2y	59	U
56	2y	62	C
56	2y	68	C
56	2y	69	G
56	2y	70	G
56	2y	71	G
56	2y	73	A

All (54) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	278	A
1	1A	548	A
1	1A	669	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	1420	U
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G

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Mol	Chain	Res	Type
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2689	U
1	1A	2756	U
1	2A	195	A
1	2A	196	A
1	2A	228	A
1	2A	249	C
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	746	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	1608	A
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2406	U
1	2A	2439	A
1	2A	2689	U
1	2A	2756	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
55	8AN	2x	76	57,63,55	17,24,25	1.12	2 (11%)	13,35,38	3.01	3 (23%)
54	4SU	1w	8	54	18,21,22	1.85	4 (22%)	25,30,33	1.80	4 (16%)
1	5MU	1A	1915	1	19,22,23	1.41	5 (26%)	27,32,35	2.21	6 (22%)
1	OMG	1A	2251	1,57,55	19,26,27	0.90	1 (5%)	21,38,41	1.12	3 (14%)
32	5MC	2a	967	32	19,22,23	1.71	3 (15%)	26,32,35	1.16	3 (11%)
43	0TD	2l	92	43	8,9,10	4.57	2 (25%)	6,11,13	4.80	2 (33%)
54	8AN	2w	76	54,1,62	17,24,25	1.38	4 (23%)	13,35,38	2.01	2 (15%)
55	PSU	2x	55	55	18,21,22	1.39	2 (11%)	21,30,33	1.99	3 (14%)
54	G7M	2w	46	54	20,26,27	1.21	1 (5%)	16,39,42	0.88	0
32	5MC	2a	1400	32	19,22,23	1.56	3 (15%)	26,32,35	1.19	3 (11%)
1	OMU	2A	2552	1,57	19,22,23	1.10	1 (5%)	25,31,34	1.79	5 (20%)
1	5MU	2A	1939	1,57	19,22,23	1.44	6 (31%)	27,32,35	2.28	6 (22%)
54	PSU	1w	55	54	18,21,22	1.40	2 (11%)	21,30,33	2.03	4 (19%)
54	PSU	2w	39	54	18,21,22	1.41	2 (11%)	21,30,33	1.85	4 (19%)
56	PSU	2y	55	56	18,21,22	1.44	3 (16%)	21,30,33	1.98	4 (19%)
1	OMG	2A	2251	1,55	19,26,27	0.91	1 (5%)	21,38,41	1.14	3 (14%)
54	PSU	2w	32	54	18,21,22	1.37	2 (11%)	21,30,33	1.84	3 (14%)
32	4OC	2a	1402	32	20,23,24	0.75	0	25,32,35	0.99	1 (4%)
1	2MA	1A	2503	1,57	18,25,26	0.70	0	20,37,40	2.11	3 (15%)
32	MA6	1a	1519	32	19,26,27	1.03	2 (10%)	18,38,41	2.09	3 (16%)
1	PSU	1A	2605	1,57	18,21,22	1.47	3 (16%)	21,30,33	1.81	3 (14%)
56	G7M	1y	46	56	20,26,27	1.30	1 (5%)	16,39,42	0.55	0
56	MIA	2y	37	56	17,24,32	1.00	1 (5%)	16,35,47	1.26	2 (12%)
1	PSU	2A	1917	1	18,21,22	1.36	2 (11%)	21,30,33	2.06	4 (19%)
56	4SU	1y	8	56	18,21,22	1.76	5 (27%)	25,30,33	1.90	5 (20%)
55	4SU	1x	8	55	18,21,22	2.17	6 (33%)	25,30,33	1.63	6 (24%)
32	M2G	2a	966	32	20,27,28	1.28	3 (15%)	19,40,43	1.07	1 (5%)
54	G7M	1w	46	54	20,26,27	1.24	2 (10%)	16,39,42	0.64	0
32	MA6	1a	1518	32	19,26,27	1.03	2 (10%)	18,38,41	1.93	3 (16%)
56	PSU	2y	39	56	18,21,22	1.41	2 (11%)	21,30,33	1.65	3 (14%)
55	4SU	2x	8	55	18,21,22	1.99	7 (38%)	25,30,33	1.33	4 (16%)
55	5MU	2x	54	55	19,22,23	1.39	5 (26%)	27,32,35	2.28	6 (22%)

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	1.44	3 (15%)	19,40,43	1.04	2 (10%)
1	PSU	2A	1911	1	18,21,22	1.35	2 (11%)	21,30,33	2.06	3 (14%)
32	MA6	2a	1519	32	19,26,27	1.03	2 (10%)	18,38,41	2.06	3 (16%)
1	5MC	2A	1962	1	19,22,23	1.60	3 (15%)	26,32,35	1.12	2 (7%)
56	4SU	2y	8	56	18,21,22	1.86	5 (27%)	25,30,33	1.85	4 (16%)
1	PSU	1A	1911	1	18,21,22	1.35	2 (11%)	21,30,33	1.99	4 (19%)
54	PSU	1w	32	54	18,21,22	1.40	3 (16%)	21,30,33	1.91	4 (19%)
32	2MG	1a	1207	32	18,26,27	0.96	1 (5%)	16,38,41	1.28	1 (6%)
1	5MC	2A	1942	1	19,22,23	1.64	3 (15%)	26,32,35	1.13	2 (7%)
1	5MU	2A	1915	1	19,22,23	1.43	5 (26%)	27,32,35	2.19	6 (22%)
1	PSU	2A	2605	1	18,21,22	1.33	2 (11%)	21,30,33	2.03	4 (19%)
32	MA6	2a	1518	32	19,26,27	0.99	2 (10%)	18,38,41	2.01	3 (16%)
32	5MC	1a	1407	32	19,22,23	1.68	2 (10%)	26,32,35	1.10	3 (11%)
32	5MC	1a	1404	32	19,22,23	1.65	3 (15%)	26,32,35	1.20	2 (7%)
56	PSU	2y	32	56	18,21,22	1.38	2 (11%)	21,30,33	2.01	4 (19%)
56	PSU	1y	55	56	18,21,22	1.34	2 (11%)	21,30,33	2.06	3 (14%)
1	OMU	1A	2552	1	19,22,23	1.21	3 (15%)	25,31,34	1.82	5 (20%)
32	2MG	2a	1207	32	18,26,27	0.91	1 (5%)	16,38,41	1.49	3 (18%)
55	5MC	2x	32	55	19,22,23	1.64	3 (15%)	26,32,35	1.28	3 (11%)
32	PSU	2a	516	32	18,21,22	1.32	2 (11%)	21,30,33	2.06	4 (19%)
54	8AN	1w	76	54,1,62	17,24,25	1.40	4 (23%)	13,35,38	2.07	2 (15%)
54	PSU	1w	39	54	18,21,22	1.35	2 (11%)	21,30,33	2.07	4 (19%)
54	5MU	1w	54	54	19,22,23	1.43	5 (26%)	27,32,35	1.96	6 (22%)
32	5MC	1a	1400	32	19,22,23	1.62	3 (15%)	26,32,35	1.23	3 (11%)
1	2MA	2A	2503	1,57	18,25,26	0.73	0	20,37,40	2.11	4 (20%)
32	4OC	1a	1402	32	20,23,24	0.76	0	25,32,35	0.96	1 (4%)
56	MIA	1y	37	56	17,24,32	1.04	1 (5%)	16,35,47	1.27	2 (12%)
54	MIA	1w	37	54	24,31,32	2.14	3 (12%)	22,44,47	2.61	7 (31%)
54	4SU	2w	8	54	18,21,22	1.81	5 (27%)	25,30,33	2.50	5 (20%)
32	G7M	2a	527	32	20,26,27	1.21	2 (10%)	16,39,42	0.56	0
32	5MC	2a	1407	57,32	19,22,23	1.69	3 (15%)	26,32,35	1.21	3 (11%)
1	PSU	1A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	2.00	5 (23%)
32	UR3	1a	1498	32	19,22,23	0.96	1 (5%)	26,32,35	1.72	4 (15%)
56	G7M	2y	46	56	20,26,27	1.34	2 (10%)	16,39,42	0.56	0
55	5MC	1x	32	55	19,22,23	1.68	3 (15%)	26,32,35	1.21	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	G7M	1a	527	57,32	20,26,27	1.22	2 (10%)	16,39,42	0.49	0
32	UR3	2a	1498	32	19,22,23	1.02	1 (5%)	26,32,35	1.75	3 (11%)
1	5MC	1A	1962	1,57	19,22,23	1.71	3 (15%)	26,32,35	1.11	3 (11%)
1	OMC	2A	1920	1	19,22,23	0.80	0	25,31,34	0.90	0
32	PSU	1a	516	32	18,21,22	1.37	2 (11%)	21,30,33	1.95	5 (23%)
54	MIA	2w	37	54	19,27,32	1.80	3 (15%)	18,39,47	1.58	5 (27%)
55	5MU	1x	54	57,55	19,22,23	1.43	5 (26%)	27,32,35	2.00	6 (22%)
32	5MC	1a	967	32	19,22,23	1.71	3 (15%)	26,32,35	1.19	2 (7%)
56	PSU	1y	32	56	18,21,22	1.35	2 (11%)	21,30,33	1.89	4 (19%)
55	PSU	1x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.03	4 (19%)
54	PSU	2w	55	54	18,21,22	1.37	2 (11%)	21,30,33	2.03	3 (14%)
56	5MU	2y	54	56	19,22,23	1.41	4 (21%)	27,32,35	1.93	5 (18%)
32	5MC	2a	1404	32	19,22,23	1.75	3 (15%)	26,32,35	1.16	2 (7%)
1	5MC	1A	1942	1	19,22,23	1.74	3 (15%)	26,32,35	1.25	3 (11%)
56	PSU	1y	39	56	18,21,22	1.46	3 (16%)	21,30,33	1.77	4 (19%)
1	5MU	1A	1939	1,57	19,22,23	1.48	6 (31%)	27,32,35	2.19	6 (22%)
55	8AN	1x	76	57,63,55	17,24,25	1.36	3 (17%)	13,35,38	3.04	3 (23%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	1.00	1 (4%)
43	0TD	1l	92	43	8,9,10	4.52	1 (12%)	6,11,13	2.59	2 (33%)
56	5MU	1y	54	56	19,22,23	1.43	5 (26%)	27,32,35	2.28	9 (33%)
54	5MU	2w	54	54	19,22,23	1.30	4 (21%)	27,32,35	2.04	7 (25%)

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
55	8AN	2x	76	57,63,55	-	3/3/25/26	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,57,55	-	0/5/27/28	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
54	8AN	2w	76	54,1,62	-	0/3/25/26	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1,57	-	0/9/27/28	0/2/2/2
1	5MU	2A	1939	1,57	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	4/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55	-	0/5/27/28	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
1	2MA	1A	2503	1,57	-	1/3/25/26	0/3/3/3
32	MA6	1a	1519	32	-	2/7/29/30	0/3/3/3
1	PSU	1A	2605	1,57	-	0/7/25/26	0/2/2/2
56	G7M	1y	46	56	-	2/3/25/26	0/3/3/3
56	MIA	2y	37	56	-	1/3/25/34	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
56	4SU	1y	8	56	-	2/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	G7M	1w	46	54	-	1/3/25/26	0/3/3/3
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	1/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/7/29/30	0/3/3/3
1	5MC	2A	1962	1	-	0/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
1	OMU	1A	2552	1	-	0/9/27/28	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	8AN	1w	76	54,1,62	-	1/3/25/26	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,57	-	2/3/25/26	0/3/3/3
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
56	MIA	1y	37	56	-	2/3/25/34	0/3/3/3
54	MIA	1w	37	54	-	1/11/33/34	0/3/3/3
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32	-	2/3/25/26	0/3/3/3
32	5MC	2a	1407	57,32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
56	G7M	2y	46	56	-	1/3/25/26	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	57,32	-	3/3/25/26	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,57	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	4/7/29/34	0/3/3/3
55	5MU	1x	54	57,55	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
56	5MU	2y	54	56	-	2/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,57	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	57,63,55	-	3/3/25/26	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
56	5MU	1y	54	56	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2

All (229) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.39	1.69	1.82
43	1l	92	0TD	CB-SB	-12.31	1.69	1.82
54	1w	37	MIA	C2-S10	-6.82	1.70	1.75
54	1w	37	MIA	C13-C14	6.74	1.52	1.32
1	1A	1942	5MC	C5-C4	6.46	1.49	1.44
32	2a	1404	5MC	C5-C4	6.43	1.49	1.44
54	2w	37	MIA	C2-S10	-6.33	1.70	1.75
32	2a	967	5MC	C5-C4	6.28	1.48	1.44
32	1a	967	5MC	C5-C4	6.27	1.48	1.44
32	1a	1407	5MC	C5-C4	6.17	1.48	1.44
1	1A	1962	5MC	C5-C4	6.14	1.48	1.44
32	2a	1407	5MC	C5-C4	6.13	1.48	1.44
55	1x	32	5MC	C5-C4	5.98	1.48	1.44
1	2A	1942	5MC	C5-C4	5.88	1.48	1.44
32	1a	1404	5MC	C5-C4	5.86	1.48	1.44
55	2x	32	5MC	C5-C4	5.84	1.48	1.44
32	1a	1400	5MC	C5-C4	5.61	1.48	1.44
1	2A	1962	5MC	C5-C4	5.57	1.48	1.44
32	2a	1400	5MC	C5-C4	5.50	1.48	1.44
55	1x	8	4SU	C4-N3	-5.20	1.32	1.37
54	2w	8	4SU	C4-S4	-5.10	1.59	1.68
54	1w	8	4SU	C4-S4	-4.88	1.60	1.68
56	2y	8	4SU	C4-S4	-4.84	1.60	1.68
56	1y	8	4SU	C4-S4	-4.51	1.60	1.68
55	2x	8	4SU	C4-N3	-4.39	1.33	1.37
55	1x	8	4SU	C4-S4	-4.36	1.61	1.68
32	1a	966	M2G	C2-N3	4.36	1.36	1.30
55	2x	8	4SU	C4-S4	-4.21	1.61	1.68
56	1y	39	PSU	C6-C5	4.18	1.39	1.35
56	2y	46	G7M	C5-C4	4.08	1.47	1.39
56	2y	39	PSU	C6-C5	4.05	1.39	1.35
56	1y	46	G7M	C5-C4	3.93	1.46	1.39
54	2w	39	PSU	C6-C5	3.92	1.39	1.35
54	1w	55	PSU	C6-C5	3.90	1.39	1.35
54	2w	55	PSU	C6-C5	3.89	1.39	1.35
56	1y	32	PSU	C6-C5	3.86	1.39	1.35
55	1x	8	4SU	C2-N3	-3.86	1.31	1.38
56	2y	32	PSU	C6-C5	3.85	1.39	1.35
56	1y	55	PSU	C6-C5	3.80	1.39	1.35
32	2a	966	M2G	C2-N3	3.74	1.35	1.30
54	2w	46	G7M	C5-C4	3.73	1.46	1.39
1	1A	1911	PSU	C6-C5	3.72	1.39	1.35
32	2a	516	PSU	C6-C5	3.70	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	55	PSU	C6-C5	3.69	1.39	1.35
32	1a	516	PSU	C6-C5	3.69	1.39	1.35
54	1w	8	4SU	C4-N3	-3.68	1.33	1.37
1	1A	2605	PSU	C6-C5	3.67	1.39	1.35
32	2a	527	G7M	C5-C4	3.65	1.46	1.39
32	1a	527	G7M	C5-C4	3.64	1.46	1.39
54	1w	46	G7M	C5-C4	3.61	1.46	1.39
54	1w	76	8AN	O4'-C1'	3.59	1.45	1.40
56	2y	55	PSU	C6-C5	3.55	1.39	1.35
55	1x	55	PSU	C6-C5	3.52	1.39	1.35
54	1w	32	PSU	C6-C5	3.49	1.39	1.35
56	2y	8	4SU	C4-N3	-3.48	1.34	1.37
54	2w	32	PSU	C6-C5	3.48	1.39	1.35
1	2A	1917	PSU	C6-C5	3.43	1.39	1.35
1	2A	1911	PSU	C6-C5	3.40	1.39	1.35
54	1w	39	PSU	C6-C5	3.25	1.38	1.35
1	2A	2605	PSU	C6-C5	3.25	1.38	1.35
1	1A	1917	PSU	C6-C5	3.21	1.38	1.35
56	1y	8	4SU	C4-N3	-3.20	1.34	1.37
54	2w	8	4SU	C4-N3	-3.14	1.34	1.37
55	2x	8	4SU	C2-N3	-3.13	1.32	1.38
55	1x	8	4SU	C5-C4	-3.12	1.38	1.42
1	1A	1962	5MC	C6-C5	3.11	1.39	1.34
32	1a	966	M2G	C2-N2	3.10	1.40	1.35
1	1A	2605	PSU	C4-N3	-3.10	1.33	1.38
56	2y	54	5MU	C6-C5	3.07	1.39	1.34
54	2w	76	8AN	O4'-C1'	3.05	1.44	1.40
32	2a	1404	5MC	C6-C5	3.04	1.39	1.34
1	2A	1942	5MC	C6-C5	3.00	1.39	1.34
56	1y	37	MIA	C2-N3	2.99	1.36	1.32
54	1w	54	5MU	C6-C5	2.99	1.39	1.34
55	2x	54	5MU	C6-C5	2.96	1.39	1.34
1	2A	1939	5MU	C6-C5	2.94	1.39	1.34
1	2A	1915	5MU	C6-C5	2.94	1.39	1.34
56	2y	37	MIA	C2-N3	2.91	1.36	1.32
54	2w	37	MIA	C6-C5	2.90	1.49	1.44
1	1A	1939	5MU	C4-N3	-2.90	1.33	1.38
55	2x	8	4SU	C5-C4	-2.90	1.39	1.42
32	1a	1400	5MC	C6-C5	2.90	1.39	1.34
55	1x	54	5MU	C6-C5	2.89	1.39	1.34
55	1x	32	5MC	C6-C5	2.89	1.39	1.34
56	1y	54	5MU	C4-C5	2.89	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1407	5MC	C6-C5	2.87	1.39	1.34
1	2A	1939	5MU	C4-N3	-2.85	1.33	1.38
32	1a	967	5MC	C6-C5	2.83	1.39	1.34
55	1x	54	5MU	C4-N3	-2.83	1.33	1.38
1	2A	1962	5MC	C6-C5	2.81	1.39	1.34
32	2a	1407	5MC	C6-C5	2.81	1.39	1.34
55	2x	32	5MC	C6-C5	2.80	1.39	1.34
54	1w	32	PSU	C4-N3	-2.77	1.33	1.38
1	1A	1915	5MU	C6-C5	2.76	1.39	1.34
1	1A	1942	5MC	C6-C5	2.75	1.39	1.34
32	1a	1404	5MC	C6-C5	2.75	1.39	1.34
56	1y	39	PSU	C4-N3	-2.75	1.33	1.38
56	1y	54	5MU	C6-C5	2.73	1.39	1.34
55	1x	76	8AN	C6-C5	-2.73	1.33	1.43
1	2A	1915	5MU	C2-N1	2.70	1.42	1.38
1	2A	1917	PSU	C4-N3	-2.69	1.33	1.38
32	2a	1400	5MC	C6-C5	2.67	1.39	1.34
56	2y	55	PSU	C4-N3	-2.66	1.33	1.38
56	1y	54	5MU	C2-N1	2.66	1.42	1.38
1	1A	1915	5MU	C2-N1	2.65	1.42	1.38
1	1A	1915	5MU	C4-C5	2.64	1.49	1.44
55	2x	76	8AN	C6-C5	-2.63	1.33	1.43
54	1w	39	PSU	C4-N3	-2.63	1.33	1.38
56	2y	39	PSU	C4-N3	-2.60	1.34	1.38
1	1A	1917	PSU	C4-N3	-2.59	1.34	1.38
1	1A	1939	5MU	C6-C5	2.59	1.38	1.34
32	1a	527	G7M	C6-N1	-2.58	1.33	1.37
55	2x	54	5MU	C4-C5	2.58	1.49	1.44
56	2y	54	5MU	C2-N1	2.57	1.42	1.38
56	2y	8	4SU	C5-C4	-2.57	1.39	1.42
54	1w	55	PSU	C4-N3	-2.57	1.34	1.38
54	1w	54	5MU	C4-N3	-2.57	1.34	1.38
54	1w	8	4SU	C5-C4	-2.56	1.39	1.42
54	2w	8	4SU	C5-C4	-2.54	1.39	1.42
54	2w	39	PSU	C4-N3	-2.54	1.34	1.38
1	2A	2251	OMG	C6-N1	-2.53	1.33	1.37
54	2w	76	8AN	C6-C5	-2.53	1.34	1.43
56	1y	8	4SU	C5-C4	-2.52	1.39	1.42
32	2a	967	5MC	C6-C5	2.52	1.38	1.34
32	2a	966	M2G	C2-N2	2.50	1.39	1.35
32	1a	966	M2G	C6-N1	-2.48	1.34	1.37
55	2x	55	PSU	C4-N3	-2.48	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	54	5MU	C6-C5	2.47	1.38	1.34
1	2A	2605	PSU	C4-N3	-2.47	1.34	1.38
54	1w	76	8AN	C6-C5	-2.45	1.34	1.43
54	2w	32	PSU	C4-N3	-2.45	1.34	1.38
55	1x	76	8AN	C2'-C3'	2.45	1.56	1.53
54	1w	54	5MU	C4-C5	2.45	1.48	1.44
1	1A	2251	OMG	C6-N1	-2.45	1.34	1.37
1	1A	1939	5MU	C2-N1	2.45	1.42	1.38
32	1a	516	PSU	C4-N3	-2.44	1.34	1.38
1	2A	1911	PSU	C4-N3	-2.43	1.34	1.38
56	1y	55	PSU	C4-N3	-2.43	1.34	1.38
32	1a	1519	MA6	C6-C5	-2.42	1.41	1.44
32	1a	1207	2MG	C6-N1	-2.42	1.34	1.37
54	2w	54	5MU	C4-C5	2.41	1.48	1.44
54	2w	37	MIA	C2-N3	2.41	1.37	1.34
55	1x	32	5MC	C6-N1	-2.41	1.33	1.38
56	2y	8	4SU	C2-N3	-2.40	1.33	1.38
32	1a	1518	MA6	C6-C5	-2.40	1.41	1.44
54	1w	8	4SU	C2-N3	-2.40	1.33	1.38
1	2A	1915	5MU	C4-N3	-2.39	1.34	1.38
55	1x	55	PSU	C4-N3	-2.39	1.34	1.38
1	1A	1939	5MU	C4-C5	2.38	1.48	1.44
32	2a	967	5MC	C6-N1	-2.38	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.38	1.33	1.38
1	1A	1939	5MU	C6-N1	-2.38	1.34	1.38
54	2w	55	PSU	C4-N3	-2.37	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.36	1.34	1.38
55	2x	8	4SU	O2-C2	2.36	1.27	1.23
55	2x	54	5MU	C2-N1	2.35	1.42	1.38
32	2a	1519	MA6	C6-C5	-2.34	1.41	1.44
56	2y	32	PSU	C4-N3	-2.34	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.34	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.34	1.34	1.38
1	1A	1915	5MU	C4-N3	-2.34	1.34	1.38
1	2A	1915	5MU	C4-C5	2.33	1.48	1.44
54	1w	54	5MU	C2-N1	2.33	1.42	1.38
56	2y	54	5MU	C4-N3	-2.32	1.34	1.38
1	2A	2552	OMU	C4-N3	-2.32	1.34	1.38
43	2l	92	0TD	CB-CA	2.32	1.55	1.54
1	2A	1939	5MU	C2-N1	2.32	1.42	1.38
56	1y	32	PSU	C4-N3	-2.32	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.31	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	54	5MU	C4-C5	2.31	1.48	1.44
55	2x	54	5MU	C4-N3	-2.30	1.34	1.38
54	1w	46	G7M	C6-N1	-2.28	1.34	1.37
32	2a	527	G7M	C6-N1	-2.28	1.34	1.37
55	1x	54	5MU	C6-N1	-2.27	1.34	1.38
1	1A	2552	OMU	C5-C4	-2.27	1.38	1.43
1	2A	1939	5MU	C4-C5	2.26	1.48	1.44
56	2y	46	G7M	C6-N1	-2.26	1.34	1.37
1	1A	1911	PSU	C4-N3	-2.26	1.34	1.38
55	1x	8	4SU	O2-C2	2.26	1.27	1.23
32	2a	966	M2G	C6-N1	-2.25	1.34	1.37
54	2w	76	8AN	C2'-C3'	-2.25	1.50	1.53
32	2a	1518	MA6	C6-C5	-2.25	1.41	1.44
56	2y	54	5MU	C4-C5	2.24	1.48	1.44
56	1y	8	4SU	C2-N1	2.24	1.42	1.38
32	2a	516	PSU	C4-N3	-2.24	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.24	1.34	1.38
54	1w	37	MIA	C6-C5	2.23	1.48	1.44
55	2x	32	5MC	C6-N1	-2.23	1.34	1.38
1	1A	2552	OMU	C4-N3	-2.22	1.34	1.38
54	2w	54	5MU	C4-N3	-2.22	1.34	1.38
32	1a	967	5MC	C6-N1	-2.22	1.34	1.38
56	2y	8	4SU	C2-N1	2.21	1.41	1.38
1	1A	1962	5MC	C6-N1	-2.21	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.20	1.34	1.38
54	2w	76	8AN	C5-N7	-2.19	1.32	1.39
1	2A	1939	5MU	C2-N3	-2.19	1.34	1.38
56	1y	54	5MU	C6-N1	-2.18	1.34	1.38
32	2a	1498	UR3	C2-N1	2.17	1.41	1.38
32	2a	1400	5MC	C6-N1	-2.17	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.17	1.34	1.38
55	1x	8	4SU	C6-C5	2.15	1.40	1.35
55	1x	54	5MU	C2-N3	-2.14	1.34	1.38
54	1w	76	8AN	C2'-C3'	-2.13	1.50	1.53
55	1x	76	8AN	C5-N7	-2.12	1.32	1.39
56	1y	39	PSU	C2-N3	-2.12	1.34	1.37
56	1y	54	5MU	C4-N3	-2.11	1.34	1.38
56	2y	55	PSU	C2-N3	-2.10	1.34	1.37
32	1a	1518	MA6	C6-N1	2.10	1.35	1.32
56	1y	8	4SU	C2-N3	-2.10	1.34	1.38
1	1A	2605	PSU	C2-N3	-2.09	1.34	1.37
1	2A	1915	5MU	C6-N1	-2.08	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	8	4SU	C2-N3	-2.08	1.34	1.38
55	2x	54	5MU	C6-N1	-2.08	1.34	1.38
54	2w	54	5MU	C2-N1	2.08	1.41	1.38
1	2A	1942	5MC	C6-N1	-2.08	1.34	1.38
54	1w	32	PSU	C2-N3	-2.07	1.34	1.37
1	1A	1915	5MU	C6-N1	-2.07	1.34	1.38
32	1a	1519	MA6	C6-N1	2.07	1.35	1.32
54	1w	76	8AN	C5-N7	-2.06	1.32	1.39
32	2a	1519	MA6	C6-N1	2.05	1.35	1.32
54	1w	54	5MU	C2-N3	-2.05	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.04	1.34	1.37
32	1a	1498	UR3	C2-N1	2.04	1.41	1.38
55	2x	76	8AN	C5-N7	-2.03	1.32	1.39
32	2a	1518	MA6	C6-N1	2.03	1.35	1.32
54	2w	8	4SU	C2-N1	2.03	1.41	1.38
55	2x	8	4SU	C6-C5	2.02	1.39	1.35
1	1A	2552	OMU	C2-N1	2.02	1.41	1.38
55	2x	8	4SU	C2-N1	2.02	1.41	1.38

All (293) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	11.38	122.83	102.36
54	1w	37	MIA	C12-C13-C14	-9.28	110.36	127.01
55	1x	76	8AN	C4'-O4'-C1'	-8.27	102.35	109.92
54	2w	8	4SU	C4-N3-C2	-7.76	119.88	127.31
1	1A	2503	2MA	C2-N3-C4	7.73	121.70	115.46
1	2A	2503	2MA	C2-N3-C4	7.54	121.55	115.46
55	2x	76	8AN	C4'-O4'-C1'	-7.45	103.11	109.92
32	2a	1498	UR3	C4-N3-C2	-6.96	118.98	124.58
32	1a	1498	UR3	C4-N3-C2	-6.82	119.09	124.58
55	2x	76	8AN	N3-C2-N1	-6.59	119.73	128.67
54	2w	8	4SU	C5-C4-N3	6.45	120.75	114.75
54	2w	76	8AN	N3-C2-N1	-6.45	119.92	128.67
1	2A	1917	PSU	N1-C2-N3	6.44	121.96	115.17
54	1w	76	8AN	N3-C2-N1	-6.44	119.93	128.67
1	2A	1911	PSU	N1-C2-N3	6.42	121.94	115.17
54	1w	39	PSU	N1-C2-N3	6.38	121.89	115.17
54	2w	55	PSU	N1-C2-N3	6.32	121.83	115.17
56	2y	32	PSU	N1-C2-N3	6.32	121.83	115.17
55	1x	76	8AN	N3-C2-N1	-6.31	120.11	128.67
55	2x	55	PSU	N1-C2-N3	6.30	121.81	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	55	PSU	N1-C2-N3	6.23	121.74	115.17
32	2a	516	PSU	N1-C2-N3	6.19	121.70	115.17
56	1y	55	PSU	N1-C2-N3	6.17	121.68	115.17
54	1w	55	PSU	N1-C2-N3	6.16	121.66	115.17
56	2y	55	PSU	N1-C2-N3	6.15	121.66	115.17
1	2A	2605	PSU	N1-C2-N3	6.05	121.55	115.17
1	1A	1911	PSU	N1-C2-N3	6.03	121.53	115.17
54	1w	32	PSU	N1-C2-N3	6.01	121.50	115.17
32	1a	516	PSU	N1-C2-N3	5.99	121.48	115.17
1	1A	1917	PSU	N1-C2-N3	5.88	121.37	115.17
32	1a	1519	MA6	N3-C2-N1	-5.83	120.75	128.67
32	2a	1519	MA6	N3-C2-N1	-5.83	120.76	128.67
54	2w	32	PSU	N1-C2-N3	5.75	121.23	115.17
32	2a	1518	MA6	N3-C2-N1	-5.71	120.92	128.67
55	2x	54	5MU	C4-N3-C2	-5.69	119.89	127.34
56	1y	54	5MU	C4-N3-C2	-5.66	119.92	127.34
1	2A	1939	5MU	C4-N3-C2	-5.64	119.95	127.34
56	1y	32	PSU	N1-C2-N3	5.62	121.09	115.17
54	2w	39	PSU	N1-C2-N3	5.62	121.09	115.17
43	1l	92	0TD	CSB-SB-CB	-5.59	92.32	102.36
1	1A	1939	5MU	C5-C4-N3	5.55	120.15	115.32
56	1y	39	PSU	N1-C2-N3	5.52	120.99	115.17
32	1a	1518	MA6	N3-C2-N1	-5.48	121.24	128.67
55	2x	54	5MU	N3-C2-N1	5.44	121.98	114.89
1	1A	1915	5MU	C4-N3-C2	-5.44	120.21	127.34
1	2A	1939	5MU	N3-C2-N1	5.41	121.94	114.89
56	2y	8	4SU	C5-C4-N3	5.41	119.78	114.75
1	1A	2605	PSU	N1-C2-N3	5.38	120.84	115.17
56	1y	54	5MU	N3-C2-N1	5.33	121.83	114.89
1	1A	1915	5MU	N3-C2-N1	5.31	121.80	114.89
1	2A	1915	5MU	C4-N3-C2	-5.28	120.42	127.34
54	1w	8	4SU	C5-C4-N3	5.22	119.60	114.75
1	1A	1939	5MU	C4-N3-C2	-5.21	120.52	127.34
56	2y	39	PSU	N1-C2-N3	5.20	120.65	115.17
56	1y	8	4SU	C4-N3-C2	-5.20	122.33	127.31
32	2a	1518	MA6	C2-N1-C6	5.16	121.90	116.84
32	1a	1519	MA6	C2-N1-C6	5.08	121.82	116.84
1	2A	1915	5MU	N3-C2-N1	5.06	121.48	114.89
55	1x	54	5MU	N3-C2-N1	5.05	121.47	114.89
1	2A	1939	5MU	C5-C4-N3	5.04	119.70	115.32
54	1w	8	4SU	C4-N3-C2	-5.00	122.52	127.31
54	1w	54	5MU	N3-C2-N1	4.95	121.34	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1518	MA6	C2-N1-C6	4.91	121.66	116.84
56	1y	8	4SU	C5-C4-N3	4.88	119.29	114.75
55	1x	54	5MU	C4-N3-C2	-4.88	120.94	127.34
32	2a	1519	MA6	C2-N1-C6	4.80	121.55	116.84
54	2w	54	5MU	C4-N3-C2	-4.76	121.09	127.34
1	2A	1915	5MU	O4-C4-C5	-4.75	119.48	124.92
54	1w	54	5MU	C4-N3-C2	-4.72	121.15	127.34
56	2y	8	4SU	C4-N3-C2	-4.69	122.82	127.31
55	2x	54	5MU	O4-C4-C5	-4.67	119.58	124.92
1	1A	2552	OMU	C4-N3-C2	-4.65	120.85	126.61
1	2A	2552	OMU	C4-N3-C2	-4.63	120.86	126.61
1	2A	1915	5MU	C5-C4-N3	4.62	119.34	115.32
55	2x	54	5MU	C5-C4-N3	4.57	119.30	115.32
56	1y	54	5MU	C5-C4-N3	4.56	119.29	115.32
54	2w	8	4SU	N3-C2-N1	4.55	120.81	114.89
54	2w	54	5MU	N3-C2-N1	4.52	120.78	114.89
56	2y	54	5MU	N3-C2-N1	4.52	120.78	114.89
1	1A	1915	5MU	C5-C4-N3	4.35	119.10	115.32
56	2y	54	5MU	C4-N3-C2	-4.34	121.64	127.34
56	2y	54	5MU	O4-C4-C5	-4.34	119.96	124.92
1	2A	1939	5MU	O4-C4-C5	-4.32	119.97	124.92
1	2A	2605	PSU	C4-N3-C2	-4.32	120.42	126.37
54	2w	54	5MU	C5-C4-N3	4.31	119.07	115.32
1	1A	1939	5MU	N3-C2-N1	4.31	120.50	114.89
32	2a	516	PSU	C4-N3-C2	-4.27	120.49	126.37
1	1A	1915	5MU	O4-C4-C5	-4.26	120.04	124.92
54	1w	37	MIA	C15-C14-C13	-4.24	109.93	122.66
1	1A	1911	PSU	C4-N3-C2	-4.24	120.53	126.37
1	2A	1917	PSU	C4-N3-C2	-4.23	120.55	126.37
1	1A	2552	OMU	N3-C2-N1	4.20	120.36	114.89
54	2w	54	5MU	O4-C4-C5	-4.19	120.13	124.92
1	2A	2552	OMU	N3-C2-N1	4.17	120.32	114.89
56	1y	55	PSU	C4-N3-C2	-4.17	120.62	126.37
32	1a	516	PSU	C4-N3-C2	-4.12	120.70	126.37
54	2w	8	4SU	C5-C4-S4	-4.11	119.61	124.31
54	1w	39	PSU	C4-N3-C2	-4.11	120.71	126.37
54	1w	54	5MU	C5-C4-N3	4.10	118.89	115.32
1	1A	1939	5MU	O4-C4-C5	-4.07	120.26	124.92
55	2x	55	PSU	C4-N3-C2	-4.04	120.80	126.37
55	1x	54	5MU	C5-C4-N3	4.02	118.82	115.32
1	2A	1911	PSU	O2-C2-N1	-4.02	118.65	122.79
1	2A	1939	5MU	C5-C6-N1	-4.01	118.96	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	1y	54	5MU	O4-C4-C5	-4.00	120.34	124.92
1	1A	1917	PSU	C4-N3-C2	-4.00	120.86	126.37
1	2A	1911	PSU	C4-N3-C2	-4.00	120.86	126.37
1	1A	1939	5MU	C5-C6-N1	-3.99	118.98	123.31
54	1w	55	PSU	C4-N3-C2	-3.98	120.89	126.37
32	1a	967	5MC	C5-C6-N1	-3.97	119.00	123.31
56	2y	54	5MU	C5-C4-N3	3.96	118.77	115.32
55	1x	55	PSU	C4-N3-C2	-3.96	120.91	126.37
56	1y	55	PSU	O2-C2-N1	-3.94	118.73	122.79
54	2w	37	MIA	C12-N6-C6	-3.93	119.21	122.85
1	1A	1917	PSU	O2-C2-N1	-3.92	118.74	122.79
54	1w	39	PSU	O2-C2-N1	-3.92	118.74	122.79
54	2w	55	PSU	C4-N3-C2	-3.91	120.99	126.37
56	2y	32	PSU	C4-N3-C2	-3.90	121.00	126.37
54	2w	55	PSU	O2-C2-N1	-3.86	118.81	122.79
54	1w	32	PSU	C4-N3-C2	-3.85	121.07	126.37
55	1x	8	4SU	C6-C5-C4	-3.84	116.63	119.95
32	2a	1404	5MC	C5-C6-N1	-3.82	119.16	123.31
56	1y	37	MIA	N3-C2-N1	-3.81	123.51	128.67
55	2x	54	5MU	C5-C6-N1	-3.79	119.19	123.31
55	1x	55	PSU	O2-C2-N1	-3.72	118.95	122.79
56	2y	55	PSU	C4-N3-C2	-3.72	121.25	126.37
54	1w	54	5MU	O4-C4-C5	-3.72	120.67	124.92
54	1w	37	MIA	C16-C14-C13	-3.71	111.52	122.66
56	2y	37	MIA	N3-C2-N1	-3.70	123.65	128.67
1	1A	2605	PSU	C4-N3-C2	-3.69	121.28	126.37
55	1x	54	5MU	C5-C6-N1	-3.68	119.31	123.31
56	1y	32	PSU	C4-N3-C2	-3.68	121.31	126.37
1	1A	1911	PSU	O2-C2-N1	-3.66	119.02	122.79
56	2y	32	PSU	O2-C2-N1	-3.65	119.03	122.79
55	1x	8	4SU	O2-C2-N1	3.64	127.54	122.80
54	2w	32	PSU	C4-N3-C2	-3.64	121.36	126.37
1	2A	1917	PSU	O2-C2-N1	-3.62	119.06	122.79
54	2w	39	PSU	C4-N3-C2	-3.59	121.43	126.37
32	2a	516	PSU	O2-C2-N1	-3.58	119.09	122.79
1	1A	2552	OMU	C5-C4-N3	3.58	119.81	114.80
1	2A	2552	OMU	C5-C4-N3	3.54	119.76	114.80
55	2x	32	5MC	C5-C6-N1	-3.53	119.48	123.31
55	1x	54	5MU	O4-C4-C5	-3.52	120.89	124.92
54	1w	55	PSU	O2-C2-N1	-3.51	119.17	122.79
1	2A	1915	5MU	C5-C6-N1	-3.50	119.51	123.31
1	2A	2552	OMU	O2-C2-N1	-3.47	118.28	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1942	5MC	C5-C6-N1	-3.45	119.57	123.31
32	1a	1400	5MC	C5-C6-N1	-3.44	119.57	123.31
1	1A	2552	OMU	O4-C4-C5	-3.44	119.22	125.16
1	2A	2605	PSU	O2-C2-N1	-3.44	119.24	122.79
32	2a	967	5MC	C5-C6-N1	-3.42	119.60	123.31
56	1y	8	4SU	N3-C2-N1	3.41	119.34	114.89
56	1y	54	5MU	C5-C6-N1	-3.41	119.61	123.31
1	1A	1915	5MU	C5-C6-N1	-3.39	119.63	123.31
32	1a	1404	5MC	C5-C6-N1	-3.37	119.65	123.31
56	1y	32	PSU	O2-C2-N1	-3.37	119.32	122.79
1	1A	1942	5MC	C5-C4-N3	-3.36	118.31	121.75
32	1a	1404	5MC	C5-C4-N3	-3.35	118.32	121.75
55	1x	32	5MC	C5-C6-N1	-3.33	119.69	123.31
32	2a	1407	5MC	C5-C4-N3	-3.29	118.38	121.75
1	1A	1942	5MC	C5-C6-N1	-3.26	119.77	123.31
54	1w	54	5MU	C5-C6-N1	-3.24	119.80	123.31
32	2a	1498	UR3	C5-C4-N3	3.24	119.30	115.04
56	1y	8	4SU	C5-C4-S4	-3.23	120.62	124.31
56	1y	39	PSU	C4-N3-C2	-3.23	121.92	126.37
54	1w	8	4SU	N3-C2-N1	3.22	119.08	114.89
1	1A	1962	5MC	C5-C6-N1	-3.20	119.83	123.31
56	2y	55	PSU	O2-C2-N1	-3.20	119.48	122.79
32	1a	1207	2MG	C8-N7-C5	3.18	107.97	102.55
32	1a	1407	5MC	C5-C6-N1	-3.18	119.86	123.31
32	2a	1400	5MC	C5-C6-N1	-3.18	119.86	123.31
32	1a	1519	MA6	C4-C5-N7	-3.17	105.99	109.34
32	2a	1407	5MC	C5-C6-N1	-3.15	119.89	123.31
55	2x	76	8AN	O4'-C1'-N9	3.13	112.90	108.75
32	2a	1519	MA6	C4-C5-N7	-3.11	106.05	109.34
1	2A	1962	5MC	C5-C6-N1	-3.07	119.98	123.31
32	1a	1498	UR3	C5-C4-N3	3.06	119.08	115.04
55	1x	32	5MC	C5-C4-N3	-3.06	118.61	121.75
55	2x	54	5MU	O2-C2-N1	-3.04	118.84	122.80
32	1a	1400	5MC	C5-C4-N3	-3.02	118.66	121.75
1	1A	2251	OMG	C8-N7-C5	3.02	107.69	102.55
32	2a	1207	2MG	N1-C2-N2	3.01	119.64	116.56
1	2A	2503	2MA	C4-C5-N7	-3.01	106.16	109.34
54	1w	37	MIA	C11-S10-C2	-3.00	100.00	102.25
55	2x	55	PSU	O2-C2-N1	-3.00	119.70	122.79
32	2a	1207	2MG	C8-N7-C5	2.98	107.61	102.55
55	1x	8	4SU	S4-C4-N3	-2.97	117.10	120.20
56	2y	54	5MU	C5-C6-N1	-2.97	120.09	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	32	5MC	C5-C4-N3	-2.96	118.72	121.75
55	2x	8	4SU	C5-C4-N3	2.96	117.50	114.75
56	2y	8	4SU	N3-C2-N1	2.95	118.73	114.89
55	1x	8	4SU	C5-C4-N3	2.94	117.48	114.75
54	2w	39	PSU	O2-C2-N1	-2.94	119.76	122.79
56	2y	39	PSU	C4-N3-C2	-2.93	122.33	126.37
1	2A	2552	OMU	O4-C4-C5	-2.91	120.14	125.16
1	2A	1942	5MC	C5-C4-N3	-2.91	118.77	121.75
32	1a	966	M2G	C8-N7-C5	2.90	107.49	102.55
54	2w	32	PSU	O2-C2-N1	-2.88	119.81	122.79
1	2A	2251	OMG	C8-N7-C5	2.88	107.45	102.55
54	1w	32	PSU	O2-C2-N1	-2.84	119.86	122.79
1	1A	1915	5MU	O2-C2-N1	-2.80	119.16	122.80
54	2w	54	5MU	C5M-C5-C4	2.78	121.75	118.78
55	2x	8	4SU	C1'-N1-C2	2.77	122.57	117.59
32	2a	1207	2MG	N2-C2-N3	-2.76	116.99	120.51
54	2w	54	5MU	O2-C2-N1	-2.76	119.20	122.80
32	2a	1518	MA6	C4-C5-N7	-2.76	106.43	109.34
1	2A	1962	5MC	C5-C4-N3	-2.73	118.96	121.75
1	1A	2552	OMU	O2-C2-N1	-2.72	119.25	122.80
56	1y	54	5MU	O2-C2-N1	-2.72	119.26	122.80
32	2a	966	M2G	C8-N7-C5	2.72	107.17	102.55
56	1y	39	PSU	O2-C2-N3	-2.71	117.05	121.86
1	1A	2503	2MA	C4-C5-N7	-2.70	106.48	109.34
55	1x	54	5MU	O2-C2-N1	-2.69	119.29	122.80
32	1a	1407	5MC	C5-C4-N3	-2.69	119.00	121.75
56	1y	8	4SU	C1'-N1-C2	2.68	122.41	117.59
54	2w	54	5MU	C5-C6-N1	-2.68	120.40	123.31
54	1w	37	MIA	C2-N1-C6	2.67	122.17	117.42
55	2x	8	4SU	C6-C5-C4	-2.67	117.64	119.95
32	1a	1400	5MC	O2-C2-N3	-2.66	118.14	122.33
56	2y	55	PSU	C6-C5-C4	-2.62	116.40	118.17
56	1y	37	MIA	C4-C5-N7	-2.62	106.57	109.34
54	2w	37	MIA	C4-C5-N7	-2.61	106.58	109.34
55	1x	76	8AN	O2'-C2'-C3'	2.61	118.49	111.61
55	2x	8	4SU	O2-C2-N1	2.60	126.18	122.80
54	2w	8	4SU	O2-C2-N1	-2.59	119.42	122.80
32	1a	1518	MA6	C4-C5-N7	-2.59	106.60	109.34
56	2y	8	4SU	C5-C4-S4	-2.59	121.35	124.31
32	2a	1404	5MC	C5-C4-N3	-2.58	119.11	121.75
1	2A	2503	2MA	C2-N1-C6	2.56	122.04	118.10
1	1A	1920	OMC	O2-C2-N3	-2.56	118.29	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	516	PSU	O2-C2-N1	-2.55	120.16	122.79
56	1y	54	5MU	C5M-C5-C4	2.55	121.50	118.78
32	2a	1400	5MC	C5-C4-N3	-2.54	119.15	121.75
1	1A	1962	5MC	C5-C4-N3	-2.53	119.16	121.75
32	2a	967	5MC	C5-C4-N3	-2.51	119.19	121.75
56	2y	37	MIA	C4-C5-N7	-2.47	106.73	109.34
1	2A	2251	OMG	C5-C6-N1	2.44	118.73	114.07
54	1w	8	4SU	C5-C4-S4	-2.44	121.52	124.31
32	2a	1407	5MC	O2-C2-N3	-2.43	118.50	122.33
55	2x	32	5MC	O2-C2-N3	-2.41	118.53	122.33
54	2w	37	MIA	C2-N1-C6	2.40	121.68	117.42
54	2w	76	8AN	C4'-O4'-C1'	-2.39	107.74	109.92
32	1a	1407	5MC	O2-C2-N3	-2.35	118.63	122.33
1	2A	1915	5MU	O2-C2-N1	-2.35	119.74	122.80
32	2a	1402	4OC	C6-C5-C4	2.35	119.83	117.00
1	1A	1942	5MC	CM5-C5-C6	-2.34	119.68	122.85
32	1a	967	5MC	C5-C4-N3	-2.34	119.35	121.75
1	1A	2503	2MA	C2-N1-C6	2.33	121.69	118.10
56	1y	32	PSU	C6-C5-C4	-2.33	116.60	118.17
32	1a	1402	4OC	C6-C5-C4	2.32	119.80	117.00
32	2a	1400	5MC	O2-C2-N3	-2.32	118.67	122.33
1	1A	1962	5MC	O2-C2-N3	-2.31	118.69	122.33
55	1x	8	4SU	O2-C2-N3	-2.31	117.23	121.49
55	1x	32	5MC	O2-C2-N3	-2.30	118.71	122.33
1	1A	1939	5MU	C5M-C5-C4	2.28	121.21	118.78
1	2A	1917	PSU	C5-C6-N1	-2.27	118.99	122.14
1	2A	1939	5MU	O2-C2-N1	-2.26	119.85	122.80
54	1w	76	8AN	O2'-C2'-C3'	-2.25	105.68	111.61
56	1y	54	5MU	C5M-C5-C6	-2.24	119.82	122.85
32	1a	516	PSU	O4'-C1'-C2'	2.24	108.25	105.15
54	1w	37	MIA	C4-C5-N7	-2.24	106.97	109.34
32	1a	516	PSU	C5-C6-N1	-2.24	119.03	122.14
43	1l	92	0TD	OD2-CG-CB	2.24	117.99	113.15
54	1w	54	5MU	O2-C2-N1	-2.24	119.88	122.80
1	2A	2503	2MA	C5-C6-N1	-2.23	118.21	120.84
1	1A	2605	PSU	C5-C6-N1	-2.22	119.05	122.14
54	2w	37	MIA	C11-S10-C2	-2.22	100.59	102.25
55	1x	8	4SU	C1'-N1-C2	2.21	121.57	117.59
1	2A	2251	OMG	O6-C6-C5	-2.20	119.96	124.32
43	2l	92	0TD	OD2-CG-CB	2.20	117.90	113.15
56	2y	32	PSU	O4'-C1'-C2'	2.20	108.19	105.15
1	2A	2605	PSU	C5-C6-N1	-2.18	119.11	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2w	39	PSU	C6-C5-C4	-2.17	116.71	118.17
32	1a	966	M2G	C5-C6-N1	2.16	118.19	114.07
55	1x	55	PSU	C5-C6-N1	-2.15	119.16	122.14
54	1w	32	PSU	C5-C6-N1	-2.15	119.16	122.14
56	1y	39	PSU	C6-C5-C4	-2.14	116.73	118.17
1	1A	2251	OMG	C5-C6-N1	2.14	118.15	114.07
32	2a	967	5MC	CM5-C5-C6	-2.14	119.95	122.85
54	1w	39	PSU	C5-C6-N1	-2.13	119.18	122.14
1	1A	2251	OMG	O6-C6-C5	-2.12	120.11	124.32
32	1a	1498	UR3	C6-N1-C2	-2.11	120.07	121.80
32	1a	1498	UR3	C3U-N3-C4	2.11	120.80	117.87
54	1w	37	MIA	N3-C2-N1	-2.11	123.17	127.03
54	1w	55	PSU	C6-C5-C4	-2.09	116.76	118.17
56	2y	39	PSU	O2-C2-N3	-2.07	118.19	121.86
1	1A	1911	PSU	C5-C6-N1	-2.06	119.28	122.14
1	1A	1917	PSU	O4'-C1'-C2'	2.06	108.00	105.15
54	2w	37	MIA	N3-C2-N1	-2.04	123.30	127.03
1	1A	1917	PSU	C5-C6-N1	-2.03	119.32	122.14
32	2a	516	PSU	O4'-C1'-C2'	2.02	107.95	105.15
56	1y	54	5MU	C1'-N1-C2	2.02	121.22	117.59
32	2a	1498	UR3	C3U-N3-C4	2.01	120.65	117.87

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	C12-C13-C14-C16
56	1y	46	G7M	C4'-C5'-O5'-P
54	2w	37	MIA	C5-C6-N6-C12
54	2w	37	MIA	N1-C6-N6-C12
54	2w	37	MIA	N1-C2-S10-C11
54	2w	37	MIA	N3-C2-S10-C11
55	2x	76	8AN	O4'-C4'-C5'-O5'
55	2x	76	8AN	C3'-C4'-C5'-O5'
56	2y	54	5MU	O4'-C4'-C5'-O5'
56	2y	55	PSU	C2'-C1'-C5-C4
55	1x	76	8AN	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
55	1x	76	8AN	O4'-C4'-C5'-O5'
56	1y	37	MIA	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
56	2y	54	5MU	C3'-C4'-C5'-O5'
56	2y	55	PSU	C3'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
56	1y	37	MIA	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
56	2y	55	PSU	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
55	2x	76	8AN	C4'-C5'-O5'-P
1	2A	2503	2MA	O4'-C4'-C5'-O5'
56	2y	37	MIA	C3'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
55	1x	76	8AN	C4'-C5'-O5'-P
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	1a	967	5MC	O4'-C4'-C5'-O5'
56	1y	46	G7M	C3'-C4'-C5'-O5'
43	1l	92	0TD	SB-CB-CG-OD1
43	2l	92	0TD	SB-CB-CG-OD1
56	1y	55	PSU	O4'-C1'-C5-C4
56	2y	55	PSU	O4'-C1'-C5-C4
54	1w	46	G7M	C4'-C5'-O5'-P
1	2A	2503	2MA	C3'-C4'-C5'-O5'
1	1A	2503	2MA	C4'-C5'-O5'-P
43	1l	92	0TD	CA-CB-SB-CSB
43	2l	92	0TD	SB-CB-CG-OD2
32	1a	527	G7M	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
56	2y	46	G7M	C4'-C5'-O5'-P
1	1A	1920	OMC	C2'-C1'-N1-C6
56	1y	8	4SU	C3'-C4'-C5'-O5'
56	1y	8	4SU	O4'-C4'-C5'-O5'
55	2x	8	4SU	C2'-C1'-N1-C2
54	1w	76	8AN	O4'-C4'-C5'-O5'

There are no ring outliers.

28 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	2x	76	8AN	2	0
1	1A	2251	OMG	1	0
32	2a	967	5MC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	2l	92	0TD	1	0
54	2w	76	8AN	1	0
54	2w	46	G7M	1	0
54	2w	39	PSU	2	0
56	2y	55	PSU	5	0
1	2A	2251	OMG	1	0
32	2a	1402	4OC	1	0
32	1a	1519	MA6	2	0
56	1y	46	G7M	1	0
56	2y	37	MIA	1	0
56	1y	8	4SU	1	0
55	1x	8	4SU	2	0
32	2a	966	M2G	1	0
32	1a	1518	MA6	2	0
56	2y	39	PSU	1	0
32	2a	1519	MA6	2	0
32	2a	1518	MA6	3	0
56	1y	55	PSU	1	0
1	2A	2503	2MA	1	0
32	1a	1402	4OC	1	0
56	1y	37	MIA	3	0
54	1w	37	MIA	1	0
56	2y	46	G7M	3	0
1	1A	1939	5MU	1	0
55	1x	76	8AN	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2794 ligands modelled in this entry, 2786 are monoatomic - leaving 8 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	$\#\|Z\|>2$
59	A1AE0	2A	3863	-	77,77,77	2.37	14 (18%)	107,113,113	2.09	16 (14%)
62	PHE	1w	109	54	10,11,12	1.60	1 (10%)	8,13,15	0.56	0
59	A1AE0	1A	4110	-	77,77,77	2.28	13 (16%)	107,113,113	2.02	24 (22%)
62	PHE	2w	108	54	10,11,12	1.63	1 (10%)	8,13,15	0.54	0
61	SF4	2d	303	35	0,12,12	-	-	-		
61	SF4	1d	302	35	0,12,12	-	-	-		
63	FME	1x	115	55	8,9,10	0.45	0	8,9,11	1.29	1 (12%)
63	FME	2x	107	55	8,9,10	0.39	0	8,9,11	1.11	0

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
59	A1AE0	2A	3863	-	-	11/88/121/121	0/6/6/6
62	PHE	1w	109	54	-	1/5/6/8	0/1/1/1
59	A1AE0	1A	4110	-	-	12/88/121/121	0/6/6/6
62	PHE	2w	108	54	-	2/5/6/8	0/1/1/1
61	SF4	2d	303	35	-	-	0/6/5/5
61	SF4	1d	302	35	-	-	0/6/5/5
63	FME	1x	115	55	-	0/7/9/11	-
63	FME	2x	107	55	-	0/7/9/11	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	2A	3863	A1AE0	CAG-CAF	-12.45	1.41	1.53
59	1A	4110	A1AE0	CAG-CAF	-11.70	1.42	1.53
59	2A	3863	A1AE0	CAB-CAF	-6.97	1.40	1.52
59	1A	4110	A1AE0	OBR-NBJ	6.66	1.56	1.40
59	2A	3863	A1AE0	CAJ-CAI	-6.21	1.38	1.51
59	1A	4110	A1AE0	CAB-CAF	-6.00	1.42	1.52
59	2A	3863	A1AE0	CCJ-CCQ	-5.84	1.39	1.48
59	1A	4110	A1AE0	CCJ-CCQ	-5.61	1.39	1.48
62	2w	108	PHE	CB-CG	-4.97	1.39	1.51
62	1w	109	PHE	CB-CG	-4.86	1.39	1.51
59	1A	4110	A1AE0	CAJ-CAI	-4.67	1.41	1.51
59	1A	4110	A1AE0	CCK-NCL	4.37	1.41	1.34
59	2A	3863	A1AE0	CCK-NCL	4.34	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	2A	3863	A1AE0	CCT-CCB	4.32	1.25	1.19
59	1A	4110	A1AE0	CAF-NBJ	4.15	1.34	1.28
59	2A	3863	A1AE0	CCF-CCI	-4.00	1.40	1.48
59	2A	3863	A1AE0	OBH-CAL	-3.91	1.41	1.47
59	1A	4110	A1AE0	CCF-CCI	-3.52	1.41	1.48
59	2A	3863	A1AE0	CAF-NBJ	3.46	1.33	1.28
59	1A	4110	A1AE0	CCG-NCL	-3.27	1.36	1.40
59	2A	3863	A1AE0	OBR-NBJ	3.15	1.48	1.40
59	2A	3863	A1AE0	CCG-NCL	-3.08	1.36	1.40
59	1A	4110	A1AE0	CCN-CCM	2.52	1.54	1.48
59	1A	4110	A1AE0	CCO-CCM	2.37	1.54	1.48
59	2A	3863	A1AE0	CAG-CAH	2.36	1.57	1.54
59	1A	4110	A1AE0	CAG-CAH	2.32	1.57	1.54
59	2A	3863	A1AE0	CCN-CCM	2.27	1.53	1.48
59	2A	3863	A1AE0	CCO-CCM	2.26	1.53	1.48
59	1A	4110	A1AE0	CAA-CAE	2.09	1.55	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	2A	3863	A1AE0	CAB-CAF-NBJ	-13.77	116.06	126.21
59	1A	4110	A1AE0	CAB-CAF-NBJ	-11.49	117.74	126.21
59	2A	3863	A1AE0	CAB-CAF-CAG	6.21	125.96	119.34
59	2A	3863	A1AE0	OBB-CBT-NBV	4.99	119.14	111.01
59	1A	4110	A1AE0	CCN-CCM-NCL	-4.77	111.33	118.87
59	1A	4110	A1AE0	CAB-CAF-CAG	4.74	124.39	119.34
59	1A	4110	A1AE0	OBB-CBT-NBV	4.72	118.70	111.01
59	1A	4110	A1AE0	CBE-CAM-CAL	-4.04	109.66	115.23
59	2A	3863	A1AE0	CBE-CAM-CAL	-3.85	109.93	115.23
59	2A	3863	A1AE0	CAE-CAA-CAB	-3.71	110.04	116.10
59	2A	3863	A1AE0	CAE-CAD-CAC	-3.67	107.93	113.54
59	1A	4110	A1AE0	CAE-CAD-CAC	-3.58	108.07	113.54
59	2A	3863	A1AE0	OBB-CBT-OBU	-3.57	119.30	124.55
59	1A	4110	A1AE0	OBH-CAL-CBG	3.49	112.96	106.80
59	2A	3863	A1AE0	CCN-CCM-NCL	-3.41	113.48	118.87
59	1A	4110	A1AE0	CCF-CCG-NCL	3.34	121.46	118.83
59	2A	3863	A1AE0	CAG-CAF-NBJ	3.29	117.79	114.40
59	1A	4110	A1AE0	CCJ-CCK-NCL	-3.02	120.80	124.42
59	1A	4110	A1AE0	OBH-CAL-CAM	2.96	112.19	105.63
59	2A	3863	A1AE0	CCJ-CCK-NCL	-2.96	120.88	124.42
59	1A	4110	A1AE0	OAO-CAD-CAE	2.94	113.28	106.44
59	2A	3863	A1AE0	CAX-CAR-CAS	-2.89	108.90	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	1A	4110	A1AE0	OBB-CBT-OBU	-2.85	120.36	124.55
59	1A	4110	A1AE0	CAX-CAR-CAS	-2.85	108.96	113.27
59	2A	3863	A1AE0	OBH-CAL-CBG	2.75	111.65	106.80
59	1A	4110	A1AE0	CAG-CAF-NBJ	2.67	117.16	114.40
59	1A	4110	A1AE0	OBU-CBT-NBV	-2.66	120.93	124.93
59	1A	4110	A1AE0	CBO-OBL-CAE	-2.61	112.21	117.51
59	1A	4110	A1AE0	OBR-NBJ-CAF	2.39	118.07	111.25
59	1A	4110	A1AE0	CBG-CAL-CAM	-2.37	108.13	112.36
63	1x	115	FME	O1-CN-N	-2.35	119.25	125.32
59	2A	3863	A1AE0	CCF-CCG-NCL	2.31	120.65	118.83
59	1A	4110	A1AE0	OAN-CAM-CBE	2.28	111.59	107.36
59	2A	3863	A1AE0	OBU-CBT-NBV	-2.26	121.53	124.93
59	1A	4110	A1AE0	CCH-CCC-CCT	-2.22	116.21	120.22
59	1A	4110	A1AE0	OAO-CAP-OAQ	-2.19	104.92	110.69
59	2A	3863	A1AE0	CCF-CCI-CCJ	2.14	118.34	115.64
59	2A	3863	A1AE0	CCG-NCL-CCM	2.06	122.02	119.88
59	1A	4110	A1AE0	CBX-CBW-NBV	-2.05	106.45	112.20
59	1A	4110	A1AE0	CBW-NBV-CBT	2.04	125.45	121.98
59	1A	4110	A1AE0	CCG-NCL-CCM	2.03	121.99	119.88

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1A	4110	A1AE0	NBJ-CAF-CAG-CBI
59	2A	3863	A1AE0	CAF-NBJ-OBR-CBS
62	1w	109	PHE	O-C-CA-CB
62	2w	108	PHE	C-CA-CB-CG
59	2A	3863	A1AE0	CBY-CBZ-CCA-CCB
59	2A	3863	A1AE0	CCI-CCJ-CCQ-OCR
59	2A	3863	A1AE0	CCI-CCJ-CCQ-OCS
59	2A	3863	A1AE0	CBW-CBX-CBY-CBZ
59	1A	4110	A1AE0	CBY-CBZ-CCA-CCB
59	2A	3863	A1AE0	OBU-CBT-OBB-CAK
59	2A	3863	A1AE0	CCK-CCJ-CCQ-OCS
59	2A	3863	A1AE0	CCK-CCJ-CCQ-OCR
59	2A	3863	A1AE0	NBV-CBT-OBB-CAK
59	1A	4110	A1AE0	CCI-CCJ-CCQ-OCS
59	1A	4110	A1AE0	CBX-CBY-CBZ-CCA
59	1A	4110	A1AE0	CCI-CCJ-CCQ-OCR
59	1A	4110	A1AE0	NBV-CBT-OBB-CAK
59	1A	4110	A1AE0	CAU-CAP-OAO-CAD

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Mol	Chain	Res	Type	Atoms
59	1A	4110	A1AE0	OBU-CBT-OBB-CAK
62	2w	108	PHE	N-CA-CB-CG
59	1A	4110	A1AE0	OAQ-CAP-OAO-CAD
59	1A	4110	A1AE0	CBW-CBX-CBY-CBZ
59	2A	3863	A1AE0	CAU-CAP-OAO-CAD
59	2A	3863	A1AE0	OAQ-CAP-OAO-CAD
59	1A	4110	A1AE0	CCK-CCJ-CCQ-OCS
59	1A	4110	A1AE0	CCK-CCJ-CCQ-OCR

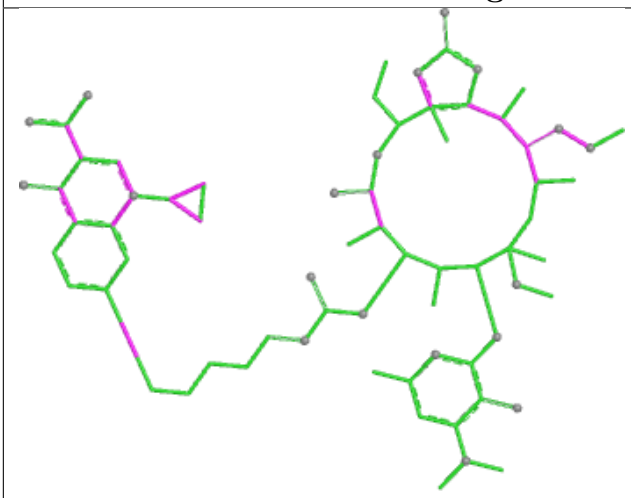
There are no ring outliers.

3 monomers are involved in 3 short contacts:

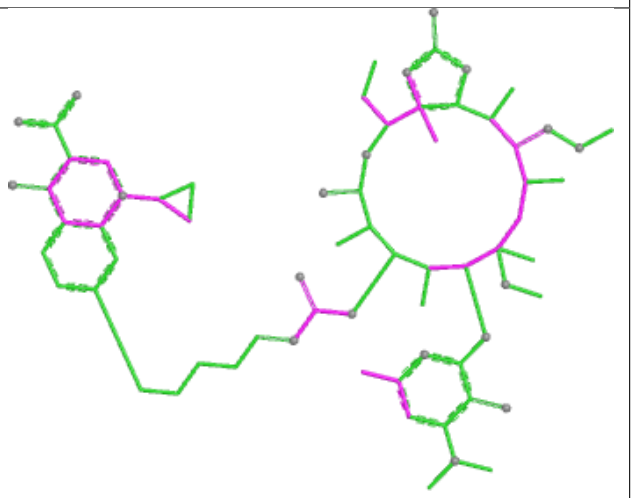
Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	1w	109	PHE	1	0
62	2w	108	PHE	1	0
61	1d	302	SF4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

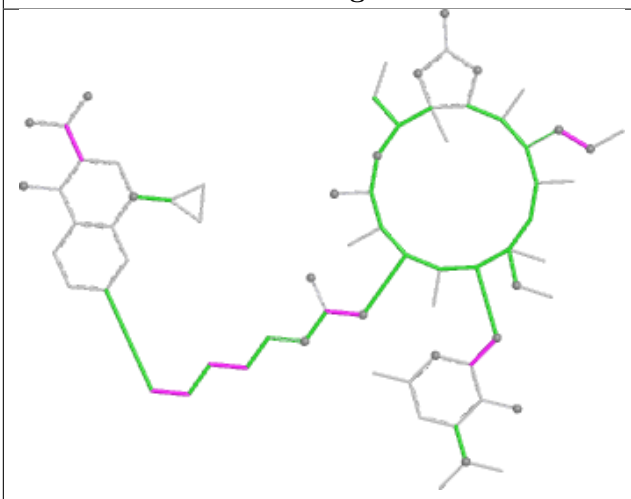
Ligand A1AE0 2A 3863



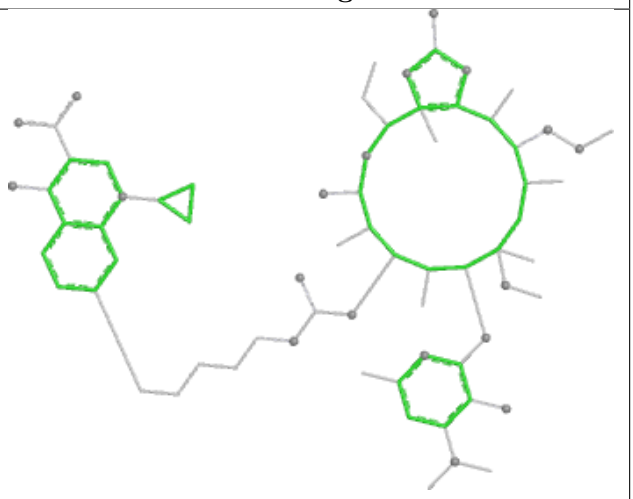
Bond lengths



Bond angles

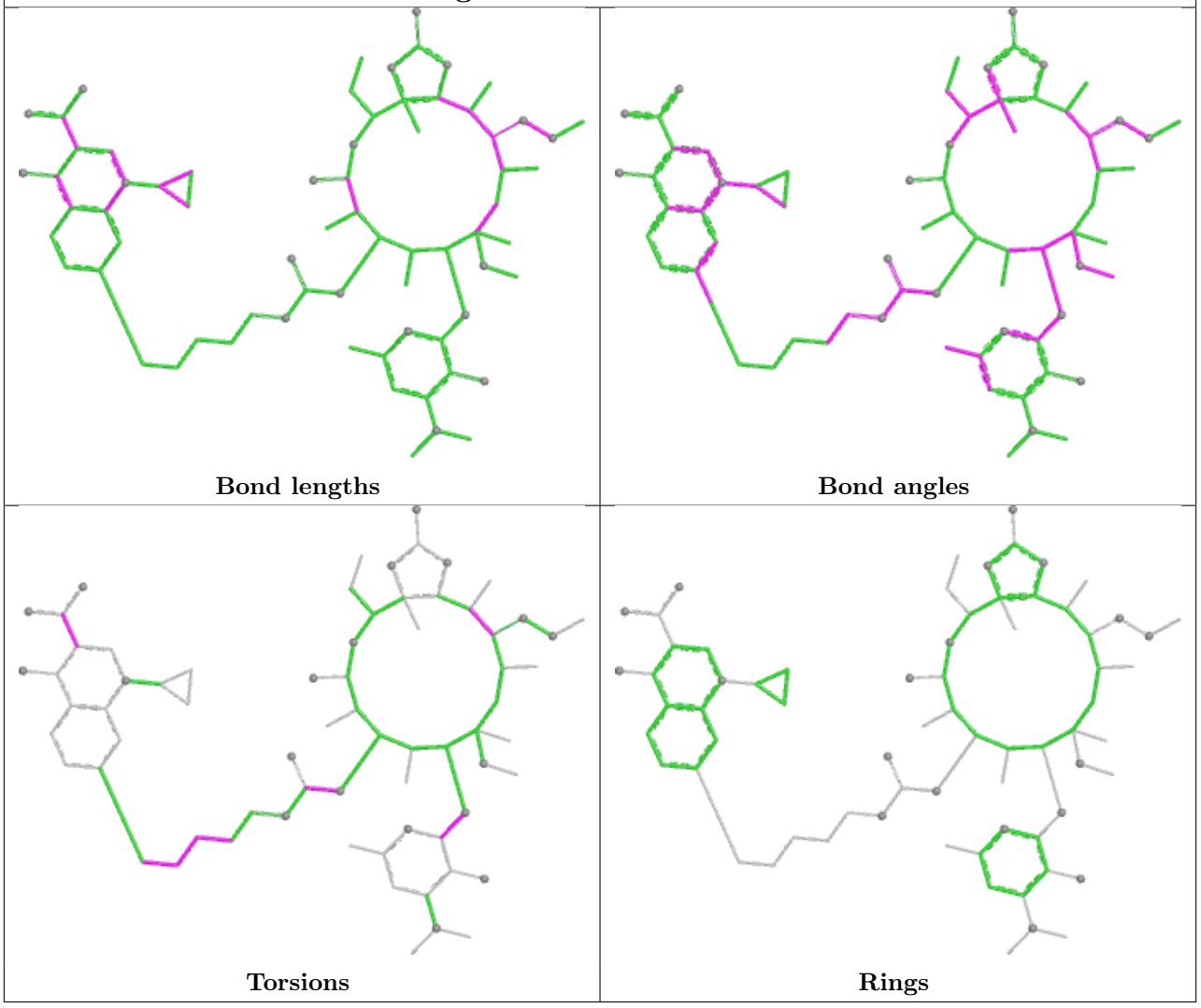


Torsions



Rings

Ligand A1AE0 1A 4110



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%)	-0.52	146 (5%) 34 39	18, 34, 91, 102	0
1	2A	2789/2915 (95%)	-0.03	139 (4%) 35 40	31, 54, 89, 104	0
2	1B	120/121 (99%)	-0.41	0 100 100	30, 47, 62, 84	0
2	2B	120/121 (99%)	0.52	0 100 100	56, 70, 78, 89	0
3	1D	275/276 (99%)	-0.28	2 (0%) 84 86	20, 36, 48, 75	0
3	2D	275/276 (99%)	0.13	3 (1%) 77 80	29, 45, 58, 78	0
4	1E	204/206 (99%)	-0.31	0 100 100	17, 37, 58, 67	0
4	2E	204/206 (99%)	0.37	3 (1%) 71 75	34, 57, 69, 78	0
5	1F	203/210 (96%)	-0.14	1 (0%) 87 90	20, 39, 62, 78	0
5	2F	203/210 (96%)	0.36	2 (0%) 79 82	33, 61, 76, 80	0
6	1G	181/182 (99%)	0.41	9 (4%) 35 40	38, 54, 68, 85	0
6	2G	181/182 (99%)	1.03	17 (9%) 15 19	52, 70, 79, 85	0
7	1H	174/180 (96%)	0.27	4 (2%) 61 65	38, 51, 63, 70	0
7	2H	174/180 (96%)	1.36	33 (18%) 4 5	68, 78, 87, 92	0
8	1I	146/148 (98%)	0.80	7 (4%) 36 42	44, 68, 76, 80	0
8	2I	146/148 (98%)	3.07	90 (61%) 0 0	52, 81, 91, 95	0
9	1N	140/140 (100%)	-0.26	1 (0%) 84 86	24, 37, 57, 72	0
9	2N	140/140 (100%)	0.68	7 (5%) 35 40	46, 61, 74, 80	0
10	1O	122/122 (100%)	-0.27	0 100 100	24, 38, 53, 61	0
10	2O	122/122 (100%)	0.35	0 100 100	46, 56, 66, 69	0
11	1P	149/150 (99%)	0.01	2 (1%) 74 77	18, 44, 65, 73	0
11	2P	149/150 (99%)	0.70	9 (6%) 29 33	35, 63, 77, 84	0
12	1Q	141/141 (100%)	-0.15	0 100 100	23, 39, 52, 66	0
12	2Q	141/141 (100%)	0.70	8 (5%) 30 34	44, 61, 72, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.40	0 100 100	24, 32, 47, 51	0
13	2R	118/118 (100%)	0.12	2 (1%) 69 72	40, 49, 59, 67	0
14	1S	110/112 (98%)	0.07	0 100 100	35, 46, 59, 64	0
14	2S	110/112 (98%)	1.03	8 (7%) 22 26	57, 66, 74, 79	0
15	1T	131/146 (89%)	-0.00	4 (3%) 51 57	28, 42, 63, 76	0
15	2T	131/146 (89%)	0.59	3 (2%) 61 65	48, 58, 71, 75	0
16	1U	116/118 (98%)	-0.52	0 100 100	19, 29, 44, 56	0
16	2U	116/118 (98%)	0.47	2 (1%) 69 72	38, 56, 69, 76	0
17	1V	101/101 (100%)	-0.39	0 100 100	22, 36, 52, 64	0
17	2V	101/101 (100%)	0.56	1 (0%) 79 82	39, 65, 72, 77	0
18	1W	112/113 (99%)	-0.45	0 100 100	21, 29, 48, 74	0
18	2W	112/113 (99%)	0.23	2 (1%) 67 71	38, 47, 62, 88	0
19	1X	95/96 (98%)	-0.14	2 (2%) 63 68	26, 37, 62, 77	0
19	2X	95/96 (98%)	0.47	4 (4%) 41 47	41, 54, 70, 82	0
20	1Y	107/110 (97%)	0.17	2 (1%) 66 69	34, 47, 64, 76	0
20	2Y	107/110 (97%)	1.19	11 (10%) 13 16	55, 67, 77, 82	0
21	1Z	154/206 (74%)	0.74	18 (11%) 10 13	36, 60, 82, 87	0
21	2Z	160/206 (77%)	1.47	35 (21%) 3 4	61, 76, 85, 91	0
22	10	83/85 (97%)	-0.15	0 100 100	22, 34, 47, 59	0
22	20	83/85 (97%)	0.70	3 (3%) 46 52	42, 57, 66, 74	0
23	11	97/98 (98%)	0.06	1 (1%) 79 82	25, 42, 67, 72	0
23	21	97/98 (98%)	0.40	5 (5%) 34 39	36, 52, 70, 74	0
24	12	70/72 (97%)	0.05	2 (2%) 54 58	33, 45, 56, 71	0
24	22	70/72 (97%)	0.50	1 (1%) 73 76	52, 64, 71, 77	0
25	13	59/60 (98%)	-0.22	1 (1%) 69 72	24, 33, 56, 74	0
25	23	59/60 (98%)	0.54	3 (5%) 34 39	50, 58, 71, 76	0
26	14	69/71 (97%)	1.09	14 (20%) 3 4	46, 70, 84, 90	0
26	24	69/71 (97%)	1.32	13 (18%) 4 5	68, 78, 86, 88	0
27	15	59/60 (98%)	-0.36	1 (1%) 69 72	18, 31, 52, 59	0
27	25	59/60 (98%)	0.10	0 100 100	35, 48, 64, 79	0
28	16	53/54 (98%)	-0.22	0 100 100	30, 40, 55, 58	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.35	1 (1%) 66 69	44, 55, 63, 67	0
29	17	48/49 (97%)	-0.26	2 (4%) 41 47	21, 27, 51, 62	0
29	27	48/49 (97%)	0.14	4 (8%) 19 22	28, 38, 59, 70	0
30	18	64/65 (98%)	-0.34	0 100 100	26, 32, 38, 53	0
30	28	64/65 (98%)	0.37	0 100 100	42, 50, 58, 61	0
31	19	37/37 (100%)	-0.10	0 100 100	27, 36, 51, 56	0
31	29	37/37 (100%)	0.89	2 (5%) 32 36	55, 63, 70, 76	0
32	1a	1488/1521 (97%)	0.20	48 (3%) 50 56	33, 61, 87, 101	0
32	2a	1491/1521 (98%)	0.44	62 (4%) 41 47	44, 69, 89, 102	0
33	1b	231/256 (90%)	1.08	30 (12%) 9 11	59, 72, 82, 88	0
33	2b	231/256 (90%)	1.31	42 (18%) 4 5	62, 77, 83, 89	0
34	1c	206/239 (86%)	0.91	19 (9%) 16 19	54, 67, 78, 83	0
34	2c	206/239 (86%)	1.44	52 (25%) 2 3	67, 75, 83, 86	0
35	1d	208/209 (99%)	1.08	21 (10%) 14 17	54, 64, 74, 83	0
35	2d	208/209 (99%)	0.66	8 (3%) 44 50	53, 63, 71, 80	0
36	1e	148/162 (91%)	0.61	9 (6%) 28 32	47, 59, 69, 78	0
36	2e	148/162 (91%)	1.02	10 (6%) 25 28	55, 68, 75, 83	0
37	1f	100/101 (99%)	0.44	0 100 100	52, 62, 70, 74	0
37	2f	100/101 (99%)	0.57	0 100 100	51, 61, 71, 79	0
38	1g	155/156 (99%)	0.68	9 (5%) 30 34	55, 66, 79, 83	0
38	2g	155/156 (99%)	1.01	18 (11%) 11 13	65, 73, 80, 84	0
39	1h	137/138 (99%)	0.57	1 (0%) 84 86	50, 61, 68, 72	0
39	2h	137/138 (99%)	0.98	9 (6%) 26 29	56, 68, 73, 80	0
40	1i	127/128 (99%)	1.20	15 (11%) 10 12	50, 71, 78, 81	0
40	2i	127/128 (99%)	1.85	50 (39%) 1 1	64, 78, 83, 85	0
41	1j	97/105 (92%)	1.38	19 (19%) 4 5	53, 72, 81, 85	0
41	2j	96/105 (91%)	1.95	39 (40%) 1 1	67, 79, 85, 90	0
42	1k	114/129 (88%)	0.53	3 (2%) 57 61	37, 62, 71, 80	0
42	2k	114/129 (88%)	0.64	5 (4%) 39 45	49, 68, 75, 78	0
43	1l	121/132 (91%)	0.24	4 (3%) 49 55	42, 50, 62, 69	0
43	2l	121/132 (91%)	0.56	7 (5%) 30 34	50, 59, 69, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.81	10 (8%) 19 23	51, 64, 73, 83	0
44	2m	122/126 (96%)	1.67	33 (27%) 2 2	64, 74, 79, 83	0
45	1n	60/61 (98%)	0.96	2 (3%) 49 55	55, 61, 69, 72	0
45	2n	60/61 (98%)	2.25	31 (51%) 0 0	68, 75, 81, 85	0
46	1o	88/89 (98%)	0.66	4 (4%) 39 44	44, 60, 70, 71	0
46	2o	88/89 (98%)	0.62	2 (2%) 61 65	53, 65, 74, 78	0
47	1p	82/88 (93%)	1.18	9 (10%) 12 14	52, 65, 72, 78	0
47	2p	82/88 (93%)	0.87	3 (3%) 45 51	57, 64, 72, 75	0
48	1q	99/105 (94%)	0.78	3 (3%) 52 58	52, 63, 72, 77	0
48	2q	99/105 (94%)	0.88	6 (6%) 28 32	56, 67, 73, 77	0
49	1r	68/88 (77%)	0.61	1 (1%) 71 75	53, 62, 73, 76	0
49	2r	68/88 (77%)	0.44	2 (2%) 54 58	54, 64, 71, 74	0
50	1s	83/93 (89%)	0.86	7 (8%) 18 22	58, 67, 75, 79	0
50	2s	83/93 (89%)	1.65	25 (30%) 1 2	71, 78, 84, 91	0
51	1t	96/106 (90%)	1.03	9 (9%) 15 19	54, 65, 73, 77	0
51	2t	96/106 (90%)	0.86	7 (7%) 22 26	56, 65, 74, 77	0
52	1u	23/27 (85%)	1.06	1 (4%) 40 46	55, 62, 66, 71	0
52	2u	23/27 (85%)	2.08	10 (43%) 1 1	68, 73, 76, 79	0
53	1v	13/24 (54%)	0.87	4 (30%) 1 1	43, 51, 89, 92	0
53	2v	13/24 (54%)	1.47	4 (30%) 1 1	60, 66, 92, 103	0
54	1w	66/76 (86%)	1.14	10 (15%) 6 8	25, 79, 92, 95	0
54	2w	64/76 (84%)	1.30	13 (20%) 3 4	44, 86, 93, 98	0
55	1x	72/77 (93%)	0.14	1 (1%) 73 76	25, 57, 77, 86	0
55	2x	72/77 (93%)	0.40	1 (1%) 73 76	40, 69, 79, 92	0
56	1y	67/76 (88%)	1.97	27 (40%) 1 1	59, 95, 98, 102	0
56	2y	66/76 (86%)	2.04	28 (42%) 1 1	69, 96, 101, 102	0
All	All	20873/21748 (95%)	0.33	1363 (6%) 26 30	17, 59, 84, 104	0

All (1363) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	10.5
44	2m	124	PRO	10.0

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Mol	Chain	Res	Type	RSRZ
8	2I	97	ILE	9.9
8	2I	107	VAL	8.8
8	2I	92	VAL	8.4
8	2I	108	THR	8.4
8	2I	98	ALA	8.3
45	2n	2	ALA	7.8
1	2A	2145	C	7.3
8	2I	120	ILE	7.2
8	2I	94	ALA	6.9
8	2I	145	VAL	6.7
7	1H	2	SER	6.6
8	2I	89	TYR	6.6
1	2A	883	G	6.6
44	2m	102	ARG	6.4
44	2m	122	LYS	6.4
8	2I	128	LEU	6.3
21	2Z	172	ALA	6.3
41	2j	32	ALA	6.2
1	1A	2115	G	6.2
1	2A	2111	C	6.1
8	2I	88	ILE	6.1
1	2A	2170	A	6.0
8	2I	136	VAL	6.0
35	1d	167	GLY	6.0
8	2I	140	LEU	5.9
8	2I	115	ALA	5.9
23	11	2	SER	5.8
1	1A	2112	G	5.8
21	2Z	174	VAL	5.8
1	1A	2145	C	5.7
1	1A	2114	A	5.7
1	2A	2117	A	5.7
8	2I	141	LYS	5.7
1	2A	884	C	5.6
8	2I	101	LEU	5.6
8	2I	138	ILE	5.6
8	2I	68	LEU	5.6
44	1m	123	ALA	5.6
8	2I	118	LYS	5.5
8	2I	99	GLU	5.5
8	2I	127	VAL	5.5
45	1n	2	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	1A	2113	U	5.4
1	2A	2146	C	5.4
38	1g	80	VAL	5.4
1	2A	2169	A	5.4
1	1A	2117	A	5.3
1	2A	2116	G	5.3
54	2w	71	G	5.3
44	1m	122	LYS	5.3
50	2s	2	PRO	5.3
8	2I	116	LEU	5.3
8	2I	95	LYS	5.3
8	2I	75	LEU	5.3
8	2I	119	PRO	5.2
41	2j	74	ILE	5.2
21	1Z	141	VAL	5.2
1	1A	2129	C	5.1
44	2m	121	LYS	5.1
1	1A	1078	U	5.1
8	2I	130	TYR	5.1
8	2I	117	GLU	5.1
1	2A	2126	A	5.1
8	2I	86	THR	5.1
33	2b	236	TYR	5.0
33	2b	237	ALA	5.0
38	2g	16	LEU	5.0
29	27	48	LYS	4.9
1	1A	2159	G	4.9
8	2I	133	HIS	4.9
8	2I	146	ALA	4.9
1	1A	2111	C	4.9
1	2A	2143	C	4.9
8	2I	111	PRO	4.8
1	2A	2115	G	4.8
15	1T	131	ALA	4.8
1	1A	2143	C	4.8
1	2A	2136	C	4.8
1	1A	2130	U	4.8
1	2A	2112	G	4.8
1	2A	2168	G	4.8
8	2I	59	ALA	4.8
8	2I	65	ALA	4.8
45	2n	3	ARG	4.8

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Mol	Chain	Res	Type	RSRZ
8	2I	79	ILE	4.7
1	1A	2160	G	4.7
1	2A	2154	G	4.7
32	2a	1032	G	4.7
33	1b	237	ALA	4.7
1	1A	2110	G	4.7
1	2A	2110	G	4.7
1	2A	896	A	4.7
1	2A	2119	A	4.7
1	2A	2127	G	4.7
1	2A	2113	U	4.6
8	2I	113	ARG	4.6
8	2I	70	GLU	4.6
1	1A	2141	G	4.6
1	2A	882	G	4.6
1	2A	2165	G	4.6
1	2A	2802	G	4.6
54	2w	70	G	4.6
1	1A	2146	C	4.6
1	2A	885	C	4.6
8	2I	142	VAL	4.6
8	2I	109	ILE	4.6
1	1A	1096	A	4.5
21	2Z	144	LEU	4.5
21	2Z	141	VAL	4.5
1	2A	2123	G	4.5
1	2A	2125	G	4.5
26	24	57	GLU	4.5
51	1t	103	GLY	4.5
8	2I	84	GLY	4.5
8	2I	87	LYS	4.5
8	2I	126	TYR	4.4
40	2i	67	GLY	4.4
1	1A	2119	A	4.4
1	1A	2135	A	4.4
8	2I	72	LEU	4.4
41	1j	45	ARG	4.4
45	2n	39	LEU	4.4
8	2I	131	LYS	4.4
53	2v	12	A	4.4
53	2v	13	A	4.4
1	1A	1064	C	4.3

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Mol	Chain	Res	Type	RSRZ
1	2A	2138	C	4.3
41	1j	4	ILE	4.3
38	2g	80	VAL	4.3
8	2I	90	GLY	4.3
1	2A	2114	A	4.3
1	2A	2147	G	4.3
8	2I	63	ALA	4.3
1	1A	2136	C	4.3
1	1A	2142	C	4.3
1	2A	2167	U	4.3
1	2A	2155	G	4.3
54	1w	70	G	4.3
45	2n	38	GLY	4.3
32	2a	1030	C	4.2
32	2a	1030(B)	C	4.2
1	1A	1094	U	4.2
40	2i	11	LYS	4.2
8	2I	129	THR	4.2
1	1A	898	C	4.2
53	1v	13	A	4.2
21	2Z	146	ILE	4.2
1	1A	2138	C	4.2
1	1A	1057	A	4.2
56	2y	36	A	4.2
7	2H	7	LEU	4.1
8	2I	103	ARG	4.1
7	2H	44	VAL	4.1
8	2I	144	VAL	4.1
45	2n	34	TYR	4.1
1	1A	885	C	4.1
7	2H	6	ARG	4.1
33	2b	17	PHE	4.1
26	24	56	VAL	4.1
32	1a	204	U	4.0
26	24	51	ASP	4.0
21	2Z	149	SER	4.0
7	2H	43	VAL	4.0
8	2I	85	GLU	4.0
3	2D	275	LYS	4.0
8	2I	110	ASP	4.0
15	1T	130	ALA	3.9
21	2Z	173	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	2A	2157	G	3.9
1	2A	2160	G	3.9
3	1D	276	LYS	3.9
8	2I	123	LEU	3.9
32	2a	1033	G	3.9
54	1w	1	G	3.9
8	2I	134	PRO	3.9
41	2j	75	ILE	3.9
34	1c	207	VAL	3.9
26	14	63	TYR	3.9
1	1A	899	A	3.9
1	2A	888	C	3.9
1	2A	2128	C	3.9
1	2A	2129	C	3.9
1	2A	2134	A	3.9
1	2A	2137	C	3.9
1	2A	2174	C	3.9
41	2j	47	PHE	3.9
8	2I	83	ALA	3.9
40	1i	8	GLY	3.9
21	2Z	171	ILE	3.9
1	1A	1068	G	3.9
1	1A	2166	G	3.9
32	2a	1030(A)	G	3.9
47	2p	82	GLN	3.9
1	2A	2164	C	3.9
1	1A	2144	U	3.9
7	2H	2	SER	3.9
8	2I	112	LYS	3.9
40	2i	14	VAL	3.8
54	2w	72	C	3.8
8	2I	64	GLU	3.8
21	2Z	136	PHE	3.8
1	2A	2120	G	3.8
33	1b	11	LEU	3.8
8	2I	137	PRO	3.8
41	1j	32	ALA	3.8
54	2w	73	A	3.8
1	1A	888	C	3.8
1	2A	2130	U	3.8
33	2b	121	LEU	3.8
21	2Z	147	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
42	2k	89	ALA	3.8
1	2A	2171	A	3.8
6	2G	52	ILE	3.8
32	2a	1035	A	3.8
1	1A	2174	C	3.8
1	2A	2144	U	3.8
56	1y	15	G	3.8
38	2g	85	TYR	3.7
34	2c	207	VAL	3.7
6	1G	50	ALA	3.7
34	2c	2	GLY	3.7
1	2A	2135	A	3.7
1	1A	897	C	3.7
1	2A	2166	G	3.7
51	2t	98	PRO	3.7
41	2j	78	ASN	3.7
8	2I	102	SER	3.7
1	1A	1066	U	3.7
1	1A	2150	U	3.7
8	2I	93	THR	3.7
38	2g	83	ALA	3.7
40	2i	102	LEU	3.7
1	1A	2118	U	3.7
26	14	56	VAL	3.7
32	2a	1002	G	3.7
45	2n	6	LEU	3.6
1	1A	2189	U	3.6
33	2b	165	VAL	3.6
45	2n	22	THR	3.6
51	2t	103	GLY	3.6
1	1A	896	A	3.6
1	1A	2169	A	3.6
8	2I	49	ALA	3.6
1	1A	2147	G	3.6
32	1a	1003	G	3.6
48	1q	100	LYS	3.6
1	1A	1065	U	3.6
1	2A	2172	U	3.6
7	2H	48	GLY	3.6
8	2I	106	GLY	3.6
43	1l	18	VAL	3.6
54	1w	72	C	3.6

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Mol	Chain	Res	Type	RSRZ
1	2A	2182	G	3.6
7	2H	45	VAL	3.6
8	2I	81	VAL	3.6
34	1c	2	GLY	3.6
38	1g	4	ARG	3.6
34	2c	200	ALA	3.6
55	2x	47	U	3.6
1	1A	1073	A	3.6
20	1Y	92	ASN	3.6
8	2I	135	GLU	3.6
23	21	2	SER	3.6
1	1A	1063	G	3.6
1	1A	2151	G	3.6
45	2n	25	VAL	3.6
50	2s	13	ASP	3.6
40	2i	126	SER	3.5
38	2g	81	GLY	3.5
1	2A	2148	G	3.5
56	2y	19	G	3.5
56	2y	34	G	3.5
1	1A	2109	U	3.5
1	2A	878	A	3.5
8	2I	67	ARG	3.5
40	2i	10	ARG	3.5
6	2G	50	ALA	3.5
1	2A	2151	G	3.5
1	2A	2159	G	3.5
8	2I	58	LEU	3.5
32	2a	1003	G	3.5
38	2g	156	TRP	3.5
40	2i	19	LEU	3.5
1	1A	1103	A	3.5
1	2A	2173	A	3.5
1	1A	2107	C	3.5
45	2n	13	THR	3.5
29	27	47	ARG	3.5
32	2a	1036	G	3.5
45	2n	55	GLY	3.5
32	2a	1030(D)	A	3.5
35	1d	164	ALA	3.5
40	2i	13	ALA	3.5
1	1A	2140	C	3.4

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Mol	Chain	Res	Type	RSRZ
1	2A	2179	C	3.4
33	1b	236	TYR	3.4
32	1a	1257	U	3.4
32	2a	1257	U	3.4
1	2A	881	G	3.4
1	2A	2124	G	3.4
12	2Q	22	LYS	3.4
41	2j	31	GLY	3.4
33	1b	188	ALA	3.4
1	1A	1088	A	3.4
35	1d	194	LEU	3.4
41	2j	65	LEU	3.4
1	2A	2139	C	3.4
56	1y	75	C	3.4
1	1A	1058	G	3.4
1	1A	2116	G	3.4
1	1A	2181	G	3.4
8	2I	114	LEU	3.4
26	14	51	ASP	3.4
1	2A	2142	C	3.4
1	2A	2183	C	3.4
1	2A	2803	C	3.4
32	1a	1027	C	3.4
38	2g	154	TYR	3.4
7	2H	49	VAL	3.4
8	2I	105	HIS	3.4
33	1b	127	ILE	3.4
40	2i	82	ALA	3.4
51	1t	10	LEU	3.4
52	2u	24	ARG	3.4
1	2A	2181	G	3.4
32	1a	1030(A)	G	3.4
54	2w	2	C	3.4
1	1A	1081	U	3.4
46	2o	89	GLY	3.4
41	2j	42	THR	3.3
33	1b	10	LEU	3.3
40	2i	66	ARG	3.3
26	24	49	PHE	3.3
33	1b	17	PHE	3.3
1	2A	898	C	3.3
21	1Z	146	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
33	1b	229	VAL	3.3
1	1A	1087	G	3.3
1	2A	2104	G	3.3
56	2y	15	G	3.3
1	1A	2170	A	3.3
8	2I	124	GLY	3.3
32	2a	1286	A	3.3
29	27	46	VAL	3.3
35	2d	5	ILE	3.3
40	2i	9	ARG	3.3
1	2A	1536	C	3.3
1	2A	2163	C	3.3
4	2E	204	ALA	3.3
15	2T	131	ALA	3.3
21	1Z	166	SER	3.3
36	2e	10	MET	3.3
50	2s	80	TYR	3.3
52	2u	2	GLY	3.3
41	1j	98	ILE	3.3
56	1y	19	G	3.3
8	1I	146	ALA	3.3
1	2A	2109	U	3.3
44	1m	124	PRO	3.3
42	1k	25	TYR	3.3
43	2l	64	TYR	3.3
34	2c	182	ILE	3.2
41	2j	50	ILE	3.2
21	2Z	164	ALA	3.2
54	1w	73	A	3.2
1	2A	2189	U	3.2
21	2Z	159	PRO	3.2
32	2a	1000	U	3.2
56	1y	18	G	3.2
8	2I	71	ILE	3.2
8	2I	121	LYS	3.2
34	2c	201	TYR	3.2
40	2i	95	LYS	3.2
7	2H	19	VAL	3.2
34	2c	75	VAL	3.2
43	2l	18	VAL	3.2
8	2I	143	SER	3.2
32	1a	1035	A	3.2

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Mol	Chain	Res	Type	RSRZ
1	1A	1091	G	3.2
1	1A	2149	G	3.2
32	2a	1034	G	3.2
21	2Z	121	HIS	3.2
45	2n	4	LYS	3.2
50	1s	8	GLY	3.2
48	1q	98	LEU	3.2
7	2H	52	VAL	3.2
34	2c	149	ALA	3.2
40	1i	2	GLU	3.2
1	2A	2150	U	3.2
1	1A	2173	A	3.2
18	2W	92	ARG	3.2
1	1A	879	G	3.2
1	1A	2120	G	3.2
6	1G	49	ASP	3.2
32	1a	1034	G	3.2
1	2A	2896	C	3.2
7	1H	174	GLY	3.2
32	2a	1038	C	3.2
50	2s	84	GLY	3.2
50	2s	15	LEU	3.2
44	2m	60	VAL	3.2
36	1e	95	ALA	3.2
51	1t	24	LEU	3.1
32	2a	630	G	3.1
32	2a	1031	G	3.1
41	2j	59	SER	3.1
3	2D	276	LYS	3.1
56	2y	33	U	3.1
44	2m	6	GLY	3.1
21	2Z	150	LEU	3.1
1	2A	2149	G	3.1
1	2A	2893	G	3.1
32	1a	1023	G	3.1
40	2i	62	TYR	3.1
1	1A	1082	U	3.1
21	1Z	150	LEU	3.1
1	1A	2790	A	3.1
33	1b	230	VAL	3.1
20	2Y	54	LYS	3.1
1	1A	2137	C	3.1

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Mol	Chain	Res	Type	RSRZ
32	2a	999	C	3.1
35	1d	201	GLN	3.1
1	1A	2133	G	3.1
1	1A	2148	G	3.1
1	1A	2152	G	3.1
26	14	66	SER	3.1
32	2a	1030(C)	G	3.1
52	2u	14	TRP	3.1
22	20	84	LEU	3.1
40	2i	91	ASP	3.1
34	2c	189	ALA	3.1
1	1A	1098	A	3.1
20	2Y	34	LYS	3.1
32	2a	1531	A	3.1
26	24	55	ARG	3.1
26	24	63	TYR	3.1
32	1a	1029	C	3.1
56	2y	75	C	3.1
1	1A	2182	G	3.0
1	2A	2184	G	3.0
19	2X	95	LEU	3.0
32	1a	1024	G	3.0
33	1b	125	PRO	3.0
41	2j	37	PRO	3.0
41	1j	33	GLN	3.0
1	1A	1095	A	3.0
1	1A	1079	C	3.0
1	1A	2161	C	3.0
35	1d	173	TRP	3.0
21	1Z	136	PHE	3.0
35	1d	110	PHE	3.0
1	2A	2133	G	3.0
54	1w	71	G	3.0
56	2y	18	G	3.0
40	2i	65	VAL	3.0
41	2j	76	ASN	3.0
7	1H	6	ARG	3.0
46	2o	88	ARG	3.0
6	2G	161	THR	3.0
52	1u	18	TYR	3.0
1	1A	278	A	3.0
21	2Z	106	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
52	2u	16	GLY	3.0
1	1A	884	C	3.0
1	1A	2108	C	3.0
1	2A	886	C	3.0
8	2I	80	PRO	3.0
8	2I	132	PRO	3.0
33	1b	232	PRO	3.0
50	1s	13	ASP	3.0
32	2a	1024	G	3.0
1	1A	2172	U	3.0
21	1Z	1	MET	3.0
50	2s	16	LEU	3.0
26	14	54	GLY	3.0
32	1a	1531	A	3.0
38	2g	82	GLY	3.0
53	2v	14	A	3.0
34	1c	65	ALA	3.0
1	2A	1026	U	3.0
40	2i	56	LEU	2.9
32	2a	1004	A	2.9
45	2n	14	PRO	2.9
53	1v	15	A	2.9
33	1b	9	GLU	2.9
41	2j	5	ARG	2.9
40	1i	13	ALA	2.9
32	2a	1018	C	2.9
20	2Y	90	LEU	2.9
6	1G	146	TYR	2.9
29	17	48	LYS	2.9
48	2q	95	TYR	2.9
33	2b	185	ILE	2.9
12	2Q	6	ARG	2.9
34	2c	190	ARG	2.9
38	1g	79	ARG	2.9
1	1A	887	A	2.9
1	2A	2158	A	2.9
20	2Y	107	ASP	2.9
32	1a	1030(D)	A	2.9
34	2c	138	VAL	2.9
50	2s	9	VAL	2.9
32	2a	1027	C	2.9
1	1A	2132	U	2.9

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Mol	Chain	Res	Type	RSRZ
45	2n	7	ILE	2.9
19	2X	94	GLY	2.9
40	2i	101	PHE	2.9
52	2u	11	GLY	2.9
26	14	55	ARG	2.9
52	2u	6	ARG	2.9
1	2A	2153	G	2.9
26	14	57	GLU	2.9
32	1a	1036	G	2.9
32	2a	1202	G	2.9
56	1y	34	G	2.9
21	1Z	165	VAL	2.9
26	14	50	VAL	2.9
44	2m	7	VAL	2.9
47	1p	82	GLN	2.9
34	2c	65	ALA	2.9
44	2m	33	ALA	2.9
1	1A	878	A	2.9
53	1v	14	A	2.9
56	1y	36	A	2.9
44	1m	121	LYS	2.9
1	1A	886	C	2.9
1	2A	2188	C	2.9
56	1y	67	C	2.9
26	24	54	GLY	2.9
38	1g	81	GLY	2.9
26	14	49	PHE	2.9
52	2u	15	ARG	2.9
6	1G	48	GLU	2.9
33	2b	93	VAL	2.9
41	2j	34	VAL	2.9
1	1A	1059	G	2.9
1	2A	2100	G	2.9
1	2A	2131	G	2.9
1	2A	2751	G	2.9
32	2a	1117	G	2.9
54	2w	5	G	2.9
15	2T	130	ALA	2.9
40	1i	64	THR	2.9
6	1G	51	ARG	2.8
7	2H	42	ARG	2.8
14	2S	35	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	2A	895	U	2.8
32	1a	1532	U	2.8
41	2j	36	GLY	2.8
34	2c	73	PRO	2.8
34	2c	128	PHE	2.8
41	2j	91	PRO	2.8
1	1A	2178	C	2.8
56	2y	67	C	2.8
45	2n	33	VAL	2.8
26	24	65	ASP	2.8
35	1d	195	ALA	2.8
32	2a	1001	A	2.8
35	2d	47	ARG	2.8
33	1b	131	PRO	2.8
36	1e	10	MET	2.8
56	1y	20	U	2.8
8	2I	96	ASP	2.8
36	1e	94	ALA	2.8
34	2c	47	LEU	2.8
26	14	58	ARG	2.8
1	1A	1062	G	2.8
7	2H	39	PRO	2.8
11	1P	44	GLY	2.8
41	1j	10	GLY	2.8
50	2s	68	GLY	2.8
1	1A	1070	A	2.8
32	1a	1447	A	2.8
56	1y	35	A	2.8
24	12	70	GLN	2.8
6	1G	149	VAL	2.8
1	1A	1072	C	2.8
32	1a	1030(B)	C	2.8
51	1t	95	ALA	2.8
54	2w	67	C	2.8
51	2t	99	LEU	2.8
47	1p	48	TRP	2.8
8	2I	82	ARG	2.8
12	2Q	10	ARG	2.8
41	2j	41	PRO	2.8
20	2Y	89	PHE	2.8
33	2b	122	PHE	2.8
40	2i	18	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	1A	1176	G	2.8
1	2A	1170	G	2.8
1	2A	2318	G	2.8
32	1a	630	G	2.8
1	1A	2134	A	2.8
6	1G	182	LYS	2.8
7	2H	63	SER	2.8
56	2y	21	A	2.8
33	2b	136	VAL	2.8
8	2I	100	ALA	2.8
34	2c	71	ALA	2.8
1	1A	2164	C	2.7
1	2A	2161	C	2.7
32	2a	1019	C	2.7
54	2w	3	C	2.7
44	1m	4	ILE	2.7
8	2I	122	GLU	2.7
35	1d	179	GLU	2.7
12	2Q	104	PHE	2.7
45	2n	17	LYS	2.7
26	24	66	SER	2.7
1	1A	2171	A	2.7
1	2A	899	A	2.7
21	1Z	105	VAL	2.7
21	2Z	105	VAL	2.7
26	24	67	TYR	2.7
40	2i	114	TYR	2.7
32	1a	202	U	2.7
56	1y	12	U	2.7
34	2c	87	LEU	2.7
45	2n	10	ALA	2.7
49	2r	66	LEU	2.7
36	2e	5	ASP	2.7
38	2g	76	ARG	2.7
21	2Z	170	THR	2.7
32	1a	1008	C	2.7
8	2I	125	GLU	2.7
18	2W	112	GLY	2.7
21	1Z	149	SER	2.7
31	29	16	VAL	2.7
45	2n	18	VAL	2.7
1	2A	2118	U	2.7

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Mol	Chain	Res	Type	RSRZ
11	2P	15	ARG	2.7
25	23	29	ARG	2.7
33	1b	120	ALA	2.7
52	2u	9	ARG	2.7
53	1v	12	A	2.7
1	2A	11	G	2.7
1	2A	2162	G	2.7
7	2H	10	PRO	2.7
33	2b	234	PRO	2.7
33	1b	134	GLU	2.7
45	2n	61	TRP	2.7
1	1A	1076	C	2.7
1	2A	2175	C	2.7
33	1b	165	VAL	2.7
40	1i	41	VAL	2.7
8	2I	55	ALA	2.7
33	2b	48	MET	2.7
38	1g	85	TYR	2.7
40	2i	45	ALA	2.7
41	1j	86	MET	2.7
44	2m	23	TYR	2.7
1	1A	271(K)	U	2.7
50	2s	12	ASP	2.7
1	1A	890	A	2.7
1	1A	1045	A	2.7
1	1A	1077	A	2.7
1	1A	1086	A	2.7
8	2I	78	THR	2.7
21	1Z	151	HIS	2.7
32	1a	1286	A	2.7
33	1b	19	HIS	2.7
34	2c	84	ILE	2.7
44	2m	113	PRO	2.7
48	2q	100	LYS	2.7
1	1A	2121	G	2.7
1	2A	1533	G	2.7
32	1a	1030(C)	G	2.7
32	1a	1033	G	2.7
32	1a	1007	C	2.7
7	2H	170	ARG	2.6
50	1s	9	VAL	2.6
50	2s	71	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
42	2k	25	TYR	2.6
26	14	69	LYS	2.6
33	2b	132	LYS	2.6
1	1A	1097	U	2.6
1	2A	2180	U	2.6
6	2G	48	GLU	2.6
24	22	11	GLU	2.6
50	1s	26	GLY	2.6
1	1A	1056	G	2.6
1	1A	2162	G	2.6
38	1g	156	TRP	2.6
41	2j	79	ARG	2.6
1	1A	2175	C	2.6
1	2A	897	C	2.6
33	1b	7	VAL	2.6
40	2i	17	VAL	2.6
8	2I	53	ALA	2.6
33	1b	186	ALA	2.6
34	2c	129	ALA	2.6
44	1m	2	ALA	2.6
42	1k	75	TYR	2.6
1	1A	1060	U	2.6
1	1A	2158	A	2.6
11	2P	79	ARG	2.6
33	2b	21	ARG	2.6
45	1n	3	ARG	2.6
1	1A	880	G	2.6
19	1X	95	LEU	2.6
32	2a	1001(A)	G	2.6
34	1c	47	LEU	2.6
39	1h	2	LEU	2.6
40	2i	99	LEU	2.6
7	2H	169	VAL	2.6
1	2A	889	C	2.6
1	2A	2804	C	2.6
54	1w	2	C	2.6
21	2Z	148	ASP	2.6
41	1j	77	PRO	2.6
50	2s	76	PRO	2.6
40	2i	27	THR	2.6
1	1A	2180	U	2.6
32	2a	1532	U	2.6

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Mol	Chain	Res	Type	RSRZ
36	1e	85	GLY	2.6
41	1j	36	GLY	2.6
43	2l	63	GLY	2.6
50	1s	84	GLY	2.6
19	2X	68	ARG	2.6
26	24	61	ARG	2.6
53	2v	15	A	2.6
56	2y	35	A	2.6
34	2c	43	LEU	2.6
7	2H	175	LYS	2.6
41	2j	80	LYS	2.6
45	2n	15	LYS	2.6
33	2b	7	VAL	2.6
11	2P	35	HIS	2.6
1	1A	652(F)	G	2.6
1	1A	882	G	2.6
1	2A	2106	G	2.6
32	2a	1224	G	2.6
38	2g	7	ALA	2.6
1	2A	652(T)	C	2.6
1	2A	2185	C	2.6
32	2a	1116	C	2.6
56	2y	25	C	2.6
25	23	60	GLU	2.6
40	2i	2	GLU	2.6
41	2j	100	THR	2.6
44	2m	105	THR	2.6
48	2q	96	GLU	2.6
33	1b	227	GLY	2.6
34	2c	74	GLY	2.6
1	2A	2122	U	2.6
11	2P	77	ARG	2.6
14	2S	32	LEU	2.5
14	2S	83	LYS	2.5
1	2A	887	A	2.5
32	1a	1001	A	2.5
41	2j	49	VAL	2.5
51	2t	97	ALA	2.5
34	2c	109	PRO	2.5
35	1d	70	ILE	2.5
6	2G	146	TYR	2.5
40	2i	7	THR	2.5

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Mol	Chain	Res	Type	RSRZ
56	1y	24	G	2.5
1	1A	2188	C	2.5
45	2n	36	PHE	2.5
1	2A	1113	U	2.5
56	1y	47	U	2.5
34	1c	178	LEU	2.5
40	1i	19	LEU	2.5
45	2n	44	LEU	2.5
9	1N	9	VAL	2.5
50	2s	11	VAL	2.5
1	1A	1054	A	2.5
21	1Z	159	PRO	2.5
20	2Y	44	ILE	2.5
21	1Z	169	GLU	2.5
34	2c	152	ILE	2.5
44	2m	100	GLY	2.5
6	2G	51	ARG	2.5
35	1d	132	ARG	2.5
40	2i	128	ARG	2.5
41	2j	46	ARG	2.5
1	2A	2805	G	2.5
32	1a	163	C	2.5
32	1a	1137	C	2.5
32	2a	1223	C	2.5
33	2b	133	LYS	2.5
56	1y	74	C	2.5
41	1j	71	LEU	2.5
41	2j	72	VAL	2.5
21	1Z	164	ALA	2.5
25	23	2	PRO	2.5
34	1c	14	ILE	2.5
44	2m	22	ILE	2.5
8	2I	54	GLN	2.5
50	2s	63	THR	2.5
11	1P	15	ARG	2.5
24	12	69	ARG	2.5
8	2I	62	LYS	2.5
14	2S	33	LYS	2.5
36	2e	133	TYR	2.5
26	14	59	PHE	2.5
46	1o	57	LEU	2.5
1	1A	1089	G	2.5

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Mol	Chain	Res	Type	RSRZ
1	2A	879	G	2.5
1	2A	1509	C	2.5
1	2A	2141	G	2.5
54	2w	68	C	2.5
56	2y	57	G	2.5
32	1a	1025	U	2.5
34	2c	195	VAL	2.5
40	2i	86	VAL	2.5
36	1e	138	ALA	2.5
8	2I	91	SER	2.5
13	2R	14	SER	2.5
33	1b	39	ILE	2.5
33	2b	134	GLU	2.5
34	1c	84	ILE	2.5
45	2n	42	ILE	2.5
26	14	52	THR	2.5
40	2i	64	THR	2.5
44	2m	29	ARG	2.5
1	1A	1067	A	2.5
56	1y	73	A	2.5
34	2c	204	LEU	2.4
35	1d	108	LEU	2.4
32	2a	1006	C	2.4
40	2i	53	VAL	2.4
56	1y	13	C	2.4
1	1A	883	G	2.4
1	1A	2101	G	2.4
1	2A	10	G	2.4
38	2g	112	PRO	2.4
41	2j	77	PRO	2.4
54	1w	44	G	2.4
40	2i	52	ALA	2.4
49	2r	20	ALA	2.4
20	2Y	91	GLU	2.4
44	2m	64	TRP	2.4
3	2D	38	LYS	2.4
9	2N	1	MET	2.4
14	2S	20	ARG	2.4
36	1e	98	THR	2.4
21	2Z	140	ASP	2.4
40	1i	105	ASP	2.4
1	2A	2801(A)	A	2.4

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Mol	Chain	Res	Type	RSRZ
14	2S	36	TYR	2.4
21	2Z	104	PHE	2.4
38	1g	84	ASN	2.4
32	2a	977	A	2.4
32	2a	1041	A	2.4
34	1c	193	TYR	2.4
40	1i	56	LEU	2.4
40	1i	85	LEU	2.4
40	2i	5	TYR	2.4
33	2b	16	HIS	2.4
5	2F	130	ALA	2.4
34	2c	137	ALA	2.4
55	1x	47	U	2.4
1	1A	2128	C	2.4
1	2A	2103	C	2.4
1	2A	2107	C	2.4
1	2A	2140	C	2.4
6	1G	52	ILE	2.4
34	2c	157	ILE	2.4
1	1A	2106	G	2.4
1	1A	2127	G	2.4
1	1A	2168	G	2.4
32	1a	216	G	2.4
54	2w	15	G	2.4
56	1y	53	G	2.4
34	1c	177	THR	2.4
36	2e	114	GLY	2.4
21	1Z	154	ASP	2.4
19	2X	92	LEU	2.4
34	2c	186	PHE	2.4
1	1A	1069	A	2.4
5	1F	89	VAL	2.4
21	2Z	158	PRO	2.4
33	1b	136	VAL	2.4
33	2b	131	PRO	2.4
42	1k	14	VAL	2.4
29	17	47	ARG	2.4
35	2d	48	ALA	2.4
50	2s	24	ALA	2.4
42	2k	48	ILE	2.4
44	2m	4	ILE	2.4
1	1A	895	U	2.4

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Mol	Chain	Res	Type	RSRZ
1	1A	2167	U	2.4
32	2a	1040	U	2.4
1	1A	1509	C	2.4
1	2A	2105	C	2.4
32	2a	1029	C	2.4
32	2a	1109	C	2.4
32	2a	1249	C	2.4
47	2p	48	TRP	2.4
7	2H	174	GLY	2.4
11	2P	118	GLY	2.4
39	2h	3	THR	2.4
1	1A	2165	G	2.4
1	2A	2156	G	2.4
32	1a	1032	G	2.4
32	2a	1042	G	2.4
33	2b	51	LEU	2.4
41	2j	90	LEU	2.4
56	1y	27	G	2.4
56	1y	69	G	2.4
26	24	59	PHE	2.4
36	1e	6	PHE	2.4
38	2g	84	ASN	2.4
9	2N	44	PRO	2.4
32	1a	1005	A	2.4
44	2m	13	LYS	2.4
56	1y	21	A	2.4
56	2y	23	A	2.4
26	24	50	VAL	2.4
34	1c	70	VAL	2.4
35	1d	88	VAL	2.4
39	2h	97	VAL	2.4
6	1G	83	ARG	2.4
7	2H	145	ALA	2.4
11	2P	75	ILE	2.4
29	27	45	ALA	2.4
41	2j	27	ALA	2.4
44	1m	5	ALA	2.4
33	2b	210	SER	2.4
34	2c	159	GLY	2.4
35	2d	6	GLY	2.4
44	1m	24	GLY	2.4
1	2A	2108	C	2.3

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Mol	Chain	Res	Type	RSRZ
32	1a	1030	C	2.3
33	1b	221	LEU	2.3
41	2j	63	PHE	2.3
47	1p	80	PHE	2.3
1	1A	2131	G	2.3
1	2A	892	G	2.3
54	1w	69	G	2.3
56	1y	1	G	2.3
9	2N	83	LYS	2.3
45	2n	11	LYS	2.3
7	2H	36	PRO	2.3
15	2T	112	ARG	2.3
41	1j	64	GLU	2.3
1	2A	652(B)	A	2.3
32	2a	1251	A	2.3
34	2c	77	ILE	2.3
45	2n	20	ALA	2.3
35	1d	87	GLY	2.3
36	1e	97	GLY	2.3
21	1Z	170	THR	2.3
8	2I	38	LEU	2.3
21	2Z	76	LEU	2.3
23	21	98	LEU	2.3
35	1d	19	LEU	2.3
40	2i	96	LEU	2.3
35	2d	110	PHE	2.3
8	2I	74	ASN	2.3
34	2c	181	ASN	2.3
1	1A	2139	C	2.3
1	1A	2794	C	2.3
1	2A	2789	C	2.3
32	2a	1037	C	2.3
6	2G	182	LYS	2.3
11	2P	78	PRO	2.3
38	1g	5	ARG	2.3
46	1o	88	ARG	2.3
32	1a	1001(A)	G	2.3
32	2a	485	G	2.3
33	2b	129	GLU	2.3
34	2c	86	VAL	2.3
40	2i	110	GLU	2.3
56	1y	57	G	2.3

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Mol	Chain	Res	Type	RSRZ
56	2y	1	G	2.3
6	2G	15	VAL	2.3
6	2G	20	ILE	2.3
9	2N	124	ALA	2.3
33	1b	200	ILE	2.3
33	2b	208	ILE	2.3
33	2b	214	ILE	2.3
34	2c	60	ALA	2.3
45	2n	5	ALA	2.3
52	2u	13	ILE	2.3
56	2y	14	A	2.3
56	2y	38	A	2.3
21	2Z	102	LEU	2.3
41	2j	48	THR	2.3
1	2A	2132	U	2.3
32	1a	203	U	2.3
6	2G	126	ASP	2.3
39	2h	98	LYS	2.3
44	2m	31	LYS	2.3
32	1a	848	C	2.3
32	1a	1028	C	2.3
38	2g	32	ARG	2.3
40	1i	4	TYR	2.3
54	1w	67	C	2.3
56	2y	43	C	2.3
56	2y	68	C	2.3
7	2H	50	VAL	2.3
23	21	62	VAL	2.3
33	2b	71	VAL	2.3
33	2b	164	VAL	2.3
40	2i	109	VAL	2.3
44	2m	53	VAL	2.3
16	2U	62	ILE	2.3
7	2H	134	SER	2.3
35	1d	137	SER	2.3
51	1t	101	GLY	2.3
1	1A	229	A	2.3
1	1A	2126	A	2.3
1	2A	900	A	2.3
1	2A	1508	A	2.3
32	2a	1357	A	2.3
50	2s	77	THR	2.3

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Mol	Chain	Res	Type	RSRZ
56	2y	31	A	2.3
1	2A	12	U	2.3
21	2Z	88	PHE	2.3
35	1d	169	LYS	2.3
41	2j	99	LYS	2.3
44	2m	120	LYS	2.3
45	2n	37	PHE	2.3
56	1y	45	U	2.3
7	2H	51	ARG	2.3
34	1c	88	ARG	2.3
34	2c	79	ARG	2.3
39	2h	18	ARG	2.3
45	2n	12	ARG	2.3
8	2I	139	GLN	2.3
1	1A	271(J)	C	2.3
1	1A	1075	C	2.3
32	2a	1043	C	2.3
34	1c	86	VAL	2.3
47	1p	2	VAL	2.3
54	2w	13	C	2.3
56	2y	13	C	2.3
50	2s	20	LEU	2.2
1	2A	2121	G	2.2
8	1I	87	LYS	2.2
20	2Y	46	LYS	2.2
32	2a	79	G	2.2
32	2a	1131	G	2.2
32	2a	1222	G	2.2
34	2c	154	SER	2.2
41	1j	30	SER	2.2
40	2i	37	PHE	2.2
50	2s	10	PHE	2.2
32	2a	1250	A	2.2
1	1A	2122	U	2.2
32	1a	182	U	2.2
40	2i	20	ARG	2.2
44	2m	104	ARG	2.2
50	2s	53	ASN	2.2
51	2t	9	ASN	2.2
7	1H	21	PRO	2.2
35	1d	29	PRO	2.2
8	1I	41	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
8	2I	60	GLU	2.2
25	13	60	GLU	2.2
35	2d	156	GLU	2.2
44	2m	101	GLN	2.2
12	2Q	109	VAL	2.2
21	2Z	139	VAL	2.2
39	2h	134	ILE	2.2
34	2c	100	ALA	2.2
40	2i	84	ALA	2.2
40	2i	94	ALA	2.2
1	1A	1052	C	2.2
56	2y	74	C	2.2
6	2G	175	LEU	2.2
33	2b	11	LEU	2.2
39	2h	2	LEU	2.2
3	1D	275	LYS	2.2
52	2u	4	GLY	2.2
43	2l	62	SER	2.2
50	2s	4	SER	2.2
8	2I	61	ARG	2.2
38	2g	79	ARG	2.2
43	2l	19	ARG	2.2
1	2A	1039	G	2.2
32	1a	1002	G	2.2
47	1p	41	PRO	2.2
1	2A	2102	U	2.2
32	1a	841	U	2.2
56	2y	26	A	2.2
33	1b	129	GLU	2.2
12	2Q	66	ILE	2.2
27	15	60	VAL	2.2
41	1j	44	VAL	2.2
50	1s	31	ILE	2.2
26	14	32	TYR	2.2
33	2b	218	ALA	2.2
49	1r	20	ALA	2.2
5	2F	24	LEU	2.2
21	2Z	156	LYS	2.2
50	2s	14	HIS	2.2
21	2Z	157	LEU	2.2
33	2b	187	LEU	2.2
34	1c	87	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
34	2c	115	LEU	2.2
44	2m	19	LEU	2.2
44	1m	26	GLY	2.2
1	1A	1104	C	2.2
1	1A	2177	C	2.2
35	1d	165	MET	2.2
56	1y	25	C	2.2
56	1y	61	C	2.2
40	1i	126	SER	2.2
41	1j	35	SER	2.2
44	2m	103	THR	2.2
15	1T	115	ARG	2.2
23	21	76	ARG	2.2
45	2n	23	ARG	2.2
47	1p	5	ARG	2.2
51	1t	8	ARG	2.2
6	2G	2	PRO	2.2
40	2i	21	PRO	2.2
46	1o	19	PRO	2.2
15	1T	38	ASN	2.2
21	2Z	168	GLU	2.2
34	1c	98	ASN	2.2
34	2c	90	GLU	2.2
1	1A	1177	A	2.2
1	2A	1171	G	2.2
1	2A	2793	G	2.2
32	1a	1009	G	2.2
32	2a	1447	A	2.2
9	2N	9	VAL	2.2
9	2N	140	VAL	2.2
33	1b	93	VAL	2.2
34	2c	5	ILE	2.2
34	2c	8	ILE	2.2
36	2e	67	VAL	2.2
41	1j	6	ILE	2.2
40	2i	92	TYR	2.2
44	2m	92	HIS	2.2
44	2m	118	ALA	2.2
45	2n	59	ALA	2.2
46	1o	69	TYR	2.2
20	2Y	67	LEU	2.2
33	2b	158	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
42	2k	102	GLY	2.2
21	2Z	103	ARG	2.2
34	2c	95	THR	2.2
1	1A	889	C	2.2
1	1A	2179	C	2.2
54	2w	4	C	2.2
56	1y	68	C	2.2
6	2G	147	ASP	2.2
33	2b	12	GLU	2.2
39	2h	54	ASP	2.2
41	1j	83	GLU	2.2
33	1b	97	TRP	2.2
1	1A	2897	U	2.2
8	1I	109	ILE	2.2
16	2U	88	ILE	2.2
32	2a	1126	U	2.2
34	2c	99	VAL	2.2
34	2c	198	VAL	2.2
36	2e	51	VAL	2.2
41	2j	14	LYS	2.2
41	2j	44	VAL	2.2
43	1l	126	LYS	2.2
1	1A	1071	G	2.2
1	2A	2176	A	2.2
33	2b	123	ALA	2.2
40	1i	84	ALA	2.2
41	2j	26	ALA	2.2
45	2n	30	ALA	2.2
56	1y	28	G	2.2
56	2y	27	G	2.2
56	2y	70	G	2.2
34	1c	81	GLY	2.1
34	2c	145	GLY	2.1
40	2i	42	ARG	2.1
44	2m	11	ARG	2.1
41	2j	87	THR	2.1
44	2m	49	THR	2.1
7	2H	53	GLU	2.1
8	2I	10	GLU	2.1
11	2P	68	GLN	2.1
32	1a	1038	C	2.1
32	2a	91	C	2.1

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Mol	Chain	Res	Type	RSRZ
36	1e	117	ASP	2.1
44	2m	12	ASN	2.1
51	1t	9	ASN	2.1
7	2H	72	ILE	2.1
7	2H	136	ILE	2.1
36	2e	13	ILE	2.1
38	2g	36	LYS	2.1
41	1j	74	ILE	2.1
43	2l	43	VAL	2.1
11	2P	134	ALA	2.1
33	2b	77	ALA	2.1
40	1i	15	ALA	2.1
20	2Y	1	MET	2.1
50	2s	22	LEU	2.1
6	2G	44	GLY	2.1
35	2d	73	ARG	2.1
40	2i	69	GLY	2.1
40	2i	120	ARG	2.1
43	1l	19	ARG	2.1
1	1A	881	G	2.1
1	1A	2207	G	2.1
1	2A	2152	G	2.1
1	2A	2319	G	2.1
32	1a	998	G	2.1
54	2w	18	G	2.1
6	2G	142	PRO	2.1
34	1c	107	GLN	2.1
41	2j	83	GLU	2.1
9	2N	118	LYS	2.1
13	2R	69	ASP	2.1
34	2c	3	ASN	2.1
1	2A	2177	C	2.1
33	2b	200	ILE	2.1
33	2b	201	ILE	2.1
35	1d	5	ILE	2.1
56	2y	2	C	2.1
7	2H	17	VAL	2.1
34	2c	55	VAL	2.1
38	2g	21	VAL	2.1
48	1q	5	VAL	2.1
4	2E	63	LEU	2.1
33	2b	221	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
50	2s	50	ALA	2.1
41	2j	29	ARG	2.1
56	1y	66	U	2.1
12	2Q	15	GLY	2.1
21	1Z	160	GLY	2.1
50	2s	72	GLY	2.1
7	2H	157	TYR	2.1
33	2b	92	TYR	2.1
35	2d	4	TYR	2.1
45	2n	21	TYR	2.1
1	1A	1174	A	2.1
1	1A	2176	A	2.1
1	2A	1460	A	2.1
32	2a	1005	A	2.1
33	1b	190	THR	2.1
7	2H	123	PHE	2.1
40	2i	98	PRO	2.1
1	1A	1093	G	2.1
32	1a	1021	G	2.1
32	2a	1021	G	2.1
20	1Y	91	GLU	2.1
40	2i	73	GLN	2.1
7	2H	9	ILE	2.1
8	1I	79	ILE	2.1
33	1b	37	ASN	2.1
40	2i	117	HIS	2.1
48	2q	90	ILE	2.1
4	2E	195	LEU	2.1
7	2H	11	VAL	2.1
21	2Z	70	LEU	2.1
23	21	94	LEU	2.1
33	1b	187	LEU	2.1
35	1d	133	VAL	2.1
39	2h	26	VAL	2.1
39	2h	79	VAL	2.1
1	2A	1043	C	2.1
32	2a	1007	C	2.1
33	2b	188	ALA	2.1
34	1c	92	ALA	2.1
54	1w	68	C	2.1
14	2S	30	ARG	2.1
40	1i	104	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
40	2i	104	ARG	2.1
50	2s	81	ARG	2.1
31	29	37	GLY	2.1
32	1a	1000	U	2.1
51	1t	69	GLY	2.1
40	2i	4	TYR	2.1
42	2k	75	TYR	2.1
33	2b	55	PHE	2.1
1	2A	1847	A	2.1
21	2Z	145	GLU	2.1
34	2c	135	LYS	2.1
36	2e	20	GLN	2.1
56	2y	58	A	2.1
1	1A	1173	G	2.1
1	1A	2157	G	2.1
1	2A	880	G	2.1
32	1a	1010	G	2.1
32	2a	976	G	2.1
32	2a	1026	G	2.1
28	26	20	ASN	2.1
33	2b	140	HIS	2.1
41	2j	38	ILE	2.1
47	1p	4	ILE	2.1
20	2Y	42	VAL	2.0
21	2Z	71	VAL	2.0
21	2Z	155	LEU	2.0
33	2b	44	LEU	2.0
43	2l	39	VAL	2.0
47	1p	49	LEU	2.0
22	20	11	ARG	2.0
33	2b	137	ARG	2.0
6	2G	163	ALA	2.0
1	2A	893	C	2.0
32	1a	1037	C	2.0
38	2g	34	GLY	2.0
51	2t	101	GLY	2.0
1	2A	272(A)	U	2.0
1	2A	2897	U	2.0
40	2i	36	TYR	2.0
43	1l	64	TYR	2.0
44	2m	59	TYR	2.0
34	2c	28	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
41	2j	33	GLN	2.0
14	2S	52	SER	2.0
32	1a	149	A	2.0
32	1a	1503	A	2.0
32	2a	983	A	2.0
32	2a	1248	A	2.0
38	1g	153	HIS	2.0
56	2y	7	A	2.0
21	1Z	120	ILE	2.0
44	1m	25	ILE	2.0
34	1c	179	ARG	2.0
35	1d	174	LEU	2.0
41	1j	8	LEU	2.0
48	2q	43	LEU	2.0
48	2q	89	LEU	2.0
50	1s	71	LEU	2.0
8	1I	136	VAL	2.0
21	2Z	86	VAL	2.0
34	2c	76	VAL	2.0
47	1p	62	VAL	2.0
1	1A	271(M)	G	2.0
1	1A	2156	G	2.0
1	2A	1112	G	2.0
1	2A	2191	G	2.0
32	2a	998	G	2.0
32	2a	1356	G	2.0
56	2y	6	G	2.0
33	2b	88	ALA	2.0
36	2e	138	ALA	2.0
44	2m	28	ALA	2.0
51	2t	94	ALA	2.0
19	1X	94	GLY	2.0
21	2Z	160	GLY	2.0
34	2c	80	GLY	2.0
40	2i	72	GLY	2.0
50	2s	8	GLY	2.0
34	2c	167	TRP	2.0
7	2H	62	LYS	2.0
8	2I	56	LYS	2.0
44	2m	27	LYS	2.0
51	1t	27	LYS	2.0
17	2V	50	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
32	1a	1446	U	2.0
6	2G	54	GLU	2.0
7	2H	47	GLU	2.0
8	1I	10	GLU	2.0
12	2Q	113	GLN	2.0
21	1Z	168	GLU	2.0
22	20	45	PHE	2.0
34	2c	48	TYR	2.0
34	2c	184	TYR	2.0
40	1i	59	PHE	2.0
41	1j	42	THR	2.0
47	2p	9	PHE	2.0
41	2j	35	SER	2.0
36	2e	11	ILE	2.0
41	2j	23	ILE	2.0
34	1c	83	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
56	MIA	2y	37	22/30	0.38	0.20	87,97,104,122	0
56	MIA	1y	37	22/30	0.39	0.18	83,90,102,115	0
56	G7M	2y	46	24/25	0.40	0.17	86,96,103,114	0
56	4SU	2y	8	20/21	0.44	0.18	89,98,105,122	0
56	5MU	2y	54	21/22	0.47	0.17	88,96,107,119	0
56	5MU	1y	54	21/22	0.48	0.16	89,94,99,112	0
56	G7M	1y	46	24/25	0.54	0.15	89,95,99,107	0
56	PSU	1y	55	20/21	0.56	0.16	90,95,98,113	0
56	PSU	2y	55	20/21	0.58	0.14	90,96,103,111	0
56	PSU	2y	32	20/21	0.60	0.15	88,92,101,116	0
56	PSU	2y	39	20/21	0.61	0.15	84,92,100,112	0
56	4SU	1y	8	20/21	0.61	0.15	90,96,113,122	0
56	PSU	1y	32	20/21	0.67	0.14	84,90,102,108	0
54	G7M	1w	46	24/25	0.68	0.15	73,80,104,124	0
54	G7M	2w	46	24/25	0.72	0.15	78,87,99,110	0
56	PSU	1y	39	20/21	0.72	0.12	79,88,95,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	4SU	2w	8	20/21	0.83	0.12	75,83,93,101	0
54	PSU	2w	55	20/21	0.85	0.11	73,79,87,88	0
55	4SU	2x	8	20/21	0.86	0.13	68,74,81,83	0
54	4SU	1w	8	20/21	0.86	0.13	69,79,85,86	0
54	5MU	2w	54	21/22	0.87	0.11	65,72,82,82	0
55	5MU	2x	54	21/22	0.88	0.14	70,76,78,79	0
32	2MG	2a	1207	24/25	0.88	0.12	62,78,81,81	0
55	PSU	1x	55	20/21	0.90	0.11	54,59,70,77	0
55	5MU	1x	54	21/22	0.90	0.10	55,62,69,76	0
54	PSU	2w	32	20/21	0.90	0.14	66,75,81,84	0
55	PSU	2x	55	20/21	0.91	0.11	68,72,82,83	0
54	MIA	2w	37	25/30	0.91	0.14	52,66,76,90	0
54	PSU	1w	55	20/21	0.91	0.09	59,66,74,76	0
43	0TD	2l	92	10/11	0.91	0.13	53,58,64,71	0
32	2MG	1a	1207	24/25	0.92	0.10	59,65,68,71	0
32	5MC	2a	967	21/22	0.92	0.14	58,61,69,73	0
55	5MC	2x	32	21/22	0.92	0.14	63,66,68,73	0
54	MIA	1w	37	29/30	0.92	0.15	38,52,64,87	0
1	PSU	2A	1917	20/21	0.93	0.10	51,60,68,69	0
32	G7M	2a	527	24/25	0.93	0.11	52,59,64,68	0
32	M2G	2a	966	25/26	0.93	0.15	51,63,75,78	0
54	PSU	1w	32	20/21	0.93	0.12	56,62,72,73	0
43	0TD	1l	92	10/11	0.93	0.11	49,51,53,68	0
32	5MC	2a	1400	21/22	0.93	0.13	60,63,68,74	0
55	4SU	1x	8	20/21	0.93	0.10	47,58,63,64	0
1	5MU	2A	1915	21/22	0.93	0.10	57,62,66,67	0
32	M2G	1a	966	25/26	0.94	0.11	43,49,56,58	0
32	5MC	2a	1404	21/22	0.94	0.10	43,50,53,55	0
32	PSU	2a	516	20/21	0.94	0.10	53,62,68,69	0
55	5MC	1x	32	21/22	0.94	0.12	49,53,59,68	0
54	5MU	1w	54	21/22	0.95	0.08	45,57,61,63	0
54	PSU	2w	39	20/21	0.95	0.11	60,70,79,80	0
54	PSU	1w	39	20/21	0.95	0.10	46,59,66,69	0
32	5MC	2a	1407	21/22	0.95	0.09	44,51,55,62	0
32	MA6	2a	1518	24/25	0.95	0.11	47,54,59,61	0
1	PSU	1A	1917	20/21	0.95	0.09	36,44,51,52	0
1	OMC	2A	1920	21/22	0.95	0.09	51,57,61,65	0
1	5MC	2A	1942	21/22	0.95	0.09	45,56,61,65	0
32	5MC	1a	1400	21/22	0.96	0.09	40,48,53,55	0
32	MA6	2a	1519	24/25	0.96	0.10	48,56,59,62	0
32	PSU	1a	516	20/21	0.96	0.09	39,51,57,57	0
1	PSU	2A	1911	20/21	0.96	0.08	46,56,59,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	8AN	2x	76	22/23	0.96	0.09	34,40,47,49	0
32	G7M	1a	527	24/25	0.96	0.09	42,46,50,53	0
1	5MU	1A	1915	21/22	0.96	0.10	43,49,52,53	0
32	5MC	1a	967	21/22	0.96	0.10	42,49,57,59	0
32	4OC	2a	1402	22/23	0.96	0.10	52,56,60,65	0
1	5MC	1A	1942	21/22	0.96	0.08	29,37,40,53	0
1	5MC	2A	1962	21/22	0.96	0.09	34,47,54,58	0
54	8AN	2w	76	22/23	0.96	0.09	29,38,42,43	0
32	UR3	2a	1498	21/22	0.97	0.09	45,50,54,55	0
1	OMU	2A	2552	21/22	0.97	0.07	39,44,47,52	0
1	PSU	2A	2605	20/21	0.97	0.07	30,36,40,40	0
55	8AN	1x	76	22/23	0.97	0.07	17,23,29,37	0
1	OMC	1A	1920	21/22	0.97	0.07	32,39,43,46	0
1	PSU	1A	1911	20/21	0.97	0.07	31,40,44,46	0
32	4OC	1a	1402	22/23	0.97	0.08	38,42,47,50	0
32	5MC	1a	1404	21/22	0.97	0.08	31,38,42,43	0
1	5MU	2A	1939	21/22	0.97	0.08	33,38,41,44	0
32	5MC	1a	1407	21/22	0.97	0.07	31,39,42,43	0
32	MA6	1a	1519	24/25	0.97	0.09	34,39,44,45	0
1	2MA	2A	2503	23/24	0.97	0.09	26,36,40,41	0
32	UR3	1a	1498	21/22	0.98	0.07	33,38,43,45	0
32	MA6	1a	1518	24/25	0.98	0.08	31,38,42,43	0
1	PSU	1A	2605	20/21	0.98	0.05	20,24,26,27	0
1	5MU	1A	1939	21/22	0.98	0.05	20,26,30,35	0
54	8AN	1w	76	22/23	0.98	0.07	17,21,23,24	0
1	5MC	1A	1962	21/22	0.98	0.06	23,31,33,41	0
1	OMG	1A	2251	24/25	0.98	0.06	20,24,25,26	0
1	2MA	1A	2503	23/24	0.98	0.06	15,19,21,23	0
1	OMG	2A	2251	24/25	0.98	0.07	35,38,42,42	0
1	OMU	1A	2552	21/22	0.99	0.06	21,26,31,31	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, 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	MG	1a	1603	1/1	0.54	0.20	67,67,67,67	0
57	MG	1B	221	1/1	0.56	0.22	66,66,66,66	0
57	MG	2y	104	1/1	0.57	0.33	86,86,86,86	0
57	MG	2A	3763	1/1	0.60	0.23	64,64,64,64	0
57	MG	2A	3544	1/1	0.60	0.24	58,58,58,58	0
57	MG	1A	3946	1/1	0.61	0.34	80,80,80,80	0
57	MG	1A	3702	1/1	0.62	0.20	56,56,56,56	0
57	MG	2w	107	1/1	0.63	0.27	78,78,78,78	0
57	MG	2A	3653	1/1	0.64	0.23	72,72,72,72	0
57	MG	2A	3168	1/1	0.64	0.25	78,78,78,78	0
57	MG	1A	3764	1/1	0.65	0.14	23,23,23,23	0
57	MG	2A	3861	1/1	0.65	0.38	81,81,81,81	0
57	MG	2A	3613	1/1	0.65	0.22	68,68,68,68	0
57	MG	2A	3182	1/1	0.65	0.27	75,75,75,75	0
57	MG	2A	3811	1/1	0.66	0.24	72,72,72,72	0
57	MG	2A	3320	1/1	0.66	0.32	72,72,72,72	0
57	MG	2A	3272	1/1	0.66	0.30	74,74,74,74	0
57	MG	2A	3597	1/1	0.66	0.20	60,60,60,60	0
57	MG	2A	3700	1/1	0.67	0.19	56,56,56,56	0
57	MG	1A	4023	1/1	0.67	0.20	57,57,57,57	0
57	MG	1A	4043	1/1	0.67	0.16	65,65,65,65	0
57	MG	2a	3168	1/1	0.68	0.24	70,70,70,70	0
57	MG	2A	3371	1/1	0.68	0.19	73,73,73,73	0
57	MG	2a	3093	1/1	0.68	0.29	82,82,82,82	0
57	MG	2A	3648	1/1	0.69	0.18	60,60,60,60	0
57	MG	2B	212	1/1	0.70	0.21	73,73,73,73	0
57	MG	2a	3015	1/1	0.70	0.19	70,70,70,70	0
57	MG	1A	4072	1/1	0.70	0.24	40,40,40,40	0
57	MG	2A	3093	1/1	0.70	0.20	78,78,78,78	0
57	MG	2a	3224	1/1	0.70	0.26	69,69,69,69	0
57	MG	1A	4099	1/1	0.70	0.20	66,66,66,66	0
57	MG	2x	106	1/1	0.70	0.28	68,68,68,68	0
57	MG	1A	3876	1/1	0.70	0.19	29,29,29,29	0
57	MG	1w	108	1/1	0.71	0.30	78,78,78,78	0
57	MG	2a	3020	1/1	0.71	0.27	71,71,71,71	0
57	MG	2A	3277	1/1	0.71	0.20	66,66,66,66	0
57	MG	2W	201	1/1	0.71	0.24	72,72,72,72	0
57	MG	2B	203	1/1	0.72	0.21	76,76,76,76	0
57	MG	1G	205	1/1	0.72	0.16	53,53,53,53	0
57	MG	2a	3215	1/1	0.72	0.17	78,78,78,78	0
57	MG	2B	215	1/1	0.72	0.26	78,78,78,78	0
57	MG	2w	102	1/1	0.72	0.24	76,76,76,76	0
57	MG	1a	1787	1/1	0.72	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
57	MG	2A	3839	1/1	0.72	0.16	85,85,85,85	0
57	MG	2A	3703	1/1	0.72	0.17	65,65,65,65	0
57	MG	2A	3832	1/1	0.73	0.20	85,85,85,85	0
57	MG	2A	3273	1/1	0.73	0.18	61,61,61,61	0
57	MG	2A	3842	1/1	0.73	0.30	71,71,71,71	0
57	MG	2A	3670	1/1	0.73	0.15	81,81,81,81	0
57	MG	25	107	1/1	0.73	0.23	76,76,76,76	0
57	MG	2A	3339	1/1	0.74	0.15	68,68,68,68	0
57	MG	1A	3525	1/1	0.74	0.15	55,55,55,55	0
57	MG	2A	3669	1/1	0.74	0.14	68,68,68,68	0
57	MG	2j	201	1/1	0.74	0.23	77,77,77,77	0
57	MG	1A	3393	1/1	0.74	0.17	61,61,61,61	0
57	MG	1A	3741	1/1	0.74	0.15	70,70,70,70	0
57	MG	1A	4016	1/1	0.74	0.12	70,70,70,70	0
57	MG	2A	3739	1/1	0.74	0.23	61,61,61,61	0
57	MG	1F	303	1/1	0.75	0.19	68,68,68,68	0
57	MG	2A	3310	1/1	0.75	0.20	64,64,64,64	0
57	MG	2A	3247	1/1	0.75	0.11	83,83,83,83	0
57	MG	2A	3634	1/1	0.75	0.22	74,74,74,74	0
57	MG	2A	3730	1/1	0.75	0.21	69,69,69,69	0
57	MG	1a	1682	1/1	0.75	0.13	68,68,68,68	0
57	MG	1A	3999	1/1	0.75	0.13	83,83,83,83	0
57	MG	1A	4078	1/1	0.76	0.29	73,73,73,73	0
57	MG	2a	3204	1/1	0.76	0.21	71,71,71,71	0
57	MG	2A	3269	1/1	0.76	0.17	68,68,68,68	0
57	MG	2A	3105	1/1	0.76	0.15	70,70,70,70	0
57	MG	18	103	1/1	0.76	0.20	59,59,59,59	0
57	MG	2A	3717	1/1	0.76	0.17	37,37,37,37	0
57	MG	2A	3086	1/1	0.76	0.15	79,79,79,79	0
57	MG	2A	3665	1/1	0.76	0.22	72,72,72,72	0
57	MG	2a	3122	1/1	0.76	0.17	73,73,73,73	0
57	MG	1A	3228	1/1	0.77	0.33	71,71,71,71	0
57	MG	2a	3115	1/1	0.77	0.26	79,79,79,79	0
57	MG	2A	3846	1/1	0.77	0.20	63,63,63,63	0
57	MG	2A	3615	1/1	0.77	0.18	67,67,67,67	0
57	MG	2a	3191	1/1	0.77	0.27	66,66,66,66	0
57	MG	1A	4083	1/1	0.77	0.17	62,62,62,62	0
57	MG	1A	3783	1/1	0.77	0.20	82,82,82,82	0
57	MG	1A	3027	1/1	0.77	0.30	67,67,67,67	0
57	MG	1B	228	1/1	0.77	0.12	70,70,70,70	0
57	MG	1A	3900	1/1	0.77	0.12	45,45,45,45	0
57	MG	2a	3013	1/1	0.77	0.12	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3504	1/1	0.77	0.15	72,72,72,72	0
57	MG	2A	3687	1/1	0.77	0.19	70,70,70,70	0
57	MG	1a	1746	1/1	0.78	0.29	61,61,61,61	0
57	MG	1A	3829	1/1	0.78	0.12	53,53,53,53	0
57	MG	1A	3969	1/1	0.78	0.18	69,69,69,69	0
57	MG	2B	204	1/1	0.78	0.18	71,71,71,71	0
57	MG	2A	3734	1/1	0.78	0.14	41,41,41,41	0
57	MG	10	107	1/1	0.78	0.29	58,58,58,58	0
57	MG	1A	4103	1/1	0.78	0.13	48,48,48,48	0
57	MG	2A	3769	1/1	0.78	0.14	55,55,55,55	0
57	MG	2p	101	1/1	0.78	0.27	71,71,71,71	0
57	MG	1A	3860	1/1	0.78	0.14	44,44,44,44	0
57	MG	1A	3922	1/1	0.78	0.13	50,50,50,50	0
57	MG	2A	3690	1/1	0.78	0.12	53,53,53,53	0
57	MG	2y	101	1/1	0.78	0.17	79,79,79,79	0
57	MG	2A	3632	1/1	0.78	0.16	65,65,65,65	0
57	MG	1A	3936	1/1	0.79	0.16	66,66,66,66	0
57	MG	2a	3028	1/1	0.79	0.27	74,74,74,74	0
57	MG	2A	3594	1/1	0.79	0.22	62,62,62,62	0
57	MG	2A	3834	1/1	0.79	0.16	55,55,55,55	0
57	MG	2A	3063	1/1	0.79	0.15	64,64,64,64	0
57	MG	2a	3155	1/1	0.79	0.12	66,66,66,66	0
57	MG	1A	3601	1/1	0.79	0.12	45,45,45,45	0
57	MG	2A	3845	1/1	0.79	0.19	62,62,62,62	0
57	MG	1A	3918	1/1	0.79	0.12	31,31,31,31	0
57	MG	2A	3713	1/1	0.79	0.17	72,72,72,72	0
57	MG	2A	3097	1/1	0.79	0.25	77,77,77,77	0
57	MG	2a	3228	1/1	0.79	0.31	71,71,71,71	0
57	MG	2A	3723	1/1	0.79	0.16	49,49,49,49	0
57	MG	1a	1708	1/1	0.79	0.34	78,78,78,78	0
57	MG	1A	3893	1/1	0.79	0.12	50,50,50,50	0
57	MG	1B	207	1/1	0.79	0.13	64,64,64,64	0
57	MG	2A	3751	1/1	0.79	0.12	39,39,39,39	0
57	MG	2A	3354	1/1	0.79	0.14	63,63,63,63	0
57	MG	2A	3224	1/1	0.79	0.26	61,61,61,61	0
57	MG	1A	3992	1/1	0.80	0.17	36,36,36,36	0
57	MG	1A	3934	1/1	0.80	0.13	30,30,30,30	0
57	MG	1a	1601	1/1	0.80	0.22	65,65,65,65	0
57	MG	2A	3417	1/1	0.80	0.24	64,64,64,64	0
57	MG	2a	3169	1/1	0.80	0.20	58,58,58,58	0
57	MG	2a	3184	1/1	0.80	0.20	70,70,70,70	0
57	MG	2A	3506	1/1	0.80	0.16	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3550	1/1	0.80	0.26	62,62,62,62	0
57	MG	2E	302	1/1	0.80	0.14	73,73,73,73	0
57	MG	2a	3217	1/1	0.80	0.15	63,63,63,63	0
57	MG	2A	3797	1/1	0.80	0.12	31,31,31,31	0
57	MG	2X	101	1/1	0.80	0.17	63,63,63,63	0
57	MG	1a	1675	1/1	0.80	0.17	68,68,68,68	0
57	MG	2a	3008	1/1	0.80	0.28	73,73,73,73	0
57	MG	1A	3727	1/1	0.80	0.19	61,61,61,61	0
57	MG	1A	3632	1/1	0.80	0.19	46,46,46,46	0
57	MG	2A	3289	1/1	0.80	0.29	76,76,76,76	0
57	MG	2A	3128	1/1	0.80	0.20	72,72,72,72	0
57	MG	1O	205	1/1	0.80	0.26	66,66,66,66	0
57	MG	1A	3675	1/1	0.81	0.16	61,61,61,61	0
57	MG	2A	3084	1/1	0.81	0.29	67,67,67,67	0
57	MG	2A	3621	1/1	0.81	0.23	68,68,68,68	0
57	MG	1A	4075	1/1	0.81	0.25	55,55,55,55	0
57	MG	1B	229	1/1	0.81	0.21	70,70,70,70	0
57	MG	1A	3475	1/1	0.81	0.13	57,57,57,57	0
57	MG	1A	4019	1/1	0.81	0.14	71,71,71,71	0
57	MG	1A	3292	1/1	0.81	0.12	61,61,61,61	0
57	MG	1A	3795	1/1	0.81	0.11	56,56,56,56	0
57	MG	2a	3225	1/1	0.81	0.19	75,75,75,75	0
57	MG	1a	1799	1/1	0.81	0.35	62,62,62,62	0
57	MG	2A	3479	1/1	0.81	0.13	35,35,35,35	0
57	MG	2A	3481	1/1	0.81	0.18	71,71,71,71	0
57	MG	1a	1805	1/1	0.81	0.15	65,65,65,65	0
57	MG	1A	4046	1/1	0.81	0.16	51,51,51,51	0
57	MG	2a	3098	1/1	0.81	0.24	68,68,68,68	0
57	MG	1x	108	1/1	0.81	0.36	72,72,72,72	0
57	MG	2A	3046	1/1	0.81	0.22	71,71,71,71	0
57	MG	2A	3684	1/1	0.82	0.18	54,54,54,54	0
57	MG	1A	3584	1/1	0.82	0.18	60,60,60,60	0
57	MG	1A	3304	1/1	0.82	0.22	50,50,50,50	0
57	MG	1A	3988	1/1	0.82	0.12	49,49,49,49	0
57	MG	1a	1772	1/1	0.82	0.13	46,46,46,46	0
57	MG	1A	3823	1/1	0.82	0.15	58,58,58,58	0
57	MG	1A	3449	1/1	0.82	0.15	64,64,64,64	0
57	MG	2A	3286	1/1	0.82	0.32	71,71,71,71	0
57	MG	2a	3197	1/1	0.82	0.26	63,63,63,63	0
57	MG	2a	3201	1/1	0.82	0.15	62,62,62,62	0
57	MG	2A	3100	1/1	0.82	0.21	65,65,65,65	0
57	MG	2A	3300	1/1	0.82	0.18	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	3216	1/1	0.82	0.27	61,61,61,61	0
57	MG	1A	3759	1/1	0.82	0.11	27,27,27,27	0
57	MG	1w	107	1/1	0.82	0.13	77,77,77,77	0
57	MG	2A	3331	1/1	0.82	0.30	64,64,64,64	0
57	MG	1a	1670	1/1	0.82	0.32	74,74,74,74	0
57	MG	2A	3341	1/1	0.82	0.20	61,61,61,61	0
57	MG	1A	3551	1/1	0.82	0.23	62,62,62,62	0
57	MG	2A	3829	1/1	0.82	0.17	67,67,67,67	0
57	MG	2A	3223	1/1	0.82	0.17	58,58,58,58	0
57	MG	2a	3041	1/1	0.82	0.17	72,72,72,72	0
57	MG	2a	3043	1/1	0.82	0.14	72,72,72,72	0
57	MG	2A	3374	1/1	0.82	0.33	75,75,75,75	0
57	MG	1A	3455	1/1	0.83	0.25	70,70,70,70	0
57	MG	2A	3667	1/1	0.83	0.19	67,67,67,67	0
57	MG	2A	3295	1/1	0.83	0.20	62,62,62,62	0
57	MG	27	102	1/1	0.83	0.15	60,60,60,60	0
57	MG	2a	3002	1/1	0.83	0.19	75,75,75,75	0
57	MG	2a	3004	1/1	0.83	0.19	60,60,60,60	0
57	MG	2A	3060	1/1	0.83	0.12	66,66,66,66	0
57	MG	2a	3012	1/1	0.83	0.22	71,71,71,71	0
57	MG	1a	1604	1/1	0.83	0.18	59,59,59,59	0
57	MG	1a	1665	1/1	0.83	0.27	62,62,62,62	0
57	MG	1a	1667	1/1	0.83	0.18	64,64,64,64	0
57	MG	1A	3686	1/1	0.83	0.15	64,64,64,64	0
57	MG	2A	3340	1/1	0.83	0.28	70,70,70,70	0
57	MG	1A	3343	1/1	0.83	0.12	60,60,60,60	0
57	MG	1a	1681	1/1	0.83	0.24	62,62,62,62	0
57	MG	1A	4031	1/1	0.83	0.11	34,34,34,34	0
57	MG	2A	3108	1/1	0.83	0.20	52,52,52,52	0
57	MG	2a	3116	1/1	0.83	0.26	58,58,58,58	0
57	MG	2A	3113	1/1	0.83	0.23	59,59,59,59	0
57	MG	2a	3140	1/1	0.83	0.12	71,71,71,71	0
57	MG	1a	1687	1/1	0.83	0.28	71,71,71,71	0
57	MG	1A	3713	1/1	0.83	0.11	47,47,47,47	0
57	MG	2A	3759	1/1	0.83	0.15	59,59,59,59	0
57	MG	2a	3171	1/1	0.83	0.21	69,69,69,69	0
57	MG	2A	3489	1/1	0.83	0.15	55,55,55,55	0
57	MG	1A	3499	1/1	0.83	0.17	55,55,55,55	0
57	MG	2A	3781	1/1	0.83	0.12	44,44,44,44	0
57	MG	2A	3187	1/1	0.83	0.17	63,63,63,63	0
57	MG	2A	3549	1/1	0.83	0.11	60,60,60,60	0
57	MG	2a	3206	1/1	0.83	0.21	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3550	1/1	0.83	0.22	72,72,72,72	0
57	MG	2A	3583	1/1	0.83	0.12	30,30,30,30	0
57	MG	2A	3584	1/1	0.83	0.14	46,46,46,46	0
57	MG	1E	305	1/1	0.83	0.17	49,49,49,49	0
57	MG	1A	3425	1/1	0.83	0.12	49,49,49,49	0
57	MG	1A	3612	1/1	0.83	0.13	67,67,67,67	0
57	MG	2A	3248	1/1	0.83	0.14	70,70,70,70	0
57	MG	1A	3367	1/1	0.83	0.33	52,52,52,52	0
57	MG	1A	4080	1/1	0.83	0.14	67,67,67,67	0
57	MG	1A	3908	1/1	0.83	0.11	26,26,26,26	0
57	MG	1A	4090	1/1	0.83	0.12	59,59,59,59	0
57	MG	2A	3649	1/1	0.83	0.30	70,70,70,70	0
57	MG	2A	3035	1/1	0.83	0.14	66,66,66,66	0
57	MG	2A	3347	1/1	0.84	0.15	65,65,65,65	0
57	MG	2A	3348	1/1	0.84	0.12	65,65,65,65	0
57	MG	2A	3173	1/1	0.84	0.18	52,52,52,52	0
57	MG	1q	201	1/1	0.84	0.14	57,57,57,57	0
57	MG	1v	101	1/1	0.84	0.31	78,78,78,78	0
57	MG	2A	3399	1/1	0.84	0.29	67,67,67,67	0
57	MG	2A	3205	1/1	0.84	0.21	71,71,71,71	0
57	MG	2a	3034	1/1	0.84	0.46	75,75,75,75	0
57	MG	1A	3402	1/1	0.84	0.14	54,54,54,54	0
57	MG	1A	3897	1/1	0.84	0.25	39,39,39,39	0
57	MG	2a	3051	1/1	0.84	0.27	72,72,72,72	0
57	MG	2a	3092	1/1	0.84	0.31	78,78,78,78	0
57	MG	1A	3635	1/1	0.84	0.15	63,63,63,63	0
57	MG	1A	3659	1/1	0.84	0.12	28,28,28,28	0
57	MG	2A	3259	1/1	0.84	0.18	71,71,71,71	0
57	MG	2A	3268	1/1	0.84	0.28	61,61,61,61	0
57	MG	2a	3118	1/1	0.84	0.29	77,77,77,77	0
57	MG	2A	3764	1/1	0.84	0.11	66,66,66,66	0
57	MG	1A	4021	1/1	0.84	0.16	50,50,50,50	0
57	MG	2a	3151	1/1	0.84	0.15	66,66,66,66	0
57	MG	1a	1668	1/1	0.84	0.21	67,67,67,67	0
57	MG	2A	3791	1/1	0.84	0.15	80,80,80,80	0
57	MG	1A	3672	1/1	0.84	0.14	47,47,47,47	0
57	MG	2A	3586	1/1	0.84	0.21	44,44,44,44	0
57	MG	2a	3182	1/1	0.84	0.16	67,67,67,67	0
57	MG	1B	214	1/1	0.84	0.13	66,66,66,66	0
57	MG	2a	3189	1/1	0.84	0.22	70,70,70,70	0
57	MG	2A	3283	1/1	0.84	0.17	58,58,58,58	0
57	MG	2A	3612	1/1	0.84	0.13	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	3200	1/1	0.84	0.15	79,79,79,79	0
57	MG	2A	3284	1/1	0.84	0.15	69,69,69,69	0
57	MG	1A	4026	1/1	0.84	0.16	57,57,57,57	0
57	MG	1A	3380	1/1	0.84	0.30	41,41,41,41	0
57	MG	2A	3625	1/1	0.84	0.16	67,67,67,67	0
57	MG	2A	3860	1/1	0.84	0.14	71,71,71,71	0
57	MG	1A	4033	1/1	0.84	0.10	58,58,58,58	0
57	MG	1A	3205	1/1	0.84	0.14	72,72,72,72	0
57	MG	1A	3690	1/1	0.84	0.10	31,31,31,31	0
57	MG	2a	3226	1/1	0.84	0.15	67,67,67,67	0
57	MG	1A	4050	1/1	0.84	0.15	37,37,37,37	0
57	MG	2A	3650	1/1	0.84	0.15	68,68,68,68	0
57	MG	2A	3322	1/1	0.84	0.20	71,71,71,71	0
57	MG	2A	3327	1/1	0.84	0.29	66,66,66,66	0
57	MG	1A	3401	1/1	0.84	0.28	71,71,71,71	0
57	MG	1A	3707	1/1	0.84	0.19	59,59,59,59	0
57	MG	2A	3166	1/1	0.84	0.20	74,74,74,74	0
57	MG	1A	3535	1/1	0.84	0.23	63,63,63,63	0
57	MG	1A	3515	1/1	0.85	0.10	67,67,67,67	0
57	MG	1a	1726	1/1	0.85	0.20	71,71,71,71	0
57	MG	1A	3766	1/1	0.85	0.12	21,21,21,21	0
57	MG	2A	3321	1/1	0.85	0.13	51,51,51,51	0
57	MG	1A	3290	1/1	0.85	0.27	51,51,51,51	0
57	MG	2a	3009	1/1	0.85	0.30	73,73,73,73	0
57	MG	2A	3157	1/1	0.85	0.19	65,65,65,65	0
57	MG	1G	203	1/1	0.85	0.08	66,66,66,66	0
57	MG	1A	4049	1/1	0.85	0.14	56,56,56,56	0
57	MG	1A	3790	1/1	0.85	0.10	19,19,19,19	0
57	MG	2A	3174	1/1	0.85	0.20	66,66,66,66	0
57	MG	2A	3689	1/1	0.85	0.13	46,46,46,46	0
57	MG	2a	3037	1/1	0.85	0.23	61,61,61,61	0
57	MG	2A	3346	1/1	0.85	0.21	71,71,71,71	0
57	MG	2a	3042	1/1	0.85	0.19	59,59,59,59	0
57	MG	1a	1817	1/1	0.85	0.13	65,65,65,65	0
57	MG	2a	3044	1/1	0.85	0.20	69,69,69,69	0
57	MG	2a	3046	1/1	0.85	0.15	79,79,79,79	0
57	MG	1A	3344	1/1	0.85	0.15	57,57,57,57	0
57	MG	2a	3067	1/1	0.85	0.25	62,62,62,62	0
57	MG	2A	3195	1/1	0.85	0.15	50,50,50,50	0
57	MG	2A	3714	1/1	0.85	0.14	62,62,62,62	0
57	MG	2A	3361	1/1	0.85	0.13	59,59,59,59	0
57	MG	2A	3367	1/1	0.85	0.16	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3977	1/1	0.85	0.14	59,59,59,59	0
57	MG	1A	3982	1/1	0.85	0.09	22,22,22,22	0
57	MG	1A	4079	1/1	0.85	0.13	54,54,54,54	0
57	MG	2A	3406	1/1	0.85	0.31	66,66,66,66	0
57	MG	2A	3242	1/1	0.85	0.19	64,64,64,64	0
57	MG	2A	3419	1/1	0.85	0.35	66,66,66,66	0
57	MG	2A	3420	1/1	0.85	0.26	60,60,60,60	0
57	MG	2A	3443	1/1	0.85	0.25	67,67,67,67	0
57	MG	2A	3770	1/1	0.85	0.14	65,65,65,65	0
57	MG	2A	3771	1/1	0.85	0.13	80,80,80,80	0
57	MG	2A	3246	1/1	0.85	0.21	75,75,75,75	0
57	MG	1x	106	1/1	0.85	0.20	57,57,57,57	0
57	MG	1A	3448	1/1	0.85	0.21	74,74,74,74	0
57	MG	2A	3254	1/1	0.85	0.19	58,58,58,58	0
57	MG	2A	3511	1/1	0.85	0.18	60,60,60,60	0
57	MG	2A	3016	1/1	0.85	0.16	59,59,59,59	0
57	MG	2A	3020	1/1	0.85	0.27	67,67,67,67	0
57	MG	2A	3836	1/1	0.85	0.12	37,37,37,37	0
57	MG	1A	3364	1/1	0.85	0.20	56,56,56,56	0
57	MG	1A	3699	1/1	0.85	0.13	32,32,32,32	0
57	MG	1A	3555	1/1	0.85	0.17	60,60,60,60	0
57	MG	2A	3275	1/1	0.85	0.17	62,62,62,62	0
57	MG	1A	3035	1/1	0.85	0.10	47,47,47,47	0
57	MG	2A	3279	1/1	0.85	0.26	71,71,71,71	0
57	MG	2A	3281	1/1	0.85	0.13	64,64,64,64	0
57	MG	2A	3282	1/1	0.85	0.22	66,66,66,66	0
57	MG	2l	203	1/1	0.85	0.10	70,70,70,70	0
57	MG	1a	1674	1/1	0.85	0.15	43,43,43,43	0
57	MG	2t	201	1/1	0.85	0.21	59,59,59,59	0
57	MG	1A	3294	1/1	0.85	0.26	60,60,60,60	0
57	MG	1A	3493	1/1	0.85	0.15	66,66,66,66	0
57	MG	1A	3068	1/1	0.85	0.12	55,55,55,55	0
57	MG	1A	3339	1/1	0.85	0.20	64,64,64,64	0
57	MG	2Z	301	1/1	0.85	0.10	75,75,75,75	0
57	MG	2A	3582	1/1	0.86	0.07	34,34,34,34	0
57	MG	1A	3602	1/1	0.86	0.09	24,24,24,24	0
57	MG	1A	4107	1/1	0.86	0.33	66,66,66,66	0
57	MG	1A	3704	1/1	0.86	0.16	53,53,53,53	0
57	MG	2A	3589	1/1	0.86	0.18	67,67,67,67	0
57	MG	1B	213	1/1	0.86	0.27	64,64,64,64	0
57	MG	1a	1679	1/1	0.86	0.11	56,56,56,56	0
57	MG	2A	3288	1/1	0.86	0.23	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	25	101	1/1	0.86	0.22	62,62,62,62	0
57	MG	1A	3944	1/1	0.86	0.09	60,60,60,60	0
57	MG	2A	3290	1/1	0.86	0.13	63,63,63,63	0
57	MG	1A	3827	1/1	0.86	0.12	37,37,37,37	0
57	MG	2A	3624	1/1	0.86	0.15	70,70,70,70	0
57	MG	2A	3110	1/1	0.86	0.32	63,63,63,63	0
57	MG	1B	224	1/1	0.86	0.12	55,55,55,55	0
57	MG	2A	3312	1/1	0.86	0.28	62,62,62,62	0
57	MG	2A	3117	1/1	0.86	0.11	68,68,68,68	0
57	MG	1A	3465	1/1	0.86	0.17	64,64,64,64	0
57	MG	1A	3971	1/1	0.86	0.11	61,61,61,61	0
57	MG	1A	3856	1/1	0.86	0.12	50,50,50,50	0
57	MG	2a	3033	1/1	0.86	0.22	63,63,63,63	0
57	MG	2A	3330	1/1	0.86	0.13	76,76,76,76	0
57	MG	1A	4051	1/1	0.86	0.14	62,62,62,62	0
57	MG	2a	3038	1/1	0.86	0.28	58,58,58,58	0
57	MG	2A	3338	1/1	0.86	0.13	65,65,65,65	0
57	MG	1A	4066	1/1	0.86	0.13	56,56,56,56	0
57	MG	2A	3676	1/1	0.86	0.15	60,60,60,60	0
57	MG	2A	3681	1/1	0.86	0.14	38,38,38,38	0
57	MG	1a	1798	1/1	0.86	0.20	73,73,73,73	0
57	MG	1A	3026	1/1	0.86	0.13	44,44,44,44	0
57	MG	2a	3054	1/1	0.86	0.14	70,70,70,70	0
57	MG	1A	3093	1/1	0.86	0.13	55,55,55,55	0
57	MG	2a	3091	1/1	0.86	0.09	69,69,69,69	0
57	MG	2A	3194	1/1	0.86	0.23	58,58,58,58	0
57	MG	1a	1809	1/1	0.86	0.15	81,81,81,81	0
57	MG	2A	3701	1/1	0.86	0.12	64,64,64,64	0
57	MG	2A	3349	1/1	0.86	0.22	54,54,54,54	0
57	MG	2A	3352	1/1	0.86	0.15	46,46,46,46	0
57	MG	1A	3100	1/1	0.86	0.14	69,69,69,69	0
57	MG	2a	3119	1/1	0.86	0.19	60,60,60,60	0
57	MG	2A	3355	1/1	0.86	0.16	70,70,70,70	0
57	MG	1f	202	1/1	0.86	0.26	65,65,65,65	0
57	MG	2a	3147	1/1	0.86	0.10	58,58,58,58	0
57	MG	1h	201	1/1	0.86	0.13	70,70,70,70	0
57	MG	2A	3232	1/1	0.86	0.09	49,49,49,49	0
57	MG	2a	3156	1/1	0.86	0.14	64,64,64,64	0
57	MG	2a	3158	1/1	0.86	0.12	64,64,64,64	0
57	MG	2a	3162	1/1	0.86	0.16	52,52,52,52	0
57	MG	2a	3165	1/1	0.86	0.13	66,66,66,66	0
57	MG	1l	202	1/1	0.86	0.10	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3393	1/1	0.86	0.19	54,54,54,54	0
57	MG	2A	3754	1/1	0.86	0.14	70,70,70,70	0
57	MG	2A	3245	1/1	0.86	0.25	67,67,67,67	0
57	MG	1A	3552	1/1	0.86	0.32	55,55,55,55	0
57	MG	1A	3400	1/1	0.86	0.15	53,53,53,53	0
57	MG	1A	3514	1/1	0.86	0.14	71,71,71,71	0
57	MG	1A	3588	1/1	0.86	0.23	50,50,50,50	0
57	MG	1a	1609	1/1	0.86	0.28	62,62,62,62	0
57	MG	2A	3779	1/1	0.86	0.17	52,52,52,52	0
57	MG	2A	3261	1/1	0.86	0.28	66,66,66,66	0
57	MG	1a	1617	1/1	0.86	0.15	61,61,61,61	0
57	MG	2A	3485	1/1	0.86	0.22	63,63,63,63	0
57	MG	2A	3801	1/1	0.86	0.12	40,40,40,40	0
57	MG	2A	3808	1/1	0.86	0.11	71,71,71,71	0
57	MG	1a	1624	1/1	0.86	0.26	68,68,68,68	0
57	MG	2A	3814	1/1	0.86	0.11	49,49,49,49	0
57	MG	2A	3495	1/1	0.86	0.09	59,59,59,59	0
57	MG	1a	1641	1/1	0.86	0.20	69,69,69,69	0
57	MG	1a	1654	1/1	0.86	0.18	57,57,57,57	0
57	MG	2A	3524	1/1	0.86	0.11	60,60,60,60	0
57	MG	1a	1657	1/1	0.86	0.19	63,63,63,63	0
57	MG	1A	4091	1/1	0.86	0.20	58,58,58,58	0
57	MG	2v	102	1/1	0.86	0.10	69,69,69,69	0
57	MG	1A	3320	1/1	0.86	0.19	51,51,51,51	0
57	MG	2A	3570	1/1	0.86	0.09	30,30,30,30	0
57	MG	2A	3858	1/1	0.86	0.10	63,63,63,63	0
57	MG	2A	3573	1/1	0.86	0.12	54,54,54,54	0
57	MG	2A	3576	1/1	0.86	0.14	55,55,55,55	0
57	MG	2A	3574	1/1	0.87	0.15	54,54,54,54	0
57	MG	2B	206	1/1	0.87	0.23	61,61,61,61	0
57	MG	2A	3054	1/1	0.87	0.31	66,66,66,66	0
57	MG	1A	4097	1/1	0.87	0.15	67,67,67,67	0
57	MG	1A	3865	1/1	0.87	0.16	32,32,32,32	0
57	MG	2U	202	1/1	0.87	0.09	57,57,57,57	0
57	MG	1A	4101	1/1	0.87	0.08	72,72,72,72	0
57	MG	1A	3872	1/1	0.87	0.15	59,59,59,59	0
57	MG	1A	3735	1/1	0.87	0.08	17,17,17,17	0
57	MG	2A	3294	1/1	0.87	0.34	54,54,54,54	0
57	MG	25	102	1/1	0.87	0.24	52,52,52,52	0
57	MG	1A	4008	1/1	0.87	0.10	39,39,39,39	0
57	MG	2A	3296	1/1	0.87	0.12	62,62,62,62	0
57	MG	2A	3098	1/1	0.87	0.20	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3614	1/1	0.87	0.13	41,41,41,41	0
57	MG	2A	3301	1/1	0.87	0.31	49,49,49,49	0
57	MG	1A	3877	1/1	0.87	0.09	25,25,25,25	0
57	MG	1A	3884	1/1	0.87	0.12	29,29,29,29	0
57	MG	1A	3890	1/1	0.87	0.17	31,31,31,31	0
57	MG	2a	3014	1/1	0.87	0.18	64,64,64,64	0
57	MG	2A	3631	1/1	0.87	0.14	61,61,61,61	0
57	MG	2a	3016	1/1	0.87	0.16	73,73,73,73	0
57	MG	2a	3018	1/1	0.87	0.25	81,81,81,81	0
57	MG	1A	3024	1/1	0.87	0.24	61,61,61,61	0
57	MG	2a	3027	1/1	0.87	0.14	75,75,75,75	0
57	MG	1a	1703	1/1	0.87	0.32	63,63,63,63	0
57	MG	2a	3030	1/1	0.87	0.20	68,68,68,68	0
57	MG	1B	225	1/1	0.87	0.11	51,51,51,51	0
57	MG	2A	3329	1/1	0.87	0.23	73,73,73,73	0
57	MG	1a	1715	1/1	0.87	0.21	63,63,63,63	0
57	MG	1A	3743	1/1	0.87	0.10	34,34,34,34	0
57	MG	2A	3663	1/1	0.87	0.12	65,65,65,65	0
57	MG	2A	3333	1/1	0.87	0.16	69,69,69,69	0
57	MG	1a	1730	1/1	0.87	0.17	65,65,65,65	0
57	MG	1A	3746	1/1	0.87	0.10	42,42,42,42	0
57	MG	2a	3045	1/1	0.87	0.18	70,70,70,70	0
57	MG	1a	1763	1/1	0.87	0.14	59,59,59,59	0
57	MG	1a	1771	1/1	0.87	0.12	65,65,65,65	0
57	MG	1A	3092	1/1	0.87	0.12	41,41,41,41	0
57	MG	2a	3057	1/1	0.87	0.19	68,68,68,68	0
57	MG	1E	311	1/1	0.87	0.19	66,66,66,66	0
57	MG	2a	3080	1/1	0.87	0.17	65,65,65,65	0
57	MG	2a	3083	1/1	0.87	0.19	58,58,58,58	0
57	MG	2A	3192	1/1	0.87	0.15	67,67,67,67	0
57	MG	1A	3594	1/1	0.87	0.10	43,43,43,43	0
57	MG	1A	3540	1/1	0.87	0.23	60,60,60,60	0
57	MG	2A	3204	1/1	0.87	0.12	54,54,54,54	0
57	MG	2a	3101	1/1	0.87	0.25	68,68,68,68	0
57	MG	2a	3106	1/1	0.87	0.32	67,67,67,67	0
57	MG	1A	3351	1/1	0.87	0.12	57,57,57,57	0
57	MG	2A	3357	1/1	0.87	0.20	60,60,60,60	0
57	MG	2A	3704	1/1	0.87	0.11	59,59,59,59	0
57	MG	2A	3219	1/1	0.87	0.23	60,60,60,60	0
57	MG	2A	3363	1/1	0.87	0.12	68,68,68,68	0
57	MG	2a	3137	1/1	0.87	0.09	89,89,89,89	0
57	MG	1A	3935	1/1	0.87	0.11	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3325	1/1	0.87	0.14	51,51,51,51	0
57	MG	13	104	1/1	0.87	0.12	53,53,53,53	0
57	MG	2A	3375	1/1	0.87	0.08	70,70,70,70	0
57	MG	2A	3380	1/1	0.87	0.18	64,64,64,64	0
57	MG	1A	3631	1/1	0.87	0.12	41,41,41,41	0
57	MG	2A	3244	1/1	0.87	0.17	75,75,75,75	0
57	MG	2a	3163	1/1	0.87	0.26	53,53,53,53	0
57	MG	1A	3463	1/1	0.87	0.29	72,72,72,72	0
57	MG	2A	3412	1/1	0.87	0.32	63,63,63,63	0
57	MG	2A	3416	1/1	0.87	0.19	57,57,57,57	0
57	MG	2a	3170	1/1	0.87	0.21	64,64,64,64	0
57	MG	1A	3953	1/1	0.87	0.10	27,27,27,27	0
57	MG	1A	3020	1/1	0.87	0.16	45,45,45,45	0
57	MG	1w	105	1/1	0.87	0.17	75,75,75,75	0
57	MG	2A	3776	1/1	0.87	0.10	57,57,57,57	0
57	MG	2a	3190	1/1	0.87	0.11	54,54,54,54	0
57	MG	2A	3424	1/1	0.87	0.30	73,73,73,73	0
57	MG	1A	3726	1/1	0.87	0.15	67,67,67,67	0
57	MG	2A	3455	1/1	0.87	0.14	70,70,70,70	0
57	MG	2A	3457	1/1	0.87	0.17	58,58,58,58	0
57	MG	1A	3575	1/1	0.87	0.13	51,51,51,51	0
57	MG	2A	3260	1/1	0.87	0.17	59,59,59,59	0
57	MG	2a	3211	1/1	0.87	0.12	69,69,69,69	0
57	MG	1x	103	1/1	0.87	0.13	59,59,59,59	0
57	MG	2A	3266	1/1	0.87	0.13	69,69,69,69	0
57	MG	2A	3490	1/1	0.87	0.16	53,53,53,53	0
57	MG	2a	3223	1/1	0.87	0.14	74,74,74,74	0
57	MG	1A	3980	1/1	0.87	0.09	26,26,26,26	0
57	MG	2A	3502	1/1	0.87	0.27	68,68,68,68	0
57	MG	1a	1630	1/1	0.87	0.15	59,59,59,59	0
57	MG	1a	1639	1/1	0.87	0.14	60,60,60,60	0
57	MG	2A	3840	1/1	0.87	0.13	51,51,51,51	0
57	MG	2A	3019	1/1	0.87	0.20	63,63,63,63	0
57	MG	1A	4084	1/1	0.87	0.15	61,61,61,61	0
57	MG	2A	3032	1/1	0.87	0.16	69,69,69,69	0
57	MG	2v	101	1/1	0.87	0.28	62,62,62,62	0
57	MG	2A	3853	1/1	0.87	0.16	56,56,56,56	0
57	MG	2w	101	1/1	0.87	0.17	56,56,56,56	0
57	MG	2A	3854	1/1	0.87	0.16	61,61,61,61	0
57	MG	2w	103	1/1	0.87	0.17	77,77,77,77	0
57	MG	2w	106	1/1	0.87	0.12	62,62,62,62	0
57	MG	1A	3728	1/1	0.87	0.10	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2x	103	1/1	0.87	0.21	62,62,62,62	0
57	MG	2A	3562	1/1	0.87	0.23	60,60,60,60	0
57	MG	1A	3985	1/1	0.87	0.21	60,60,60,60	0
57	MG	2A	3053	1/1	0.87	0.16	62,62,62,62	0
57	MG	2A	3674	1/1	0.88	0.09	31,31,31,31	0
57	MG	1A	3677	1/1	0.88	0.08	41,41,41,41	0
57	MG	1A	3289	1/1	0.88	0.13	44,44,44,44	0
57	MG	2A	3404	1/1	0.88	0.18	57,57,57,57	0
57	MG	2a	3021	1/1	0.88	0.17	68,68,68,68	0
57	MG	2A	3090	1/1	0.88	0.13	40,40,40,40	0
57	MG	1A	3424	1/1	0.88	0.12	49,49,49,49	0
57	MG	1A	4045	1/1	0.88	0.08	13,13,13,13	0
57	MG	2A	3699	1/1	0.88	0.14	71,71,71,71	0
57	MG	1a	1741	1/1	0.88	0.26	76,76,76,76	0
57	MG	1A	3486	1/1	0.88	0.10	55,55,55,55	0
57	MG	1a	1761	1/1	0.88	0.12	77,77,77,77	0
57	MG	1A	3050	1/1	0.88	0.15	45,45,45,45	0
57	MG	2A	3285	1/1	0.88	0.24	74,74,74,74	0
57	MG	2A	3445	1/1	0.88	0.14	62,62,62,62	0
57	MG	2A	3716	1/1	0.88	0.16	65,65,65,65	0
57	MG	2A	3452	1/1	0.88	0.10	53,53,53,53	0
57	MG	1N	201	1/1	0.88	0.21	70,70,70,70	0
57	MG	2A	3727	1/1	0.88	0.20	56,56,56,56	0
57	MG	1A	3937	1/1	0.88	0.16	55,55,55,55	0
57	MG	2A	3471	1/1	0.88	0.18	50,50,50,50	0
57	MG	2A	3473	1/1	0.88	0.26	64,64,64,64	0
57	MG	2A	3741	1/1	0.88	0.20	55,55,55,55	0
57	MG	2A	3478	1/1	0.88	0.11	46,46,46,46	0
57	MG	2a	3087	1/1	0.88	0.27	63,63,63,63	0
57	MG	2a	3088	1/1	0.88	0.21	60,60,60,60	0
57	MG	2a	3089	1/1	0.88	0.16	51,51,51,51	0
57	MG	1A	3618	1/1	0.88	0.15	54,54,54,54	0
57	MG	2A	3119	1/1	0.88	0.25	62,62,62,62	0
57	MG	2A	3761	1/1	0.88	0.14	53,53,53,53	0
57	MG	1A	4060	1/1	0.88	0.10	54,54,54,54	0
57	MG	2a	3099	1/1	0.88	0.15	59,59,59,59	0
57	MG	1A	3825	1/1	0.88	0.14	59,59,59,59	0
57	MG	2A	3768	1/1	0.88	0.09	73,73,73,73	0
57	MG	2a	3107	1/1	0.88	0.08	61,61,61,61	0
57	MG	1A	3951	1/1	0.88	0.09	37,37,37,37	0
57	MG	1A	3625	1/1	0.88	0.09	20,20,20,20	0
57	MG	1A	3446	1/1	0.88	0.14	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3773	1/1	0.88	0.12	48,48,48,48	0
57	MG	2A	3303	1/1	0.88	0.17	61,61,61,61	0
57	MG	2a	3131	1/1	0.88	0.13	75,75,75,75	0
57	MG	2a	3132	1/1	0.88	0.11	72,72,72,72	0
57	MG	1A	3718	1/1	0.88	0.12	55,55,55,55	0
57	MG	2A	3512	1/1	0.88	0.10	35,35,35,35	0
57	MG	1A	3972	1/1	0.88	0.10	63,63,63,63	0
57	MG	1A	3975	1/1	0.88	0.10	61,61,61,61	0
57	MG	1m	3002	1/1	0.88	0.14	53,53,53,53	0
57	MG	1A	3719	1/1	0.88	0.12	69,69,69,69	0
57	MG	2A	3560	1/1	0.88	0.10	73,73,73,73	0
57	MG	2A	3326	1/1	0.88	0.17	72,72,72,72	0
57	MG	1A	3391	1/1	0.88	0.08	41,41,41,41	0
57	MG	2A	3572	1/1	0.88	0.18	66,66,66,66	0
57	MG	2A	3196	1/1	0.88	0.10	52,52,52,52	0
57	MG	2A	3197	1/1	0.88	0.16	52,52,52,52	0
57	MG	1A	3868	1/1	0.88	0.32	35,35,35,35	0
57	MG	1A	3347	1/1	0.88	0.13	62,62,62,62	0
57	MG	2a	3174	1/1	0.88	0.27	56,56,56,56	0
57	MG	2a	3179	1/1	0.88	0.24	67,67,67,67	0
57	MG	2A	3337	1/1	0.88	0.10	58,58,58,58	0
57	MG	2a	3183	1/1	0.88	0.16	66,66,66,66	0
57	MG	2A	3844	1/1	0.88	0.14	66,66,66,66	0
57	MG	2a	3185	1/1	0.88	0.17	80,80,80,80	0
57	MG	2a	3186	1/1	0.88	0.18	54,54,54,54	0
57	MG	2A	3216	1/1	0.88	0.22	62,62,62,62	0
57	MG	1A	3636	1/1	0.88	0.12	60,60,60,60	0
57	MG	1A	3637	1/1	0.88	0.12	22,22,22,22	0
57	MG	1A	3998	1/1	0.88	0.08	61,61,61,61	0
57	MG	2A	3856	1/1	0.88	0.12	59,59,59,59	0
57	MG	2A	3225	1/1	0.88	0.27	40,40,40,40	0
57	MG	2A	3604	1/1	0.88	0.17	42,42,42,42	0
57	MG	1A	3646	1/1	0.88	0.12	44,44,44,44	0
57	MG	2a	3208	1/1	0.88	0.14	50,50,50,50	0
57	MG	2a	3209	1/1	0.88	0.23	72,72,72,72	0
57	MG	2B	201	1/1	0.88	0.17	70,70,70,70	0
57	MG	1x	112	1/1	0.88	0.12	66,66,66,66	0
57	MG	2A	3012	1/1	0.88	0.12	68,68,68,68	0
57	MG	2A	3351	1/1	0.88	0.08	70,70,70,70	0
57	MG	2a	3222	1/1	0.88	0.16	61,61,61,61	0
57	MG	1A	4002	1/1	0.88	0.07	23,23,23,23	0
57	MG	1a	1671	1/1	0.88	0.13	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3252	1/1	0.88	0.12	56,56,56,56	0
57	MG	2R	201	1/1	0.88	0.11	55,55,55,55	0
57	MG	2S	3900	1/1	0.88	0.12	69,69,69,69	0
57	MG	2a	3237	1/1	0.88	0.15	58,58,58,58	0
57	MG	2A	3627	1/1	0.88	0.13	67,67,67,67	0
57	MG	1A	3283	1/1	0.88	0.14	57,57,57,57	0
57	MG	2A	3360	1/1	0.88	0.11	61,61,61,61	0
57	MG	1B	216	1/1	0.88	0.14	48,48,48,48	0
57	MG	2A	3646	1/1	0.88	0.13	60,60,60,60	0
57	MG	2A	3038	1/1	0.88	0.20	55,55,55,55	0
57	MG	1A	3748	1/1	0.88	0.09	23,23,23,23	0
57	MG	1A	3752	1/1	0.88	0.08	16,16,16,16	0
57	MG	1A	3905	1/1	0.88	0.14	30,30,30,30	0
57	MG	1a	1691	1/1	0.88	0.28	61,61,61,61	0
57	MG	2A	3377	1/1	0.88	0.11	67,67,67,67	0
57	MG	2A	3666	1/1	0.88	0.11	49,49,49,49	0
57	MG	1A	3589	1/1	0.88	0.23	59,59,59,59	0
57	MG	2A	3381	1/1	0.88	0.14	64,64,64,64	0
57	MG	2y	102	1/1	0.88	0.11	74,74,74,74	0
57	MG	2A	3392	1/1	0.88	0.22	36,36,36,36	0
57	MG	2A	3642	1/1	0.89	0.13	52,52,52,52	0
57	MG	2a	3011	1/1	0.89	0.29	66,66,66,66	0
57	MG	2A	3645	1/1	0.89	0.13	46,46,46,46	0
57	MG	2A	3155	1/1	0.89	0.19	57,57,57,57	0
57	MG	1a	1732	1/1	0.89	0.14	62,62,62,62	0
57	MG	1a	1733	1/1	0.89	0.08	54,54,54,54	0
57	MG	1a	1740	1/1	0.89	0.08	66,66,66,66	0
57	MG	1A	3494	1/1	0.89	0.13	63,63,63,63	0
57	MG	2A	3655	1/1	0.89	0.15	60,60,60,60	0
57	MG	2A	3660	1/1	0.89	0.15	43,43,43,43	0
57	MG	2a	3026	1/1	0.89	0.37	62,62,62,62	0
57	MG	1A	3751	1/1	0.89	0.11	43,43,43,43	0
57	MG	1a	1748	1/1	0.89	0.15	51,51,51,51	0
57	MG	1B	230	1/1	0.89	0.08	67,67,67,67	0
57	MG	2a	3032	1/1	0.89	0.17	70,70,70,70	0
57	MG	2A	3189	1/1	0.89	0.17	66,66,66,66	0
57	MG	1a	1762	1/1	0.89	0.09	76,76,76,76	0
57	MG	2a	3035	1/1	0.89	0.26	66,66,66,66	0
57	MG	2a	3036	1/1	0.89	0.12	55,55,55,55	0
57	MG	2A	3359	1/1	0.89	0.21	60,60,60,60	0
57	MG	1D	312	1/1	0.89	0.18	40,40,40,40	0
57	MG	1A	3055	1/1	0.89	0.11	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3679	1/1	0.89	0.12	62,62,62,62	0
57	MG	2A	3683	1/1	0.89	0.15	50,50,50,50	0
57	MG	2A	3366	1/1	0.89	0.10	51,51,51,51	0
57	MG	2A	3686	1/1	0.89	0.13	56,56,56,56	0
57	MG	1a	1778	1/1	0.89	0.07	65,65,65,65	0
57	MG	2A	3200	1/1	0.89	0.15	66,66,66,66	0
57	MG	2a	3052	1/1	0.89	0.20	74,74,74,74	0
57	MG	1A	4032	1/1	0.89	0.23	61,61,61,61	0
57	MG	1a	1789	1/1	0.89	0.09	64,64,64,64	0
57	MG	1a	1792	1/1	0.89	0.12	59,59,59,59	0
57	MG	2a	3069	1/1	0.89	0.18	71,71,71,71	0
57	MG	1A	3761	1/1	0.89	0.09	38,38,38,38	0
57	MG	1G	204	1/1	0.89	0.09	71,71,71,71	0
57	MG	2A	3383	1/1	0.89	0.09	69,69,69,69	0
57	MG	2A	3709	1/1	0.89	0.10	73,73,73,73	0
57	MG	1a	1801	1/1	0.89	0.15	58,58,58,58	0
57	MG	1A	3909	1/1	0.89	0.10	30,30,30,30	0
57	MG	2A	3394	1/1	0.89	0.25	48,48,48,48	0
57	MG	1A	3246	1/1	0.89	0.09	57,57,57,57	0
57	MG	2a	3094	1/1	0.89	0.09	69,69,69,69	0
57	MG	2A	3238	1/1	0.89	0.13	58,58,58,58	0
57	MG	1a	1813	1/1	0.89	0.15	73,73,73,73	0
57	MG	1A	3089	1/1	0.89	0.15	51,51,51,51	0
57	MG	1Y	201	1/1	0.89	0.13	52,52,52,52	0
57	MG	2A	3736	1/1	0.89	0.15	67,67,67,67	0
57	MG	1Z	303	1/1	0.89	0.12	49,49,49,49	0
57	MG	1A	3124	1/1	0.89	0.12	49,49,49,49	0
57	MG	1A	3517	1/1	0.89	0.10	61,61,61,61	0
57	MG	2A	3250	1/1	0.89	0.32	64,64,64,64	0
57	MG	1A	3792	1/1	0.89	0.08	39,39,39,39	0
57	MG	2a	3127	1/1	0.89	0.09	67,67,67,67	0
57	MG	2A	3255	1/1	0.89	0.18	64,64,64,64	0
57	MG	2A	3257	1/1	0.89	0.32	70,70,70,70	0
57	MG	2A	3258	1/1	0.89	0.19	62,62,62,62	0
57	MG	1A	3160	1/1	0.89	0.20	58,58,58,58	0
57	MG	1A	4061	1/1	0.89	0.08	20,20,20,20	0
57	MG	1A	3801	1/1	0.89	0.14	52,52,52,52	0
57	MG	1A	3705	1/1	0.89	0.12	49,49,49,49	0
57	MG	1A	3528	1/1	0.89	0.16	44,44,44,44	0
57	MG	1A	3626	1/1	0.89	0.17	55,55,55,55	0
57	MG	2a	3159	1/1	0.89	0.10	62,62,62,62	0
57	MG	1A	3828	1/1	0.89	0.08	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1638	1/1	0.89	0.37	62,62,62,62	0
57	MG	1A	3399	1/1	0.89	0.23	44,44,44,44	0
57	MG	2a	3166	1/1	0.89	0.29	67,67,67,67	0
57	MG	2A	3493	1/1	0.89	0.21	71,71,71,71	0
57	MG	1A	3830	1/1	0.89	0.14	55,55,55,55	0
57	MG	2A	3018	1/1	0.89	0.18	48,48,48,48	0
57	MG	1A	3840	1/1	0.89	0.08	56,56,56,56	0
57	MG	1A	3849	1/1	0.89	0.10	26,26,26,26	0
57	MG	2A	3817	1/1	0.89	0.06	49,49,49,49	0
57	MG	1a	1658	1/1	0.89	0.11	52,52,52,52	0
57	MG	1a	1664	1/1	0.89	0.24	59,59,59,59	0
57	MG	2A	3543	1/1	0.89	0.16	72,72,72,72	0
57	MG	1A	3850	1/1	0.89	0.07	33,33,33,33	0
57	MG	1A	3178	1/1	0.89	0.24	49,49,49,49	0
57	MG	2a	3187	1/1	0.89	0.14	60,60,60,60	0
57	MG	1A	3984	1/1	0.89	0.10	28,28,28,28	0
57	MG	1A	3857	1/1	0.89	0.12	67,67,67,67	0
57	MG	2A	3058	1/1	0.89	0.20	55,55,55,55	0
57	MG	2a	3192	1/1	0.89	0.21	63,63,63,63	0
57	MG	2a	3196	1/1	0.89	0.12	62,62,62,62	0
57	MG	2A	3569	1/1	0.89	0.18	61,61,61,61	0
57	MG	1A	3464	1/1	0.89	0.13	58,58,58,58	0
57	MG	2A	3849	1/1	0.89	0.12	55,55,55,55	0
57	MG	2a	3202	1/1	0.89	0.30	67,67,67,67	0
57	MG	2A	3851	1/1	0.89	0.14	59,59,59,59	0
57	MG	1A	4105	1/1	0.89	0.13	55,55,55,55	0
57	MG	2A	3064	1/1	0.89	0.10	45,45,45,45	0
57	MG	2A	3070	1/1	0.89	0.22	70,70,70,70	0
57	MG	2a	3210	1/1	0.89	0.33	65,65,65,65	0
57	MG	2A	3575	1/1	0.89	0.15	62,62,62,62	0
57	MG	1A	3181	1/1	0.89	0.15	65,65,65,65	0
57	MG	2A	3578	1/1	0.89	0.11	39,39,39,39	0
57	MG	2A	3862	1/1	0.89	0.09	70,70,70,70	0
57	MG	2A	3579	1/1	0.89	0.10	61,61,61,61	0
57	MG	2A	3302	1/1	0.89	0.14	53,53,53,53	0
57	MG	1A	3062	1/1	0.89	0.08	52,52,52,52	0
57	MG	2A	3307	1/1	0.89	0.15	66,66,66,66	0
57	MG	1A	3731	1/1	0.89	0.07	48,48,48,48	0
57	MG	2B	213	1/1	0.89	0.18	64,64,64,64	0
57	MG	1A	3421	1/1	0.89	0.20	64,64,64,64	0
57	MG	2A	3318	1/1	0.89	0.13	57,57,57,57	0
57	MG	1a	1685	1/1	0.89	0.27	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3492	1/1	0.89	0.09	58,58,58,58	0
57	MG	2r	101	1/1	0.89	0.19	72,72,72,72	0
57	MG	1B	217	1/1	0.89	0.08	50,50,50,50	0
57	MG	1a	1701	1/1	0.89	0.28	61,61,61,61	0
57	MG	1B	220	1/1	0.89	0.08	59,59,59,59	0
57	MG	1A	4012	1/1	0.89	0.11	56,56,56,56	0
57	MG	1B	223	1/1	0.89	0.14	54,54,54,54	0
57	MG	1a	1720	1/1	0.89	0.21	37,37,37,37	0
57	MG	1A	3423	1/1	0.89	0.12	52,52,52,52	0
57	MG	1A	3674	1/1	0.89	0.10	30,30,30,30	0
57	MG	2x	102	1/1	0.89	0.13	66,66,66,66	0
57	MG	2A	3135	1/1	0.89	0.12	60,60,60,60	0
57	MG	2A	3138	1/1	0.89	0.22	51,51,51,51	0
57	MG	2a	3005	1/1	0.89	0.21	69,69,69,69	0
57	MG	2a	3007	1/1	0.89	0.26	69,69,69,69	0
57	MG	2A	3148	1/1	0.89	0.21	69,69,69,69	0
57	MG	1A	3349	1/1	0.90	0.11	73,73,73,73	0
57	MG	1A	3802	1/1	0.90	0.15	49,49,49,49	0
57	MG	2A	3677	1/1	0.90	0.18	68,68,68,68	0
57	MG	2a	3023	1/1	0.90	0.11	56,56,56,56	0
57	MG	1A	3809	1/1	0.90	0.10	49,49,49,49	0
57	MG	1A	3820	1/1	0.90	0.13	51,51,51,51	0
57	MG	1A	4044	1/1	0.90	0.17	60,60,60,60	0
57	MG	2A	3685	1/1	0.90	0.09	44,44,44,44	0
57	MG	2A	3405	1/1	0.90	0.36	60,60,60,60	0
57	MG	1A	3633	1/1	0.90	0.09	20,20,20,20	0
57	MG	2A	3411	1/1	0.90	0.21	52,52,52,52	0
57	MG	1B	231	1/1	0.90	0.10	56,56,56,56	0
57	MG	2A	3024	1/1	0.90	0.21	57,57,57,57	0
57	MG	1A	3169	1/1	0.90	0.09	43,43,43,43	0
57	MG	1A	3473	1/1	0.90	0.19	34,34,34,34	0
57	MG	2A	3702	1/1	0.90	0.09	37,37,37,37	0
57	MG	1A	3291	1/1	0.90	0.09	61,61,61,61	0
57	MG	1a	1692	1/1	0.90	0.22	53,53,53,53	0
57	MG	2A	3429	1/1	0.90	0.31	44,44,44,44	0
57	MG	1E	313	1/1	0.90	0.12	55,55,55,55	0
57	MG	1A	3476	1/1	0.90	0.18	57,57,57,57	0
57	MG	2a	3047	1/1	0.90	0.14	66,66,66,66	0
57	MG	2A	3447	1/1	0.90	0.28	60,60,60,60	0
57	MG	1A	3479	1/1	0.90	0.12	38,38,38,38	0
57	MG	1A	3836	1/1	0.90	0.08	67,67,67,67	0
57	MG	2A	3061	1/1	0.90	0.20	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	3058	1/1	0.90	0.07	60,60,60,60	0
57	MG	2A	3728	1/1	0.90	0.12	60,60,60,60	0
57	MG	1A	3970	1/1	0.90	0.11	40,40,40,40	0
57	MG	2a	3072	1/1	0.90	0.20	48,48,48,48	0
57	MG	2a	3077	1/1	0.90	0.20	55,55,55,55	0
57	MG	2a	3079	1/1	0.90	0.26	64,64,64,64	0
57	MG	1a	1722	1/1	0.90	0.15	56,56,56,56	0
57	MG	2A	3069	1/1	0.90	0.09	47,47,47,47	0
57	MG	2a	3085	1/1	0.90	0.15	78,78,78,78	0
57	MG	1A	4068	1/1	0.90	0.14	38,38,38,38	0
57	MG	2A	3480	1/1	0.90	0.21	57,57,57,57	0
57	MG	2A	3075	1/1	0.90	0.15	48,48,48,48	0
57	MG	2A	3081	1/1	0.90	0.11	55,55,55,55	0
57	MG	2A	3757	1/1	0.90	0.11	64,64,64,64	0
57	MG	2A	3488	1/1	0.90	0.11	59,59,59,59	0
57	MG	1O	204	1/1	0.90	0.11	63,63,63,63	0
57	MG	2a	3096	1/1	0.90	0.10	60,60,60,60	0
57	MG	1A	3331	1/1	0.90	0.08	52,52,52,52	0
57	MG	2A	3491	1/1	0.90	0.12	59,59,59,59	0
57	MG	2A	3287	1/1	0.90	0.22	59,59,59,59	0
57	MG	2a	3102	1/1	0.90	0.17	68,68,68,68	0
57	MG	2A	3494	1/1	0.90	0.07	35,35,35,35	0
57	MG	1T	202	1/1	0.90	0.13	49,49,49,49	0
57	MG	2a	3110	1/1	0.90	0.13	59,59,59,59	0
57	MG	1a	1739	1/1	0.90	0.19	59,59,59,59	0
57	MG	2A	3772	1/1	0.90	0.10	44,44,44,44	0
57	MG	2A	3095	1/1	0.90	0.15	55,55,55,55	0
57	MG	2A	3096	1/1	0.90	0.20	69,69,69,69	0
57	MG	1A	3377	1/1	0.90	0.11	55,55,55,55	0
57	MG	2a	3123	1/1	0.90	0.19	61,61,61,61	0
57	MG	2a	3125	1/1	0.90	0.20	66,66,66,66	0
57	MG	2A	3517	1/1	0.90	0.10	42,42,42,42	0
57	MG	1A	3974	1/1	0.90	0.08	66,66,66,66	0
57	MG	10	102	1/1	0.90	0.18	46,46,46,46	0
57	MG	2A	3800	1/1	0.90	0.09	63,63,63,63	0
57	MG	10	104	1/1	0.90	0.14	62,62,62,62	0
57	MG	2a	3141	1/1	0.90	0.08	53,53,53,53	0
57	MG	2A	3805	1/1	0.90	0.09	64,64,64,64	0
57	MG	2A	3548	1/1	0.90	0.14	45,45,45,45	0
57	MG	2a	3154	1/1	0.90	0.09	67,67,67,67	0
57	MG	2A	3810	1/1	0.90	0.13	42,42,42,42	0
57	MG	1a	1759	1/1	0.90	0.17	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3256	1/1	0.90	0.12	63,63,63,63	0
57	MG	11	103	1/1	0.90	0.07	69,69,69,69	0
57	MG	2A	3819	1/1	0.90	0.14	55,55,55,55	0
57	MG	2A	3824	1/1	0.90	0.12	60,60,60,60	0
57	MG	2A	3826	1/1	0.90	0.11	57,57,57,57	0
57	MG	2A	3828	1/1	0.90	0.08	43,43,43,43	0
57	MG	12	101	1/1	0.90	0.12	55,55,55,55	0
57	MG	1A	3445	1/1	0.90	0.13	62,62,62,62	0
57	MG	2A	3315	1/1	0.90	0.15	58,58,58,58	0
57	MG	17	104	1/1	0.90	0.13	51,51,51,51	0
57	MG	18	101	1/1	0.90	0.10	48,48,48,48	0
57	MG	1A	3244	1/1	0.90	0.14	55,55,55,55	0
57	MG	1A	3682	1/1	0.90	0.10	32,32,32,32	0
57	MG	1A	3501	1/1	0.90	0.14	51,51,51,51	0
57	MG	1A	3753	1/1	0.90	0.13	46,46,46,46	0
57	MG	1A	3689	1/1	0.90	0.10	34,34,34,34	0
57	MG	2A	3581	1/1	0.90	0.15	57,57,57,57	0
57	MG	1A	3991	1/1	0.90	0.12	55,55,55,55	0
57	MG	1A	3301	1/1	0.90	0.30	53,53,53,53	0
57	MG	1a	1806	1/1	0.90	0.10	60,60,60,60	0
57	MG	2A	3336	1/1	0.90	0.08	59,59,59,59	0
57	MG	2A	3180	1/1	0.90	0.17	59,59,59,59	0
57	MG	2a	3193	1/1	0.90	0.12	67,67,67,67	0
57	MG	1A	3695	1/1	0.90	0.08	24,24,24,24	0
57	MG	1A	3883	1/1	0.90	0.11	25,25,25,25	0
57	MG	2A	3188	1/1	0.90	0.26	60,60,60,60	0
57	MG	1A	3395	1/1	0.90	0.15	46,46,46,46	0
57	MG	1b	301	1/1	0.90	0.12	64,64,64,64	0
57	MG	1e	201	1/1	0.90	0.11	67,67,67,67	0
57	MG	1B	202	1/1	0.90	0.29	60,60,60,60	0
57	MG	2B	210	1/1	0.90	0.08	70,70,70,70	0
57	MG	2A	3618	1/1	0.90	0.26	65,65,65,65	0
57	MG	2A	3619	1/1	0.90	0.15	41,41,41,41	0
57	MG	1a	1644	1/1	0.90	0.14	60,60,60,60	0
57	MG	2a	3214	1/1	0.90	0.21	60,60,60,60	0
57	MG	1l	201	1/1	0.90	0.08	61,61,61,61	0
57	MG	2E	306	1/1	0.90	0.14	56,56,56,56	0
57	MG	1a	1650	1/1	0.90	0.26	62,62,62,62	0
57	MG	2a	3220	1/1	0.90	0.10	72,72,72,72	0
57	MG	2R	202	1/1	0.90	0.12	56,56,56,56	0
57	MG	1a	1652	1/1	0.90	0.18	45,45,45,45	0
57	MG	2U	201	1/1	0.90	0.22	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3773	1/1	0.90	0.12	32,32,32,32	0
57	MG	2A	3211	1/1	0.90	0.18	61,61,61,61	0
57	MG	2a	3227	1/1	0.90	0.20	61,61,61,61	0
57	MG	1t	201	1/1	0.90	0.15	56,56,56,56	0
57	MG	2a	3235	1/1	0.90	0.09	80,80,80,80	0
57	MG	1A	3452	1/1	0.90	0.10	44,44,44,44	0
57	MG	21	102	1/1	0.90	0.36	51,51,51,51	0
57	MG	1A	3785	1/1	0.90	0.13	55,55,55,55	0
57	MG	1A	3453	1/1	0.90	0.18	56,56,56,56	0
57	MG	1A	3791	1/1	0.90	0.10	38,38,38,38	0
57	MG	26	101	1/1	0.90	0.11	57,57,57,57	0
57	MG	2A	3226	1/1	0.90	0.17	55,55,55,55	0
57	MG	2A	3370	1/1	0.90	0.29	62,62,62,62	0
57	MG	1x	101	1/1	0.90	0.29	62,62,62,62	0
57	MG	2A	3372	1/1	0.90	0.16	63,63,63,63	0
57	MG	1A	3098	1/1	0.90	0.13	63,63,63,63	0
57	MG	2A	3239	1/1	0.90	0.17	63,63,63,63	0
57	MG	1x	104	1/1	0.90	0.17	62,62,62,62	0
57	MG	2A	3243	1/1	0.90	0.20	61,61,61,61	0
57	MG	1x	105	1/1	0.90	0.21	56,56,56,56	0
57	MG	2A	3668	1/1	0.90	0.12	61,61,61,61	0
57	MG	1A	3348	1/1	0.90	0.17	61,61,61,61	0
57	MG	2A	3384	1/1	0.90	0.16	59,59,59,59	0
57	MG	2A	3671	1/1	0.90	0.13	64,64,64,64	0
59	A1AE0	1A	4110	72/72	0.90	0.14	14,30,64,67	0
57	MG	1A	3467	1/1	0.91	0.14	49,49,49,49	0
57	MG	2A	3609	1/1	0.91	0.15	48,48,48,48	0
57	MG	2A	3611	1/1	0.91	0.11	39,39,39,39	0
57	MG	1A	4000	1/1	0.91	0.17	43,43,43,43	0
57	MG	2A	3102	1/1	0.91	0.09	52,52,52,52	0
57	MG	1A	3853	1/1	0.91	0.09	45,45,45,45	0
57	MG	1E	309	1/1	0.91	0.09	26,26,26,26	0
57	MG	1A	4005	1/1	0.91	0.08	24,24,24,24	0
57	MG	29	101	1/1	0.91	0.24	68,68,68,68	0
57	MG	1A	4007	1/1	0.91	0.08	40,40,40,40	0
57	MG	2A	3114	1/1	0.91	0.17	58,58,58,58	0
57	MG	1A	3470	1/1	0.91	0.18	39,39,39,39	0
57	MG	1F	311	1/1	0.91	0.25	37,37,37,37	0
57	MG	2A	3121	1/1	0.91	0.08	56,56,56,56	0
57	MG	1F	312	1/1	0.91	0.11	45,45,45,45	0
57	MG	2A	3132	1/1	0.91	0.14	50,50,50,50	0
57	MG	1a	1751	1/1	0.91	0.14	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3636	1/1	0.91	0.12	52,52,52,52	0
57	MG	1A	4010	1/1	0.91	0.12	45,45,45,45	0
57	MG	2A	3146	1/1	0.91	0.20	48,48,48,48	0
57	MG	1A	3231	1/1	0.91	0.10	64,64,64,64	0
57	MG	1A	3859	1/1	0.91	0.10	45,45,45,45	0
57	MG	1A	4018	1/1	0.91	0.10	47,47,47,47	0
57	MG	1a	1767	1/1	0.91	0.10	66,66,66,66	0
57	MG	2a	3022	1/1	0.91	0.30	68,68,68,68	0
57	MG	1A	3729	1/1	0.91	0.08	53,53,53,53	0
57	MG	2a	3024	1/1	0.91	0.12	58,58,58,58	0
57	MG	2a	3025	1/1	0.91	0.18	58,58,58,58	0
57	MG	2A	3654	1/1	0.91	0.15	44,44,44,44	0
57	MG	1A	3863	1/1	0.91	0.18	36,36,36,36	0
57	MG	2A	3658	1/1	0.91	0.12	53,53,53,53	0
57	MG	2A	3659	1/1	0.91	0.11	50,50,50,50	0
57	MG	2a	3031	1/1	0.91	0.22	59,59,59,59	0
57	MG	1A	3306	1/1	0.91	0.20	55,55,55,55	0
57	MG	2A	3176	1/1	0.91	0.13	56,56,56,56	0
57	MG	1a	1780	1/1	0.91	0.11	76,76,76,76	0
57	MG	1A	3316	1/1	0.91	0.10	50,50,50,50	0
57	MG	2A	3362	1/1	0.91	0.09	64,64,64,64	0
57	MG	2A	3184	1/1	0.91	0.11	59,59,59,59	0
57	MG	2A	3186	1/1	0.91	0.18	65,65,65,65	0
57	MG	2a	3039	1/1	0.91	0.12	64,64,64,64	0
57	MG	1Z	301	1/1	0.91	0.14	55,55,55,55	0
57	MG	2A	3369	1/1	0.91	0.17	52,52,52,52	0
57	MG	1A	4030	1/1	0.91	0.13	55,55,55,55	0
57	MG	2A	3675	1/1	0.91	0.17	66,66,66,66	0
57	MG	1A	3243	1/1	0.91	0.14	53,53,53,53	0
57	MG	1A	3125	1/1	0.91	0.11	42,42,42,42	0
57	MG	1A	3179	1/1	0.91	0.16	55,55,55,55	0
57	MG	1a	1803	1/1	0.91	0.19	51,51,51,51	0
57	MG	11	102	1/1	0.91	0.09	46,46,46,46	0
57	MG	1A	3880	1/1	0.91	0.09	36,36,36,36	0
57	MG	2A	3198	1/1	0.91	0.11	53,53,53,53	0
57	MG	1A	3336	1/1	0.91	0.16	59,59,59,59	0
57	MG	2a	3064	1/1	0.91	0.20	58,58,58,58	0
57	MG	1A	3407	1/1	0.91	0.11	62,62,62,62	0
57	MG	1a	1814	1/1	0.91	0.08	61,61,61,61	0
57	MG	2a	3070	1/1	0.91	0.09	66,66,66,66	0
57	MG	2A	3691	1/1	0.91	0.10	42,42,42,42	0
57	MG	2A	3696	1/1	0.91	0.11	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3207	1/1	0.91	0.23	61,61,61,61	0
57	MG	2A	3210	1/1	0.91	0.15	58,58,58,58	0
57	MG	2A	3396	1/1	0.91	0.22	56,56,56,56	0
57	MG	2A	3398	1/1	0.91	0.15	62,62,62,62	0
57	MG	2a	3086	1/1	0.91	0.30	63,63,63,63	0
57	MG	15	3205	1/1	0.91	0.14	33,33,33,33	0
57	MG	2A	3214	1/1	0.91	0.13	60,60,60,60	0
57	MG	2A	3705	1/1	0.91	0.12	40,40,40,40	0
57	MG	2A	3706	1/1	0.91	0.11	57,57,57,57	0
57	MG	1A	3886	1/1	0.91	0.07	30,30,30,30	0
57	MG	2A	3218	1/1	0.91	0.29	59,59,59,59	0
57	MG	2A	3410	1/1	0.91	0.19	53,53,53,53	0
57	MG	1d	301	1/1	0.91	0.38	64,64,64,64	0
57	MG	1A	3411	1/1	0.91	0.12	53,53,53,53	0
57	MG	2A	3720	1/1	0.91	0.10	35,35,35,35	0
57	MG	2A	3722	1/1	0.91	0.18	39,39,39,39	0
57	MG	2A	3413	1/1	0.91	0.19	55,55,55,55	0
57	MG	18	102	1/1	0.91	0.10	34,34,34,34	0
57	MG	1A	3415	1/1	0.91	0.24	55,55,55,55	0
57	MG	2A	3729	1/1	0.91	0.14	52,52,52,52	0
57	MG	1A	3145	1/1	0.91	0.24	32,32,32,32	0
57	MG	1A	3508	1/1	0.91	0.25	44,44,44,44	0
57	MG	2A	3421	1/1	0.91	0.28	56,56,56,56	0
57	MG	2A	3738	1/1	0.91	0.09	63,63,63,63	0
57	MG	2A	3423	1/1	0.91	0.14	53,53,53,53	0
57	MG	1A	3904	1/1	0.91	0.11	29,29,29,29	0
57	MG	2A	3427	1/1	0.91	0.21	61,61,61,61	0
57	MG	1a	1605	1/1	0.91	0.10	58,58,58,58	0
57	MG	2A	3440	1/1	0.91	0.16	56,56,56,56	0
57	MG	2A	3758	1/1	0.91	0.12	64,64,64,64	0
57	MG	1A	3657	1/1	0.91	0.11	50,50,50,50	0
57	MG	1A	3765	1/1	0.91	0.09	50,50,50,50	0
57	MG	2A	3446	1/1	0.91	0.21	59,59,59,59	0
57	MG	1a	1622	1/1	0.91	0.16	55,55,55,55	0
57	MG	2A	3767	1/1	0.91	0.10	63,63,63,63	0
57	MG	2A	3450	1/1	0.91	0.08	53,53,53,53	0
57	MG	1w	106	1/1	0.91	0.20	65,65,65,65	0
57	MG	1A	3342	1/1	0.91	0.23	62,62,62,62	0
57	MG	1a	1628	1/1	0.91	0.25	54,54,54,54	0
57	MG	2A	3467	1/1	0.91	0.11	47,47,47,47	0
57	MG	1A	4073	1/1	0.91	0.11	55,55,55,55	0
57	MG	2A	3249	1/1	0.91	0.10	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3475	1/1	0.91	0.10	48,48,48,48	0
57	MG	2A	3477	1/1	0.91	0.08	45,45,45,45	0
57	MG	1A	3910	1/1	0.91	0.12	34,34,34,34	0
57	MG	2A	3794	1/1	0.91	0.08	52,52,52,52	0
57	MG	1A	3663	1/1	0.91	0.09	31,31,31,31	0
57	MG	1A	3182	1/1	0.91	0.08	31,31,31,31	0
57	MG	2a	3172	1/1	0.91	0.10	66,66,66,66	0
57	MG	1A	3260	1/1	0.91	0.06	45,45,45,45	0
57	MG	2A	3804	1/1	0.91	0.10	56,56,56,56	0
57	MG	1A	3521	1/1	0.91	0.09	44,44,44,44	0
57	MG	1A	3439	1/1	0.91	0.13	42,42,42,42	0
57	MG	1A	3443	1/1	0.91	0.15	52,52,52,52	0
57	MG	1A	3534	1/1	0.91	0.17	52,52,52,52	0
57	MG	1A	4096	1/1	0.91	0.14	55,55,55,55	0
57	MG	1A	3683	1/1	0.91	0.12	19,19,19,19	0
57	MG	1A	3947	1/1	0.91	0.11	57,57,57,57	0
57	MG	2A	3822	1/1	0.91	0.09	56,56,56,56	0
57	MG	1a	1666	1/1	0.91	0.22	60,60,60,60	0
57	MG	1A	3263	1/1	0.91	0.15	48,48,48,48	0
57	MG	2A	3033	1/1	0.91	0.16	52,52,52,52	0
57	MG	2A	3507	1/1	0.91	0.10	53,53,53,53	0
57	MG	2A	3510	1/1	0.91	0.10	44,44,44,44	0
57	MG	2A	3276	1/1	0.91	0.09	51,51,51,51	0
57	MG	1A	3537	1/1	0.91	0.10	52,52,52,52	0
57	MG	2A	3838	1/1	0.91	0.10	57,57,57,57	0
57	MG	2A	3516	1/1	0.91	0.10	51,51,51,51	0
57	MG	2a	3205	1/1	0.91	0.11	69,69,69,69	0
57	MG	1A	3954	1/1	0.91	0.11	45,45,45,45	0
57	MG	1A	3819	1/1	0.91	0.07	41,41,41,41	0
57	MG	2A	3050	1/1	0.91	0.21	64,64,64,64	0
57	MG	2A	3052	1/1	0.91	0.23	63,63,63,63	0
57	MG	1A	4108	1/1	0.91	0.26	59,59,59,59	0
57	MG	2a	3213	1/1	0.91	0.25	59,59,59,59	0
57	MG	1A	3185	1/1	0.91	0.11	40,40,40,40	0
57	MG	2A	3850	1/1	0.91	0.12	54,54,54,54	0
57	MG	1A	3821	1/1	0.91	0.14	48,48,48,48	0
57	MG	1A	3189	1/1	0.91	0.10	47,47,47,47	0
57	MG	1A	3019	1/1	0.91	0.16	49,49,49,49	0
57	MG	2A	3565	1/1	0.91	0.10	63,63,63,63	0
57	MG	2A	3568	1/1	0.91	0.15	57,57,57,57	0
57	MG	2A	3859	1/1	0.91	0.15	79,79,79,79	0
57	MG	1a	1684	1/1	0.91	0.31	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3363	1/1	0.91	0.16	51,51,51,51	0
57	MG	1A	3214	1/1	0.91	0.09	48,48,48,48	0
57	MG	1a	1688	1/1	0.91	0.36	62,62,62,62	0
57	MG	2a	3229	1/1	0.91	0.23	65,65,65,65	0
57	MG	1a	1689	1/1	0.91	0.19	58,58,58,58	0
57	MG	2A	3298	1/1	0.91	0.14	49,49,49,49	0
57	MG	2g	201	1/1	0.91	0.20	69,69,69,69	0
57	MG	2A	3078	1/1	0.91	0.21	60,60,60,60	0
57	MG	2A	3079	1/1	0.91	0.12	49,49,49,49	0
57	MG	1A	3365	1/1	0.91	0.12	54,54,54,54	0
57	MG	1A	3582	1/1	0.91	0.15	60,60,60,60	0
57	MG	2B	214	1/1	0.91	0.08	63,63,63,63	0
57	MG	2A	3306	1/1	0.91	0.11	64,64,64,64	0
57	MG	2D	305	1/1	0.91	0.24	55,55,55,55	0
57	MG	1A	3831	1/1	0.91	0.09	42,42,42,42	0
57	MG	1A	3220	1/1	0.91	0.14	39,39,39,39	0
57	MG	2F	308	1/1	0.91	0.20	62,62,62,62	0
57	MG	2P	201	1/1	0.91	0.18	48,48,48,48	0
57	MG	1A	3221	1/1	0.91	0.14	43,43,43,43	0
57	MG	2A	3587	1/1	0.91	0.07	41,41,41,41	0
57	MG	1A	3846	1/1	0.91	0.10	61,61,61,61	0
57	MG	2T	202	1/1	0.91	0.14	66,66,66,66	0
57	MG	1A	3847	1/1	0.91	0.08	59,59,59,59	0
57	MG	1A	3082	1/1	0.91	0.09	35,35,35,35	0
57	MG	2y	103	1/1	0.91	0.11	84,84,84,84	0
57	MG	2V	201	1/1	0.91	0.20	42,42,42,42	0
57	MG	2A	3598	1/1	0.91	0.15	37,37,37,37	0
57	MG	2A	3292	1/1	0.92	0.19	65,65,65,65	0
57	MG	2E	303	1/1	0.92	0.13	53,53,53,53	0
57	MG	2A	3293	1/1	0.92	0.25	61,61,61,61	0
57	MG	2F	302	1/1	0.92	0.09	64,64,64,64	0
57	MG	2F	305	1/1	0.92	0.12	53,53,53,53	0
57	MG	1a	1660	1/1	0.92	0.10	54,54,54,54	0
57	MG	2G	201	1/1	0.92	0.18	68,68,68,68	0
57	MG	1a	1662	1/1	0.92	0.15	57,57,57,57	0
57	MG	1A	3916	1/1	0.92	0.09	54,54,54,54	0
57	MG	2A	3297	1/1	0.92	0.13	55,55,55,55	0
57	MG	2A	3055	1/1	0.92	0.13	46,46,46,46	0
57	MG	1A	4086	1/1	0.92	0.09	35,35,35,35	0
57	MG	1A	3358	1/1	0.92	0.14	51,51,51,51	0
57	MG	1A	3503	1/1	0.92	0.14	58,58,58,58	0
57	MG	1A	3932	1/1	0.92	0.11	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1669	1/1	0.92	0.33	64,64,64,64	0
57	MG	1A	3168	1/1	0.92	0.12	54,54,54,54	0
57	MG	2A	3308	1/1	0.92	0.17	56,56,56,56	0
57	MG	1A	3319	1/1	0.92	0.13	54,54,54,54	0
57	MG	1A	3643	1/1	0.92	0.14	60,60,60,60	0
57	MG	2A	3314	1/1	0.92	0.14	55,55,55,55	0
57	MG	25	103	1/1	0.92	0.12	63,63,63,63	0
57	MG	25	106	1/1	0.92	0.10	52,52,52,52	0
57	MG	1A	3511	1/1	0.92	0.11	54,54,54,54	0
57	MG	2A	3316	1/1	0.92	0.12	69,69,69,69	0
57	MG	1A	3654	1/1	0.92	0.07	27,27,27,27	0
57	MG	28	103	1/1	0.92	0.21	46,46,46,46	0
57	MG	1A	4106	1/1	0.92	0.13	49,49,49,49	0
57	MG	1A	3945	1/1	0.92	0.09	53,53,53,53	0
57	MG	2a	3003	1/1	0.92	0.09	71,71,71,71	0
57	MG	2A	3620	1/1	0.92	0.11	47,47,47,47	0
57	MG	1A	3656	1/1	0.92	0.09	54,54,54,54	0
57	MG	1A	3431	1/1	0.92	0.11	61,61,61,61	0
57	MG	1A	3950	1/1	0.92	0.07	42,42,42,42	0
57	MG	1A	3001	1/1	0.92	0.11	38,38,38,38	0
57	MG	1A	3442	1/1	0.92	0.16	69,69,69,69	0
57	MG	1A	3671	1/1	0.92	0.07	25,25,25,25	0
57	MG	2A	3332	1/1	0.92	0.13	62,62,62,62	0
57	MG	2A	3635	1/1	0.92	0.07	31,31,31,31	0
57	MG	1A	3957	1/1	0.92	0.13	53,53,53,53	0
57	MG	1a	1693	1/1	0.92	0.09	47,47,47,47	0
57	MG	1a	1695	1/1	0.92	0.23	60,60,60,60	0
57	MG	2A	3103	1/1	0.92	0.20	51,51,51,51	0
57	MG	1A	3964	1/1	0.92	0.11	51,51,51,51	0
57	MG	2A	3106	1/1	0.92	0.24	57,57,57,57	0
57	MG	1A	3818	1/1	0.92	0.08	28,28,28,28	0
57	MG	2A	3342	1/1	0.92	0.40	66,66,66,66	0
57	MG	1A	3323	1/1	0.92	0.13	49,49,49,49	0
57	MG	1a	1709	1/1	0.92	0.08	55,55,55,55	0
57	MG	2A	3656	1/1	0.92	0.09	67,67,67,67	0
57	MG	1a	1711	1/1	0.92	0.24	64,64,64,64	0
57	MG	1a	1714	1/1	0.92	0.22	54,54,54,54	0
57	MG	1A	3368	1/1	0.92	0.11	48,48,48,48	0
57	MG	1A	3372	1/1	0.92	0.12	48,48,48,48	0
57	MG	2A	3124	1/1	0.92	0.14	58,58,58,58	0
57	MG	1A	3529	1/1	0.92	0.17	48,48,48,48	0
57	MG	1a	1724	1/1	0.92	0.08	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3531	1/1	0.92	0.13	36,36,36,36	0
57	MG	2A	3137	1/1	0.92	0.18	57,57,57,57	0
57	MG	1A	3264	1/1	0.92	0.18	64,64,64,64	0
57	MG	2A	3142	1/1	0.92	0.13	51,51,51,51	0
57	MG	2a	3040	1/1	0.92	0.28	71,71,71,71	0
57	MG	2A	3143	1/1	0.92	0.24	62,62,62,62	0
57	MG	1A	3378	1/1	0.92	0.39	49,49,49,49	0
57	MG	1A	3685	1/1	0.92	0.09	29,29,29,29	0
57	MG	1a	1736	1/1	0.92	0.24	65,65,65,65	0
57	MG	2A	3679	1/1	0.92	0.13	59,59,59,59	0
57	MG	1A	3536	1/1	0.92	0.12	51,51,51,51	0
57	MG	2A	3682	1/1	0.92	0.08	38,38,38,38	0
57	MG	2a	3049	1/1	0.92	0.12	64,64,64,64	0
57	MG	2a	3050	1/1	0.92	0.09	61,61,61,61	0
57	MG	2A	3160	1/1	0.92	0.21	68,68,68,68	0
57	MG	2A	3164	1/1	0.92	0.08	62,62,62,62	0
57	MG	1A	3077	1/1	0.92	0.25	42,42,42,42	0
57	MG	1A	3987	1/1	0.92	0.10	56,56,56,56	0
57	MG	2A	3376	1/1	0.92	0.14	60,60,60,60	0
57	MG	1a	1745	1/1	0.92	0.11	48,48,48,48	0
57	MG	2A	3378	1/1	0.92	0.11	63,63,63,63	0
57	MG	1A	3834	1/1	0.92	0.22	55,55,55,55	0
57	MG	2A	3695	1/1	0.92	0.10	56,56,56,56	0
57	MG	1A	3538	1/1	0.92	0.07	53,53,53,53	0
57	MG	2a	3073	1/1	0.92	0.26	63,63,63,63	0
57	MG	1A	3693	1/1	0.92	0.17	54,54,54,54	0
57	MG	1A	3844	1/1	0.92	0.09	20,20,20,20	0
57	MG	2A	3391	1/1	0.92	0.23	54,54,54,54	0
57	MG	1a	1760	1/1	0.92	0.08	55,55,55,55	0
57	MG	2A	3185	1/1	0.92	0.24	63,63,63,63	0
57	MG	1A	3334	1/1	0.92	0.14	42,42,42,42	0
57	MG	1A	3547	1/1	0.92	0.30	49,49,49,49	0
57	MG	1A	3392	1/1	0.92	0.10	34,34,34,34	0
57	MG	1A	3703	1/1	0.92	0.10	52,52,52,52	0
57	MG	2A	3710	1/1	0.92	0.13	58,58,58,58	0
57	MG	1a	1768	1/1	0.92	0.10	38,38,38,38	0
57	MG	1A	3457	1/1	0.92	0.13	68,68,68,68	0
57	MG	2A	3715	1/1	0.92	0.11	76,76,76,76	0
57	MG	1A	3285	1/1	0.92	0.12	53,53,53,53	0
57	MG	2A	3407	1/1	0.92	0.30	57,57,57,57	0
57	MG	2A	3718	1/1	0.92	0.14	54,54,54,54	0
57	MG	2a	3100	1/1	0.92	0.19	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1S	202	1/1	0.92	0.10	47,47,47,47	0
57	MG	2A	3721	1/1	0.92	0.11	54,54,54,54	0
57	MG	1A	3554	1/1	0.92	0.11	41,41,41,41	0
57	MG	1V	202	1/1	0.92	0.25	41,41,41,41	0
57	MG	2a	3109	1/1	0.92	0.15	65,65,65,65	0
57	MG	1V	207	1/1	0.92	0.11	55,55,55,55	0
57	MG	2A	3202	1/1	0.92	0.11	54,54,54,54	0
57	MG	2A	3203	1/1	0.92	0.07	49,49,49,49	0
57	MG	1A	3002	1/1	0.92	0.10	50,50,50,50	0
57	MG	2A	3731	1/1	0.92	0.13	61,61,61,61	0
57	MG	2a	3120	1/1	0.92	0.27	66,66,66,66	0
57	MG	2a	3121	1/1	0.92	0.23	58,58,58,58	0
57	MG	1A	4013	1/1	0.92	0.09	64,64,64,64	0
57	MG	1A	3569	1/1	0.92	0.09	31,31,31,31	0
57	MG	1A	3861	1/1	0.92	0.13	40,40,40,40	0
57	MG	1A	3862	1/1	0.92	0.21	37,37,37,37	0
57	MG	1a	1804	1/1	0.92	0.18	56,56,56,56	0
57	MG	1A	3398	1/1	0.92	0.21	49,49,49,49	0
57	MG	2A	3437	1/1	0.92	0.12	56,56,56,56	0
57	MG	1A	3581	1/1	0.92	0.09	44,44,44,44	0
57	MG	1A	3217	1/1	0.92	0.11	45,45,45,45	0
57	MG	2A	3220	1/1	0.92	0.09	57,57,57,57	0
57	MG	1A	3869	1/1	0.92	0.09	33,33,33,33	0
57	MG	2a	3152	1/1	0.92	0.08	68,68,68,68	0
57	MG	2A	3762	1/1	0.92	0.12	42,42,42,42	0
57	MG	1A	3468	1/1	0.92	0.50	51,51,51,51	0
57	MG	2A	3448	1/1	0.92	0.10	45,45,45,45	0
57	MG	2A	3765	1/1	0.92	0.10	58,58,58,58	0
57	MG	2A	3766	1/1	0.92	0.12	68,68,68,68	0
57	MG	14	101	1/1	0.92	0.14	70,70,70,70	0
57	MG	2A	3451	1/1	0.92	0.06	33,33,33,33	0
57	MG	2a	3164	1/1	0.92	0.19	58,58,58,58	0
57	MG	1A	3873	1/1	0.92	0.11	34,34,34,34	0
57	MG	2A	3453	1/1	0.92	0.25	65,65,65,65	0
57	MG	15	3207	1/1	0.92	0.12	36,36,36,36	0
57	MG	2A	3236	1/1	0.92	0.14	58,58,58,58	0
57	MG	2A	3458	1/1	0.92	0.10	53,53,53,53	0
57	MG	2A	3462	1/1	0.92	0.09	48,48,48,48	0
57	MG	2A	3464	1/1	0.92	0.10	54,54,54,54	0
57	MG	1A	3875	1/1	0.92	0.08	31,31,31,31	0
57	MG	2A	3785	1/1	0.92	0.14	50,50,50,50	0
57	MG	2a	3181	1/1	0.92	0.12	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3788	1/1	0.92	0.08	48,48,48,48	0
57	MG	1A	4036	1/1	0.92	0.12	30,30,30,30	0
57	MG	1A	4037	1/1	0.92	0.10	23,23,23,23	0
57	MG	1A	3586	1/1	0.92	0.27	66,66,66,66	0
57	MG	19	101	1/1	0.92	0.19	49,49,49,49	0
57	MG	1A	3247	1/1	0.92	0.13	54,54,54,54	0
57	MG	2A	3803	1/1	0.92	0.17	63,63,63,63	0
57	MG	1A	3879	1/1	0.92	0.13	25,25,25,25	0
57	MG	1A	3250	1/1	0.92	0.09	20,20,20,20	0
57	MG	1A	3738	1/1	0.92	0.06	17,17,17,17	0
57	MG	1w	102	1/1	0.92	0.13	75,75,75,75	0
57	MG	1w	104	1/1	0.92	0.20	51,51,51,51	0
57	MG	2A	3251	1/1	0.92	0.12	61,61,61,61	0
57	MG	2A	3816	1/1	0.92	0.09	34,34,34,34	0
57	MG	1a	1607	1/1	0.92	0.10	54,54,54,54	0
57	MG	1a	1608	1/1	0.92	0.09	51,51,51,51	0
57	MG	1A	3148	1/1	0.92	0.10	41,41,41,41	0
57	MG	1a	1614	1/1	0.92	0.09	51,51,51,51	0
57	MG	1A	3885	1/1	0.92	0.12	23,23,23,23	0
57	MG	1a	1619	1/1	0.92	0.17	49,49,49,49	0
57	MG	2A	3503	1/1	0.92	0.07	33,33,33,33	0
57	MG	2A	3830	1/1	0.92	0.12	60,60,60,60	0
57	MG	2A	3831	1/1	0.92	0.21	46,46,46,46	0
57	MG	2A	3505	1/1	0.92	0.18	58,58,58,58	0
57	MG	2A	3833	1/1	0.92	0.14	48,48,48,48	0
57	MG	1A	3405	1/1	0.92	0.24	58,58,58,58	0
57	MG	2A	3265	1/1	0.92	0.14	57,57,57,57	0
57	MG	1A	3477	1/1	0.92	0.09	48,48,48,48	0
57	MG	2a	3218	1/1	0.92	0.12	54,54,54,54	0
57	MG	1a	1625	1/1	0.92	0.29	61,61,61,61	0
57	MG	1A	3040	1/1	0.92	0.22	59,59,59,59	0
57	MG	2A	3515	1/1	0.92	0.10	39,39,39,39	0
57	MG	2A	3843	1/1	0.92	0.16	64,64,64,64	0
57	MG	2A	3271	1/1	0.92	0.17	54,54,54,54	0
57	MG	1x	111	1/1	0.92	0.19	67,67,67,67	0
57	MG	1A	4067	1/1	0.92	0.10	49,49,49,49	0
57	MG	2A	3528	1/1	0.92	0.08	51,51,51,51	0
57	MG	2A	3530	1/1	0.92	0.12	42,42,42,42	0
57	MG	2a	3234	1/1	0.92	0.13	64,64,64,64	0
57	MG	2A	3537	1/1	0.92	0.10	31,31,31,31	0
57	MG	2A	3539	1/1	0.92	0.08	32,32,32,32	0
57	MG	2A	3542	1/1	0.92	0.08	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1635	1/1	0.92	0.16	66,66,66,66	0
57	MG	1A	3894	1/1	0.92	0.09	56,56,56,56	0
57	MG	1A	3408	1/1	0.92	0.07	42,42,42,42	0
57	MG	2q	201	1/1	0.92	0.09	72,72,72,72	0
57	MG	2q	202	1/1	0.92	0.12	67,67,67,67	0
57	MG	1A	3257	1/1	0.92	0.17	62,62,62,62	0
57	MG	2A	3280	1/1	0.92	0.09	56,56,56,56	0
57	MG	2A	3558	1/1	0.92	0.13	66,66,66,66	0
57	MG	1A	3258	1/1	0.92	0.11	54,54,54,54	0
57	MG	2B	202	1/1	0.92	0.13	59,59,59,59	0
57	MG	1a	1646	1/1	0.92	0.22	61,61,61,61	0
57	MG	1A	3755	1/1	0.92	0.11	20,20,20,20	0
57	MG	1A	3630	1/1	0.92	0.11	47,47,47,47	0
57	MG	2B	209	1/1	0.92	0.16	53,53,53,53	0
57	MG	1A	3419	1/1	0.92	0.09	51,51,51,51	0
57	MG	1a	1655	1/1	0.92	0.10	55,55,55,55	0
57	MG	2A	3039	1/1	0.92	0.16	67,67,67,67	0
57	MG	1A	4082	1/1	0.92	0.18	58,58,58,58	0
57	MG	2A	3049	1/1	0.92	0.10	62,62,62,62	0
57	MG	2B	218	1/1	0.92	0.10	55,55,55,55	0
57	MG	2B	219	1/1	0.92	0.24	65,65,65,65	0
57	MG	1A	3353	1/1	0.92	0.10	52,52,52,52	0
59	A1AE0	2A	3863	72/72	0.92	0.15	32,46,68,77	0
57	MG	1A	3760	1/1	0.93	0.09	23,23,23,23	0
57	MG	1A	3116	1/1	0.93	0.07	33,33,33,33	0
57	MG	2F	303	1/1	0.93	0.17	52,52,52,52	0
57	MG	2A	3305	1/1	0.93	0.09	59,59,59,59	0
57	MG	1a	1661	1/1	0.93	0.14	56,56,56,56	0
57	MG	2A	3588	1/1	0.93	0.11	40,40,40,40	0
57	MG	2O	202	1/1	0.93	0.15	60,60,60,60	0
57	MG	2A	3062	1/1	0.93	0.26	50,50,50,50	0
57	MG	2A	3591	1/1	0.93	0.15	61,61,61,61	0
57	MG	1A	3763	1/1	0.93	0.06	29,29,29,29	0
57	MG	2A	3595	1/1	0.93	0.11	49,49,49,49	0
57	MG	1A	3297	1/1	0.93	0.18	43,43,43,43	0
57	MG	2A	3311	1/1	0.93	0.13	60,60,60,60	0
57	MG	1A	4089	1/1	0.93	0.12	58,58,58,58	0
57	MG	2A	3607	1/1	0.93	0.09	50,50,50,50	0
57	MG	1A	3496	1/1	0.93	0.08	44,44,44,44	0
57	MG	1A	3498	1/1	0.93	0.09	44,44,44,44	0
57	MG	1A	4094	1/1	0.93	0.07	41,41,41,41	0
57	MG	1A	3919	1/1	0.93	0.09	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	21	103	1/1	0.93	0.08	51,51,51,51	0
57	MG	2A	3319	1/1	0.93	0.22	68,68,68,68	0
57	MG	1A	3770	1/1	0.93	0.08	38,38,38,38	0
57	MG	2A	3616	1/1	0.93	0.12	44,44,44,44	0
57	MG	25	105	1/1	0.93	0.10	48,48,48,48	0
57	MG	2A	3617	1/1	0.93	0.13	58,58,58,58	0
57	MG	2A	3083	1/1	0.93	0.10	50,50,50,50	0
57	MG	1A	3199	1/1	0.93	0.06	42,42,42,42	0
57	MG	2A	3323	1/1	0.93	0.11	53,53,53,53	0
57	MG	1A	3302	1/1	0.93	0.09	63,63,63,63	0
57	MG	1A	4102	1/1	0.93	0.08	54,54,54,54	0
57	MG	1A	3248	1/1	0.93	0.07	59,59,59,59	0
57	MG	1A	3366	1/1	0.93	0.14	45,45,45,45	0
57	MG	1A	3507	1/1	0.93	0.25	43,43,43,43	0
57	MG	1A	3941	1/1	0.93	0.07	56,56,56,56	0
57	MG	2a	3006	1/1	0.93	0.08	64,64,64,64	0
57	MG	2A	3633	1/1	0.93	0.10	59,59,59,59	0
57	MG	1A	3204	1/1	0.93	0.17	53,53,53,53	0
57	MG	1A	3793	1/1	0.93	0.06	49,49,49,49	0
57	MG	2a	3010	1/1	0.93	0.22	60,60,60,60	0
57	MG	1A	3440	1/1	0.93	0.16	63,63,63,63	0
57	MG	2A	3637	1/1	0.93	0.09	52,52,52,52	0
57	MG	1A	3639	1/1	0.93	0.07	27,27,27,27	0
57	MG	1a	1690	1/1	0.93	0.22	57,57,57,57	0
57	MG	1A	3512	1/1	0.93	0.13	61,61,61,61	0
57	MG	1A	3806	1/1	0.93	0.14	42,42,42,42	0
57	MG	1A	3513	1/1	0.93	0.11	43,43,43,43	0
57	MG	2A	3344	1/1	0.93	0.18	63,63,63,63	0
57	MG	2A	3345	1/1	0.93	0.13	63,63,63,63	0
57	MG	2A	3111	1/1	0.93	0.25	58,58,58,58	0
57	MG	1A	3811	1/1	0.93	0.09	51,51,51,51	0
57	MG	1a	1699	1/1	0.93	0.29	56,56,56,56	0
57	MG	1A	3647	1/1	0.93	0.07	35,35,35,35	0
57	MG	2A	3350	1/1	0.93	0.07	61,61,61,61	0
57	MG	1B	222	1/1	0.93	0.10	53,53,53,53	0
57	MG	2A	3120	1/1	0.93	0.07	48,48,48,48	0
57	MG	2A	3353	1/1	0.93	0.16	58,58,58,58	0
57	MG	1a	1704	1/1	0.93	0.21	48,48,48,48	0
57	MG	1A	3441	1/1	0.93	0.17	33,33,33,33	0
57	MG	2A	3356	1/1	0.93	0.29	61,61,61,61	0
57	MG	1A	3966	1/1	0.93	0.07	52,52,52,52	0
57	MG	1A	3655	1/1	0.93	0.06	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1B	226	1/1	0.93	0.08	42,42,42,42	0
57	MG	1A	3162	1/1	0.93	0.24	32,32,32,32	0
57	MG	1a	1717	1/1	0.93	0.11	56,56,56,56	0
57	MG	2A	3141	1/1	0.93	0.29	72,72,72,72	0
57	MG	2A	3365	1/1	0.93	0.29	64,64,64,64	0
57	MG	2A	3678	1/1	0.93	0.12	56,56,56,56	0
57	MG	1A	3164	1/1	0.93	0.17	33,33,33,33	0
57	MG	1A	3519	1/1	0.93	0.08	47,47,47,47	0
57	MG	2A	3368	1/1	0.93	0.08	53,53,53,53	0
57	MG	1A	3375	1/1	0.93	0.11	35,35,35,35	0
57	MG	1B	235	1/1	0.93	0.08	42,42,42,42	0
57	MG	2A	3151	1/1	0.93	0.10	49,49,49,49	0
57	MG	1a	1727	1/1	0.93	0.12	54,54,54,54	0
57	MG	1D	309	1/1	0.93	0.12	48,48,48,48	0
57	MG	1A	3118	1/1	0.93	0.15	41,41,41,41	0
57	MG	1A	3527	1/1	0.93	0.14	38,38,38,38	0
57	MG	1A	3978	1/1	0.93	0.15	60,60,60,60	0
57	MG	2a	3055	1/1	0.93	0.11	58,58,58,58	0
57	MG	2A	3167	1/1	0.93	0.13	66,66,66,66	0
57	MG	1A	3322	1/1	0.93	0.08	46,46,46,46	0
57	MG	2a	3061	1/1	0.93	0.14	49,49,49,49	0
57	MG	1A	3119	1/1	0.93	0.11	53,53,53,53	0
57	MG	1E	314	1/1	0.93	0.08	39,39,39,39	0
57	MG	2A	3175	1/1	0.93	0.24	65,65,65,65	0
57	MG	2A	3388	1/1	0.93	0.23	46,46,46,46	0
57	MG	2A	3389	1/1	0.93	0.16	38,38,38,38	0
57	MG	2A	3390	1/1	0.93	0.20	44,44,44,44	0
57	MG	2a	3074	1/1	0.93	0.22	50,50,50,50	0
57	MG	2a	3075	1/1	0.93	0.21	61,61,61,61	0
57	MG	1A	3832	1/1	0.93	0.10	39,39,39,39	0
57	MG	2A	3177	1/1	0.93	0.22	56,56,56,56	0
57	MG	1A	3384	1/1	0.93	0.45	42,42,42,42	0
57	MG	1A	3532	1/1	0.93	0.29	51,51,51,51	0
57	MG	1a	1750	1/1	0.93	0.17	61,61,61,61	0
57	MG	1G	202	1/1	0.93	0.17	59,59,59,59	0
57	MG	1a	1756	1/1	0.93	0.15	51,51,51,51	0
57	MG	1A	3087	1/1	0.93	0.16	45,45,45,45	0
57	MG	1A	3989	1/1	0.93	0.13	38,38,38,38	0
57	MG	2a	3090	1/1	0.93	0.10	57,57,57,57	0
57	MG	1A	3841	1/1	0.93	0.13	51,51,51,51	0
57	MG	2A	3190	1/1	0.93	0.13	59,59,59,59	0
57	MG	2A	3408	1/1	0.93	0.18	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3842	1/1	0.93	0.11	63,63,63,63	0
57	MG	2A	3193	1/1	0.93	0.16	53,53,53,53	0
57	MG	2A	3726	1/1	0.93	0.09	53,53,53,53	0
57	MG	1N	206	1/1	0.93	0.15	44,44,44,44	0
57	MG	1O	201	1/1	0.93	0.12	51,51,51,51	0
57	MG	2A	3414	1/1	0.93	0.12	66,66,66,66	0
57	MG	1A	3993	1/1	0.93	0.07	13,13,13,13	0
57	MG	2a	3103	1/1	0.93	0.17	69,69,69,69	0
57	MG	1a	1769	1/1	0.93	0.08	50,50,50,50	0
57	MG	2A	3733	1/1	0.93	0.10	40,40,40,40	0
57	MG	1A	3997	1/1	0.93	0.07	56,56,56,56	0
57	MG	2A	3735	1/1	0.93	0.16	62,62,62,62	0
57	MG	1R	205	1/1	0.93	0.16	32,32,32,32	0
57	MG	2A	3737	1/1	0.93	0.07	55,55,55,55	0
57	MG	1a	1773	1/1	0.93	0.10	47,47,47,47	0
57	MG	2A	3422	1/1	0.93	0.21	51,51,51,51	0
57	MG	1A	3454	1/1	0.93	0.12	59,59,59,59	0
57	MG	1A	3223	1/1	0.93	0.16	61,61,61,61	0
57	MG	2A	3752	1/1	0.93	0.14	67,67,67,67	0
57	MG	2A	3425	1/1	0.93	0.14	55,55,55,55	0
57	MG	1A	3227	1/1	0.93	0.08	48,48,48,48	0
57	MG	1A	3461	1/1	0.93	0.10	52,52,52,52	0
57	MG	2A	3209	1/1	0.93	0.26	74,74,74,74	0
57	MG	1A	3539	1/1	0.93	0.08	53,53,53,53	0
57	MG	1A	3851	1/1	0.93	0.08	46,46,46,46	0
57	MG	1Z	302	1/1	0.93	0.08	62,62,62,62	0
57	MG	2A	3215	1/1	0.93	0.16	57,57,57,57	0
57	MG	1A	3335	1/1	0.93	0.14	57,57,57,57	0
57	MG	1a	1802	1/1	0.93	0.15	58,58,58,58	0
57	MG	2A	3449	1/1	0.93	0.16	62,62,62,62	0
57	MG	1A	3541	1/1	0.93	0.16	35,35,35,35	0
57	MG	1A	3543	1/1	0.93	0.10	42,42,42,42	0
57	MG	1A	3546	1/1	0.93	0.11	35,35,35,35	0
57	MG	1A	3268	1/1	0.93	0.11	52,52,52,52	0
57	MG	1a	1808	1/1	0.93	0.11	60,60,60,60	0
57	MG	1A	4017	1/1	0.93	0.07	58,58,58,58	0
57	MG	2A	3229	1/1	0.93	0.29	47,47,47,47	0
57	MG	2A	3230	1/1	0.93	0.12	58,58,58,58	0
57	MG	2A	3463	1/1	0.93	0.08	53,53,53,53	0
57	MG	2A	3784	1/1	0.93	0.16	46,46,46,46	0
57	MG	1A	3549	1/1	0.93	0.20	40,40,40,40	0
57	MG	2A	3233	1/1	0.93	0.08	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	13	103	1/1	0.93	0.12	46,46,46,46	0
57	MG	1A	3270	1/1	0.93	0.07	38,38,38,38	0
57	MG	1A	4020	1/1	0.93	0.09	51,51,51,51	0
57	MG	2A	3799	1/1	0.93	0.07	44,44,44,44	0
57	MG	2a	3178	1/1	0.93	0.14	60,60,60,60	0
57	MG	1A	3276	1/1	0.93	0.29	34,34,34,34	0
57	MG	1A	3864	1/1	0.93	0.05	38,38,38,38	0
57	MG	16	102	1/1	0.93	0.10	52,52,52,52	0
57	MG	1A	3006	1/1	0.93	0.12	48,48,48,48	0
57	MG	1A	4028	1/1	0.93	0.06	41,41,41,41	0
57	MG	2A	3482	1/1	0.93	0.10	37,37,37,37	0
57	MG	2A	3809	1/1	0.93	0.08	50,50,50,50	0
57	MG	1A	3866	1/1	0.93	0.19	36,36,36,36	0
57	MG	2a	3188	1/1	0.93	0.23	54,54,54,54	0
57	MG	1A	3469	1/1	0.93	0.13	51,51,51,51	0
57	MG	2A	3813	1/1	0.93	0.06	33,33,33,33	0
57	MG	1A	3140	1/1	0.93	0.09	35,35,35,35	0
57	MG	1A	3560	1/1	0.93	0.14	50,50,50,50	0
57	MG	1A	3562	1/1	0.93	0.22	52,52,52,52	0
57	MG	2a	3195	1/1	0.93	0.11	62,62,62,62	0
57	MG	2A	3252	1/1	0.93	0.09	52,52,52,52	0
57	MG	1w	101	1/1	0.93	0.12	43,43,43,43	0
57	MG	2a	3199	1/1	0.93	0.08	59,59,59,59	0
57	MG	1A	3403	1/1	0.93	0.10	50,50,50,50	0
57	MG	2A	3498	1/1	0.93	0.07	39,39,39,39	0
57	MG	2A	3827	1/1	0.93	0.16	60,60,60,60	0
57	MG	2a	3203	1/1	0.93	0.19	51,51,51,51	0
57	MG	2A	3256	1/1	0.93	0.10	55,55,55,55	0
57	MG	1A	3570	1/1	0.93	0.21	33,33,33,33	0
57	MG	1A	3345	1/1	0.93	0.09	56,56,56,56	0
57	MG	1A	3232	1/1	0.93	0.15	25,25,25,25	0
57	MG	1A	3057	1/1	0.93	0.09	45,45,45,45	0
57	MG	1A	4048	1/1	0.93	0.09	44,44,44,44	0
57	MG	2A	3262	1/1	0.93	0.12	52,52,52,52	0
57	MG	2A	3835	1/1	0.93	0.08	56,56,56,56	0
57	MG	1A	3882	1/1	0.93	0.08	38,38,38,38	0
57	MG	2A	3513	1/1	0.93	0.05	44,44,44,44	0
57	MG	1a	1618	1/1	0.93	0.10	56,56,56,56	0
57	MG	1A	3110	1/1	0.93	0.11	39,39,39,39	0
57	MG	1a	1621	1/1	0.93	0.08	49,49,49,49	0
57	MG	1A	3480	1/1	0.93	0.09	53,53,53,53	0
57	MG	1A	4054	1/1	0.93	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3485	1/1	0.93	0.11	53,53,53,53	0
57	MG	1A	3412	1/1	0.93	0.21	58,58,58,58	0
57	MG	2A	3001	1/1	0.93	0.22	54,54,54,54	0
57	MG	1A	4062	1/1	0.93	0.11	59,59,59,59	0
57	MG	1a	1632	1/1	0.93	0.15	62,62,62,62	0
57	MG	1A	3887	1/1	0.93	0.07	15,15,15,15	0
57	MG	1a	1637	1/1	0.93	0.19	55,55,55,55	0
57	MG	1A	3750	1/1	0.93	0.10	49,49,49,49	0
57	MG	1A	3487	1/1	0.93	0.17	55,55,55,55	0
57	MG	2a	3236	1/1	0.93	0.18	70,70,70,70	0
57	MG	2A	3551	1/1	0.93	0.07	29,29,29,29	0
57	MG	2d	302	1/1	0.93	0.14	66,66,66,66	0
57	MG	2f	202	1/1	0.93	0.15	62,62,62,62	0
57	MG	2A	3554	1/1	0.93	0.17	55,55,55,55	0
57	MG	2A	3029	1/1	0.93	0.21	54,54,54,54	0
57	MG	1a	1640	1/1	0.93	0.17	58,58,58,58	0
57	MG	2A	3561	1/1	0.93	0.07	45,45,45,45	0
57	MG	1A	4069	1/1	0.93	0.10	30,30,30,30	0
57	MG	1A	3598	1/1	0.93	0.10	26,26,26,26	0
57	MG	2A	3037	1/1	0.93	0.23	57,57,57,57	0
57	MG	1a	1645	1/1	0.93	0.27	61,61,61,61	0
57	MG	2B	207	1/1	0.93	0.10	63,63,63,63	0
57	MG	2B	208	1/1	0.93	0.29	61,61,61,61	0
57	MG	1A	3490	1/1	0.93	0.19	46,46,46,46	0
57	MG	2A	3571	1/1	0.93	0.23	72,72,72,72	0
57	MG	2A	3040	1/1	0.93	0.10	60,60,60,60	0
57	MG	2w	104	1/1	0.93	0.23	51,51,51,51	0
57	MG	2w	105	1/1	0.93	0.14	62,62,62,62	0
57	MG	1A	3899	1/1	0.93	0.11	55,55,55,55	0
57	MG	2A	3047	1/1	0.93	0.09	48,48,48,48	0
57	MG	1A	4077	1/1	0.93	0.07	45,45,45,45	0
57	MG	2B	216	1/1	0.93	0.16	60,60,60,60	0
57	MG	2x	105	1/1	0.93	0.17	60,60,60,60	0
57	MG	1a	1653	1/1	0.93	0.25	55,55,55,55	0
57	MG	1A	3245	1/1	0.93	0.21	39,39,39,39	0
57	MG	2D	301	1/1	0.93	0.15	47,47,47,47	0
57	MG	1A	3902	1/1	0.93	0.13	52,52,52,52	0
57	MG	1a	1656	1/1	0.93	0.11	48,48,48,48	0
57	MG	1A	3606	1/1	0.93	0.09	42,42,42,42	0
57	MG	2E	305	1/1	0.93	0.11	33,33,33,33	0
57	MG	1A	4029	1/1	0.94	0.07	46,46,46,46	0
57	MG	2A	3127	1/1	0.94	0.08	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1X	106	1/1	0.94	0.15	46,46,46,46	0
57	MG	2A	3130	1/1	0.94	0.07	42,42,42,42	0
57	MG	1X	108	1/1	0.94	0.13	69,69,69,69	0
57	MG	2T	201	1/1	0.94	0.10	63,63,63,63	0
57	MG	1A	3757	1/1	0.94	0.06	25,25,25,25	0
57	MG	1A	3041	1/1	0.94	0.07	30,30,30,30	0
57	MG	2A	3622	1/1	0.94	0.11	54,54,54,54	0
57	MG	2A	3623	1/1	0.94	0.20	50,50,50,50	0
57	MG	1A	3338	1/1	0.94	0.17	34,34,34,34	0
57	MG	2A	3140	1/1	0.94	0.22	49,49,49,49	0
57	MG	2Y	201	1/1	0.94	0.19	63,63,63,63	0
57	MG	2A	3626	1/1	0.94	0.13	49,49,49,49	0
57	MG	20	102	1/1	0.94	0.15	70,70,70,70	0
57	MG	21	101	1/1	0.94	0.07	59,59,59,59	0
57	MG	1a	1753	1/1	0.94	0.07	58,58,58,58	0
57	MG	1a	1755	1/1	0.94	0.10	53,53,53,53	0
57	MG	1A	3076	1/1	0.94	0.16	45,45,45,45	0
57	MG	2A	3145	1/1	0.94	0.20	52,52,52,52	0
57	MG	1A	4034	1/1	0.94	0.07	35,35,35,35	0
57	MG	1A	3281	1/1	0.94	0.17	40,40,40,40	0
57	MG	1A	3230	1/1	0.94	0.26	48,48,48,48	0
57	MG	2A	3152	1/1	0.94	0.10	35,35,35,35	0
57	MG	2A	3638	1/1	0.94	0.09	56,56,56,56	0
57	MG	10	108	1/1	0.94	0.09	47,47,47,47	0
57	MG	2A	3644	1/1	0.94	0.12	35,35,35,35	0
57	MG	10	109	1/1	0.94	0.08	41,41,41,41	0
57	MG	11	101	1/1	0.94	0.20	33,33,33,33	0
57	MG	2A	3161	1/1	0.94	0.27	61,61,61,61	0
57	MG	2A	3162	1/1	0.94	0.10	40,40,40,40	0
57	MG	1A	3417	1/1	0.94	0.14	37,37,37,37	0
57	MG	2A	3165	1/1	0.94	0.12	64,64,64,64	0
57	MG	1A	3418	1/1	0.94	0.09	43,43,43,43	0
57	MG	1A	3895	1/1	0.94	0.15	56,56,56,56	0
57	MG	1A	3034	1/1	0.94	0.27	34,34,34,34	0
57	MG	2A	3657	1/1	0.94	0.10	47,47,47,47	0
57	MG	2A	3171	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3287	1/1	0.94	0.08	45,45,45,45	0
57	MG	1A	3776	1/1	0.94	0.10	26,26,26,26	0
57	MG	2A	3661	1/1	0.94	0.07	69,69,69,69	0
57	MG	1A	3780	1/1	0.94	0.04	32,32,32,32	0
57	MG	1a	1786	1/1	0.94	0.10	71,71,71,71	0
57	MG	1A	3422	1/1	0.94	0.09	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3097	1/1	0.94	0.11	50,50,50,50	0
57	MG	1A	3642	1/1	0.94	0.07	48,48,48,48	0
57	MG	1a	1795	1/1	0.94	0.09	48,48,48,48	0
57	MG	2A	3379	1/1	0.94	0.07	57,57,57,57	0
57	MG	1A	3240	1/1	0.94	0.09	42,42,42,42	0
57	MG	2A	3673	1/1	0.94	0.07	58,58,58,58	0
57	MG	1A	3128	1/1	0.94	0.09	37,37,37,37	0
57	MG	2A	3382	1/1	0.94	0.13	42,42,42,42	0
57	MG	1A	4064	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	4065	1/1	0.94	0.11	40,40,40,40	0
57	MG	1A	3912	1/1	0.94	0.07	30,30,30,30	0
57	MG	1a	1602	1/1	0.94	0.06	58,58,58,58	0
57	MG	1A	3915	1/1	0.94	0.10	38,38,38,38	0
57	MG	1A	3350	1/1	0.94	0.10	44,44,44,44	0
57	MG	1a	1807	1/1	0.94	0.09	58,58,58,58	0
57	MG	1A	3652	1/1	0.94	0.07	27,27,27,27	0
57	MG	1A	3653	1/1	0.94	0.07	23,23,23,23	0
57	MG	1a	1812	1/1	0.94	0.21	59,59,59,59	0
57	MG	1A	3435	1/1	0.94	0.16	39,39,39,39	0
57	MG	2A	3199	1/1	0.94	0.14	58,58,58,58	0
57	MG	2A	3400	1/1	0.94	0.24	46,46,46,46	0
57	MG	2A	3403	1/1	0.94	0.28	59,59,59,59	0
57	MG	1A	3924	1/1	0.94	0.07	37,37,37,37	0
57	MG	1a	1816	1/1	0.94	0.12	53,53,53,53	0
57	MG	1a	1611	1/1	0.94	0.15	44,44,44,44	0
57	MG	1A	3803	1/1	0.94	0.11	35,35,35,35	0
57	MG	1A	3078	1/1	0.94	0.06	24,24,24,24	0
57	MG	2a	3048	1/1	0.94	0.09	67,67,67,67	0
57	MG	1A	3807	1/1	0.94	0.13	51,51,51,51	0
57	MG	2A	3208	1/1	0.94	0.08	62,62,62,62	0
57	MG	1A	3352	1/1	0.94	0.12	54,54,54,54	0
57	MG	1A	3081	1/1	0.94	0.18	39,39,39,39	0
57	MG	2a	3053	1/1	0.94	0.16	58,58,58,58	0
57	MG	1A	3815	1/1	0.94	0.07	26,26,26,26	0
57	MG	2A	3212	1/1	0.94	0.15	44,44,44,44	0
57	MG	1A	3816	1/1	0.94	0.07	33,33,33,33	0
57	MG	2A	3711	1/1	0.94	0.09	58,58,58,58	0
57	MG	2a	3059	1/1	0.94	0.22	58,58,58,58	0
57	MG	1A	3354	1/1	0.94	0.09	44,44,44,44	0
57	MG	1n	101	1/1	0.94	0.33	59,59,59,59	0
57	MG	2a	3066	1/1	0.94	0.28	71,71,71,71	0
57	MG	1n	102	1/1	0.94	0.15	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1626	1/1	0.94	0.16	61,61,61,61	0
57	MG	1A	3661	1/1	0.94	0.07	18,18,18,18	0
57	MG	2a	3071	1/1	0.94	0.12	52,52,52,52	0
57	MG	1a	1629	1/1	0.94	0.12	49,49,49,49	0
57	MG	1A	3355	1/1	0.94	0.09	51,51,51,51	0
57	MG	1a	1631	1/1	0.94	0.18	54,54,54,54	0
57	MG	1A	3949	1/1	0.94	0.10	49,49,49,49	0
57	MG	2a	3076	1/1	0.94	0.14	60,60,60,60	0
57	MG	2A	3430	1/1	0.94	0.17	51,51,51,51	0
57	MG	2a	3078	1/1	0.94	0.20	47,47,47,47	0
57	MG	2A	3724	1/1	0.94	0.10	49,49,49,49	0
57	MG	2A	3431	1/1	0.94	0.10	60,60,60,60	0
57	MG	2a	3082	1/1	0.94	0.27	52,52,52,52	0
57	MG	2A	3435	1/1	0.94	0.10	68,68,68,68	0
57	MG	2A	3436	1/1	0.94	0.22	63,63,63,63	0
57	MG	2A	3227	1/1	0.94	0.15	46,46,46,46	0
57	MG	2A	3439	1/1	0.94	0.14	42,42,42,42	0
57	MG	1A	3668	1/1	0.94	0.09	24,24,24,24	0
57	MG	2A	3732	1/1	0.94	0.10	33,33,33,33	0
57	MG	1A	3357	1/1	0.94	0.18	42,42,42,42	0
57	MG	2A	3231	1/1	0.94	0.10	56,56,56,56	0
57	MG	1A	3952	1/1	0.94	0.09	54,54,54,54	0
57	MG	1A	3824	1/1	0.94	0.07	47,47,47,47	0
57	MG	2A	3234	1/1	0.94	0.10	46,46,46,46	0
57	MG	1A	3191	1/1	0.94	0.20	33,33,33,33	0
57	MG	2A	3237	1/1	0.94	0.18	44,44,44,44	0
57	MG	1x	102	1/1	0.94	0.22	55,55,55,55	0
57	MG	2A	3743	1/1	0.94	0.12	46,46,46,46	0
57	MG	2A	3746	1/1	0.94	0.07	56,56,56,56	0
57	MG	2A	3749	1/1	0.94	0.17	61,61,61,61	0
57	MG	1A	3956	1/1	0.94	0.08	53,53,53,53	0
57	MG	2A	3240	1/1	0.94	0.10	46,46,46,46	0
57	MG	1A	3362	1/1	0.94	0.24	36,36,36,36	0
57	MG	1A	4104	1/1	0.94	0.08	35,35,35,35	0
57	MG	1A	3959	1/1	0.94	0.10	37,37,37,37	0
57	MG	2a	3111	1/1	0.94	0.08	55,55,55,55	0
57	MG	1a	1647	1/1	0.94	0.20	52,52,52,52	0
57	MG	1x	110	1/1	0.94	0.10	23,23,23,23	0
57	MG	1A	3961	1/1	0.94	0.15	55,55,55,55	0
57	MG	1A	3298	1/1	0.94	0.32	55,55,55,55	0
57	MG	1x	113	1/1	0.94	0.07	53,53,53,53	0
57	MG	1A	3450	1/1	0.94	0.14	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3002	1/1	0.94	0.19	54,54,54,54	0
57	MG	2A	3476	1/1	0.94	0.11	60,60,60,60	0
57	MG	1B	201	1/1	0.94	0.16	54,54,54,54	0
57	MG	1A	3195	1/1	0.94	0.08	33,33,33,33	0
57	MG	2a	3128	1/1	0.94	0.09	70,70,70,70	0
57	MG	1A	3109	1/1	0.94	0.13	35,35,35,35	0
57	MG	1A	3303	1/1	0.94	0.09	56,56,56,56	0
57	MG	1A	3152	1/1	0.94	0.26	35,35,35,35	0
57	MG	1A	3251	1/1	0.94	0.07	49,49,49,49	0
57	MG	2A	3484	1/1	0.94	0.11	21,21,21,21	0
57	MG	2a	3146	1/1	0.94	0.10	66,66,66,66	0
57	MG	2A	3778	1/1	0.94	0.10	64,64,64,64	0
57	MG	1A	3837	1/1	0.94	0.07	58,58,58,58	0
57	MG	1A	3838	1/1	0.94	0.14	54,54,54,54	0
57	MG	1a	1663	1/1	0.94	0.17	55,55,55,55	0
57	MG	1A	3307	1/1	0.94	0.26	58,58,58,58	0
57	MG	2A	3786	1/1	0.94	0.08	38,38,38,38	0
57	MG	2A	3787	1/1	0.94	0.10	51,51,51,51	0
57	MG	2A	3263	1/1	0.94	0.14	60,60,60,60	0
57	MG	2A	3789	1/1	0.94	0.10	37,37,37,37	0
57	MG	2A	3264	1/1	0.94	0.11	63,63,63,63	0
57	MG	1A	3374	1/1	0.94	0.09	63,63,63,63	0
57	MG	2A	3796	1/1	0.94	0.09	57,57,57,57	0
57	MG	1A	3308	1/1	0.94	0.07	33,33,33,33	0
57	MG	2A	3798	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3309	1/1	0.94	0.10	52,52,52,52	0
57	MG	2A	3501	1/1	0.94	0.09	54,54,54,54	0
57	MG	1A	3310	1/1	0.94	0.09	48,48,48,48	0
57	MG	2A	3042	1/1	0.94	0.11	43,43,43,43	0
57	MG	2a	3173	1/1	0.94	0.21	58,58,58,58	0
57	MG	1A	3986	1/1	0.94	0.10	48,48,48,48	0
57	MG	2a	3177	1/1	0.94	0.10	58,58,58,58	0
57	MG	1B	227	1/1	0.94	0.07	38,38,38,38	0
57	MG	2A	3048	1/1	0.94	0.22	66,66,66,66	0
57	MG	1A	3153	1/1	0.94	0.11	40,40,40,40	0
57	MG	1A	3382	1/1	0.94	0.08	54,54,54,54	0
57	MG	1A	3317	1/1	0.94	0.17	50,50,50,50	0
57	MG	1A	3471	1/1	0.94	0.10	42,42,42,42	0
57	MG	2A	3514	1/1	0.94	0.08	36,36,36,36	0
57	MG	1B	233	1/1	0.94	0.14	65,65,65,65	0
57	MG	1A	3561	1/1	0.94	0.25	38,38,38,38	0
57	MG	2A	3056	1/1	0.94	0.16	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3821	1/1	0.94	0.13	46,46,46,46	0
57	MG	1A	3855	1/1	0.94	0.12	52,52,52,52	0
57	MG	2A	3526	1/1	0.94	0.10	36,36,36,36	0
57	MG	2A	3527	1/1	0.94	0.12	39,39,39,39	0
57	MG	1A	3385	1/1	0.94	0.09	49,49,49,49	0
57	MG	1A	3390	1/1	0.94	0.21	34,34,34,34	0
57	MG	2A	3531	1/1	0.94	0.11	62,62,62,62	0
57	MG	2A	3535	1/1	0.94	0.09	32,32,32,32	0
57	MG	1E	308	1/1	0.94	0.06	47,47,47,47	0
57	MG	1A	3211	1/1	0.94	0.07	44,44,44,44	0
57	MG	2A	3541	1/1	0.94	0.15	56,56,56,56	0
57	MG	1A	3059	1/1	0.94	0.07	36,36,36,36	0
57	MG	2A	3067	1/1	0.94	0.19	48,48,48,48	0
57	MG	1A	3577	1/1	0.94	0.15	50,50,50,50	0
57	MG	1A	4003	1/1	0.94	0.05	22,22,22,22	0
57	MG	1A	4004	1/1	0.94	0.10	34,34,34,34	0
57	MG	2a	3207	1/1	0.94	0.14	57,57,57,57	0
57	MG	1F	304	1/1	0.94	0.08	37,37,37,37	0
57	MG	2A	3841	1/1	0.94	0.10	36,36,36,36	0
57	MG	1a	1696	1/1	0.94	0.12	58,58,58,58	0
57	MG	2A	3552	1/1	0.94	0.08	51,51,51,51	0
57	MG	2A	3080	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3478	1/1	0.94	0.14	47,47,47,47	0
57	MG	1A	3216	1/1	0.94	0.09	44,44,44,44	0
57	MG	2A	3847	1/1	0.94	0.08	57,57,57,57	0
57	MG	2A	3848	1/1	0.94	0.10	52,52,52,52	0
57	MG	1A	3114	1/1	0.94	0.18	25,25,25,25	0
57	MG	2A	3085	1/1	0.94	0.09	48,48,48,48	0
57	MG	2a	3221	1/1	0.94	0.09	59,59,59,59	0
57	MG	1A	3482	1/1	0.94	0.19	49,49,49,49	0
57	MG	2A	3852	1/1	0.94	0.14	64,64,64,64	0
57	MG	2A	3567	1/1	0.94	0.08	47,47,47,47	0
57	MG	2A	3304	1/1	0.94	0.12	54,54,54,54	0
57	MG	2A	3087	1/1	0.94	0.11	59,59,59,59	0
57	MG	2A	3089	1/1	0.94	0.16	48,48,48,48	0
57	MG	1A	3397	1/1	0.94	0.11	43,43,43,43	0
57	MG	2A	3091	1/1	0.94	0.09	43,43,43,43	0
57	MG	2A	3309	1/1	0.94	0.20	57,57,57,57	0
57	MG	1A	3054	1/1	0.94	0.07	51,51,51,51	0
57	MG	1a	1710	1/1	0.94	0.38	62,62,62,62	0
57	MG	1I	201	1/1	0.94	0.07	61,61,61,61	0
57	MG	2d	301	1/1	0.94	0.08	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3577	1/1	0.94	0.15	62,62,62,62	0
57	MG	1A	3329	1/1	0.94	0.10	51,51,51,51	0
57	MG	2B	205	1/1	0.94	0.17	59,59,59,59	0
57	MG	1A	3330	1/1	0.94	0.18	53,53,53,53	0
57	MG	2l	201	1/1	0.94	0.12	57,57,57,57	0
57	MG	1A	3167	1/1	0.94	0.26	34,34,34,34	0
57	MG	2A	3317	1/1	0.94	0.26	49,49,49,49	0
57	MG	2A	3101	1/1	0.94	0.20	69,69,69,69	0
57	MG	1A	3333	1/1	0.94	0.12	45,45,45,45	0
57	MG	2B	211	1/1	0.94	0.19	60,60,60,60	0
57	MG	1A	3267	1/1	0.94	0.14	43,43,43,43	0
57	MG	1a	1723	1/1	0.94	0.07	61,61,61,61	0
57	MG	1P	201	1/1	0.94	0.40	30,30,30,30	0
57	MG	1a	1725	1/1	0.94	0.09	54,54,54,54	0
57	MG	2A	3590	1/1	0.94	0.11	44,44,44,44	0
57	MG	2B	217	1/1	0.94	0.16	63,63,63,63	0
57	MG	2A	3325	1/1	0.94	0.12	66,66,66,66	0
57	MG	1A	3608	1/1	0.94	0.05	30,30,30,30	0
57	MG	1A	3609	1/1	0.94	0.09	10,10,10,10	0
57	MG	1S	203	1/1	0.94	0.06	51,51,51,51	0
57	MG	2x	101	1/1	0.94	0.18	65,65,65,65	0
57	MG	1T	201	1/1	0.94	0.08	61,61,61,61	0
57	MG	2A	3601	1/1	0.94	0.10	51,51,51,51	0
57	MG	2x	104	1/1	0.94	0.07	44,44,44,44	0
57	MG	2E	304	1/1	0.94	0.11	42,42,42,42	0
57	MG	1A	3117	1/1	0.94	0.24	46,46,46,46	0
57	MG	2A	3118	1/1	0.94	0.19	54,54,54,54	0
57	MG	1U	204	1/1	0.94	0.28	48,48,48,48	0
57	MG	2A	3334	1/1	0.94	0.08	48,48,48,48	0
57	MG	1A	3756	1/1	0.94	0.07	41,41,41,41	0
57	MG	1V	205	1/1	0.94	0.23	56,56,56,56	0
57	MG	2A	3122	1/1	0.94	0.09	60,60,60,60	0
57	MG	2E	301	1/1	0.95	0.09	53,53,53,53	0
57	MG	2A	3014	1/1	0.95	0.13	48,48,48,48	0
57	MG	1A	3300	1/1	0.95	0.06	45,45,45,45	0
57	MG	1A	3149	1/1	0.95	0.05	29,29,29,29	0
57	MG	1A	3099	1/1	0.95	0.08	50,50,50,50	0
57	MG	1a	1623	1/1	0.95	0.07	46,46,46,46	0
57	MG	2A	3022	1/1	0.95	0.10	42,42,42,42	0
57	MG	1A	3229	1/1	0.95	0.12	43,43,43,43	0
57	MG	2F	304	1/1	0.95	0.07	42,42,42,42	0
57	MG	2A	3025	1/1	0.95	0.14	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3027	1/1	0.95	0.10	55,55,55,55	0
57	MG	2A	3028	1/1	0.95	0.13	41,41,41,41	0
57	MG	1A	3370	1/1	0.95	0.09	49,49,49,49	0
57	MG	1A	3025	1/1	0.95	0.15	33,33,33,33	0
57	MG	2P	202	1/1	0.95	0.10	56,56,56,56	0
57	MG	2Q	202	1/1	0.95	0.16	48,48,48,48	0
57	MG	1a	1627	1/1	0.95	0.17	52,52,52,52	0
57	MG	1A	4071	1/1	0.95	0.10	42,42,42,42	0
57	MG	1A	3891	1/1	0.95	0.09	47,47,47,47	0
57	MG	2A	3592	1/1	0.95	0.08	37,37,37,37	0
57	MG	1A	3737	1/1	0.95	0.08	23,23,23,23	0
57	MG	1A	3563	1/1	0.95	0.10	35,35,35,35	0
57	MG	2A	3596	1/1	0.95	0.07	46,46,46,46	0
57	MG	1A	3739	1/1	0.95	0.17	43,43,43,43	0
57	MG	2V	202	1/1	0.95	0.10	55,55,55,55	0
57	MG	1a	1634	1/1	0.95	0.20	49,49,49,49	0
57	MG	2W	202	1/1	0.95	0.09	54,54,54,54	0
57	MG	1A	3305	1/1	0.95	0.25	49,49,49,49	0
57	MG	2A	3602	1/1	0.95	0.12	60,60,60,60	0
57	MG	1A	3154	1/1	0.95	0.14	43,43,43,43	0
57	MG	20	101	1/1	0.95	0.09	51,51,51,51	0
57	MG	1A	3744	1/1	0.95	0.09	51,51,51,51	0
57	MG	1A	3156	1/1	0.95	0.12	27,27,27,27	0
57	MG	1A	3103	1/1	0.95	0.07	26,26,26,26	0
57	MG	1A	3749	1/1	0.95	0.12	52,52,52,52	0
57	MG	1a	1642	1/1	0.95	0.21	57,57,57,57	0
57	MG	1A	3578	1/1	0.95	0.12	39,39,39,39	0
57	MG	1A	3580	1/1	0.95	0.16	33,33,33,33	0
57	MG	25	104	1/1	0.95	0.14	53,53,53,53	0
57	MG	2A	3313	1/1	0.95	0.07	36,36,36,36	0
57	MG	1A	3161	1/1	0.95	0.17	36,36,36,36	0
57	MG	1A	3106	1/1	0.95	0.27	37,37,37,37	0
57	MG	1A	3913	1/1	0.95	0.09	68,68,68,68	0
57	MG	1a	1651	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	4095	1/1	0.95	0.06	56,56,56,56	0
57	MG	1A	3313	1/1	0.95	0.12	60,60,60,60	0
57	MG	1A	3315	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	4098	1/1	0.95	0.11	66,66,66,66	0
57	MG	1A	3587	1/1	0.95	0.19	50,50,50,50	0
57	MG	1A	3474	1/1	0.95	0.08	34,34,34,34	0
57	MG	2A	3071	1/1	0.95	0.08	44,44,44,44	0
57	MG	2A	3628	1/1	0.95	0.09	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3388	1/1	0.95	0.19	30,30,30,30	0
57	MG	2A	3076	1/1	0.95	0.06	46,46,46,46	0
57	MG	2A	3328	1/1	0.95	0.22	68,68,68,68	0
57	MG	1a	1659	1/1	0.95	0.20	66,66,66,66	0
57	MG	1A	3590	1/1	0.95	0.09	44,44,44,44	0
57	MG	1A	3593	1/1	0.95	0.07	53,53,53,53	0
57	MG	1A	3108	1/1	0.95	0.07	40,40,40,40	0
57	MG	1A	3596	1/1	0.95	0.06	37,37,37,37	0
57	MG	1A	3165	1/1	0.95	0.17	51,51,51,51	0
57	MG	2a	3017	1/1	0.95	0.10	63,63,63,63	0
57	MG	2A	3643	1/1	0.95	0.09	63,63,63,63	0
57	MG	2a	3019	1/1	0.95	0.09	57,57,57,57	0
57	MG	1A	3767	1/1	0.95	0.05	24,24,24,24	0
57	MG	1A	4109	1/1	0.95	0.26	56,56,56,56	0
57	MG	1A	3938	1/1	0.95	0.08	60,60,60,60	0
57	MG	2A	3647	1/1	0.95	0.13	61,61,61,61	0
57	MG	1A	3940	1/1	0.95	0.07	60,60,60,60	0
57	MG	1A	3599	1/1	0.95	0.06	39,39,39,39	0
57	MG	1B	208	1/1	0.95	0.14	59,59,59,59	0
57	MG	2A	3652	1/1	0.95	0.13	56,56,56,56	0
57	MG	2A	3092	1/1	0.95	0.07	56,56,56,56	0
57	MG	2a	3029	1/1	0.95	0.20	46,46,46,46	0
57	MG	1B	209	1/1	0.95	0.10	44,44,44,44	0
57	MG	2A	3094	1/1	0.95	0.08	49,49,49,49	0
57	MG	1a	1672	1/1	0.95	0.15	55,55,55,55	0
57	MG	1B	211	1/1	0.95	0.13	48,48,48,48	0
57	MG	1B	212	1/1	0.95	0.15	60,60,60,60	0
57	MG	1A	3600	1/1	0.95	0.07	28,28,28,28	0
57	MG	1a	1680	1/1	0.95	0.32	59,59,59,59	0
57	MG	1A	3318	1/1	0.95	0.14	36,36,36,36	0
57	MG	1A	3029	1/1	0.95	0.07	39,39,39,39	0
57	MG	1A	3781	1/1	0.95	0.06	47,47,47,47	0
57	MG	2A	3104	1/1	0.95	0.13	42,42,42,42	0
57	MG	1A	3394	1/1	0.95	0.06	46,46,46,46	0
57	MG	1a	1686	1/1	0.95	0.22	57,57,57,57	0
57	MG	1A	3607	1/1	0.95	0.08	24,24,24,24	0
57	MG	2A	3109	1/1	0.95	0.25	67,67,67,67	0
57	MG	1A	3786	1/1	0.95	0.09	51,51,51,51	0
57	MG	1A	3481	1/1	0.95	0.10	57,57,57,57	0
57	MG	2A	3112	1/1	0.95	0.09	50,50,50,50	0
57	MG	1A	3033	1/1	0.95	0.40	33,33,33,33	0
57	MG	2A	3364	1/1	0.95	0.09	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3611	1/1	0.95	0.05	24,24,24,24	0
57	MG	2A	3116	1/1	0.95	0.11	41,41,41,41	0
57	MG	1A	3484	1/1	0.95	0.06	41,41,41,41	0
57	MG	1A	3613	1/1	0.95	0.11	28,28,28,28	0
57	MG	1A	3614	1/1	0.95	0.06	30,30,30,30	0
57	MG	1A	3615	1/1	0.95	0.08	29,29,29,29	0
57	MG	1a	1697	1/1	0.95	0.22	60,60,60,60	0
57	MG	1a	1698	1/1	0.95	0.06	50,50,50,50	0
57	MG	2A	3373	1/1	0.95	0.24	49,49,49,49	0
57	MG	2a	3060	1/1	0.95	0.16	56,56,56,56	0
57	MG	1A	3962	1/1	0.95	0.15	55,55,55,55	0
57	MG	2A	3125	1/1	0.95	0.11	41,41,41,41	0
57	MG	2A	3126	1/1	0.95	0.17	45,45,45,45	0
57	MG	1A	3396	1/1	0.95	0.09	44,44,44,44	0
57	MG	2A	3693	1/1	0.95	0.15	57,57,57,57	0
57	MG	1a	1702	1/1	0.95	0.06	43,43,43,43	0
57	MG	2A	3129	1/1	0.95	0.04	37,37,37,37	0
57	MG	1A	3624	1/1	0.95	0.07	22,22,22,22	0
57	MG	1B	234	1/1	0.95	0.11	57,57,57,57	0
57	MG	2A	3133	1/1	0.95	0.14	40,40,40,40	0
57	MG	1a	1705	1/1	0.95	0.12	35,35,35,35	0
57	MG	1a	1707	1/1	0.95	0.10	59,59,59,59	0
57	MG	1A	3967	1/1	0.95	0.07	68,68,68,68	0
57	MG	1B	236	1/1	0.95	0.07	41,41,41,41	0
57	MG	1A	3968	1/1	0.95	0.09	66,66,66,66	0
57	MG	2A	3707	1/1	0.95	0.10	50,50,50,50	0
57	MG	2A	3708	1/1	0.95	0.13	53,53,53,53	0
57	MG	1A	3249	1/1	0.95	0.19	42,42,42,42	0
57	MG	1a	1713	1/1	0.95	0.15	51,51,51,51	0
57	MG	1A	3112	1/1	0.95	0.17	35,35,35,35	0
57	MG	1E	307	1/1	0.95	0.08	48,48,48,48	0
57	MG	2A	3395	1/1	0.95	0.21	48,48,48,48	0
57	MG	2A	3147	1/1	0.95	0.20	51,51,51,51	0
57	MG	2A	3397	1/1	0.95	0.19	33,33,33,33	0
57	MG	1A	3324	1/1	0.95	0.13	48,48,48,48	0
57	MG	2A	3149	1/1	0.95	0.09	55,55,55,55	0
57	MG	2A	3719	1/1	0.95	0.12	57,57,57,57	0
57	MG	2A	3150	1/1	0.95	0.11	53,53,53,53	0
57	MG	2A	3402	1/1	0.95	0.20	47,47,47,47	0
57	MG	1a	1718	1/1	0.95	0.06	52,52,52,52	0
57	MG	1A	3812	1/1	0.95	0.07	38,38,38,38	0
57	MG	2A	3153	1/1	0.95	0.13	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3725	1/1	0.95	0.21	62,62,62,62	0
57	MG	1A	3813	1/1	0.95	0.06	23,23,23,23	0
57	MG	1E	312	1/1	0.95	0.14	33,33,33,33	0
57	MG	2a	3104	1/1	0.95	0.15	67,67,67,67	0
57	MG	2a	3105	1/1	0.95	0.22	56,56,56,56	0
57	MG	1A	3058	1/1	0.95	0.06	29,29,29,29	0
57	MG	1A	3327	1/1	0.95	0.12	46,46,46,46	0
57	MG	2a	3108	1/1	0.95	0.13	52,52,52,52	0
57	MG	1F	302	1/1	0.95	0.19	32,32,32,32	0
57	MG	2A	3163	1/1	0.95	0.12	44,44,44,44	0
57	MG	1A	3084	1/1	0.95	0.20	39,39,39,39	0
57	MG	2a	3113	1/1	0.95	0.28	65,65,65,65	0
57	MG	2a	3114	1/1	0.95	0.19	49,49,49,49	0
57	MG	1A	3253	1/1	0.95	0.10	31,31,31,31	0
57	MG	1a	1731	1/1	0.95	0.12	54,54,54,54	0
57	MG	2a	3117	1/1	0.95	0.21	55,55,55,55	0
57	MG	1F	309	1/1	0.95	0.08	48,48,48,48	0
57	MG	2A	3418	1/1	0.95	0.17	42,42,42,42	0
57	MG	1A	3497	1/1	0.95	0.08	40,40,40,40	0
57	MG	2A	3170	1/1	0.95	0.07	48,48,48,48	0
57	MG	1A	3255	1/1	0.95	0.12	44,44,44,44	0
57	MG	1F	313	1/1	0.95	0.15	53,53,53,53	0
57	MG	2a	3124	1/1	0.95	0.10	59,59,59,59	0
57	MG	1A	3822	1/1	0.95	0.18	43,43,43,43	0
57	MG	2a	3126	1/1	0.95	0.09	61,61,61,61	0
57	MG	1A	3086	1/1	0.95	0.10	38,38,38,38	0
57	MG	1A	3043	1/1	0.95	0.23	34,34,34,34	0
57	MG	2A	3750	1/1	0.95	0.08	64,64,64,64	0
57	MG	1A	3409	1/1	0.95	0.07	53,53,53,53	0
57	MG	2a	3133	1/1	0.95	0.13	60,60,60,60	0
57	MG	2a	3134	1/1	0.95	0.11	59,59,59,59	0
57	MG	2a	3136	1/1	0.95	0.10	71,71,71,71	0
57	MG	2A	3428	1/1	0.95	0.09	54,54,54,54	0
57	MG	2A	3179	1/1	0.95	0.13	44,44,44,44	0
57	MG	2A	3755	1/1	0.95	0.06	42,42,42,42	0
57	MG	1A	3645	1/1	0.95	0.09	41,41,41,41	0
57	MG	1a	1749	1/1	0.95	0.10	58,58,58,58	0
57	MG	2a	3149	1/1	0.95	0.11	49,49,49,49	0
57	MG	1A	3410	1/1	0.95	0.11	47,47,47,47	0
57	MG	1N	202	1/1	0.95	0.18	42,42,42,42	0
57	MG	1N	203	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3088	1/1	0.95	0.10	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3259	1/1	0.95	0.17	56,56,56,56	0
57	MG	2a	3157	1/1	0.95	0.14	53,53,53,53	0
57	MG	1a	1758	1/1	0.95	0.06	60,60,60,60	0
57	MG	1A	3509	1/1	0.95	0.18	36,36,36,36	0
57	MG	2a	3160	1/1	0.95	0.12	46,46,46,46	0
57	MG	2a	3161	1/1	0.95	0.07	51,51,51,51	0
57	MG	1A	3413	1/1	0.95	0.06	46,46,46,46	0
57	MG	1A	3833	1/1	0.95	0.06	35,35,35,35	0
57	MG	1P	203	1/1	0.95	0.13	37,37,37,37	0
57	MG	1Q	203	1/1	0.95	0.11	60,60,60,60	0
57	MG	1a	1764	1/1	0.95	0.08	51,51,51,51	0
57	MG	2a	3167	1/1	0.95	0.20	49,49,49,49	0
57	MG	1R	202	1/1	0.95	0.10	42,42,42,42	0
57	MG	1A	3120	1/1	0.95	0.16	37,37,37,37	0
57	MG	1A	4001	1/1	0.95	0.05	30,30,30,30	0
57	MG	1A	3060	1/1	0.95	0.20	56,56,56,56	0
57	MG	1A	3049	1/1	0.95	0.05	13,13,13,13	0
57	MG	1A	3265	1/1	0.95	0.20	48,48,48,48	0
57	MG	2A	3460	1/1	0.95	0.08	46,46,46,46	0
57	MG	1U	202	1/1	0.95	0.17	38,38,38,38	0
57	MG	1A	3839	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	3516	1/1	0.95	0.14	70,70,70,70	0
57	MG	2a	3180	1/1	0.95	0.09	62,62,62,62	0
57	MG	2A	3465	1/1	0.95	0.22	52,52,52,52	0
57	MG	2A	3466	1/1	0.95	0.36	63,63,63,63	0
57	MG	1A	3198	1/1	0.95	0.11	31,31,31,31	0
57	MG	2A	3469	1/1	0.95	0.08	51,51,51,51	0
57	MG	1A	3126	1/1	0.95	0.11	66,66,66,66	0
57	MG	1V	208	1/1	0.95	0.11	46,46,46,46	0
57	MG	2A	3474	1/1	0.95	0.09	54,54,54,54	0
57	MG	1a	1794	1/1	0.95	0.06	59,59,59,59	0
57	MG	1W	202	1/1	0.95	0.09	44,44,44,44	0
57	MG	1a	1796	1/1	0.95	0.17	59,59,59,59	0
57	MG	1a	1797	1/1	0.95	0.19	62,62,62,62	0
57	MG	1W	204	1/1	0.95	0.09	34,34,34,34	0
57	MG	2A	3217	1/1	0.95	0.23	57,57,57,57	0
57	MG	1W	205	1/1	0.95	0.15	22,22,22,22	0
57	MG	1a	1800	1/1	0.95	0.11	58,58,58,58	0
57	MG	1A	4011	1/1	0.95	0.05	50,50,50,50	0
57	MG	2A	3221	1/1	0.95	0.16	37,37,37,37	0
57	MG	2A	3222	1/1	0.95	0.12	54,54,54,54	0
57	MG	1A	3346	1/1	0.95	0.10	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3524	1/1	0.95	0.24	37,37,37,37	0
57	MG	1Y	202	1/1	0.95	0.23	52,52,52,52	0
57	MG	1A	3202	1/1	0.95	0.23	48,48,48,48	0
57	MG	1A	3203	1/1	0.95	0.08	46,46,46,46	0
57	MG	1A	3427	1/1	0.95	0.07	40,40,40,40	0
57	MG	2A	3823	1/1	0.95	0.08	53,53,53,53	0
57	MG	2A	3497	1/1	0.95	0.06	42,42,42,42	0
57	MG	10	101	1/1	0.95	0.12	45,45,45,45	0
57	MG	1A	3428	1/1	0.95	0.17	43,43,43,43	0
57	MG	1A	3429	1/1	0.95	0.11	48,48,48,48	0
57	MG	10	105	1/1	0.95	0.10	46,46,46,46	0
57	MG	1A	3854	1/1	0.95	0.09	43,43,43,43	0
57	MG	1A	4022	1/1	0.95	0.07	37,37,37,37	0
57	MG	1A	3065	1/1	0.95	0.10	46,46,46,46	0
57	MG	2A	3509	1/1	0.95	0.08	40,40,40,40	0
57	MG	1A	4025	1/1	0.95	0.07	51,51,51,51	0
57	MG	1A	3533	1/1	0.95	0.16	51,51,51,51	0
57	MG	1A	3131	1/1	0.95	0.10	52,52,52,52	0
57	MG	2A	3241	1/1	0.95	0.21	57,57,57,57	0
57	MG	1e	202	1/1	0.95	0.16	51,51,51,51	0
57	MG	1A	3858	1/1	0.95	0.07	21,21,21,21	0
57	MG	1A	3206	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	3286	1/1	0.95	0.12	53,53,53,53	0
57	MG	2A	3520	1/1	0.95	0.13	54,54,54,54	0
57	MG	1A	3691	1/1	0.95	0.08	24,24,24,24	0
57	MG	15	3202	1/1	0.95	0.19	34,34,34,34	0
57	MG	2a	3232	1/1	0.95	0.07	47,47,47,47	0
57	MG	2a	3233	1/1	0.95	0.10	43,43,43,43	0
57	MG	15	3203	1/1	0.95	0.22	43,43,43,43	0
57	MG	1A	3209	1/1	0.95	0.07	35,35,35,35	0
57	MG	2A	3529	1/1	0.95	0.07	30,30,30,30	0
57	MG	1A	3135	1/1	0.95	0.17	44,44,44,44	0
57	MG	2a	3238	1/1	0.95	0.08	59,59,59,59	0
57	MG	15	3208	1/1	0.95	0.07	46,46,46,46	0
57	MG	2A	3533	1/1	0.95	0.08	34,34,34,34	0
57	MG	2e	201	1/1	0.95	0.09	63,63,63,63	0
57	MG	16	101	1/1	0.95	0.14	48,48,48,48	0
57	MG	1A	3698	1/1	0.95	0.08	28,28,28,28	0
57	MG	1A	3138	1/1	0.95	0.08	42,42,42,42	0
57	MG	2A	3540	1/1	0.95	0.19	59,59,59,59	0
57	MG	2l	202	1/1	0.95	0.07	65,65,65,65	0
57	MG	1A	4039	1/1	0.95	0.05	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4041	1/1	0.95	0.06	45,45,45,45	0
57	MG	1A	3444	1/1	0.95	0.18	51,51,51,51	0
57	MG	1A	3139	1/1	0.95	0.07	43,43,43,43	0
57	MG	2A	3545	1/1	0.95	0.11	42,42,42,42	0
57	MG	2A	3546	1/1	0.95	0.07	35,35,35,35	0
57	MG	1A	3094	1/1	0.95	0.17	36,36,36,36	0
57	MG	1A	3870	1/1	0.95	0.14	31,31,31,31	0
57	MG	1A	3447	1/1	0.95	0.08	48,48,48,48	0
57	MG	1A	3361	1/1	0.95	0.15	44,44,44,44	0
57	MG	1A	3711	1/1	0.95	0.11	49,49,49,49	0
57	MG	1A	3144	1/1	0.95	0.19	42,42,42,42	0
57	MG	2A	3555	1/1	0.95	0.14	55,55,55,55	0
57	MG	1A	3714	1/1	0.95	0.13	37,37,37,37	0
57	MG	1A	4055	1/1	0.95	0.10	58,58,58,58	0
57	MG	1x	109	1/1	0.95	0.23	59,59,59,59	0
57	MG	1A	4058	1/1	0.95	0.11	13,13,13,13	0
57	MG	1a	1612	1/1	0.95	0.31	64,64,64,64	0
57	MG	1A	3015	1/1	0.95	0.08	32,32,32,32	0
57	MG	1a	1615	1/1	0.95	0.08	57,57,57,57	0
57	MG	1a	1616	1/1	0.95	0.22	60,60,60,60	0
57	MG	1A	3053	1/1	0.95	0.10	45,45,45,45	0
57	MG	2A	3003	1/1	0.95	0.11	46,46,46,46	0
57	MG	2A	3004	1/1	0.95	0.12	51,51,51,51	0
57	MG	2A	3007	1/1	0.95	0.13	51,51,51,51	0
57	MG	1A	3720	1/1	0.95	0.12	43,43,43,43	0
57	MG	2D	306	1/1	0.95	0.15	55,55,55,55	0
62	PHE	2w	108	11/12	0.95	0.11	36,39,42,44	0
57	MG	1A	3462	1/1	0.96	0.09	46,46,46,46	0
57	MG	1A	4074	1/1	0.96	0.13	49,49,49,49	0
57	MG	15	3206	1/1	0.96	0.11	36,36,36,36	0
57	MG	1A	3127	1/1	0.96	0.12	38,38,38,38	0
57	MG	1A	4076	1/1	0.96	0.06	37,37,37,37	0
57	MG	28	101	1/1	0.96	0.28	53,53,53,53	0
57	MG	1A	3789	1/1	0.96	0.09	20,20,20,20	0
57	MG	2A	3386	1/1	0.96	0.15	37,37,37,37	0
57	MG	2a	3001	1/1	0.96	0.09	63,63,63,63	0
57	MG	2A	3387	1/1	0.96	0.15	48,48,48,48	0
57	MG	2A	3169	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3648	1/1	0.96	0.09	46,46,46,46	0
57	MG	17	101	1/1	0.96	0.11	34,34,34,34	0
57	MG	17	102	1/1	0.96	0.18	30,30,30,30	0
57	MG	2A	3662	1/1	0.96	0.07	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3042	1/1	0.96	0.06	22,22,22,22	0
57	MG	1A	3299	1/1	0.96	0.24	54,54,54,54	0
57	MG	1A	4081	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	3200	1/1	0.96	0.09	21,21,21,21	0
57	MG	1A	3794	1/1	0.96	0.05	43,43,43,43	0
57	MG	1a	1810	1/1	0.96	0.06	56,56,56,56	0
57	MG	2A	3181	1/1	0.96	0.07	48,48,48,48	0
57	MG	1a	1811	1/1	0.96	0.07	52,52,52,52	0
57	MG	2A	3183	1/1	0.96	0.11	42,42,42,42	0
57	MG	1A	3071	1/1	0.96	0.09	29,29,29,29	0
57	MG	1A	3797	1/1	0.96	0.04	19,19,19,19	0
57	MG	1A	3132	1/1	0.96	0.08	26,26,26,26	0
57	MG	1A	3073	1/1	0.96	0.11	44,44,44,44	0
57	MG	1A	3075	1/1	0.96	0.05	31,31,31,31	0
57	MG	1A	3943	1/1	0.96	0.07	50,50,50,50	0
57	MG	1A	3805	1/1	0.96	0.08	57,57,57,57	0
57	MG	2A	3409	1/1	0.96	0.19	53,53,53,53	0
57	MG	2A	3191	1/1	0.96	0.22	55,55,55,55	0
57	MG	1A	3004	1/1	0.96	0.05	23,23,23,23	0
57	MG	1A	3207	1/1	0.96	0.12	41,41,41,41	0
57	MG	1f	201	1/1	0.96	0.18	44,44,44,44	0
57	MG	1A	3808	1/1	0.96	0.12	23,23,23,23	0
57	MG	1A	3047	1/1	0.96	0.06	38,38,38,38	0
57	MG	1A	4100	1/1	0.96	0.10	63,63,63,63	0
57	MG	1A	3810	1/1	0.96	0.18	30,30,30,30	0
57	MG	1A	3669	1/1	0.96	0.04	19,19,19,19	0
57	MG	1A	3210	1/1	0.96	0.07	40,40,40,40	0
57	MG	1A	3170	1/1	0.96	0.08	38,38,38,38	0
57	MG	1a	1620	1/1	0.96	0.09	43,43,43,43	0
57	MG	1A	3212	1/1	0.96	0.11	34,34,34,34	0
57	MG	1A	3312	1/1	0.96	0.22	35,35,35,35	0
57	MG	1A	3175	1/1	0.96	0.11	21,21,21,21	0
57	MG	2A	3426	1/1	0.96	0.22	40,40,40,40	0
57	MG	1A	3215	1/1	0.96	0.11	29,29,29,29	0
57	MG	1w	103	1/1	0.96	0.07	60,60,60,60	0
57	MG	1A	3960	1/1	0.96	0.07	30,30,30,30	0
57	MG	1A	3261	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3483	1/1	0.96	0.13	42,42,42,42	0
57	MG	2A	3213	1/1	0.96	0.17	45,45,45,45	0
57	MG	1B	203	1/1	0.96	0.08	42,42,42,42	0
57	MG	1A	3963	1/1	0.96	0.09	43,43,43,43	0
57	MG	2A	3438	1/1	0.96	0.10	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3684	1/1	0.96	0.07	19,19,19,19	0
57	MG	1A	3965	1/1	0.96	0.13	60,60,60,60	0
57	MG	2A	3441	1/1	0.96	0.11	38,38,38,38	0
57	MG	1B	210	1/1	0.96	0.12	48,48,48,48	0
57	MG	2A	3444	1/1	0.96	0.05	25,25,25,25	0
57	MG	1A	3176	1/1	0.96	0.06	34,34,34,34	0
57	MG	2a	3056	1/1	0.96	0.13	39,39,39,39	0
57	MG	1A	3572	1/1	0.96	0.14	61,61,61,61	0
57	MG	1A	3687	1/1	0.96	0.08	26,26,26,26	0
57	MG	1x	107	1/1	0.96	0.19	51,51,51,51	0
57	MG	1A	3826	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3048	1/1	0.96	0.12	30,30,30,30	0
57	MG	1A	3079	1/1	0.96	0.13	39,39,39,39	0
57	MG	1B	218	1/1	0.96	0.15	41,41,41,41	0
57	MG	1B	219	1/1	0.96	0.06	40,40,40,40	0
57	MG	2a	3068	1/1	0.96	0.18	56,56,56,56	0
57	MG	2A	3454	1/1	0.96	0.10	45,45,45,45	0
57	MG	2A	3228	1/1	0.96	0.28	51,51,51,51	0
57	MG	2A	3456	1/1	0.96	0.15	55,55,55,55	0
57	MG	1a	1643	1/1	0.96	0.15	48,48,48,48	0
57	MG	1y	101	1/1	0.96	0.10	58,58,58,58	0
57	MG	2A	3459	1/1	0.96	0.08	38,38,38,38	0
57	MG	1A	3369	1/1	0.96	0.21	33,33,33,33	0
57	MG	1A	3692	1/1	0.96	0.08	21,21,21,21	0
57	MG	1A	3426	1/1	0.96	0.12	36,36,36,36	0
57	MG	1A	3976	1/1	0.96	0.07	49,49,49,49	0
57	MG	2A	3235	1/1	0.96	0.10	41,41,41,41	0
57	MG	1A	3694	1/1	0.96	0.09	29,29,29,29	0
57	MG	2A	3008	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3491	1/1	0.96	0.18	36,36,36,36	0
57	MG	2a	3084	1/1	0.96	0.19	34,34,34,34	0
57	MG	2A	3744	1/1	0.96	0.10	62,62,62,62	0
57	MG	2A	3013	1/1	0.96	0.16	40,40,40,40	0
57	MG	1A	3979	1/1	0.96	0.13	24,24,24,24	0
57	MG	2A	3015	1/1	0.96	0.06	32,32,32,32	0
57	MG	1A	3266	1/1	0.96	0.12	49,49,49,49	0
57	MG	1A	3371	1/1	0.96	0.08	44,44,44,44	0
57	MG	2A	3753	1/1	0.96	0.07	58,58,58,58	0
57	MG	1A	3701	1/1	0.96	0.08	30,30,30,30	0
57	MG	1A	3585	1/1	0.96	0.10	38,38,38,38	0
57	MG	2A	3021	1/1	0.96	0.08	51,51,51,51	0
57	MG	1A	3080	1/1	0.96	0.12	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	3097	1/1	0.96	0.11	56,56,56,56	0
57	MG	1B	232	1/1	0.96	0.09	57,57,57,57	0
57	MG	1A	3495	1/1	0.96	0.09	55,55,55,55	0
57	MG	1A	3430	1/1	0.96	0.10	61,61,61,61	0
57	MG	1A	3706	1/1	0.96	0.05	62,62,62,62	0
57	MG	1A	3990	1/1	0.96	0.05	43,43,43,43	0
57	MG	2A	3030	1/1	0.96	0.10	44,44,44,44	0
57	MG	1D	302	1/1	0.96	0.28	49,49,49,49	0
57	MG	1D	303	1/1	0.96	0.16	36,36,36,36	0
57	MG	1D	305	1/1	0.96	0.04	32,32,32,32	0
57	MG	2A	3036	1/1	0.96	0.07	42,42,42,42	0
57	MG	1A	3222	1/1	0.96	0.06	33,33,33,33	0
57	MG	1D	310	1/1	0.96	0.19	30,30,30,30	0
57	MG	1A	3708	1/1	0.96	0.05	13,13,13,13	0
57	MG	2A	3500	1/1	0.96	0.08	32,32,32,32	0
57	MG	2A	3775	1/1	0.96	0.05	45,45,45,45	0
57	MG	1E	302	1/1	0.96	0.07	44,44,44,44	0
57	MG	2A	3777	1/1	0.96	0.08	51,51,51,51	0
57	MG	1A	3709	1/1	0.96	0.08	49,49,49,49	0
57	MG	2A	3043	1/1	0.96	0.18	53,53,53,53	0
57	MG	2A	3504	1/1	0.96	0.07	65,65,65,65	0
57	MG	2A	3044	1/1	0.96	0.13	42,42,42,42	0
57	MG	2A	3045	1/1	0.96	0.12	26,26,26,26	0
57	MG	2A	3267	1/1	0.96	0.11	55,55,55,55	0
57	MG	2A	3508	1/1	0.96	0.09	56,56,56,56	0
57	MG	1A	3848	1/1	0.96	0.08	19,19,19,19	0
57	MG	1A	3432	1/1	0.96	0.12	36,36,36,36	0
57	MG	2A	3790	1/1	0.96	0.06	36,36,36,36	0
57	MG	1a	1673	1/1	0.96	0.11	43,43,43,43	0
57	MG	1A	3591	1/1	0.96	0.07	30,30,30,30	0
57	MG	2A	3795	1/1	0.96	0.05	65,65,65,65	0
57	MG	1A	3433	1/1	0.96	0.14	32,32,32,32	0
57	MG	2A	3051	1/1	0.96	0.06	38,38,38,38	0
57	MG	1a	1677	1/1	0.96	0.22	64,64,64,64	0
57	MG	1A	3716	1/1	0.96	0.09	50,50,50,50	0
57	MG	2A	3278	1/1	0.96	0.16	51,51,51,51	0
57	MG	1A	3500	1/1	0.96	0.10	24,24,24,24	0
57	MG	2a	3139	1/1	0.96	0.11	67,67,67,67	0
57	MG	2A	3523	1/1	0.96	0.12	47,47,47,47	0
57	MG	1A	3595	1/1	0.96	0.07	21,21,21,21	0
57	MG	2a	3142	1/1	0.96	0.08	51,51,51,51	0
57	MG	2A	3525	1/1	0.96	0.11	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3807	1/1	0.96	0.06	21,21,21,21	0
57	MG	2a	3148	1/1	0.96	0.08	75,75,75,75	0
57	MG	1A	3434	1/1	0.96	0.16	46,46,46,46	0
57	MG	1a	1683	1/1	0.96	0.21	47,47,47,47	0
57	MG	2A	3059	1/1	0.96	0.13	64,64,64,64	0
57	MG	2a	3153	1/1	0.96	0.08	69,69,69,69	0
57	MG	1A	3723	1/1	0.96	0.05	37,37,37,37	0
57	MG	1A	4006	1/1	0.96	0.04	36,36,36,36	0
57	MG	1F	306	1/1	0.96	0.14	28,28,28,28	0
57	MG	2A	3532	1/1	0.96	0.08	58,58,58,58	0
57	MG	1A	3597	1/1	0.96	0.08	40,40,40,40	0
57	MG	2A	3534	1/1	0.96	0.08	56,56,56,56	0
57	MG	1A	3063	1/1	0.96	0.20	52,52,52,52	0
57	MG	1A	3436	1/1	0.96	0.26	32,32,32,32	0
57	MG	2A	3538	1/1	0.96	0.08	46,46,46,46	0
57	MG	2A	3068	1/1	0.96	0.08	48,48,48,48	0
57	MG	2A	3825	1/1	0.96	0.08	51,51,51,51	0
57	MG	2A	3291	1/1	0.96	0.20	73,73,73,73	0
57	MG	1A	3505	1/1	0.96	0.25	30,30,30,30	0
57	MG	1A	3437	1/1	0.96	0.11	40,40,40,40	0
57	MG	1A	3732	1/1	0.96	0.05	41,41,41,41	0
57	MG	1A	4014	1/1	0.96	0.09	50,50,50,50	0
57	MG	1a	1694	1/1	0.96	0.15	55,55,55,55	0
57	MG	1A	3733	1/1	0.96	0.06	47,47,47,47	0
57	MG	2A	3547	1/1	0.96	0.10	31,31,31,31	0
57	MG	1A	3438	1/1	0.96	0.16	34,34,34,34	0
57	MG	2A	3299	1/1	0.96	0.18	67,67,67,67	0
57	MG	2a	3175	1/1	0.96	0.10	68,68,68,68	0
57	MG	2a	3176	1/1	0.96	0.13	58,58,58,58	0
57	MG	1A	3603	1/1	0.96	0.07	49,49,49,49	0
57	MG	1A	3867	1/1	0.96	0.20	33,33,33,33	0
57	MG	1A	3605	1/1	0.96	0.10	39,39,39,39	0
57	MG	2A	3553	1/1	0.96	0.13	55,55,55,55	0
57	MG	1N	205	1/1	0.96	0.16	45,45,45,45	0
57	MG	1A	3272	1/1	0.96	0.10	50,50,50,50	0
57	MG	2A	3556	1/1	0.96	0.11	60,60,60,60	0
57	MG	1N	207	1/1	0.96	0.13	50,50,50,50	0
57	MG	1A	3510	1/1	0.96	0.10	29,29,29,29	0
57	MG	1O	203	1/1	0.96	0.06	46,46,46,46	0
57	MG	1A	3742	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	3326	1/1	0.96	0.15	42,42,42,42	0
57	MG	2A	3566	1/1	0.96	0.09	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3874	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	3183	1/1	0.96	0.15	46,46,46,46	0
57	MG	1A	3381	1/1	0.96	0.07	26,26,26,26	0
57	MG	1Q	205	1/1	0.96	0.11	48,48,48,48	0
57	MG	1Q	206	1/1	0.96	0.14	43,43,43,43	0
57	MG	1A	3123	1/1	0.96	0.18	29,29,29,29	0
57	MG	1a	1716	1/1	0.96	0.07	50,50,50,50	0
57	MG	2a	3198	1/1	0.96	0.07	54,54,54,54	0
57	MG	2A	3099	1/1	0.96	0.05	26,26,26,26	0
57	MG	1A	3878	1/1	0.96	0.09	27,27,27,27	0
57	MG	1A	3282	1/1	0.96	0.18	43,43,43,43	0
57	MG	1A	3187	1/1	0.96	0.11	34,34,34,34	0
57	MG	1A	3387	1/1	0.96	0.21	48,48,48,48	0
57	MG	1A	3617	1/1	0.96	0.07	47,47,47,47	0
57	MG	2A	3580	1/1	0.96	0.09	60,60,60,60	0
57	MG	1A	3518	1/1	0.96	0.07	62,62,62,62	0
57	MG	2A	3324	1/1	0.96	0.11	50,50,50,50	0
57	MG	1U	203	1/1	0.96	0.17	31,31,31,31	0
57	MG	2A	3107	1/1	0.96	0.18	37,37,37,37	0
57	MG	2A	3585	1/1	0.96	0.08	47,47,47,47	0
57	MG	1A	4038	1/1	0.96	0.05	34,34,34,34	0
57	MG	2a	3212	1/1	0.96	0.20	54,54,54,54	0
57	MG	1U	206	1/1	0.96	0.26	34,34,34,34	0
57	MG	1U	207	1/1	0.96	0.27	32,32,32,32	0
57	MG	1A	3622	1/1	0.96	0.05	32,32,32,32	0
57	MG	1A	3284	1/1	0.96	0.11	40,40,40,40	0
57	MG	1V	206	1/1	0.96	0.06	29,29,29,29	0
57	MG	1A	4042	1/1	0.96	0.08	28,28,28,28	0
57	MG	2a	3219	1/1	0.96	0.11	57,57,57,57	0
57	MG	1A	3520	1/1	0.96	0.08	44,44,44,44	0
57	MG	2A	3335	1/1	0.96	0.21	48,48,48,48	0
57	MG	1W	201	1/1	0.96	0.17	45,45,45,45	0
57	MG	1A	3888	1/1	0.96	0.11	66,66,66,66	0
57	MG	1A	3889	1/1	0.96	0.04	33,33,33,33	0
57	MG	2D	302	1/1	0.96	0.21	55,55,55,55	0
57	MG	2A	3600	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	3758	1/1	0.96	0.07	35,35,35,35	0
57	MG	1X	103	1/1	0.96	0.09	39,39,39,39	0
57	MG	1X	105	1/1	0.96	0.15	38,38,38,38	0
57	MG	2a	3230	1/1	0.96	0.07	68,68,68,68	0
57	MG	2a	3231	1/1	0.96	0.07	62,62,62,62	0
57	MG	2A	3606	1/1	0.96	0.06	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3036	1/1	0.96	0.06	32,32,32,32	0
57	MG	1A	3629	1/1	0.96	0.08	55,55,55,55	0
57	MG	1A	3066	1/1	0.96	0.10	35,35,35,35	0
57	MG	2E	307	1/1	0.96	0.13	37,37,37,37	0
57	MG	2F	301	1/1	0.96	0.11	38,38,38,38	0
57	MG	1a	1754	1/1	0.96	0.11	48,48,48,48	0
57	MG	1A	3192	1/1	0.96	0.17	33,33,33,33	0
57	MG	1A	4052	1/1	0.96	0.04	31,31,31,31	0
57	MG	1a	1757	1/1	0.96	0.08	72,72,72,72	0
57	MG	2F	306	1/1	0.96	0.17	42,42,42,42	0
57	MG	2A	3131	1/1	0.96	0.10	45,45,45,45	0
57	MG	1A	3526	1/1	0.96	0.21	43,43,43,43	0
57	MG	1A	3898	1/1	0.96	0.18	17,17,17,17	0
57	MG	1A	4057	1/1	0.96	0.10	45,45,45,45	0
57	MG	1A	3238	1/1	0.96	0.27	38,38,38,38	0
57	MG	2Q	201	1/1	0.96	0.10	51,51,51,51	0
57	MG	10	103	1/1	0.96	0.13	40,40,40,40	0
57	MG	2A	3139	1/1	0.96	0.08	40,40,40,40	0
57	MG	1A	3193	1/1	0.96	0.10	45,45,45,45	0
57	MG	1A	3341	1/1	0.96	0.10	40,40,40,40	0
57	MG	1a	1766	1/1	0.96	0.07	63,63,63,63	0
57	MG	1A	3903	1/1	0.96	0.06	38,38,38,38	0
57	MG	2T	203	1/1	0.96	0.14	48,48,48,48	0
57	MG	2T	204	1/1	0.96	0.07	65,65,65,65	0
57	MG	2A	3144	1/1	0.96	0.15	38,38,38,38	0
57	MG	1A	4063	1/1	0.96	0.05	38,38,38,38	0
57	MG	2A	3629	1/1	0.96	0.15	56,56,56,56	0
57	MG	1A	3769	1/1	0.96	0.10	54,54,54,54	0
57	MG	1A	3241	1/1	0.96	0.24	50,50,50,50	0
57	MG	1A	3771	1/1	0.96	0.06	27,27,27,27	0
57	MG	1A	3194	1/1	0.96	0.14	34,34,34,34	0
57	MG	11	104	1/1	0.96	0.07	34,34,34,34	0
57	MG	1A	3640	1/1	0.96	0.08	29,29,29,29	0
57	MG	12	102	1/1	0.96	0.06	41,41,41,41	0
57	MG	13	102	1/1	0.96	0.12	39,39,39,39	0
57	MG	2A	3154	1/1	0.96	0.12	60,60,60,60	0
57	MG	1A	3458	1/1	0.96	0.13	33,33,33,33	0
57	MG	1A	4070	1/1	0.96	0.05	31,31,31,31	0
57	MG	2A	3159	1/1	0.96	0.09	40,40,40,40	0
57	MG	1a	1793	1/1	0.96	0.09	60,60,60,60	0
57	MG	1A	3460	1/1	0.96	0.07	46,46,46,46	0
60	ZN	24	501	1/1	0.96	0.08	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
62	PHE	1w	109	11/12	0.96	0.09	17,21,26,26	0
57	MG	1A	3085	1/1	0.96	0.25	31,31,31,31	0
63	FME	2x	107	10/11	0.96	0.10	37,44,50,51	0
57	MG	1R	203	1/1	0.97	0.19	37,37,37,37	0
57	MG	1A	3213	1/1	0.97	0.12	31,31,31,31	0
57	MG	2A	3712	1/1	0.97	0.15	32,32,32,32	0
57	MG	1A	3466	1/1	0.97	0.08	54,54,54,54	0
57	MG	1A	4047	1/1	0.97	0.08	50,50,50,50	0
57	MG	2A	3057	1/1	0.97	0.09	49,49,49,49	0
57	MG	1A	3641	1/1	0.97	0.06	29,29,29,29	0
57	MG	1A	3892	1/1	0.97	0.08	21,21,21,21	0
57	MG	1A	3762	1/1	0.97	0.12	24,24,24,24	0
57	MG	1A	3052	1/1	0.97	0.13	23,23,23,23	0
57	MG	1A	3134	1/1	0.97	0.07	44,44,44,44	0
57	MG	1U	205	1/1	0.97	0.18	37,37,37,37	0
57	MG	1A	4053	1/1	0.97	0.03	19,19,19,19	0
57	MG	2A	3483	1/1	0.97	0.08	39,39,39,39	0
57	MG	2A	3270	1/1	0.97	0.15	56,56,56,56	0
57	MG	1a	1712	1/1	0.97	0.10	55,55,55,55	0
57	MG	2A	3486	1/1	0.97	0.11	40,40,40,40	0
57	MG	1A	3644	1/1	0.97	0.06	33,33,33,33	0
57	MG	1V	201	1/1	0.97	0.11	26,26,26,26	0
57	MG	1A	3332	1/1	0.97	0.06	34,34,34,34	0
57	MG	1V	203	1/1	0.97	0.25	35,35,35,35	0
57	MG	2A	3492	1/1	0.97	0.08	31,31,31,31	0
57	MG	2A	3074	1/1	0.97	0.13	28,28,28,28	0
57	MG	1V	204	1/1	0.97	0.11	25,25,25,25	0
57	MG	1A	3542	1/1	0.97	0.14	25,25,25,25	0
57	MG	2A	3496	1/1	0.97	0.07	37,37,37,37	0
57	MG	2A	3077	1/1	0.97	0.06	46,46,46,46	0
57	MG	1A	3172	1/1	0.97	0.13	32,32,32,32	0
57	MG	2A	3499	1/1	0.97	0.05	45,45,45,45	0
57	MG	1A	3544	1/1	0.97	0.18	31,31,31,31	0
57	MG	1A	3650	1/1	0.97	0.10	46,46,46,46	0
57	MG	2A	3742	1/1	0.97	0.12	67,67,67,67	0
57	MG	1A	3651	1/1	0.97	0.06	26,26,26,26	0
57	MG	2A	3082	1/1	0.97	0.08	48,48,48,48	0
57	MG	2A	3745	1/1	0.97	0.05	54,54,54,54	0
57	MG	1A	3775	1/1	0.97	0.09	55,55,55,55	0
57	MG	2A	3748	1/1	0.97	0.06	49,49,49,49	0
57	MG	1A	3545	1/1	0.97	0.10	27,27,27,27	0
57	MG	1A	3779	1/1	0.97	0.06	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1728	1/1	0.97	0.04	39,39,39,39	0
57	MG	1a	1729	1/1	0.97	0.07	39,39,39,39	0
57	MG	2a	3062	1/1	0.97	0.15	46,46,46,46	0
57	MG	2a	3063	1/1	0.97	0.14	44,44,44,44	0
57	MG	1W	206	1/1	0.97	0.06	45,45,45,45	0
57	MG	2a	3065	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3173	1/1	0.97	0.05	35,35,35,35	0
57	MG	1X	104	1/1	0.97	0.07	43,43,43,43	0
57	MG	1A	3911	1/1	0.97	0.21	56,56,56,56	0
57	MG	1a	1734	1/1	0.97	0.07	42,42,42,42	0
57	MG	1a	1735	1/1	0.97	0.08	48,48,48,48	0
57	MG	2A	3760	1/1	0.97	0.14	50,50,50,50	0
57	MG	1A	3271	1/1	0.97	0.06	37,37,37,37	0
57	MG	1a	1738	1/1	0.97	0.08	47,47,47,47	0
57	MG	1X	107	1/1	0.97	0.06	31,31,31,31	0
57	MG	2A	3518	1/1	0.97	0.08	40,40,40,40	0
57	MG	2A	3519	1/1	0.97	0.10	39,39,39,39	0
57	MG	1A	3782	1/1	0.97	0.07	18,18,18,18	0
57	MG	1A	3218	1/1	0.97	0.04	39,39,39,39	0
57	MG	1a	1742	1/1	0.97	0.07	63,63,63,63	0
57	MG	1A	3273	1/1	0.97	0.07	33,33,33,33	0
57	MG	2a	3081	1/1	0.97	0.13	47,47,47,47	0
57	MG	1A	3917	1/1	0.97	0.06	52,52,52,52	0
57	MG	1A	3275	1/1	0.97	0.11	28,28,28,28	0
57	MG	1A	3090	1/1	0.97	0.07	45,45,45,45	0
57	MG	1A	3921	1/1	0.97	0.05	42,42,42,42	0
57	MG	1A	3660	1/1	0.97	0.05	26,26,26,26	0
57	MG	1A	3277	1/1	0.97	0.10	31,31,31,31	0
57	MG	1A	3927	1/1	0.97	0.04	28,28,28,28	0
57	MG	1A	3280	1/1	0.97	0.19	39,39,39,39	0
57	MG	1A	3665	1/1	0.97	0.09	18,18,18,18	0
57	MG	2A	3780	1/1	0.97	0.05	32,32,32,32	0
57	MG	1A	3666	1/1	0.97	0.09	24,24,24,24	0
57	MG	2A	3782	1/1	0.97	0.08	40,40,40,40	0
57	MG	2A	3783	1/1	0.97	0.07	34,34,34,34	0
57	MG	2a	3095	1/1	0.97	0.06	55,55,55,55	0
57	MG	2A	3536	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3558	1/1	0.97	0.07	20,20,20,20	0
57	MG	1A	3796	1/1	0.97	0.06	19,19,19,19	0
57	MG	1A	3136	1/1	0.97	0.07	29,29,29,29	0
57	MG	2A	3115	1/1	0.97	0.08	30,30,30,30	0
57	MG	1A	4085	1/1	0.97	0.11	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3798	1/1	0.97	0.04	41,41,41,41	0
57	MG	1A	3799	1/1	0.97	0.05	26,26,26,26	0
57	MG	1A	3942	1/1	0.97	0.05	56,56,56,56	0
57	MG	1A	3800	1/1	0.97	0.27	23,23,23,23	0
57	MG	1A	4093	1/1	0.97	0.05	53,53,53,53	0
57	MG	1A	3177	1/1	0.97	0.11	37,37,37,37	0
57	MG	1A	3414	1/1	0.97	0.07	48,48,48,48	0
57	MG	1a	1770	1/1	0.97	0.07	61,61,61,61	0
57	MG	1A	3673	1/1	0.97	0.08	50,50,50,50	0
57	MG	1A	3804	1/1	0.97	0.08	44,44,44,44	0
57	MG	2a	3112	1/1	0.97	0.16	40,40,40,40	0
57	MG	1A	3948	1/1	0.97	0.05	47,47,47,47	0
57	MG	1A	3137	1/1	0.97	0.07	14,14,14,14	0
57	MG	1a	1779	1/1	0.97	0.06	41,41,41,41	0
57	MG	2A	3806	1/1	0.97	0.06	62,62,62,62	0
57	MG	1A	3565	1/1	0.97	0.09	40,40,40,40	0
57	MG	1a	1783	1/1	0.97	0.08	71,71,71,71	0
57	MG	1a	1785	1/1	0.97	0.08	81,81,81,81	0
57	MG	2A	3134	1/1	0.97	0.14	37,37,37,37	0
57	MG	1A	3676	1/1	0.97	0.06	20,20,20,20	0
57	MG	2A	3136	1/1	0.97	0.21	38,38,38,38	0
57	MG	1A	3111	1/1	0.97	0.05	32,32,32,32	0
57	MG	2A	3815	1/1	0.97	0.11	39,39,39,39	0
57	MG	1a	1788	1/1	0.97	0.06	64,64,64,64	0
57	MG	1A	3678	1/1	0.97	0.06	22,22,22,22	0
57	MG	2A	3818	1/1	0.97	0.07	53,53,53,53	0
57	MG	1A	3180	1/1	0.97	0.07	48,48,48,48	0
57	MG	2a	3129	1/1	0.97	0.06	51,51,51,51	0
57	MG	2A	3820	1/1	0.97	0.04	57,57,57,57	0
57	MG	1A	3680	1/1	0.97	0.06	21,21,21,21	0
57	MG	17	103	1/1	0.97	0.10	38,38,38,38	0
57	MG	1A	3681	1/1	0.97	0.06	24,24,24,24	0
57	MG	1A	3958	1/1	0.97	0.08	23,23,23,23	0
57	MG	1A	3091	1/1	0.97	0.07	23,23,23,23	0
57	MG	1A	3814	1/1	0.97	0.03	30,30,30,30	0
57	MG	1A	3573	1/1	0.97	0.08	39,39,39,39	0
57	MG	1A	3420	1/1	0.97	0.07	39,39,39,39	0
57	MG	1A	3817	1/1	0.97	0.06	33,33,33,33	0
57	MG	2a	3143	1/1	0.97	0.15	52,52,52,52	0
57	MG	2a	3145	1/1	0.97	0.07	61,61,61,61	0
57	MG	1B	204	1/1	0.97	0.17	49,49,49,49	0
57	MG	1A	3576	1/1	0.97	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
57	MG	1A	3488	1/1	0.97	0.22	28,28,28,28	0
57	MG	1a	1606	1/1	0.97	0.09	45,45,45,45	0
57	MG	1A	3489	1/1	0.97	0.11	28,28,28,28	0
57	MG	1A	3688	1/1	0.97	0.05	35,35,35,35	0
57	MG	2A	3156	1/1	0.97	0.06	48,48,48,48	0
57	MG	2A	3837	1/1	0.97	0.13	54,54,54,54	0
57	MG	1A	3113	1/1	0.97	0.11	40,40,40,40	0
57	MG	2A	3158	1/1	0.97	0.12	53,53,53,53	0
57	MG	1a	1610	1/1	0.97	0.07	50,50,50,50	0
57	MG	1A	3288	1/1	0.97	0.18	23,23,23,23	0
57	MG	1A	3141	1/1	0.97	0.14	27,27,27,27	0
57	MG	1a	1613	1/1	0.97	0.09	28,28,28,28	0
57	MG	1A	3583	1/1	0.97	0.21	30,30,30,30	0
57	MG	1A	3142	1/1	0.97	0.11	31,31,31,31	0
57	MG	2A	3593	1/1	0.97	0.05	35,35,35,35	0
57	MG	1A	3233	1/1	0.97	0.10	30,30,30,30	0
57	MG	1A	3234	1/1	0.97	0.07	47,47,47,47	0
57	MG	1A	3696	1/1	0.97	0.06	12,12,12,12	0
57	MG	1A	3697	1/1	0.97	0.07	43,43,43,43	0
57	MG	1A	3356	1/1	0.97	0.14	38,38,38,38	0
57	MG	1A	3235	1/1	0.97	0.07	28,28,28,28	0
57	MG	1A	3700	1/1	0.97	0.05	30,30,30,30	0
57	MG	2A	3172	1/1	0.97	0.09	29,29,29,29	0
57	MG	1A	3981	1/1	0.97	0.08	28,28,28,28	0
57	MG	2A	3605	1/1	0.97	0.14	43,43,43,43	0
57	MG	1A	3236	1/1	0.97	0.10	33,33,33,33	0
57	MG	1A	3359	1/1	0.97	0.18	40,40,40,40	0
57	MG	2A	3608	1/1	0.97	0.07	37,37,37,37	0
57	MG	1A	3186	1/1	0.97	0.14	36,36,36,36	0
57	MG	2A	3610	1/1	0.97	0.06	50,50,50,50	0
57	MG	1m	3001	1/1	0.97	0.09	45,45,45,45	0
57	MG	2A	3178	1/1	0.97	0.08	44,44,44,44	0
57	MG	1A	3239	1/1	0.97	0.12	43,43,43,43	0
57	MG	1A	3028	1/1	0.97	0.22	26,26,26,26	0
57	MG	1A	3045	1/1	0.97	0.08	32,32,32,32	0
57	MG	2A	3385	1/1	0.97	0.09	55,55,55,55	0
57	MG	1A	3242	1/1	0.97	0.09	44,44,44,44	0
57	MG	1A	3506	1/1	0.97	0.22	37,37,37,37	0
57	MG	1A	3843	1/1	0.97	0.15	40,40,40,40	0
57	MG	1A	3146	1/1	0.97	0.17	31,31,31,31	0
57	MG	1A	3845	1/1	0.97	0.12	37,37,37,37	0
57	MG	1a	1636	1/1	0.97	0.09	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3994	1/1	0.97	0.22	25,25,25,25	0
57	MG	1D	301	1/1	0.97	0.10	27,27,27,27	0
57	MG	1A	3147	1/1	0.97	0.14	32,32,32,32	0
57	MG	2a	3194	1/1	0.97	0.20	51,51,51,51	0
57	MG	1A	3712	1/1	0.97	0.16	42,42,42,42	0
57	MG	1D	304	1/1	0.97	0.07	19,19,19,19	0
57	MG	1A	3046	1/1	0.97	0.04	24,24,24,24	0
57	MG	1A	3007	1/1	0.97	0.04	33,33,33,33	0
57	MG	2A	3630	1/1	0.97	0.09	48,48,48,48	0
57	MG	1A	3069	1/1	0.97	0.09	21,21,21,21	0
57	MG	1A	3717	1/1	0.97	0.08	49,49,49,49	0
57	MG	1A	3852	1/1	0.97	0.25	33,33,33,33	0
57	MG	1A	3197	1/1	0.97	0.06	33,33,33,33	0
57	MG	1A	3030	1/1	0.97	0.13	26,26,26,26	0
57	MG	1A	3121	1/1	0.97	0.25	33,33,33,33	0
57	MG	2A	3201	1/1	0.97	0.08	51,51,51,51	0
57	MG	1A	3722	1/1	0.97	0.07	38,38,38,38	0
57	MG	2A	3639	1/1	0.97	0.08	44,44,44,44	0
57	MG	2A	3641	1/1	0.97	0.09	39,39,39,39	0
57	MG	1A	3155	1/1	0.97	0.11	26,26,26,26	0
57	MG	1A	3201	1/1	0.97	0.05	30,30,30,30	0
57	MG	1A	3314	1/1	0.97	0.07	39,39,39,39	0
57	MG	2A	3206	1/1	0.97	0.06	53,53,53,53	0
57	MG	1A	3005	1/1	0.97	0.07	45,45,45,45	0
57	MG	1x	114	1/1	0.97	0.12	45,45,45,45	0
57	MG	1F	301	1/1	0.97	0.10	32,32,32,32	0
57	MG	2A	3415	1/1	0.97	0.15	42,42,42,42	0
57	MG	1A	3254	1/1	0.97	0.05	34,34,34,34	0
57	MG	2A	3651	1/1	0.97	0.09	38,38,38,38	0
57	MG	1A	3730	1/1	0.97	0.04	38,38,38,38	0
57	MG	1A	4015	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3158	1/1	0.97	0.24	31,31,31,31	0
57	MG	2A	3005	1/1	0.97	0.07	36,36,36,36	0
57	MG	2A	3006	1/1	0.97	0.11	52,52,52,52	0
57	MG	1A	3101	1/1	0.97	0.05	26,26,26,26	0
57	MG	1F	310	1/1	0.97	0.14	26,26,26,26	0
57	MG	2A	3010	1/1	0.97	0.12	38,38,38,38	0
57	MG	2A	3011	1/1	0.97	0.05	44,44,44,44	0
57	MG	1A	3522	1/1	0.97	0.24	39,39,39,39	0
57	MG	1A	3616	1/1	0.97	0.09	30,30,30,30	0
57	MG	1A	3736	1/1	0.97	0.08	31,31,31,31	0
57	MG	2A	3664	1/1	0.97	0.05	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1G	201	1/1	0.97	0.15	44,44,44,44	0
57	MG	1A	3523	1/1	0.97	0.20	32,32,32,32	0
57	MG	1A	3102	1/1	0.97	0.14	36,36,36,36	0
57	MG	2A	3433	1/1	0.97	0.19	45,45,45,45	0
57	MG	1A	3619	1/1	0.97	0.08	22,22,22,22	0
57	MG	1A	3871	1/1	0.97	0.13	32,32,32,32	0
57	MG	1A	3074	1/1	0.97	0.04	31,31,31,31	0
57	MG	2A	3672	1/1	0.97	0.05	56,56,56,56	0
57	MG	1A	3321	1/1	0.97	0.06	31,31,31,31	0
57	MG	2f	201	1/1	0.97	0.13	39,39,39,39	0
57	MG	1A	3389	1/1	0.97	0.04	27,27,27,27	0
57	MG	23	101	1/1	0.97	0.11	50,50,50,50	0
57	MG	23	102	1/1	0.97	0.05	49,49,49,49	0
57	MG	1A	3456	1/1	0.97	0.16	40,40,40,40	0
57	MG	2A	3026	1/1	0.97	0.16	42,42,42,42	0
57	MG	2A	3442	1/1	0.97	0.12	68,68,68,68	0
57	MG	1a	1676	1/1	0.97	0.07	60,60,60,60	0
57	MG	1N	204	1/1	0.97	0.05	27,27,27,27	0
57	MG	1a	1678	1/1	0.97	0.08	59,59,59,59	0
57	MG	1A	3745	1/1	0.97	0.05	44,44,44,44	0
57	MG	1A	3627	1/1	0.97	0.09	32,32,32,32	0
57	MG	27	101	1/1	0.97	0.12	38,38,38,38	0
57	MG	1A	3628	1/1	0.97	0.06	19,19,19,19	0
57	MG	1A	3163	1/1	0.97	0.05	25,25,25,25	0
57	MG	1O	202	1/1	0.97	0.09	43,43,43,43	0
57	MG	1A	4035	1/1	0.97	0.11	32,32,32,32	0
57	MG	1A	3530	1/1	0.97	0.05	27,27,27,27	0
57	MG	1A	3105	1/1	0.97	0.29	41,41,41,41	0
57	MG	1A	3017	1/1	0.97	0.06	44,44,44,44	0
57	MG	2A	3692	1/1	0.97	0.11	43,43,43,43	0
57	MG	2A	3041	1/1	0.97	0.12	67,67,67,67	0
57	MG	2A	3694	1/1	0.97	0.06	33,33,33,33	0
57	MG	1A	3262	1/1	0.97	0.10	38,38,38,38	0
57	MG	1P	204	1/1	0.97	0.30	29,29,29,29	0
57	MG	2A	3698	1/1	0.97	0.08	52,52,52,52	0
57	MG	1P	205	1/1	0.97	0.22	23,23,23,23	0
57	MG	1P	206	1/1	0.97	0.08	39,39,39,39	0
57	MG	1Q	201	1/1	0.97	0.06	29,29,29,29	0
57	MG	2A	3461	1/1	0.97	0.13	40,40,40,40	0
57	MG	1Q	202	1/1	0.97	0.04	37,37,37,37	0
58	K	2A	3432	1/1	0.97	0.06	49,49,49,49	0
57	MG	1A	3129	1/1	0.97	0.04	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1Q	204	1/1	0.97	0.04	49,49,49,49	0
57	MG	1A	3061	1/1	0.97	0.08	25,25,25,25	0
57	MG	1A	3328	1/1	0.97	0.11	41,41,41,41	0
57	MG	1A	3638	1/1	0.97	0.05	26,26,26,26	0
63	FME	1x	115	10/11	0.97	0.13	16,19,24,30	10
57	MG	2A	3468	1/1	0.97	0.14	40,40,40,40	0
57	MG	1A	3734	1/1	0.98	0.04	47,47,47,47	0
57	MG	2O	201	1/1	0.98	0.08	55,55,55,55	0
57	MG	1A	3662	1/1	0.98	0.05	28,28,28,28	0
57	MG	1a	1743	1/1	0.98	0.06	52,52,52,52	0
57	MG	1a	1744	1/1	0.98	0.05	45,45,45,45	0
57	MG	1A	3104	1/1	0.98	0.04	27,27,27,27	0
57	MG	2A	3747	1/1	0.98	0.05	50,50,50,50	0
57	MG	1A	4087	1/1	0.98	0.05	44,44,44,44	0
57	MG	1a	1747	1/1	0.98	0.05	50,50,50,50	0
57	MG	1A	3896	1/1	0.98	0.05	41,41,41,41	0
57	MG	1A	3269	1/1	0.98	0.08	30,30,30,30	0
57	MG	2A	3599	1/1	0.98	0.08	56,56,56,56	0
57	MG	2A	3031	1/1	0.98	0.13	33,33,33,33	0
57	MG	1A	3174	1/1	0.98	0.06	28,28,28,28	0
57	MG	2a	3130	1/1	0.98	0.04	72,72,72,72	0
57	MG	1A	4092	1/1	0.98	0.04	31,31,31,31	0
57	MG	2A	3603	1/1	0.98	0.09	32,32,32,32	0
57	MG	1A	3667	1/1	0.98	0.05	20,20,20,20	0
57	MG	1A	3740	1/1	0.98	0.07	50,50,50,50	0
57	MG	1P	202	1/1	0.98	0.13	28,28,28,28	0
57	MG	1A	3039	1/1	0.98	0.28	32,32,32,32	0
57	MG	1A	3022	1/1	0.98	0.06	40,40,40,40	0
57	MG	2X	102	1/1	0.98	0.12	42,42,42,42	0
57	MG	1A	3670	1/1	0.98	0.03	18,18,18,18	0
57	MG	1A	3107	1/1	0.98	0.32	30,30,30,30	0
57	MG	1A	3311	1/1	0.98	0.15	26,26,26,26	0
57	MG	1A	3051	1/1	0.98	0.11	22,22,22,22	0
57	MG	1A	3604	1/1	0.98	0.05	26,26,26,26	0
57	MG	1A	3151	1/1	0.98	0.07	40,40,40,40	0
57	MG	1A	3064	1/1	0.98	0.13	37,37,37,37	0
57	MG	1A	3278	1/1	0.98	0.17	25,25,25,25	0
57	MG	2a	3150	1/1	0.98	0.08	60,60,60,60	0
57	MG	1R	201	1/1	0.98	0.11	28,28,28,28	0
57	MG	1A	3279	1/1	0.98	0.15	32,32,32,32	0
57	MG	1A	3008	1/1	0.98	0.11	18,18,18,18	0
57	MG	2A	3774	1/1	0.98	0.09	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1R	204	1/1	0.98	0.26	38,38,38,38	0
57	MG	1A	3835	1/1	0.98	0.08	29,29,29,29	0
57	MG	1S	201	1/1	0.98	0.10	34,34,34,34	0
57	MG	1A	3130	1/1	0.98	0.06	31,31,31,31	0
57	MG	1a	1774	1/1	0.98	0.05	68,68,68,68	0
57	MG	1a	1775	1/1	0.98	0.05	54,54,54,54	0
57	MG	1a	1776	1/1	0.98	0.05	52,52,52,52	0
57	MG	1A	3032	1/1	0.98	0.18	21,21,21,21	0
57	MG	28	102	1/1	0.98	0.06	42,42,42,42	0
57	MG	1A	3920	1/1	0.98	0.06	35,35,35,35	0
57	MG	1a	1649	1/1	0.98	0.14	44,44,44,44	0
57	MG	1a	1782	1/1	0.98	0.04	39,39,39,39	0
57	MG	1A	3184	1/1	0.98	0.20	38,38,38,38	0
57	MG	1U	201	1/1	0.98	0.13	27,27,27,27	0
57	MG	1A	3095	1/1	0.98	0.04	34,34,34,34	0
57	MG	2A	3065	1/1	0.98	0.06	28,28,28,28	0
57	MG	2A	3066	1/1	0.98	0.08	50,50,50,50	0
57	MG	1A	3923	1/1	0.98	0.05	12,12,12,12	0
57	MG	2A	3792	1/1	0.98	0.04	41,41,41,41	0
57	MG	2A	3793	1/1	0.98	0.04	56,56,56,56	0
57	MG	1B	205	1/1	0.98	0.05	40,40,40,40	0
57	MG	2A	3343	1/1	0.98	0.07	53,53,53,53	0
57	MG	1B	206	1/1	0.98	0.04	46,46,46,46	0
57	MG	2A	3640	1/1	0.98	0.06	58,58,58,58	0
57	MG	1a	1790	1/1	0.98	0.04	58,58,58,58	0
57	MG	1A	3451	1/1	0.98	0.11	50,50,50,50	0
57	MG	2A	3072	1/1	0.98	0.10	37,37,37,37	0
57	MG	2A	3073	1/1	0.98	0.07	39,39,39,39	0
57	MG	1A	3925	1/1	0.98	0.03	51,51,51,51	0
57	MG	1A	3404	1/1	0.98	0.10	31,31,31,31	0
57	MG	1A	3928	1/1	0.98	0.07	24,24,24,24	0
57	MG	1A	3929	1/1	0.98	0.09	51,51,51,51	0
57	MG	1A	3930	1/1	0.98	0.06	29,29,29,29	0
57	MG	1A	3931	1/1	0.98	0.03	46,46,46,46	0
57	MG	1A	3502	1/1	0.98	0.23	44,44,44,44	0
57	MG	1B	215	1/1	0.98	0.05	46,46,46,46	0
57	MG	1A	3933	1/1	0.98	0.05	43,43,43,43	0
57	MG	2A	3812	1/1	0.98	0.04	48,48,48,48	0
57	MG	1A	4027	1/1	0.98	0.05	37,37,37,37	0
57	MG	1A	3360	1/1	0.98	0.14	48,48,48,48	0
57	MG	1A	3556	1/1	0.98	0.04	27,27,27,27	0
57	MG	1A	3620	1/1	0.98	0.04	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3621	1/1	0.98	0.03	25,25,25,25	0
57	MG	2A	3088	1/1	0.98	0.20	43,43,43,43	0
57	MG	1X	102	1/1	0.98	0.28	37,37,37,37	0
57	MG	1A	3557	1/1	0.98	0.09	31,31,31,31	0
57	MG	1A	3939	1/1	0.98	0.04	43,43,43,43	0
57	MG	1A	3406	1/1	0.98	0.13	37,37,37,37	0
57	MG	1A	3157	1/1	0.98	0.04	27,27,27,27	0
57	MG	1A	3133	1/1	0.98	0.25	34,34,34,34	0
57	MG	1A	3096	1/1	0.98	0.15	21,21,21,21	0
57	MG	1A	3190	1/1	0.98	0.27	38,38,38,38	0
57	MG	1a	1815	1/1	0.98	0.11	54,54,54,54	0
57	MG	1A	3774	1/1	0.98	0.05	45,45,45,45	0
57	MG	1A	4040	1/1	0.98	0.06	36,36,36,36	0
57	MG	2A	3521	1/1	0.98	0.10	28,28,28,28	0
57	MG	2A	3522	1/1	0.98	0.07	35,35,35,35	0
57	MG	1A	3564	1/1	0.98	0.10	42,42,42,42	0
57	MG	1A	3459	1/1	0.98	0.09	37,37,37,37	0
57	MG	1A	3566	1/1	0.98	0.16	31,31,31,31	0
57	MG	1A	3567	1/1	0.98	0.29	34,34,34,34	0
57	MG	1A	3568	1/1	0.98	0.06	41,41,41,41	0
57	MG	1A	3016	1/1	0.98	0.17	45,45,45,45	0
57	MG	1A	3115	1/1	0.98	0.08	35,35,35,35	0
57	MG	10	106	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3784	1/1	0.98	0.07	44,44,44,44	0
57	MG	1A	3571	1/1	0.98	0.10	34,34,34,34	0
57	MG	1A	3955	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	3225	1/1	0.98	0.08	27,27,27,27	0
57	MG	1D	306	1/1	0.98	0.05	29,29,29,29	0
57	MG	1D	307	1/1	0.98	0.13	33,33,33,33	0
57	MG	1D	308	1/1	0.98	0.17	46,46,46,46	0
57	MG	1A	3787	1/1	0.98	0.04	18,18,18,18	0
57	MG	1A	3083	1/1	0.98	0.10	25,25,25,25	0
57	MG	2A	3253	1/1	0.98	0.05	47,47,47,47	0
57	MG	1D	311	1/1	0.98	0.05	39,39,39,39	0
57	MG	1A	3574	1/1	0.98	0.12	37,37,37,37	0
57	MG	1a	1700	1/1	0.98	0.13	36,36,36,36	0
57	MG	1A	3293	1/1	0.98	0.13	35,35,35,35	0
57	MG	1E	304	1/1	0.98	0.13	30,30,30,30	0
57	MG	1A	4056	1/1	0.98	0.05	40,40,40,40	0
57	MG	2A	3123	1/1	0.98	0.12	50,50,50,50	0
57	MG	2A	3401	1/1	0.98	0.28	59,59,59,59	0
57	MG	1E	306	1/1	0.98	0.04	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3044	1/1	0.98	0.06	35,35,35,35	0
57	MG	1a	1706	1/1	0.98	0.08	32,32,32,32	0
57	MG	1A	3710	1/1	0.98	0.09	30,30,30,30	0
57	MG	1A	3295	1/1	0.98	0.10	30,30,30,30	0
57	MG	1E	310	1/1	0.98	0.08	19,19,19,19	0
57	MG	1A	3009	1/1	0.98	0.04	18,18,18,18	0
57	MG	1A	3373	1/1	0.98	0.14	24,24,24,24	0
57	MG	16	103	1/1	0.98	0.09	38,38,38,38	0
57	MG	2A	3559	1/1	0.98	0.07	62,62,62,62	0
57	MG	1A	3196	1/1	0.98	0.15	22,22,22,22	0
57	MG	1A	3715	1/1	0.98	0.05	18,18,18,18	0
57	MG	1A	3166	1/1	0.98	0.07	14,14,14,14	0
57	MG	2A	3564	1/1	0.98	0.04	33,33,33,33	0
57	MG	1A	3376	1/1	0.98	0.05	44,44,44,44	0
57	MG	2A	3274	1/1	0.98	0.10	53,53,53,53	0
57	MG	1A	3649	1/1	0.98	0.07	38,38,38,38	0
57	MG	1A	3472	1/1	0.98	0.09	41,41,41,41	0
57	MG	1F	305	1/1	0.98	0.06	36,36,36,36	0
57	MG	1A	3010	1/1	0.98	0.07	25,25,25,25	0
57	MG	19	102	1/1	0.98	0.18	33,33,33,33	0
57	MG	1F	307	1/1	0.98	0.09	28,28,28,28	0
57	MG	1F	308	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3973	1/1	0.98	0.04	33,33,33,33	0
57	MG	2D	303	1/1	0.98	0.07	28,28,28,28	0
57	MG	2D	304	1/1	0.98	0.15	36,36,36,36	0
57	MG	1A	3721	1/1	0.98	0.07	42,42,42,42	0
57	MG	1A	3337	1/1	0.98	0.24	33,33,33,33	0
57	MG	1A	3379	1/1	0.98	0.08	31,31,31,31	0
57	MG	1A	3724	1/1	0.98	0.04	20,20,20,20	0
57	MG	1A	3011	1/1	0.98	0.04	36,36,36,36	0
57	MG	1A	3038	1/1	0.98	0.15	27,27,27,27	0
57	MG	1A	3340	1/1	0.98	0.16	31,31,31,31	0
57	MG	1A	3383	1/1	0.98	0.29	38,38,38,38	0
57	MG	1A	3658	1/1	0.98	0.08	37,37,37,37	0
58	K	1A	3553	1/1	0.98	0.04	36,36,36,36	0
57	MG	2A	3434	1/1	0.98	0.10	21,21,21,21	0
57	MG	1A	3983	1/1	0.98	0.04	22,22,22,22	0
57	MG	2A	3017	1/1	0.98	0.09	24,24,24,24	0
60	ZN	1n	103	1/1	0.98	0.03	56,56,56,56	0
60	ZN	2Y	202	1/1	0.98	0.04	83,83,83,83	0
57	MG	1A	3143	1/1	0.98	0.06	31,31,31,31	0
60	ZN	29	102	1/1	0.98	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
60	ZN	2n	501	1/1	0.98	0.05	85,85,85,85	0
61	SF4	1d	302	8/8	0.98	0.05	59,62,66,68	0
57	MG	1A	3122	1/1	0.98	0.14	34,34,34,34	0
57	MG	2A	3740	1/1	0.98	0.07	46,46,46,46	0
57	MG	2F	307	1/1	0.98	0.13	45,45,45,45	0
57	MG	1A	3386	1/1	0.98	0.07	52,52,52,52	0
57	MG	1E	301	1/1	0.99	0.13	30,30,30,30	0
57	MG	1A	3219	1/1	0.99	0.06	34,34,34,34	0
57	MG	2A	3487	1/1	0.99	0.06	39,39,39,39	0
57	MG	1E	303	1/1	0.99	0.15	31,31,31,31	0
57	MG	1A	3559	1/1	0.99	0.10	34,34,34,34	0
57	MG	1a	1633	1/1	0.99	0.15	24,24,24,24	0
57	MG	1A	4009	1/1	0.99	0.04	30,30,30,30	0
57	MG	1A	4059	1/1	0.99	0.08	29,29,29,29	0
57	MG	13	101	1/1	0.99	0.07	27,27,27,27	0
57	MG	1A	3018	1/1	0.99	0.08	20,20,20,20	0
57	MG	1A	3014	1/1	0.99	0.03	21,21,21,21	0
57	MG	1a	1765	1/1	0.99	0.05	50,50,50,50	0
57	MG	1A	3003	1/1	0.99	0.05	23,23,23,23	0
57	MG	1A	3171	1/1	0.99	0.21	31,31,31,31	0
57	MG	15	3201	1/1	0.99	0.12	25,25,25,25	0
57	MG	1A	3592	1/1	0.99	0.11	37,37,37,37	0
57	MG	1A	3623	1/1	0.99	0.04	17,17,17,17	0
57	MG	15	3204	1/1	0.99	0.19	25,25,25,25	0
57	MG	1A	3224	1/1	0.99	0.08	24,24,24,24	0
57	MG	1A	3188	1/1	0.99	0.17	27,27,27,27	0
57	MG	1A	3226	1/1	0.99	0.08	33,33,33,33	0
57	MG	1a	1648	1/1	0.99	0.10	39,39,39,39	0
57	MG	2a	3135	1/1	0.99	0.03	57,57,57,57	0
57	MG	1A	3926	1/1	0.99	0.04	32,32,32,32	0
57	MG	1a	1777	1/1	0.99	0.09	51,51,51,51	0
57	MG	2a	3138	1/1	0.99	0.05	55,55,55,55	0
57	MG	1A	3881	1/1	0.99	0.05	48,48,48,48	0
57	MG	2A	3358	1/1	0.99	0.04	42,42,42,42	0
57	MG	1A	3725	1/1	0.99	0.03	23,23,23,23	0
57	MG	1A	3021	1/1	0.99	0.09	21,21,21,21	0
57	MG	1a	1781	1/1	0.99	0.04	62,62,62,62	0
57	MG	2a	3144	1/1	0.99	0.02	51,51,51,51	0
57	MG	1A	3037	1/1	0.99	0.13	20,20,20,20	0
57	MG	1A	4024	1/1	0.99	0.03	25,25,25,25	0
57	MG	2A	3756	1/1	0.99	0.03	47,47,47,47	0
57	MG	1a	1784	1/1	0.99	0.04	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3416	1/1	0.99	0.13	37,37,37,37	0
57	MG	1A	3296	1/1	0.99	0.04	22,22,22,22	0
57	MG	1A	3208	1/1	0.99	0.13	30,30,30,30	0
57	MG	1a	1719	1/1	0.99	0.04	35,35,35,35	0
57	MG	1A	3664	1/1	0.99	0.05	37,37,37,37	0
57	MG	1a	1721	1/1	0.99	0.07	40,40,40,40	0
57	MG	1a	1791	1/1	0.99	0.04	63,63,63,63	0
57	MG	1A	3768	1/1	0.99	0.03	30,30,30,30	0
57	MG	1A	3274	1/1	0.99	0.09	20,20,20,20	0
57	MG	1A	3056	1/1	0.99	0.03	27,27,27,27	0
57	MG	2A	3009	1/1	0.99	0.08	42,42,42,42	0
57	MG	1A	3634	1/1	0.99	0.04	12,12,12,12	0
57	MG	2A	3688	1/1	0.99	0.03	48,48,48,48	0
57	MG	1A	3772	1/1	0.99	0.03	20,20,20,20	0
57	MG	2A	3855	1/1	0.99	0.03	59,59,59,59	0
57	MG	1W	203	1/1	0.99	0.10	31,31,31,31	0
57	MG	2A	3857	1/1	0.99	0.05	41,41,41,41	0
57	MG	1A	3159	1/1	0.99	0.17	47,47,47,47	0
57	MG	1A	3067	1/1	0.99	0.07	26,26,26,26	0
57	MG	1A	3548	1/1	0.99	0.06	40,40,40,40	0
57	MG	1X	101	1/1	0.99	0.03	29,29,29,29	0
57	MG	1A	3012	1/1	0.99	0.03	27,27,27,27	0
57	MG	1A	4088	1/1	0.99	0.06	40,40,40,40	0
57	MG	2A	3697	1/1	0.99	0.07	38,38,38,38	0
57	MG	1A	3777	1/1	0.99	0.03	58,58,58,58	0
57	MG	1A	3778	1/1	0.99	0.05	39,39,39,39	0
57	MG	1A	3023	1/1	0.99	0.04	12,12,12,12	0
57	MG	1a	1737	1/1	0.99	0.17	42,42,42,42	0
57	MG	2A	3023	1/1	0.99	0.12	32,32,32,32	0
57	MG	1A	3579	1/1	0.99	0.04	37,37,37,37	0
57	MG	1A	3070	1/1	0.99	0.08	13,13,13,13	0
57	MG	1A	3610	1/1	0.99	0.04	29,29,29,29	0
57	MG	1A	3995	1/1	0.99	0.07	17,17,17,17	0
57	MG	1A	3996	1/1	0.99	0.03	32,32,32,32	0
57	MG	2A	3470	1/1	0.99	0.04	61,61,61,61	0
57	MG	1A	3031	1/1	0.99	0.09	31,31,31,31	0
57	MG	2A	3472	1/1	0.99	0.10	56,56,56,56	0
57	MG	1A	3906	1/1	0.99	0.04	31,31,31,31	0
57	MG	1A	3907	1/1	0.99	0.04	28,28,28,28	0
57	MG	1A	3237	1/1	0.99	0.18	28,28,28,28	0
57	MG	1A	3150	1/1	0.99	0.10	33,33,33,33	0
60	ZN	1Y	203	1/1	0.99	0.02	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	ZN	14	102	1/1	0.99	0.04	83,83,83,83	0
60	ZN	16	104	1/1	0.99	0.07	51,51,51,51	0
57	MG	2A	3034	1/1	0.99	0.07	21,21,21,21	0
57	MG	1A	3072	1/1	0.99	0.04	13,13,13,13	0
57	MG	1A	3747	1/1	0.99	0.05	13,13,13,13	0
60	ZN	25	108	1/1	0.99	0.03	61,61,61,61	0
60	ZN	26	102	1/1	0.99	0.04	60,60,60,60	0
57	MG	2A	3557	1/1	0.99	0.06	33,33,33,33	0
57	MG	1A	3788	1/1	0.99	0.04	16,16,16,16	0
57	MG	1A	3013	1/1	0.99	0.07	22,22,22,22	0
61	SF4	2d	303	8/8	0.99	0.04	62,66,72,77	0
57	MG	1a	1752	1/1	0.99	0.05	47,47,47,47	0
57	MG	1A	3914	1/1	0.99	0.07	37,37,37,37	0
57	MG	1D	313	1/1	0.99	0.16	29,29,29,29	0
57	MG	2A	3563	1/1	0.99	0.06	33,33,33,33	0
57	MG	2A	3680	1/1	1.00	0.03	27,27,27,27	0
57	MG	1A	3754	1/1	1.00	0.08	35,35,35,35	0
60	ZN	15	3209	1/1	1.00	0.02	45,45,45,45	0
57	MG	2A	3802	1/1	1.00	0.05	28,28,28,28	0
60	ZN	19	103	1/1	1.00	0.06	41,41,41,41	0
57	MG	1A	3901	1/1	1.00	0.04	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.