Full wwPDB X-ray Structure Validation Report (i)

Mar 6, 2026 – 09:33 AM UTC

PDB ID	:	8CVJ / pdb_00008cvj
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with mRNA, aminoacylated A-site Phe-NH-tRNAphe, peptidyl P-site fMSEAC-NH-tRNAmet, and deacylated E-site tRNAphe at 2.40A resolution
Authors	:	Syroegin, E.A.; Aleksandrova, E.V.; Polikanov, Y.S.
Deposited on	:	2022-05-18
Resolution	:	2.40 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:

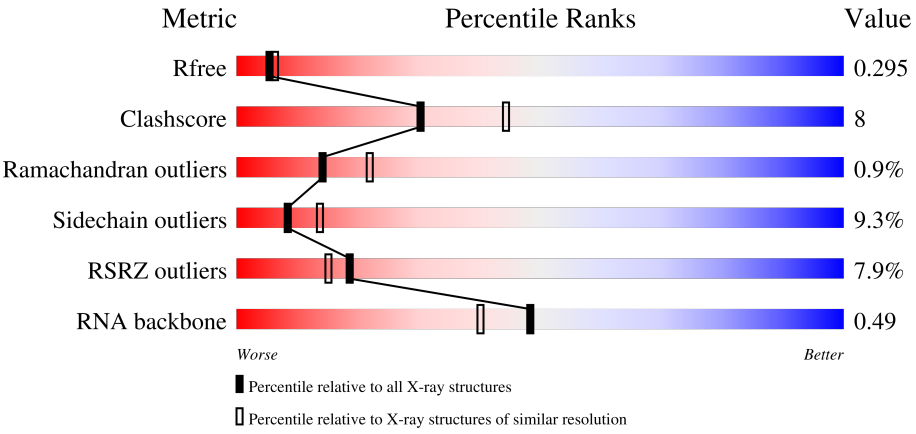
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)
RNA backbone	3983	1155 (2.70-2.10)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	6% 66% 26% 6% ·
1	2A	2915	5% 59% 31% 6% ·
2	1B	121	72% 27% ·
2	2B	121	2% 52% 40% 7% ·

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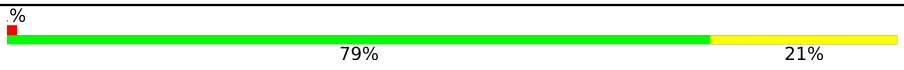
Mol	Chain	Length	Quality of chain
3	1D	276	
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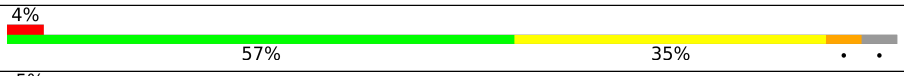
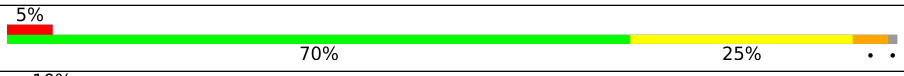
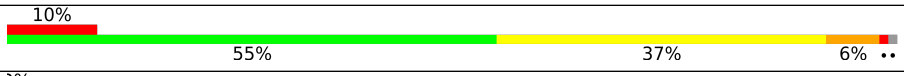
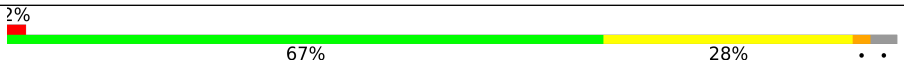
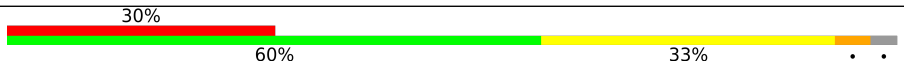
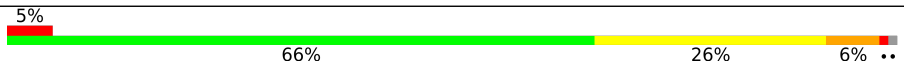
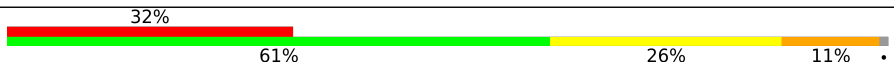
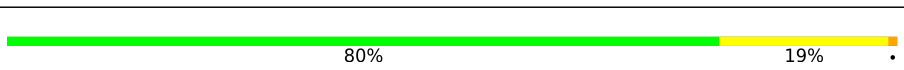
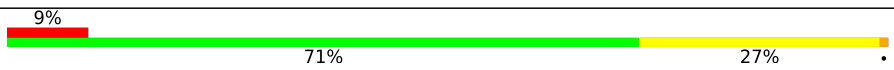
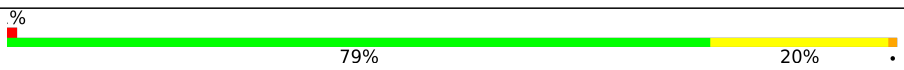
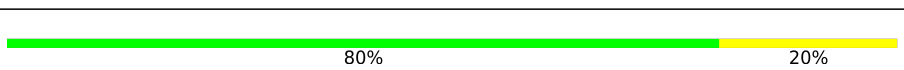
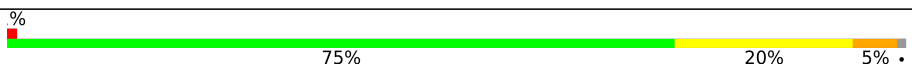
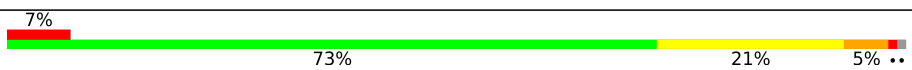
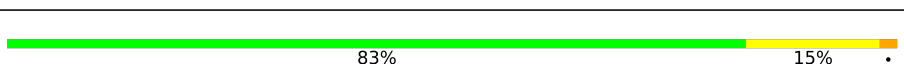
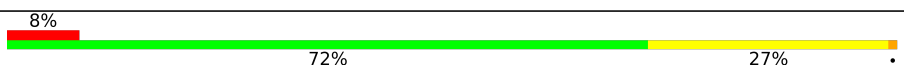
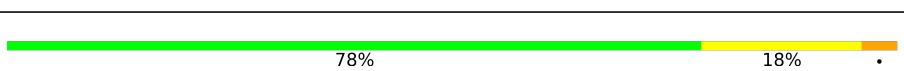
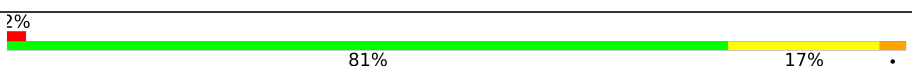
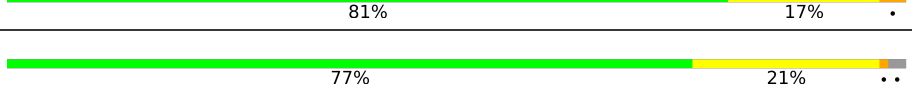
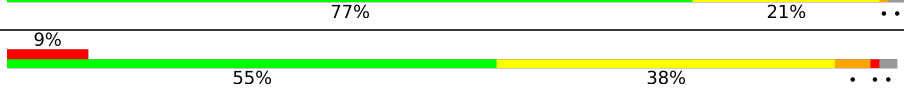
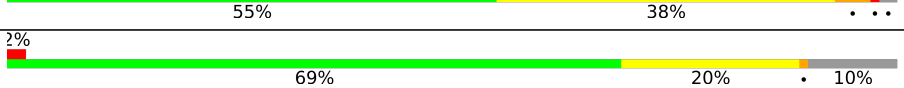
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

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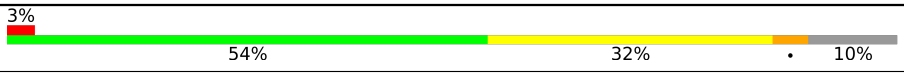
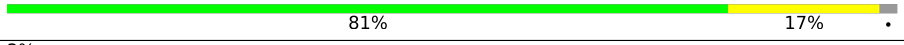
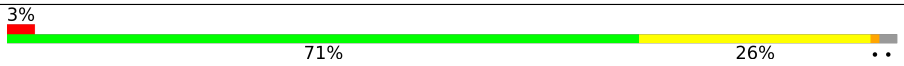
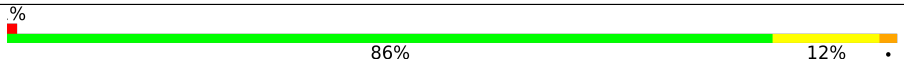
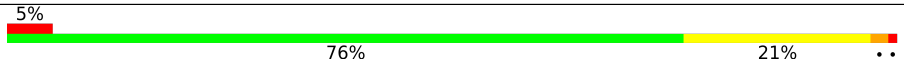
Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
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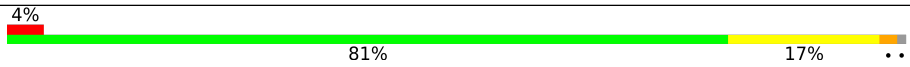
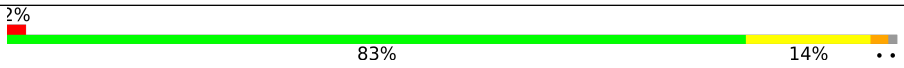
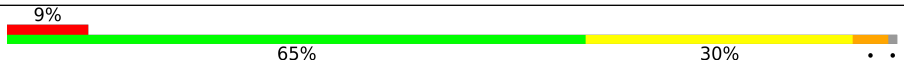
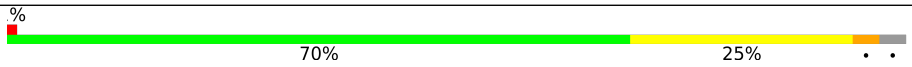
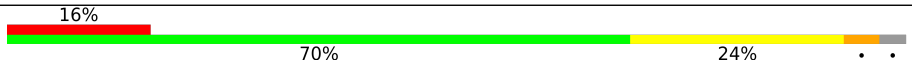
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
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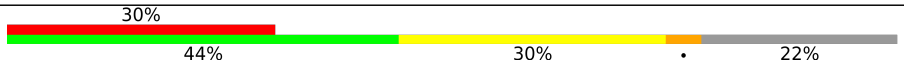
21	2Z	206	
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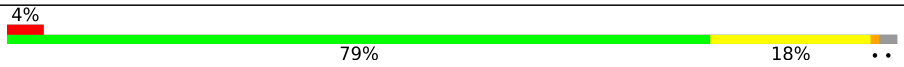
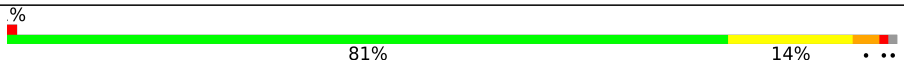
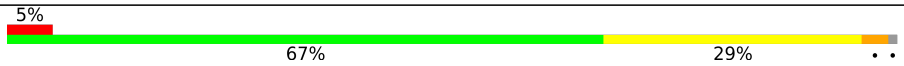
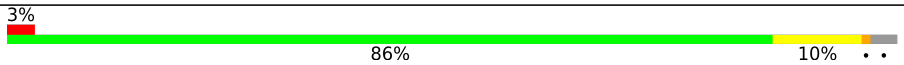
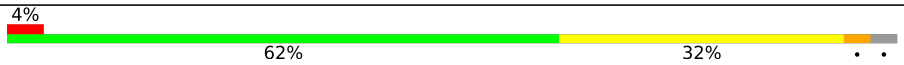
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
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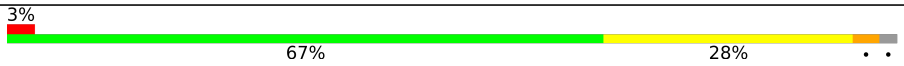
25	23	60	
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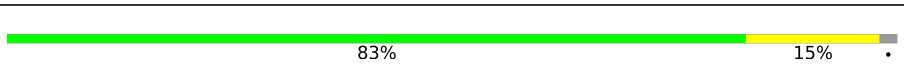
27	25	60	

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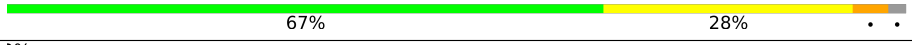
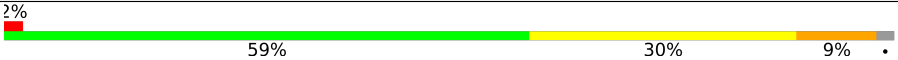
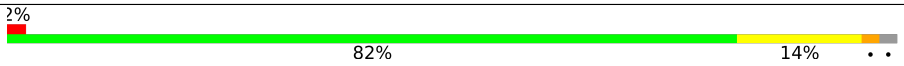
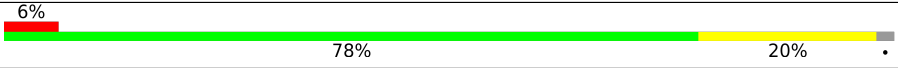
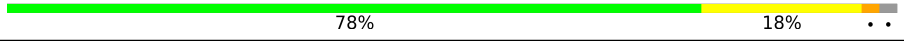
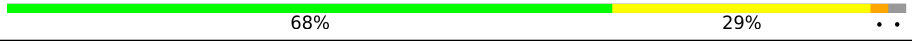
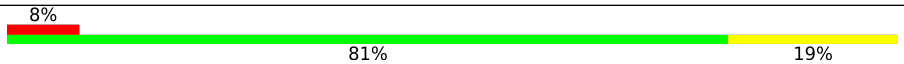
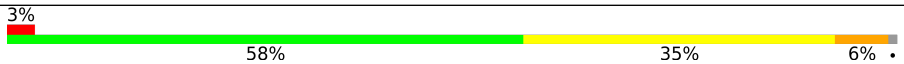
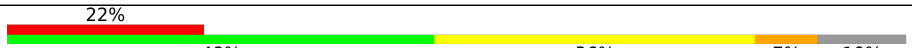
Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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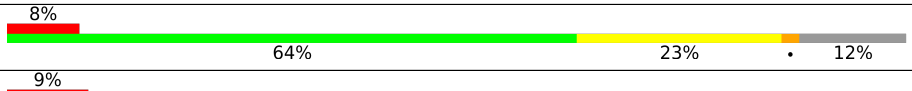
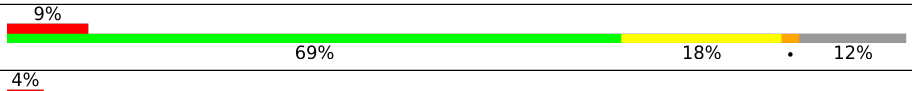
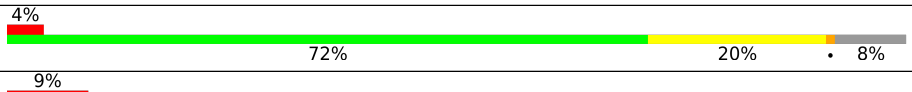
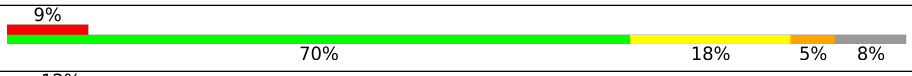
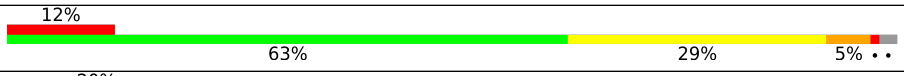
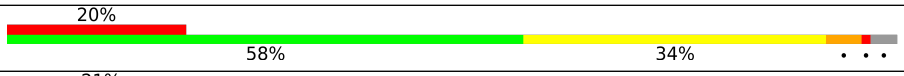
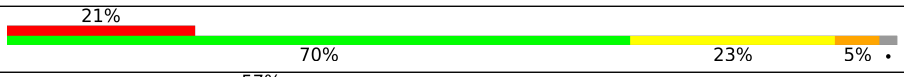
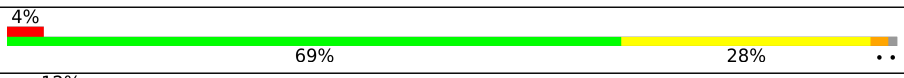
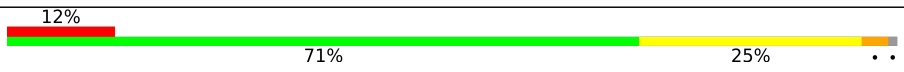
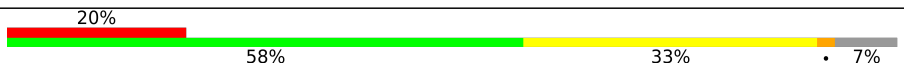
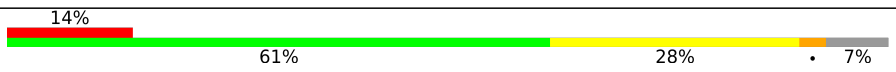
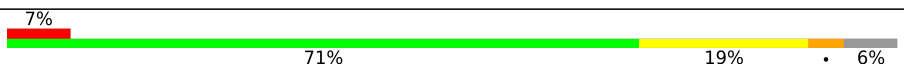
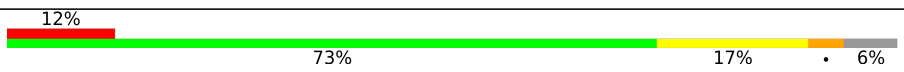
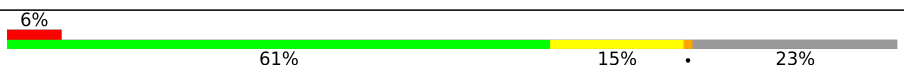
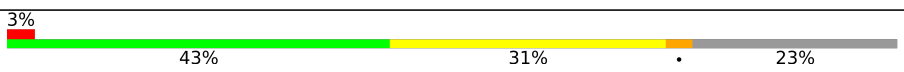
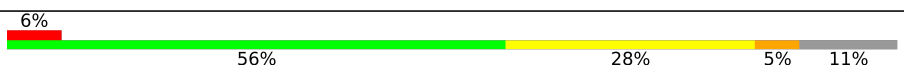
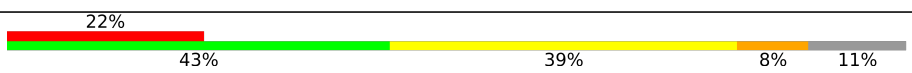
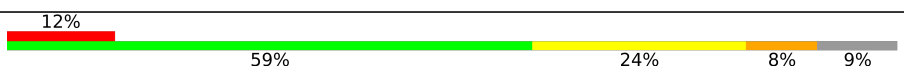
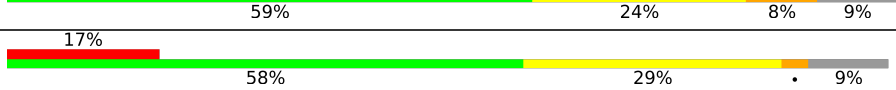
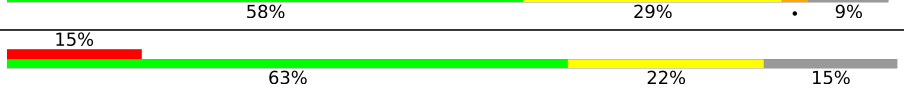
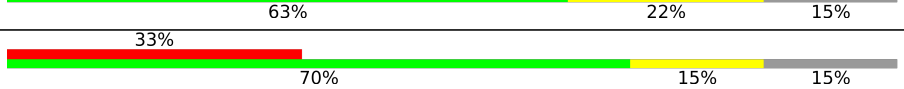
Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	
52	2u	27	

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Mol	Chain	Length	Quality of chain
53	1v	24	12% 42% 12% 46%
53	2v	24	17% 46% 8% 46%
54	1w	76	11% 42% 45% 9%
54	2w	76	20% 34% 39% 20% 5%
55	1x	77	% 62% 34%
55	2x	77	3% 57% 39%
56	1z	5	80% 20%
56	2z	5	40% 20% 40%
57	1y	76	41% 41% 32% 22%
57	2y	76	41% 33% 50% 13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	PSU	2y	55	-	-	X	-
61	SF4	1d	302	-	-	X	-

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 299959 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	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
5	2F	202	Total	C	N	O	S	0	0	0
			1579	1007	296	274	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1423	913	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1097	701	191	204	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	1			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total 873	C 550	N 174	O 149	0	0	0
14	2S	110	Total 870	C 549	N 173	O 148	0	0	0

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1548	973	301	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			810	514	144	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			983	623	193	167			
40	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			709	440	138	131			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	131			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

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

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

- Molecule 53 is a RNA chain called MF-mRNA.

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

- Molecule 54 is a RNA chain called A-site Aminoacyl-tRNA Phe-NH-tRNAphe.

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

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA fMSEAC-NH-tRNAmet RNA-part.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1z	4	Total	C	N	O	S	0	0	0
			26	14	4	7	1			
56	2z	3	Total	C	N	O	S	0	0	0
			20	11	3	5	1			

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1108	Total	Mg	0	0
			1108	1108		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1B	38	Total Mg 38 38	0	0
58	1D	10	Total Mg 10 10	0	0
58	1E	14	Total Mg 14 14	0	0
58	1F	14	Total Mg 14 14	0	0
58	1G	5	Total Mg 5 5	0	0
58	1H	1	Total Mg 1 1	0	0
58	1I	1	Total Mg 1 1	0	0
58	1N	5	Total Mg 5 5	0	0
58	1O	5	Total Mg 5 5	0	0
58	1P	4	Total Mg 4 4	0	0
58	1Q	8	Total Mg 8 8	0	0
58	1R	3	Total Mg 3 3	0	0
58	1S	3	Total Mg 3 3	0	0
58	1T	3	Total Mg 3 3	0	0
58	1U	11	Total Mg 11 11	0	0
58	1V	6	Total Mg 6 6	0	0
58	1W	4	Total Mg 4 4	0	0
58	1X	6	Total Mg 6 6	0	0
58	1Y	3	Total Mg 3 3	0	0
58	1Z	3	Total Mg 3 3	0	0
58	10	7	Total Mg 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	11	6	Total Mg 6 6	0	0
58	12	2	Total Mg 2 2	0	0
58	13	6	Total Mg 6 6	0	0
58	14	1	Total Mg 1 1	0	0
58	15	7	Total Mg 7 7	0	0
58	16	2	Total Mg 2 2	0	0
58	17	5	Total Mg 5 5	0	0
58	18	5	Total Mg 5 5	0	0
58	19	1	Total Mg 1 1	0	0
58	1a	213	Total Mg 213 213	0	0
58	1b	1	Total Mg 1 1	0	0
58	1d	1	Total Mg 1 1	0	0
58	1e	2	Total Mg 2 2	0	0
58	1f	2	Total Mg 2 2	0	0
58	1k	1	Total Mg 1 1	0	0
58	1l	2	Total Mg 2 2	0	0
58	1m	1	Total Mg 1 1	0	0
58	1n	2	Total Mg 2 2	0	0
58	1t	1	Total Mg 1 1	0	0
58	1v	1	Total Mg 1 1	0	0
58	1w	9	Total Mg 9 9	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1x	12	Total Mg 12 12	0	0
58	2A	869	Total Mg 869 869	0	0
58	2B	19	Total Mg 19 19	0	0
58	2D	7	Total Mg 7 7	0	0
58	2E	8	Total Mg 8 8	0	0
58	2F	6	Total Mg 6 6	0	0
58	2G	1	Total Mg 1 1	0	0
58	2O	1	Total Mg 1 1	0	0
58	2P	1	Total Mg 1 1	0	0
58	2Q	2	Total Mg 2 2	0	0
58	2R	2	Total Mg 2 2	0	0
58	2T	3	Total Mg 3 3	0	0
58	2U	2	Total Mg 2 2	0	0
58	2V	2	Total Mg 2 2	0	0
58	2W	2	Total Mg 2 2	0	0
58	2X	2	Total Mg 2 2	0	0
58	2Y	1	Total Mg 1 1	0	0
58	2Z	1	Total Mg 1 1	0	0
58	20	3	Total Mg 3 3	0	0
58	21	1	Total Mg 1 1	0	0
58	23	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	25	6	Total Mg 6 6	0	0
58	27	3	Total Mg 3 3	0	0
58	28	3	Total Mg 3 3	0	0
58	2a	235	Total Mg 235 235	0	0
58	2d	2	Total Mg 2 2	0	0
58	2e	1	Total Mg 1 1	0	0
58	2f	2	Total Mg 2 2	0	0
58	2g	1	Total Mg 1 1	0	0
58	2i	1	Total Mg 1 1	0	0
58	2j	1	Total Mg 1 1	0	0
58	2k	1	Total Mg 1 1	0	0
58	2l	4	Total Mg 4 4	0	0
58	2n	1	Total Mg 1 1	0	0
58	2p	1	Total Mg 1 1	0	0
58	2q	2	Total Mg 2 2	0	0
58	2r	1	Total Mg 1 1	0	0
58	2t	1	Total Mg 1 1	0	0
58	2v	4	Total Mg 4 4	0	0
58	2w	4	Total Mg 4 4	0	0
58	2x	6	Total Mg 6 6	0	0
58	2y	1	Total Mg 1 1	0	0

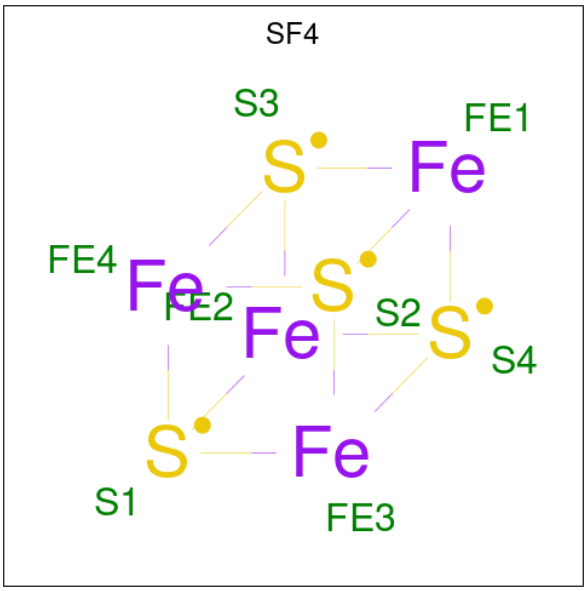
- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

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

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

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

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



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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1A	1956	Total O 1956 1956	0	0
62	1B	62	Total O 62 62	0	0
62	1D	27	Total O 27 27	0	0
62	1E	28	Total O 28 28	0	0
62	1F	22	Total O 22 22	0	0
62	1G	3	Total O 3 3	0	0
62	1H	2	Total O 2 2	0	0
62	1N	4	Total O 4 4	0	0
62	1O	5	Total O 5 5	0	0
62	1P	21	Total O 21 21	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1Q	6	Total O 6 6	0	0
62	1R	11	Total O 11 11	0	0
62	1S	4	Total O 4 4	0	0
62	1T	7	Total O 7 7	0	0
62	1U	11	Total O 11 11	0	0
62	1V	8	Total O 8 8	0	0
62	1W	8	Total O 8 8	0	0
62	1X	5	Total O 5 5	0	0
62	1Y	3	Total O 3 3	0	0
62	1Z	1	Total O 1 1	0	0
62	10	13	Total O 13 13	0	0
62	11	12	Total O 12 12	0	0
62	12	3	Total O 3 3	0	0
62	13	4	Total O 4 4	0	0
62	14	1	Total O 1 1	0	0
62	15	6	Total O 6 6	0	0
62	16	2	Total O 2 2	0	0
62	17	10	Total O 10 10	0	0
62	18	8	Total O 8 8	0	0
62	1a	326	Total O 326 326	0	0
62	1b	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1e	1	Total O 1 1	0	0
62	1f	1	Total O 1 1	0	0
62	1g	1	Total O 1 1	0	0
62	1i	1	Total O 1 1	0	0
62	1l	4	Total O 4 4	0	0
62	1m	1	Total O 1 1	0	0
62	1o	1	Total O 1 1	0	0
62	1p	1	Total O 1 1	0	0
62	1q	2	Total O 2 2	0	0
62	1u	1	Total O 1 1	0	0
62	1v	5	Total O 5 5	0	0
62	1w	8	Total O 8 8	0	0
62	1x	9	Total O 9 9	0	0
62	1z	1	Total O 1 1	0	0
62	1y	1	Total O 1 1	0	0
62	2A	1067	Total O 1067 1067	0	0
62	2B	22	Total O 22 22	0	0
62	2D	26	Total O 26 26	0	0
62	2E	17	Total O 17 17	0	0
62	2F	13	Total O 13 13	0	0
62	2N	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2O	1	Total O 1 1	0	0
62	2P	10	Total O 10 10	0	0
62	2Q	2	Total O 2 2	0	0
62	2R	4	Total O 4 4	0	0
62	2T	4	Total O 4 4	0	0
62	2U	2	Total O 2 2	0	0
62	2W	2	Total O 2 2	0	0
62	2X	4	Total O 4 4	0	0
62	2Y	1	Total O 1 1	0	0
62	2Z	1	Total O 1 1	0	0
62	20	3	Total O 3 3	0	0
62	21	10	Total O 10 10	0	0
62	22	1	Total O 1 1	0	0
62	23	1	Total O 1 1	0	0
62	25	2	Total O 2 2	0	0
62	27	4	Total O 4 4	0	0
62	28	3	Total O 3 3	0	0
62	29	1	Total O 1 1	0	0
62	2a	225	Total O 225 225	0	0
62	2c	1	Total O 1 1	0	0
62	2d	1	Total O 1 1	0	0

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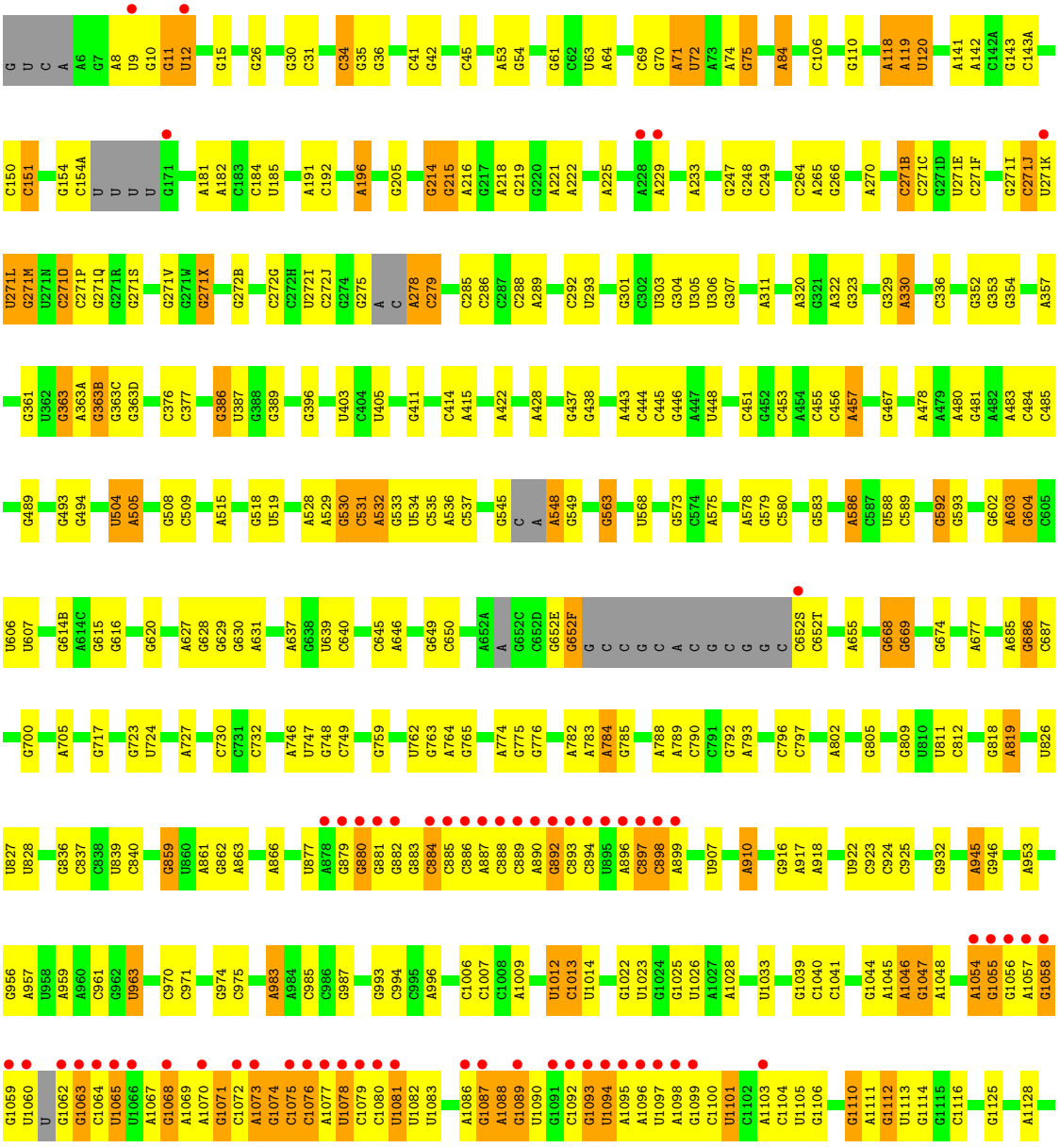
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2e	2	Total O 2 2	0	0
62	2i	1	Total O 1 1	0	0
62	2j	3	Total O 3 3	0	0
62	2l	6	Total O 6 6	0	0
62	2p	2	Total O 2 2	0	0
62	2r	1	Total O 1 1	0	0
62	2t	2	Total O 2 2	0	0
62	2v	1	Total O 1 1	0	0
62	2w	5	Total O 5 5	0	0
62	2x	3	Total O 3 3	0	0
62	2z	1	Total O 1 1	0	0

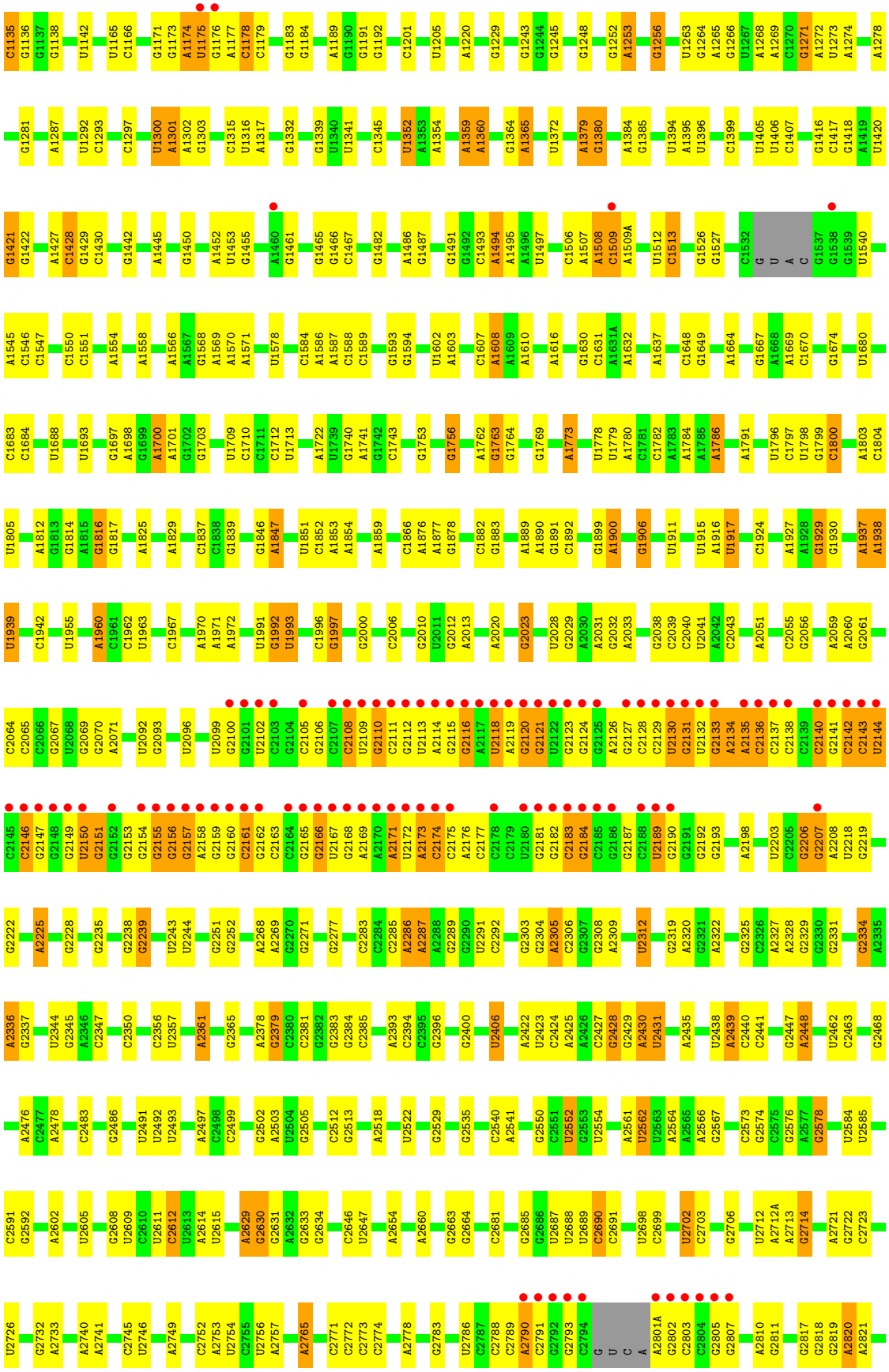
3 Residue-property plots (i)

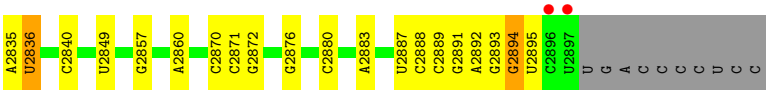
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S Ribosomal RNA

Chain 1A:

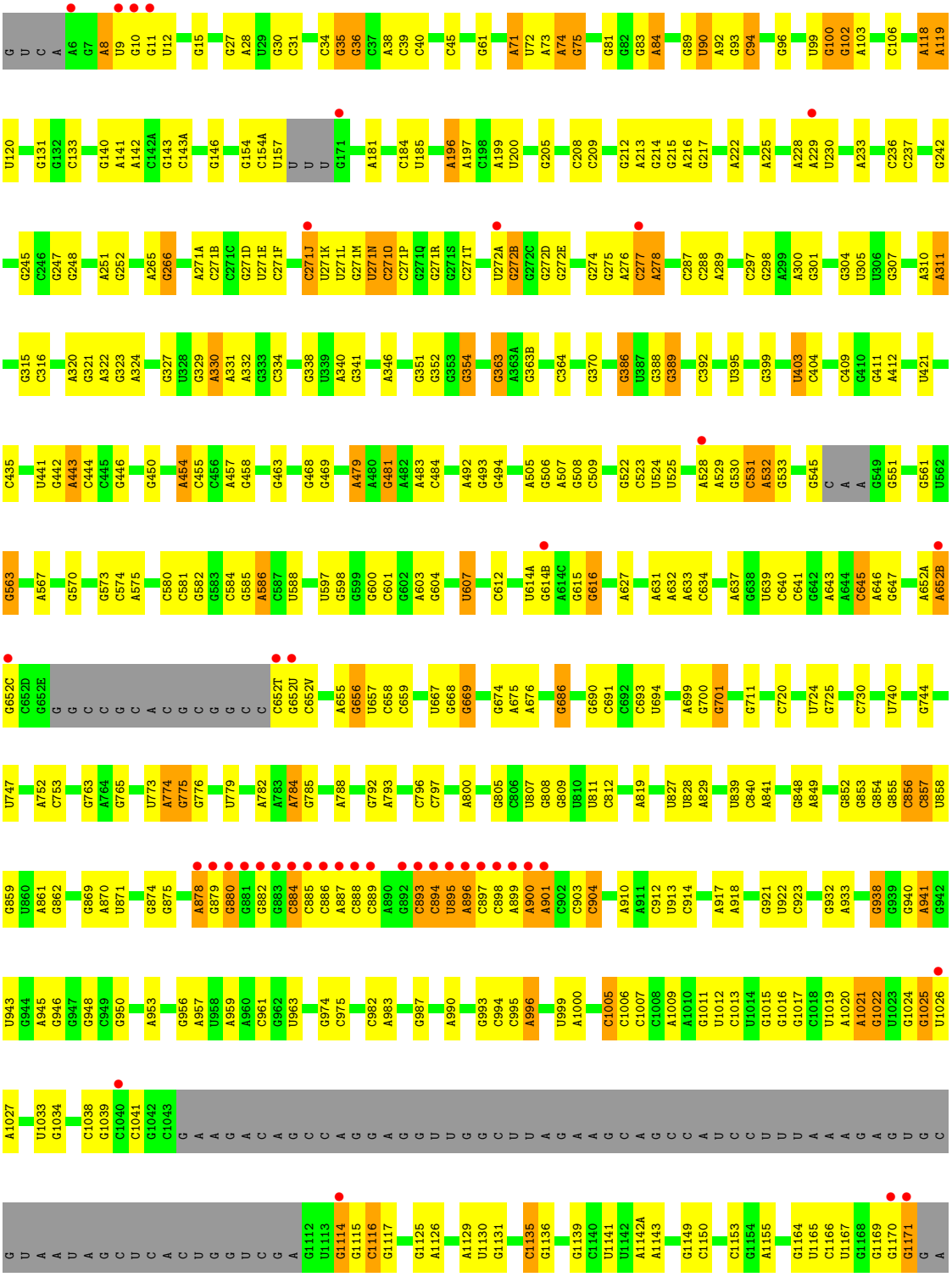


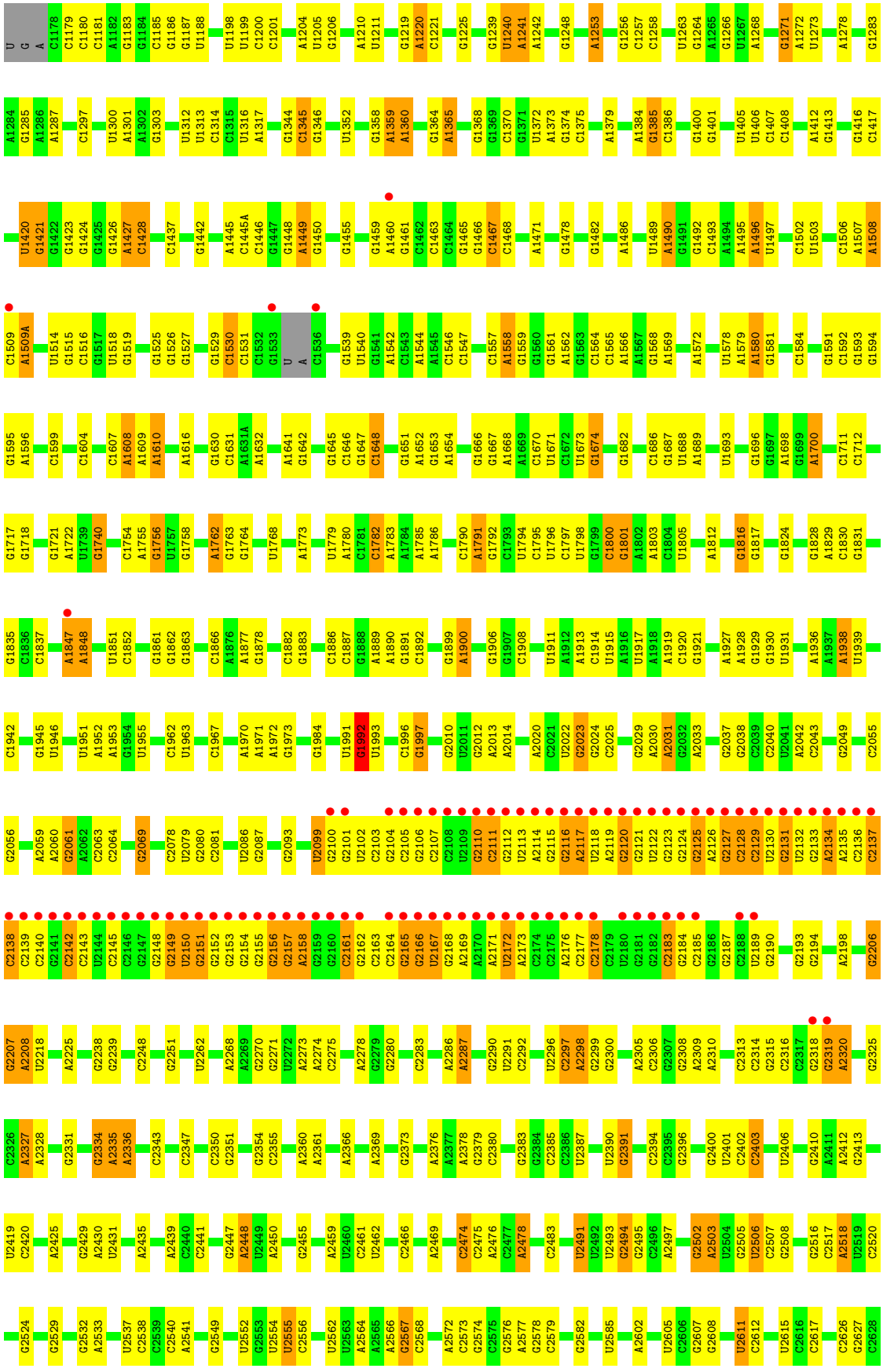


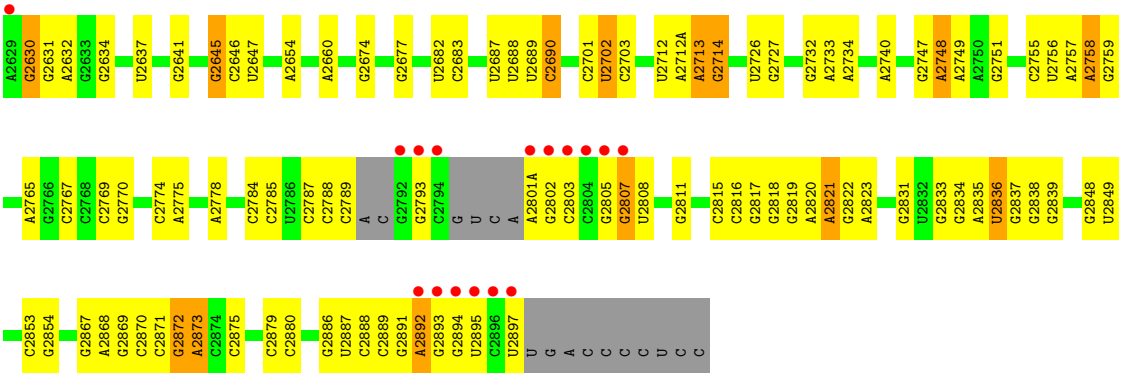


• Molecule 1: 23S Ribosomal RNA

Chain 2A:





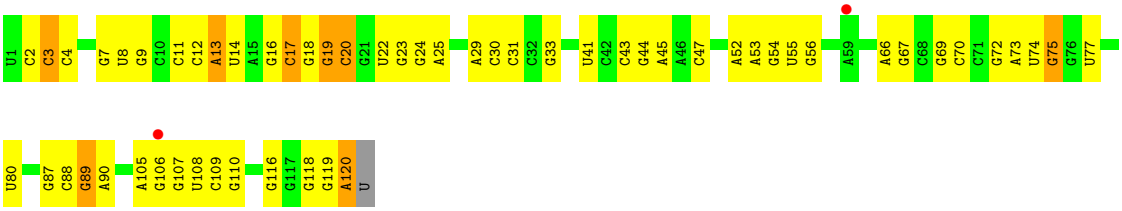


• Molecule 2: 5S Ribosomal RNA

Chain 1B:

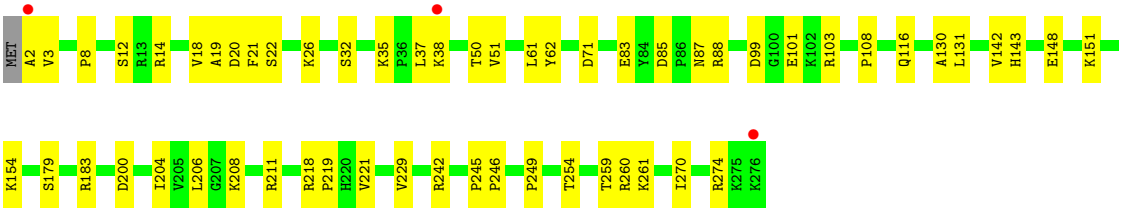
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



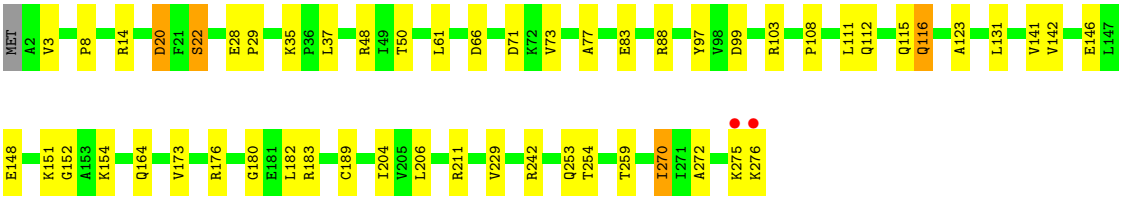
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



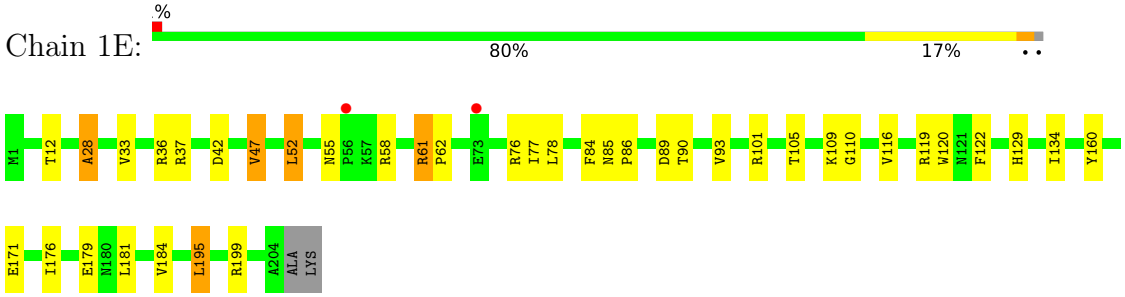
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



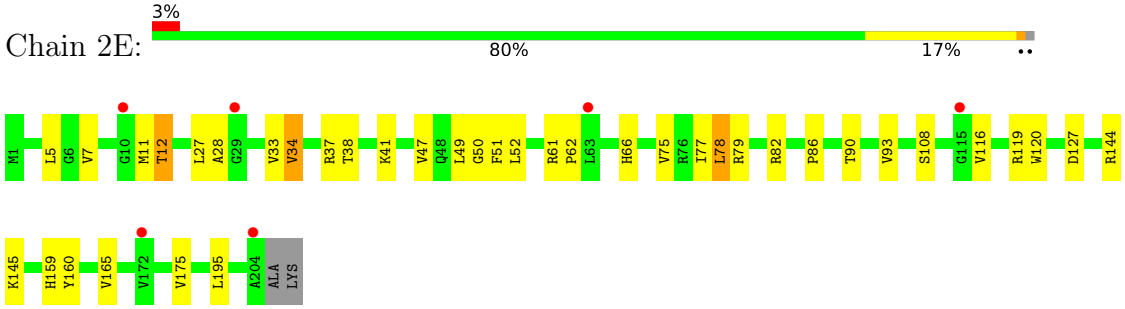
• Molecule 4: 50S ribosomal protein L3

Chain 1E:



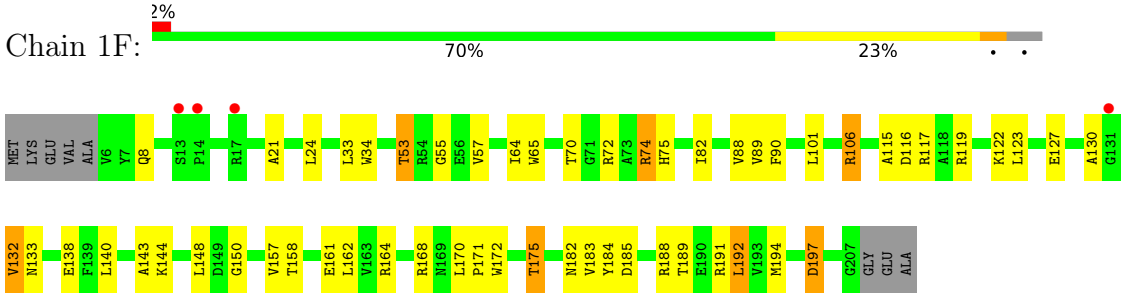
• Molecule 4: 50S ribosomal protein L3

Chain 2E:



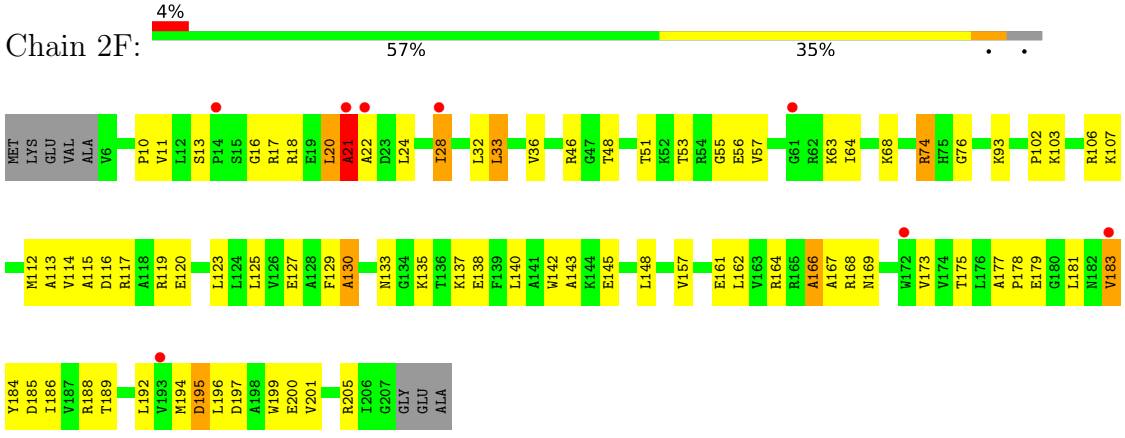
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



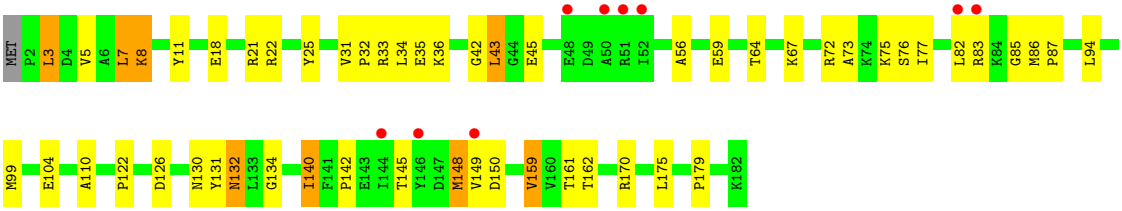
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



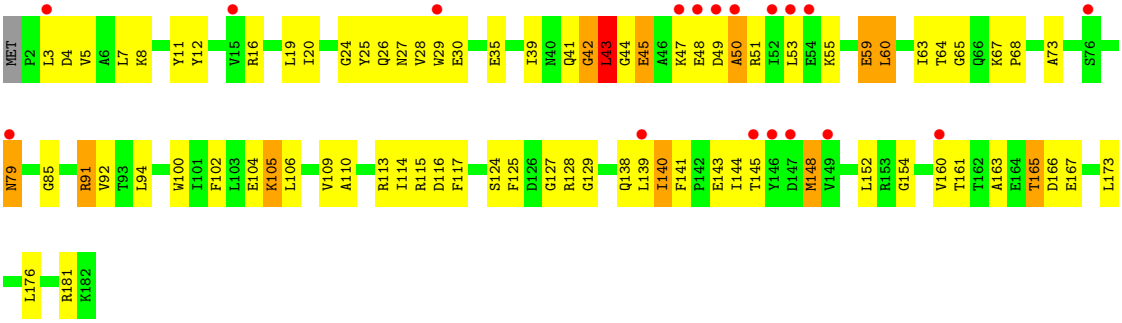
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



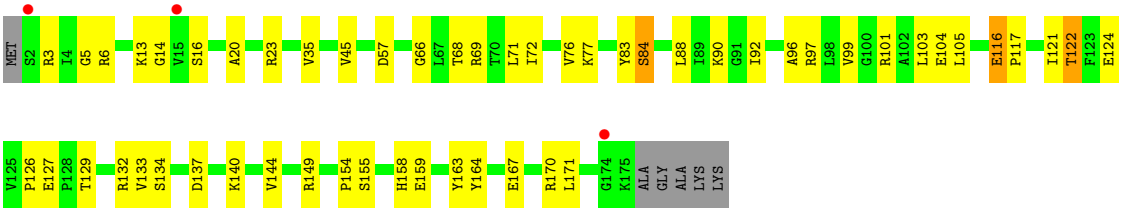
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



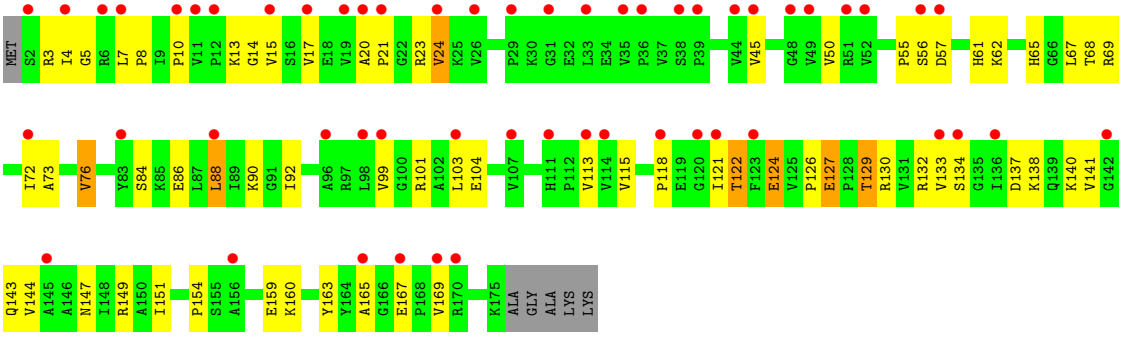
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



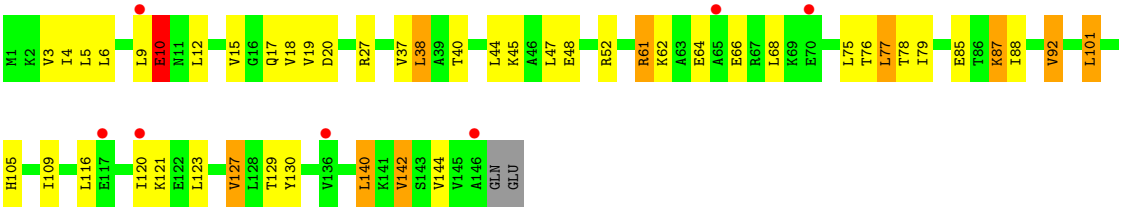
• Molecule 7: 50S ribosomal protein L6

Chain 2H:

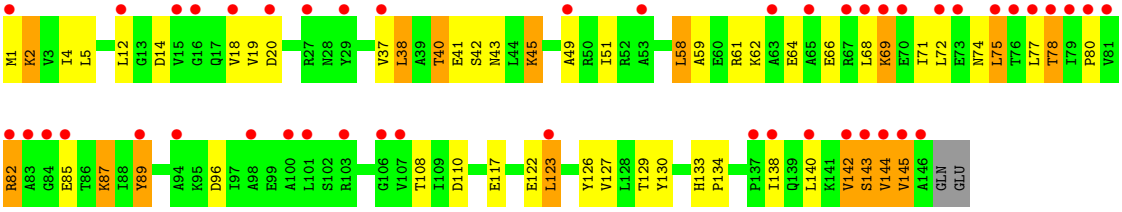


• Molecule 8: 50S ribosomal protein L9

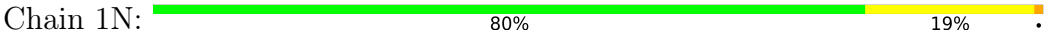
Chain 1I:

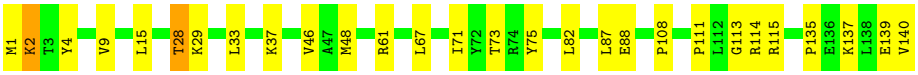


• Molecule 8: 50S ribosomal protein L9



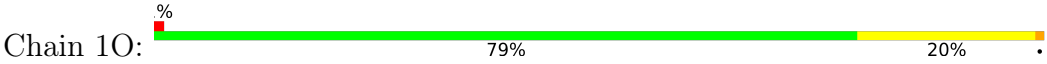
• Molecule 9: 50S ribosomal protein L13

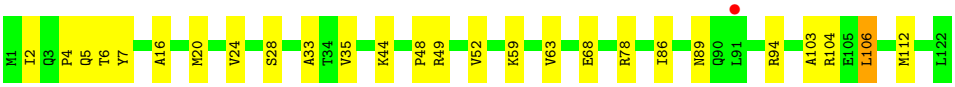




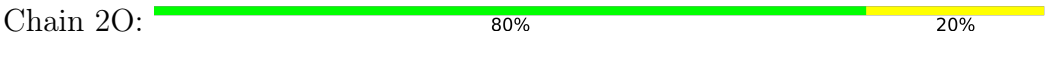
• Molecule 9: 50S ribosomal protein L13

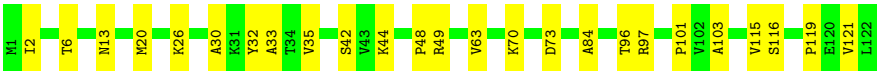
• Molecule 10: 50S ribosomal protein L14





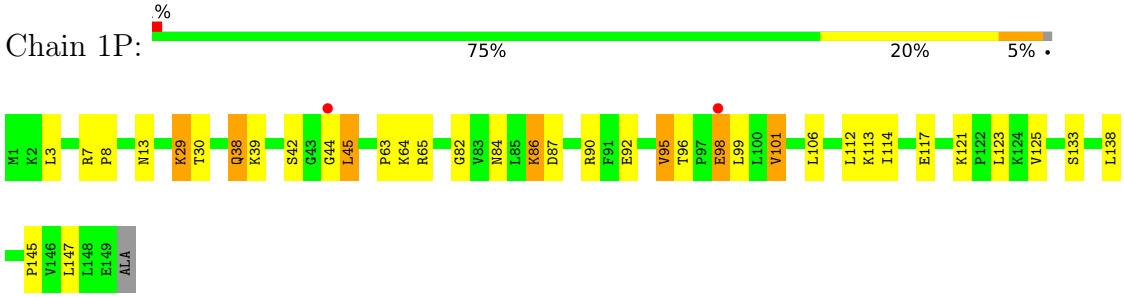
• Molecule 10: 50S ribosomal protein L14





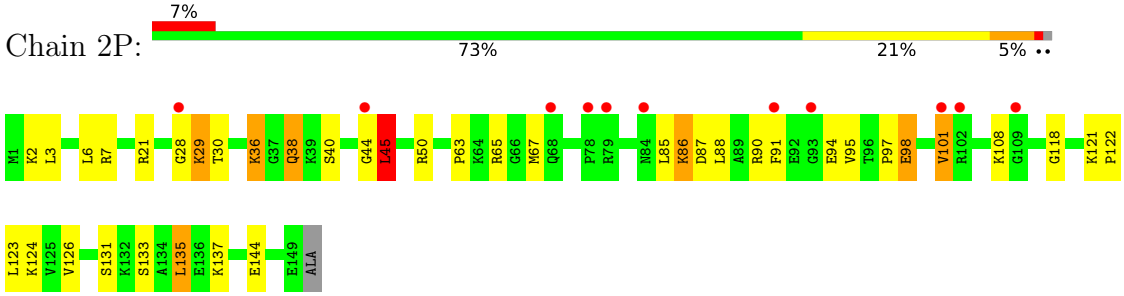
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



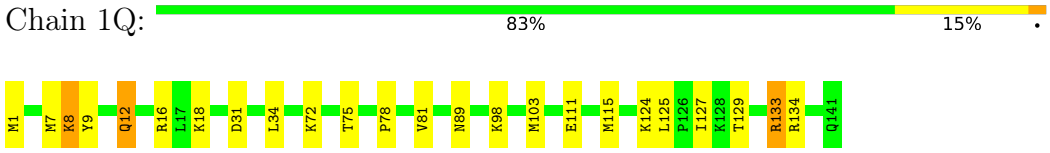
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



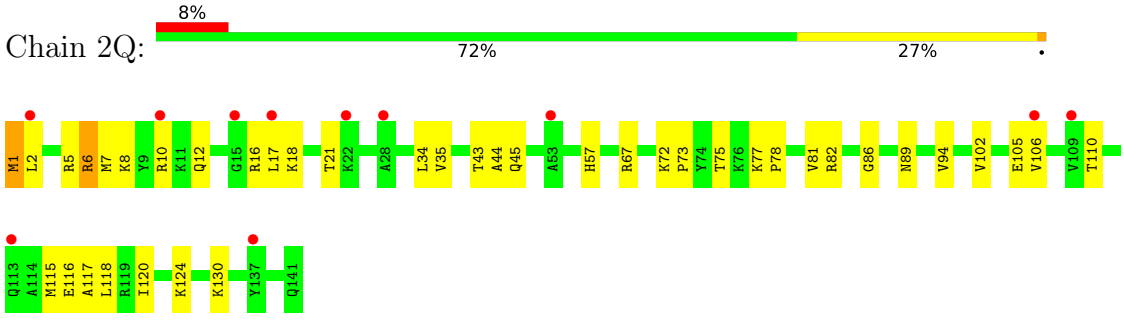
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



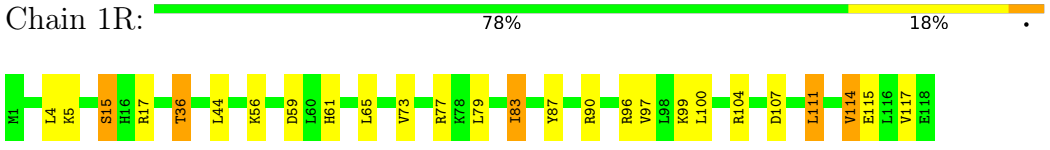
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



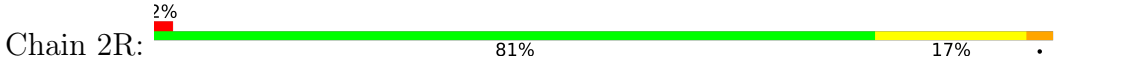
• Molecule 13: 50S ribosomal protein L17

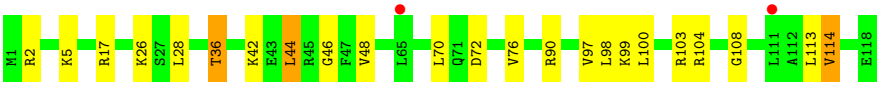
Chain 1R:



• Molecule 13: 50S ribosomal protein L17

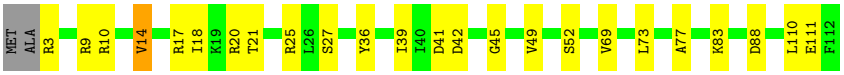
Chain 2R:





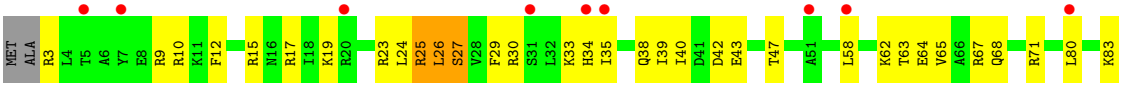
• Molecule 14: 50S ribosomal protein L18

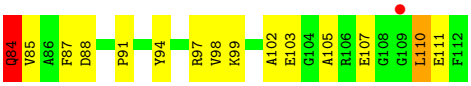
Chain 1S:



• Molecule 14: 50S ribosomal protein L18

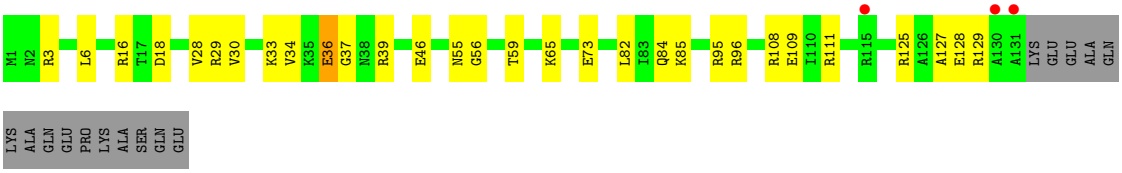
Chain 2S:





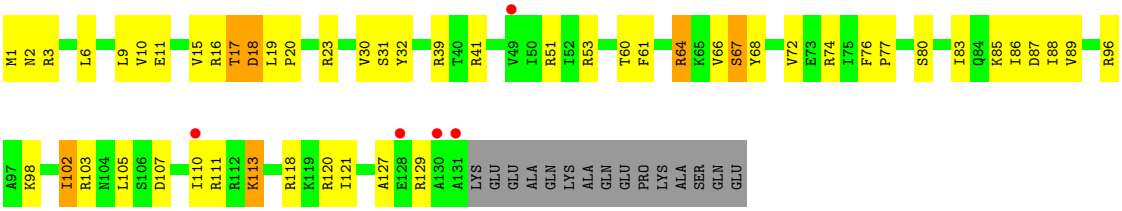
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



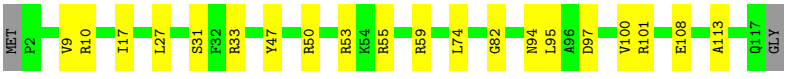
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



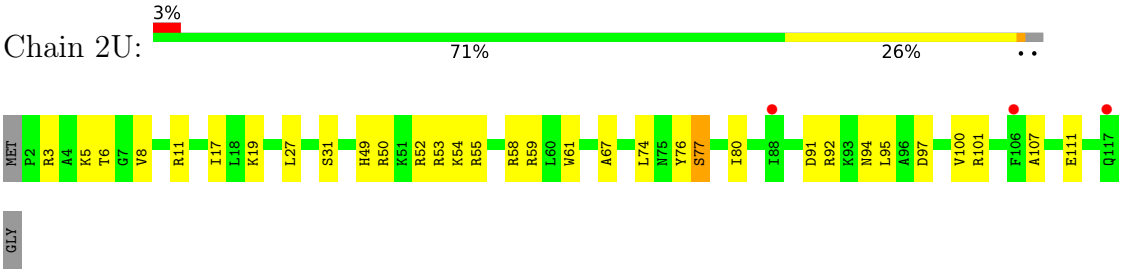
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



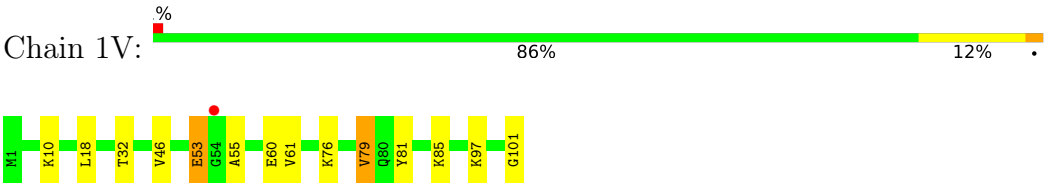
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



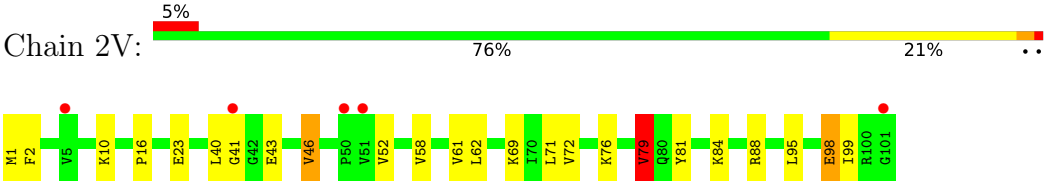
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



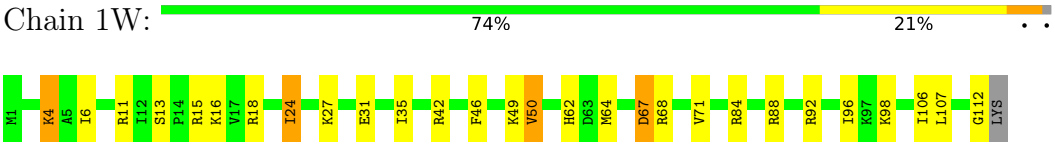
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



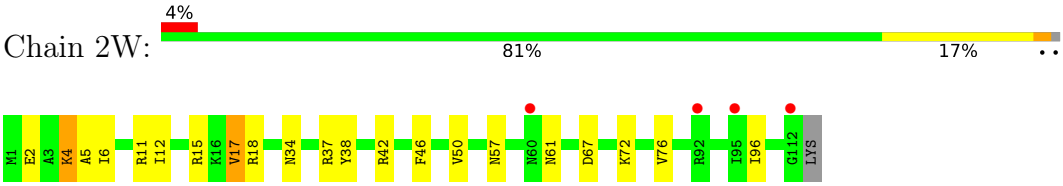
• Molecule 18: 50S ribosomal protein L22

Chain 1W:



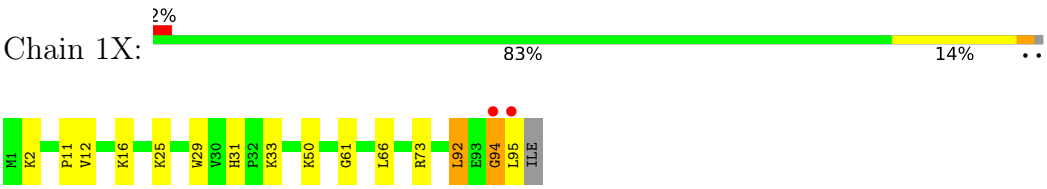
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



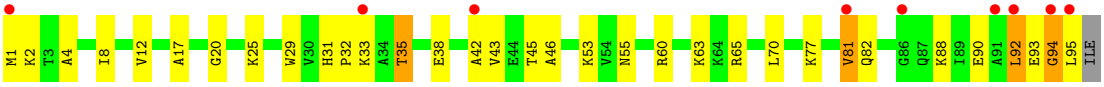
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



• Molecule 19: 50S ribosomal protein L23

Chain 2X:

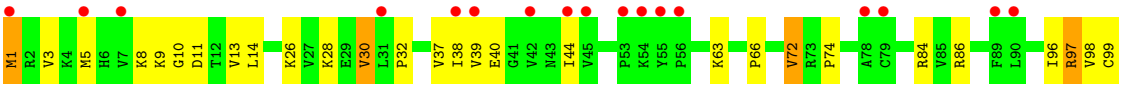


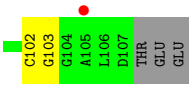
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:

• Molecule 20: 50S ribosomal protein L24

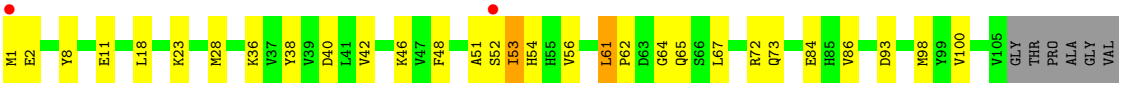
Chain 2Y:

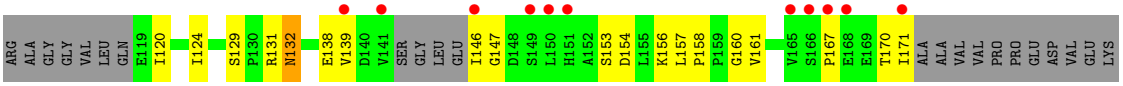




• Molecule 21: 50S ribosomal protein L25

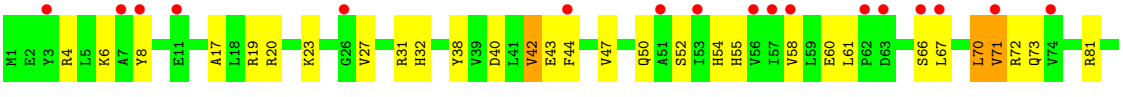
Chain 1Z:

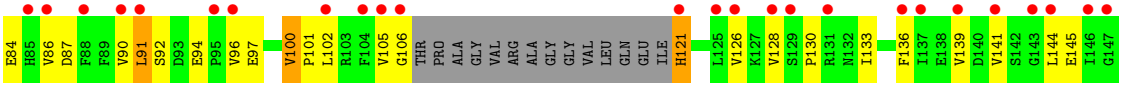


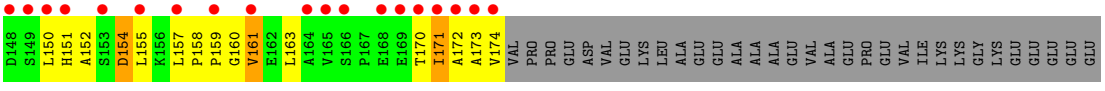


• Molecule 21: 50S ribosomal protein L25

Chain 2Z:

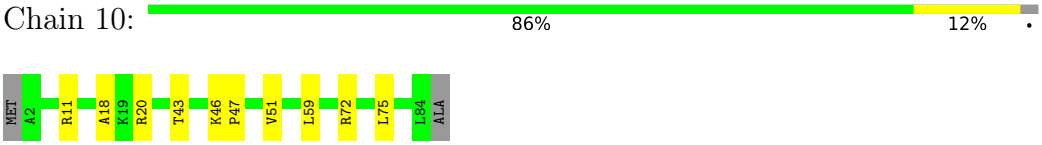






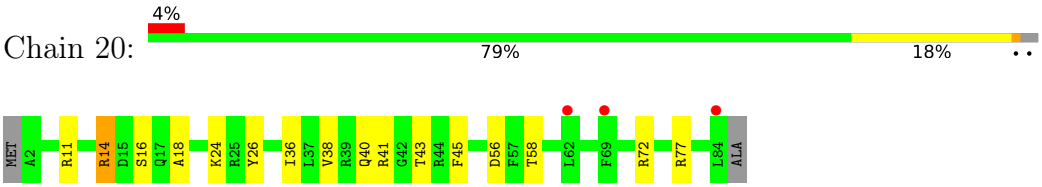
• Molecule 22: 50S ribosomal protein L27

Chain 10:



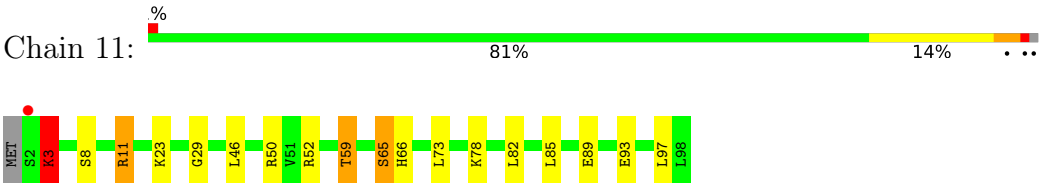
• Molecule 22: 50S ribosomal protein L27

Chain 20:



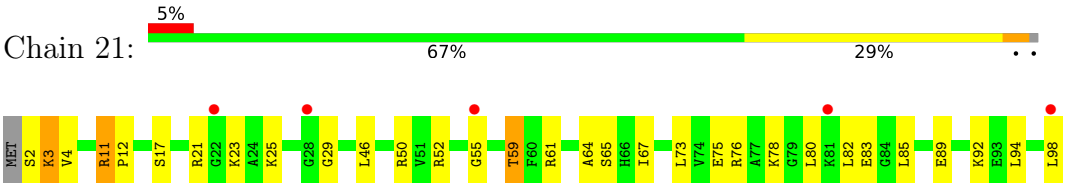
• Molecule 23: 50S ribosomal protein L28

Chain 11:



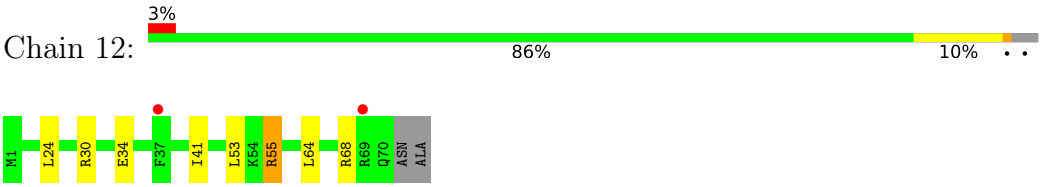
• Molecule 23: 50S ribosomal protein L28

Chain 21:



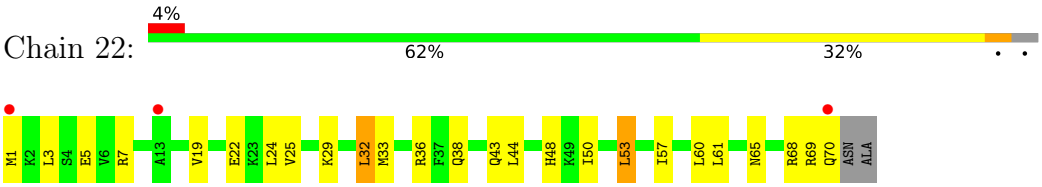
• Molecule 24: 50S ribosomal protein L29

Chain 12:



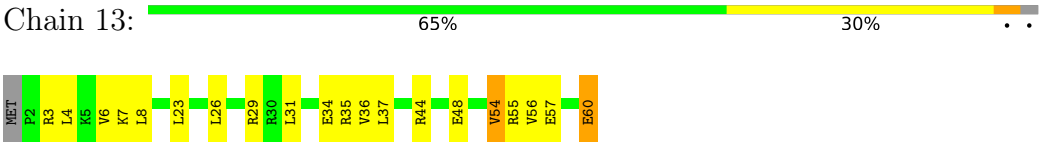
• Molecule 24: 50S ribosomal protein L29

Chain 22:



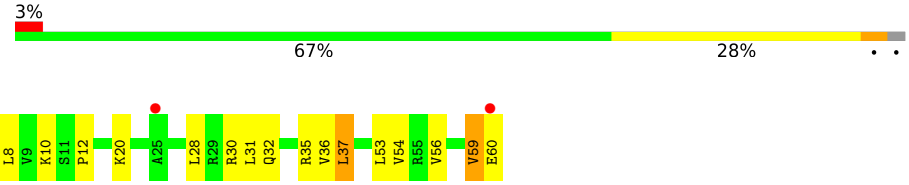
• Molecule 25: 50S ribosomal protein L30

Chain 13:



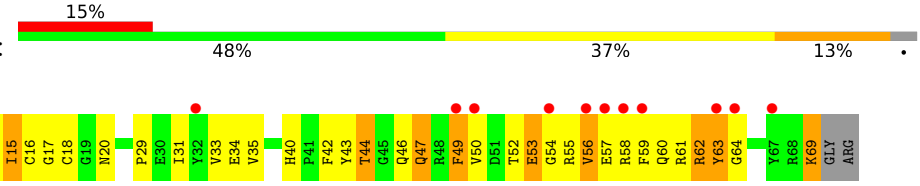
• Molecule 25: 50S ribosomal protein L30

Chain 23:



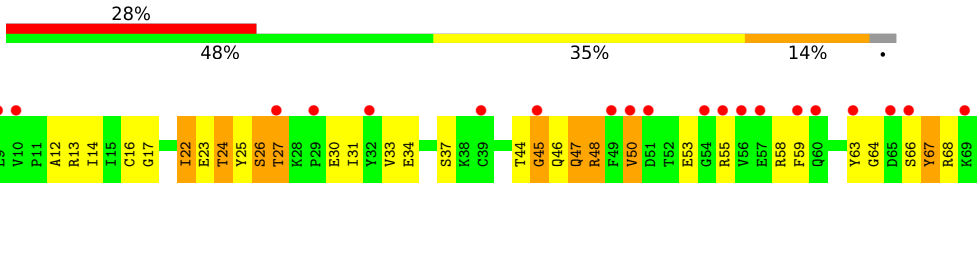
• Molecule 26: 50S ribosomal protein L31

Chain 14:



• Molecule 26: 50S ribosomal protein L31

Chain 24:

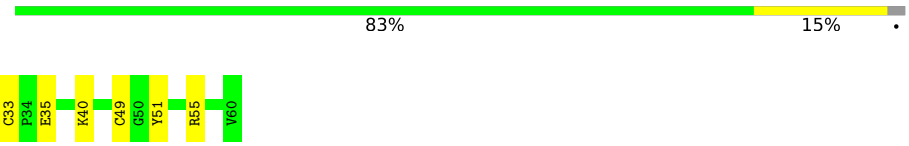


• Molecule 27: 50S ribosomal protein L32

Chain 15:

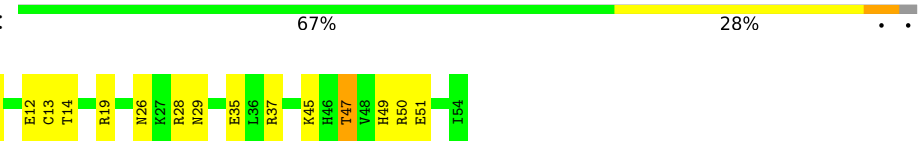
• Molecule 27: 50S ribosomal protein L32

Chain 25:



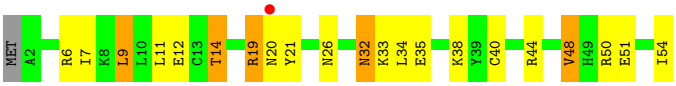
• Molecule 28: 50S ribosomal protein L33

Chain 16:



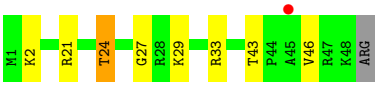
• Molecule 28: 50S ribosomal protein L33

Chain 26:



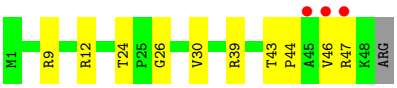
• Molecule 29: 50S ribosomal protein L34

Chain 17:



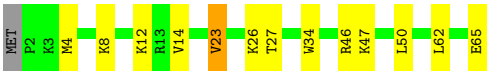
• Molecule 29: 50S ribosomal protein L34

Chain 27:



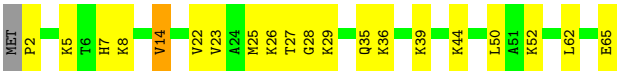
• Molecule 30: 50S ribosomal protein L35

Chain 18:



• Molecule 30: 50S ribosomal protein L35

Chain 28:

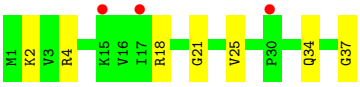


• Molecule 31: 50S ribosomal protein L36

Chain 19:

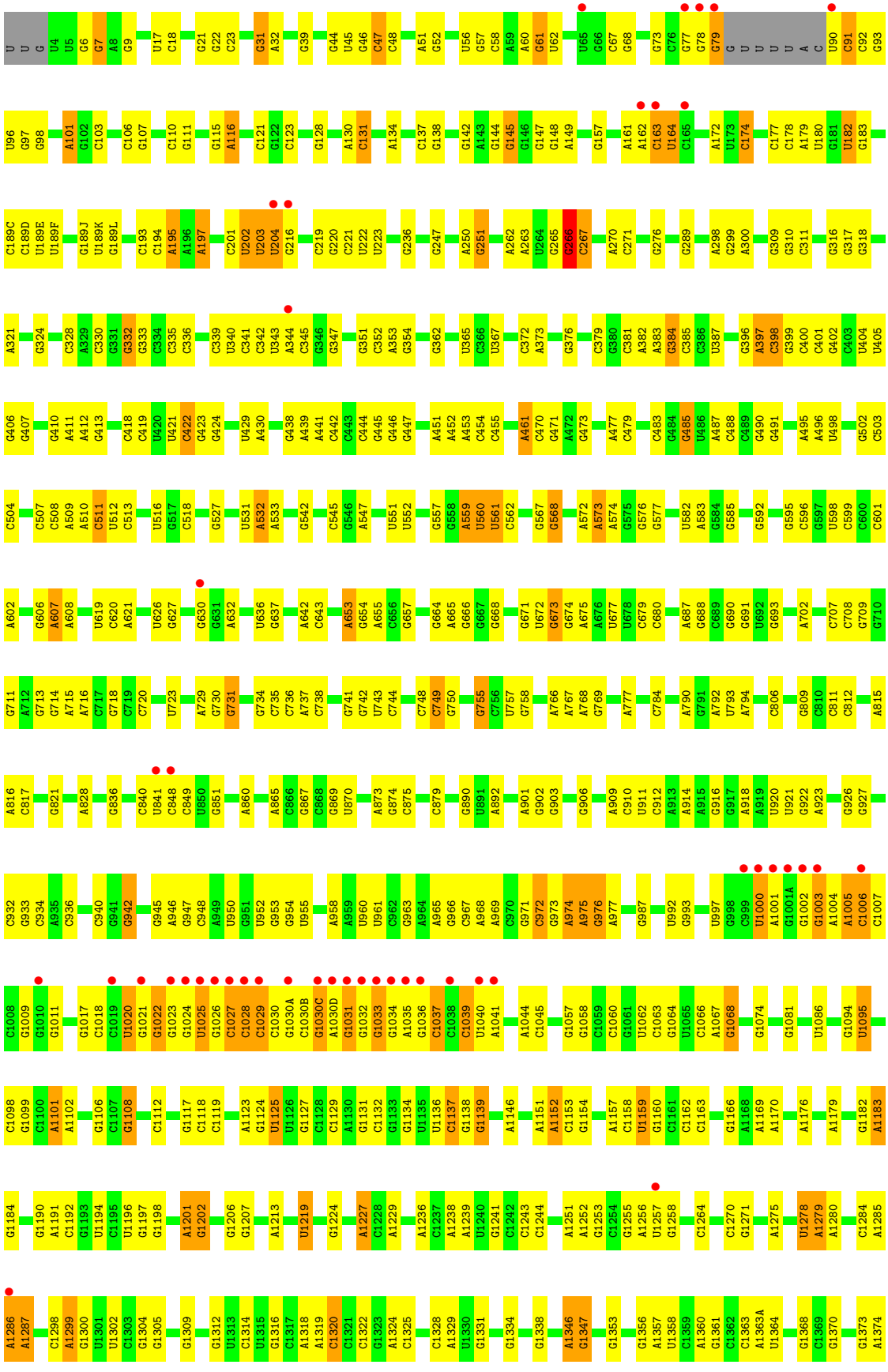
• Molecule 31: 50S ribosomal protein L36

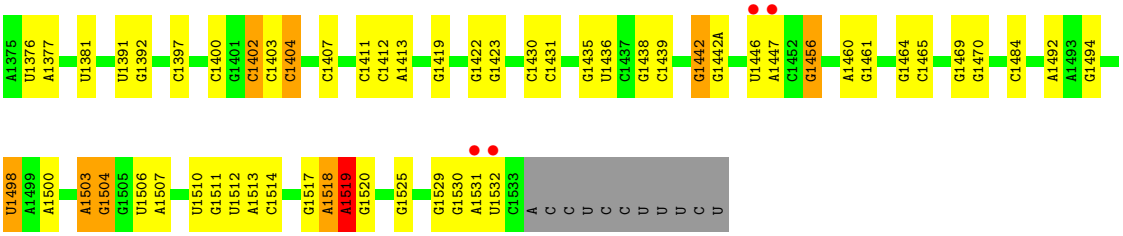
Chain 29:



• Molecule 32: 16S Ribosomal RNA

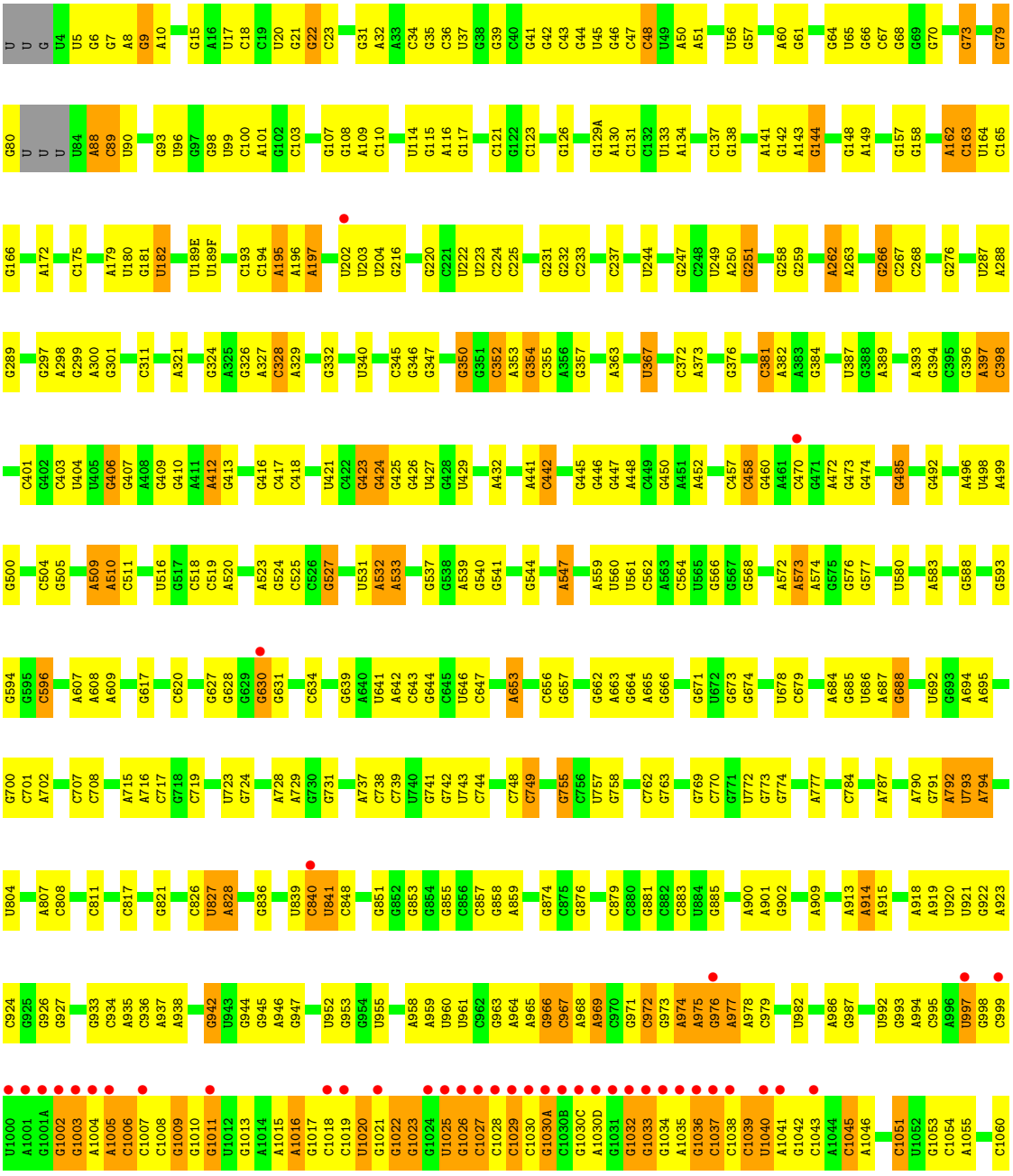
Chain 1a:

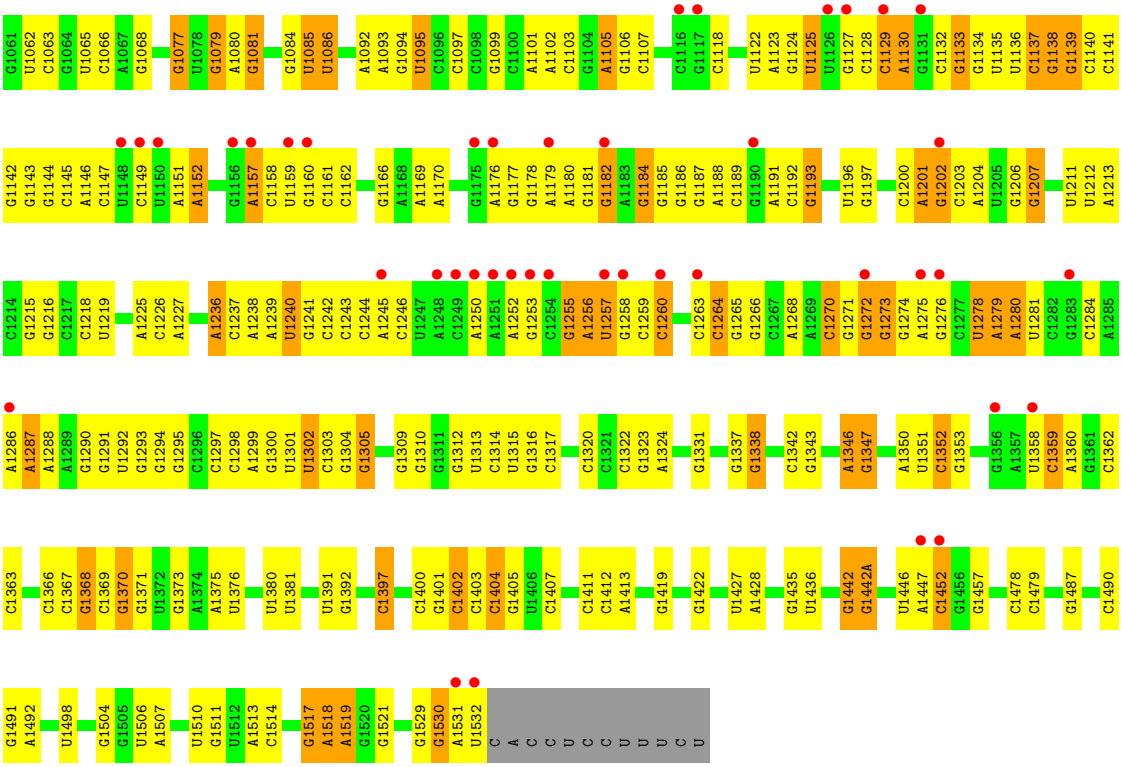




• Molecule 32: 16S Ribosomal RNA

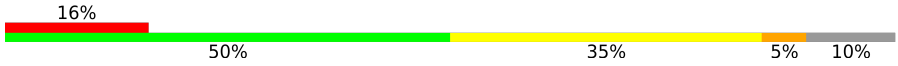
Chain 2a:

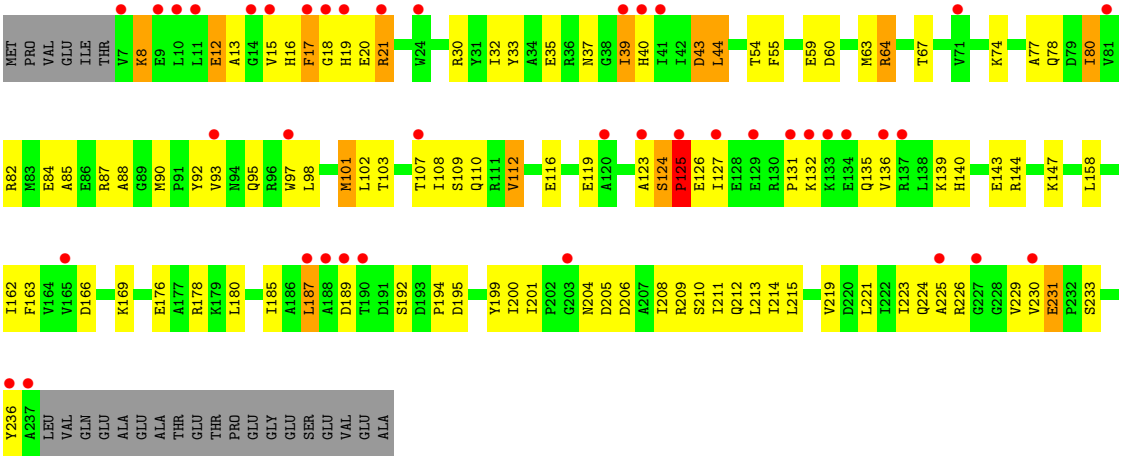




• Molecule 33: 30S ribosomal protein S2

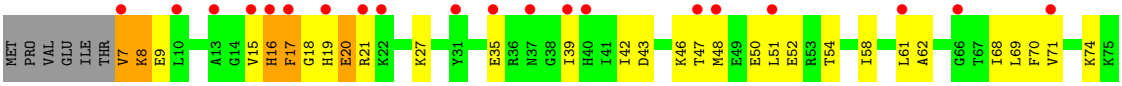
Chain 1b:

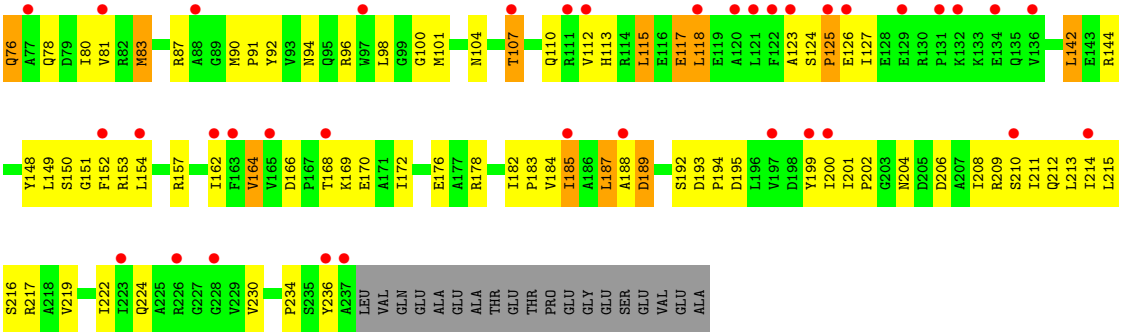




• Molecule 33: 30S ribosomal protein S2

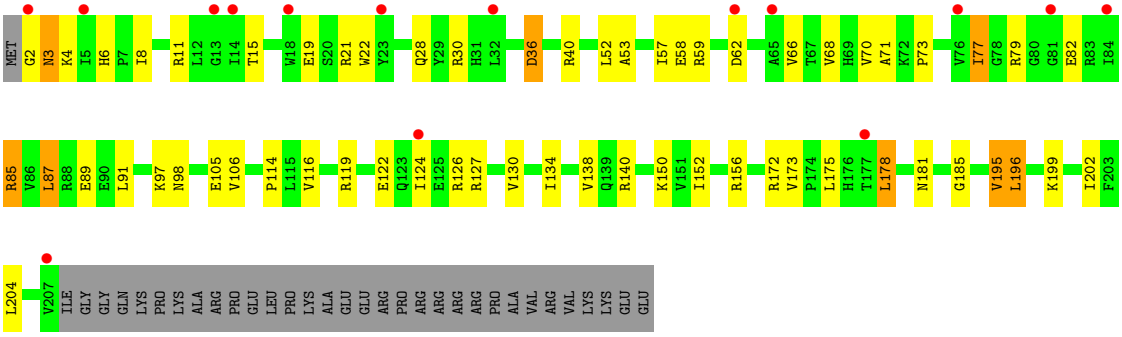
Chain 2b:





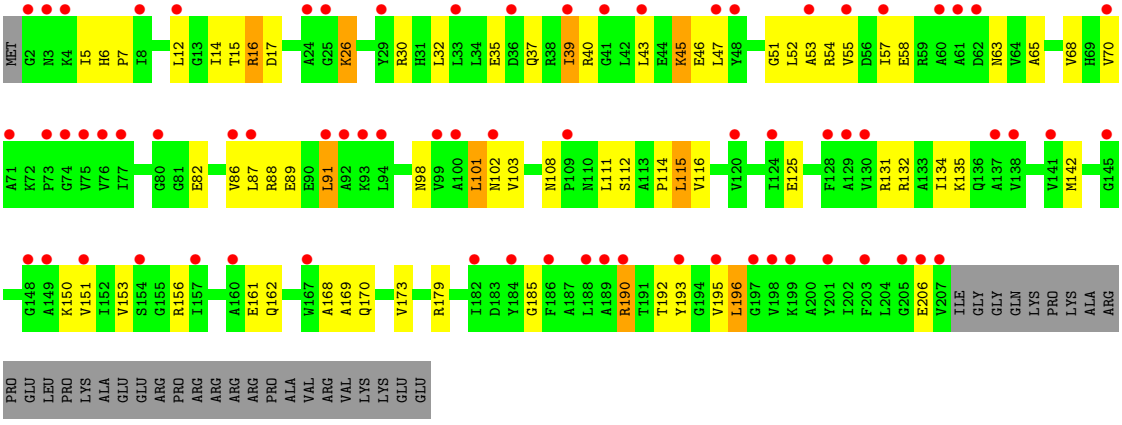
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



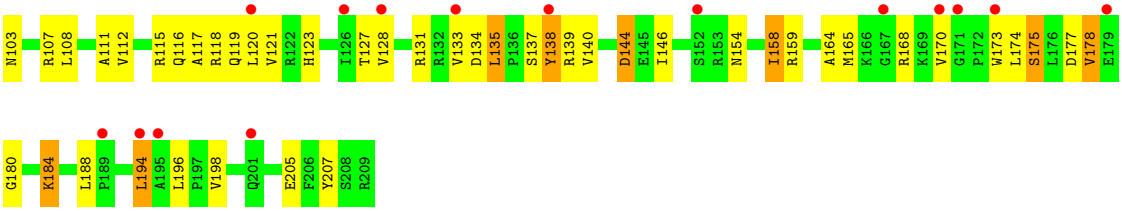
• Molecule 34: 30S ribosomal protein S3

Chain 2c:

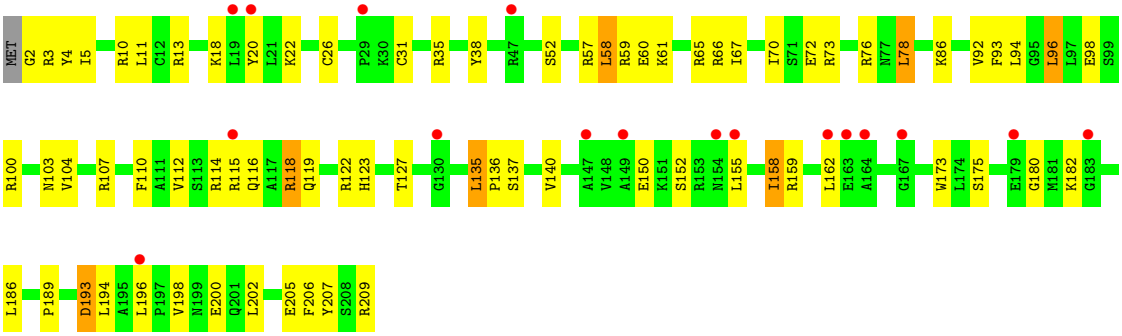


• Molecule 35: 30S ribosomal protein S4

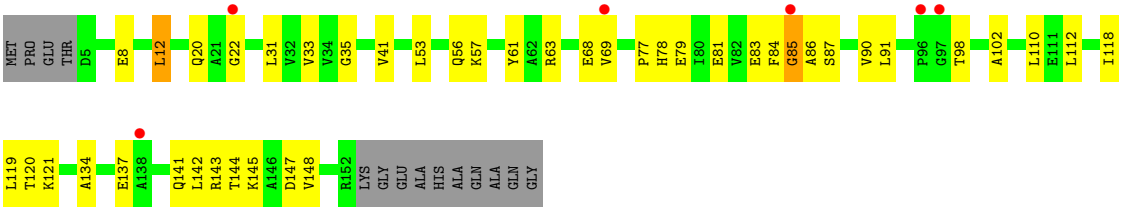
Chain 1d:



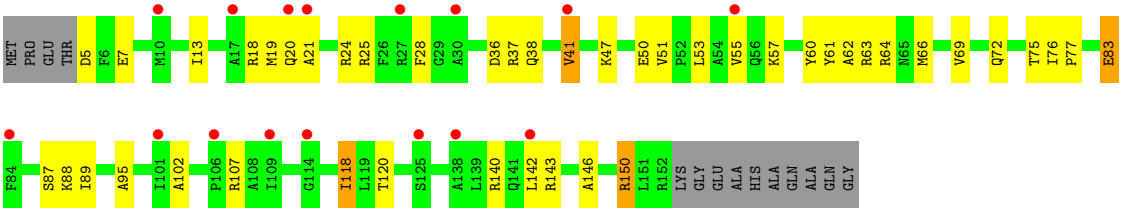
• Molecule 35: 30S ribosomal protein S4



• Molecule 36: 30S ribosomal protein S5



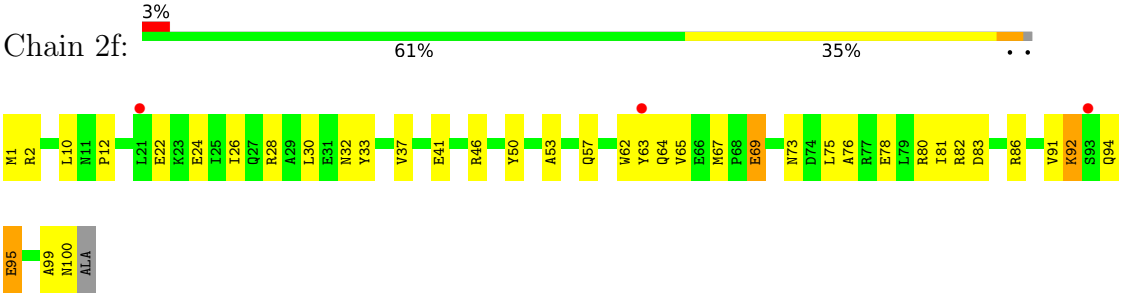
• Molecule 36: 30S ribosomal protein S5



• Molecule 37: 30S ribosomal protein S6

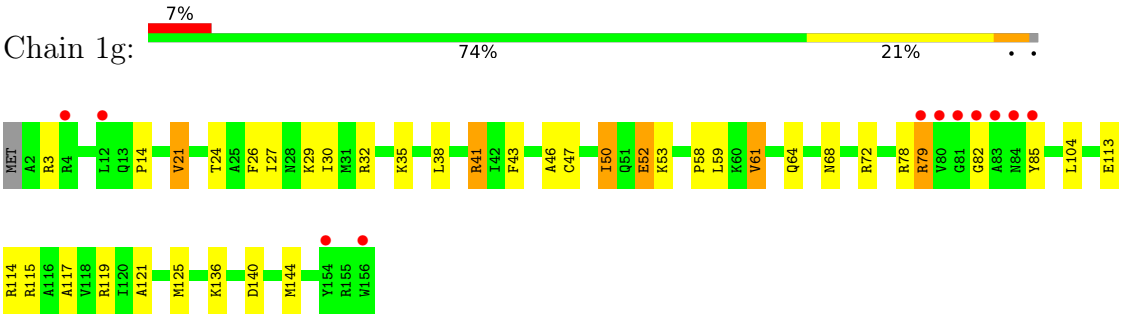
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



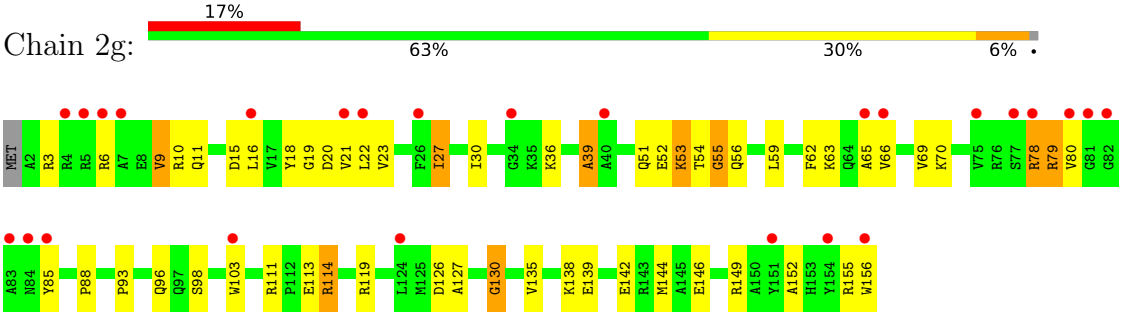
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



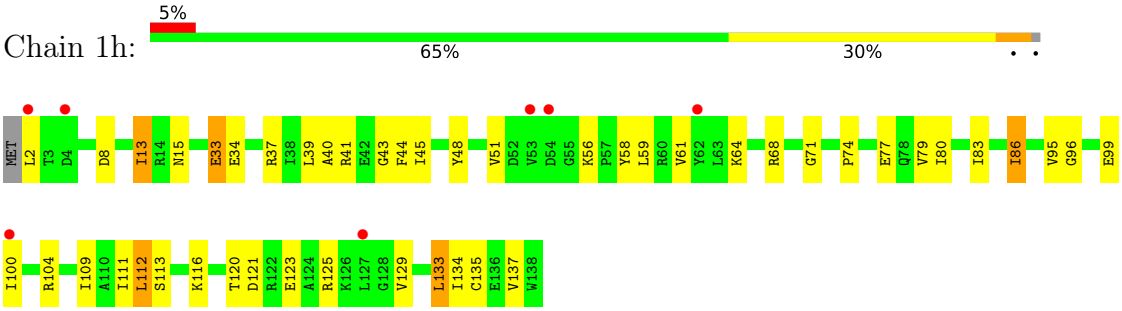
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



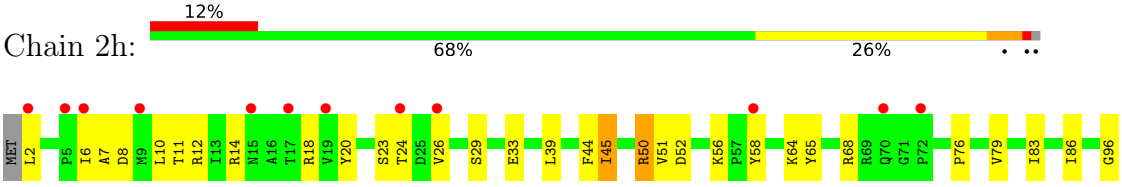
• Molecule 39: 30S ribosomal protein S8

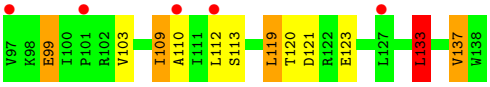
Chain 1h:



• Molecule 39: 30S ribosomal protein S8

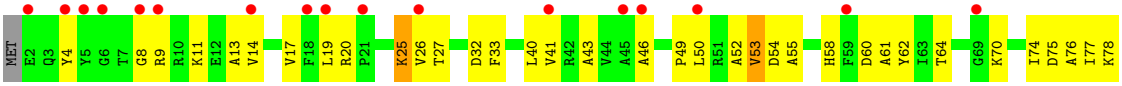
Chain 2h:

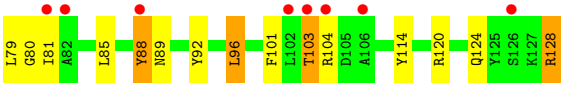




• Molecule 40: 30S ribosomal protein S9

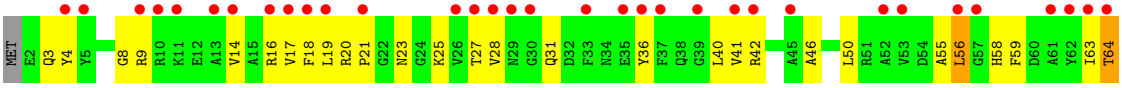
Chain 1i:

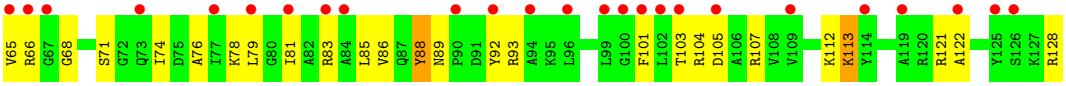




• Molecule 40: 30S ribosomal protein S9

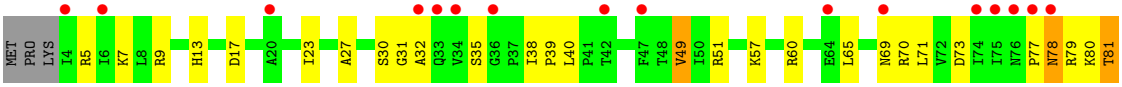
Chain 2i:

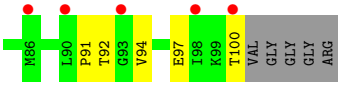




• Molecule 41: 30S ribosomal protein S10

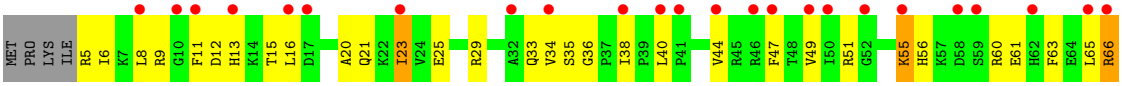
Chain 1j:

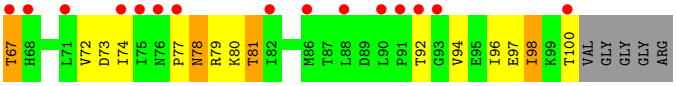




• Molecule 41: 30S ribosomal protein S10

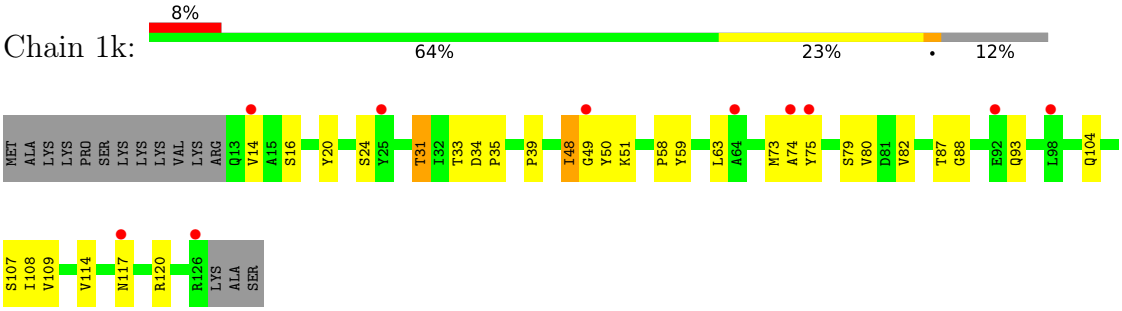
Chain 2j:





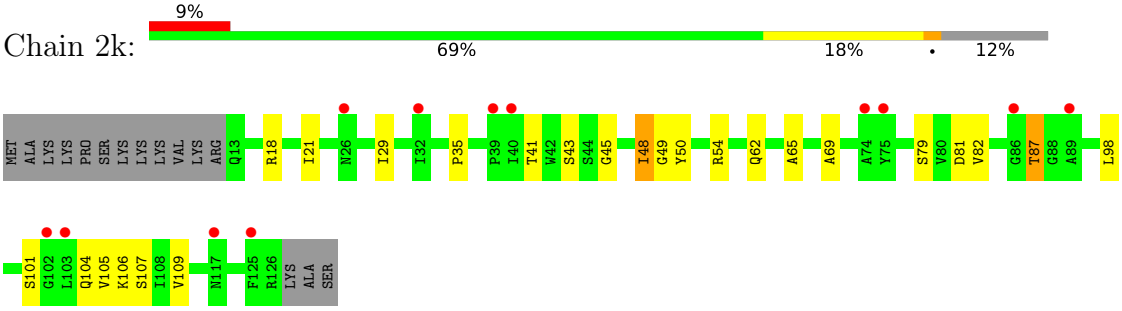
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



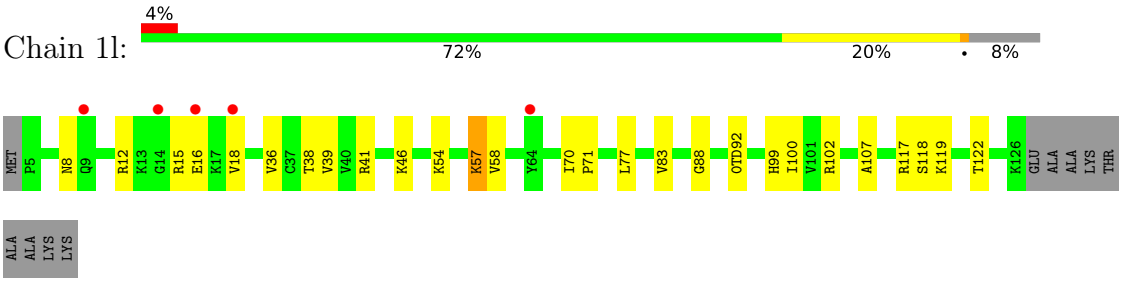
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



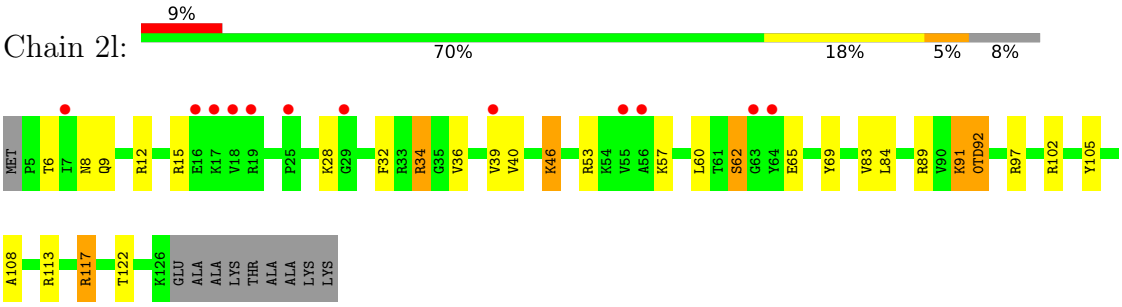
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



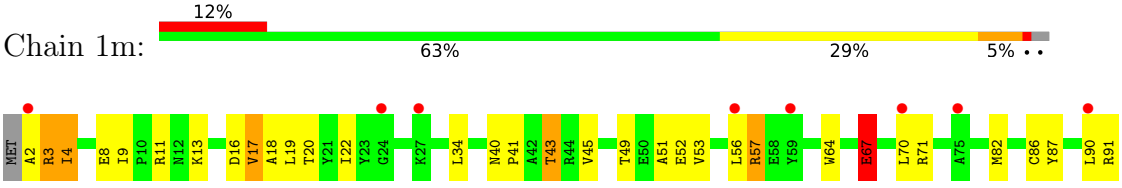
• Molecule 43: 30S ribosomal protein S12

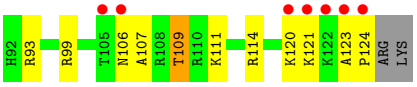
Chain 2l:



• Molecule 44: 30S ribosomal protein S13

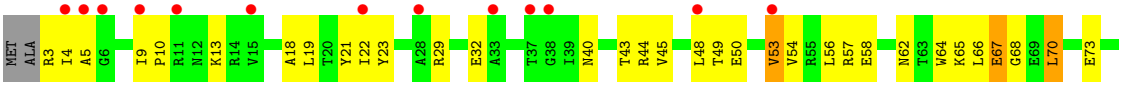
Chain 1m:

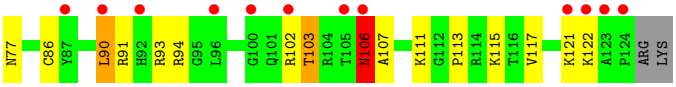




• Molecule 44: 30S ribosomal protein S13

Chain 2m:



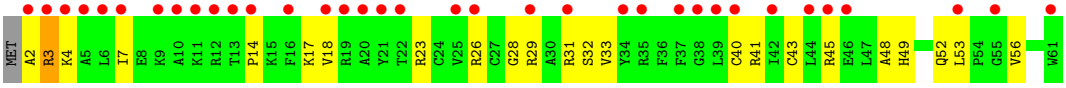


• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:

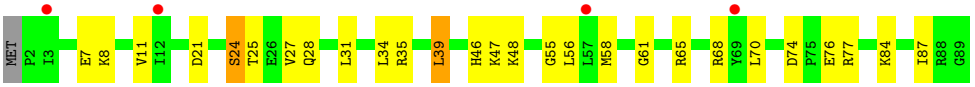
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



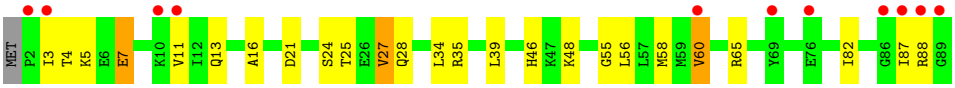
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



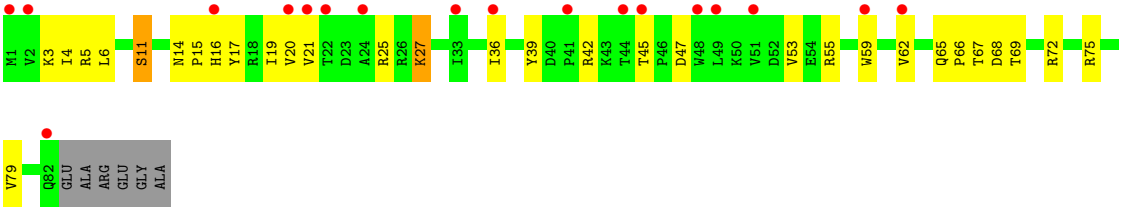
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



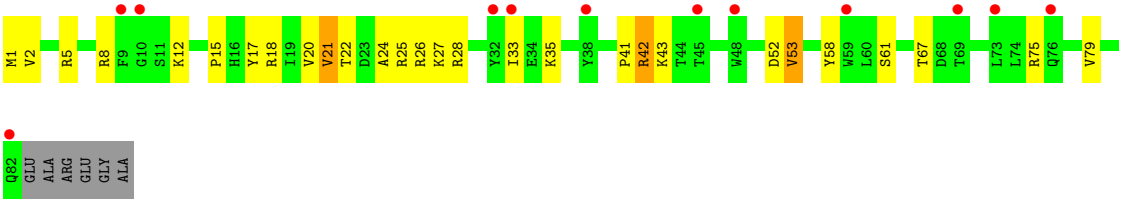
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



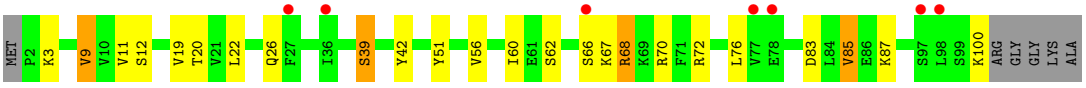
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



• Molecule 48: 30S ribosomal protein S17

Chain 1q:

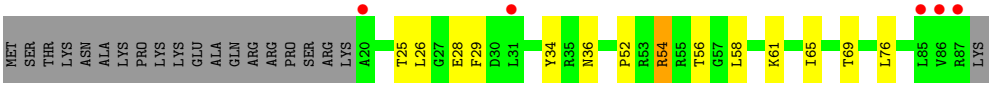


• Molecule 48: 30S ribosomal protein S17

Chain 2q:

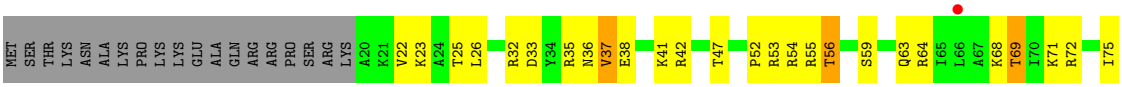
• Molecule 49: 30S ribosomal protein S18

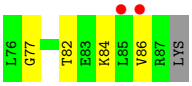
Chain 1r:



• Molecule 49: 30S ribosomal protein S18

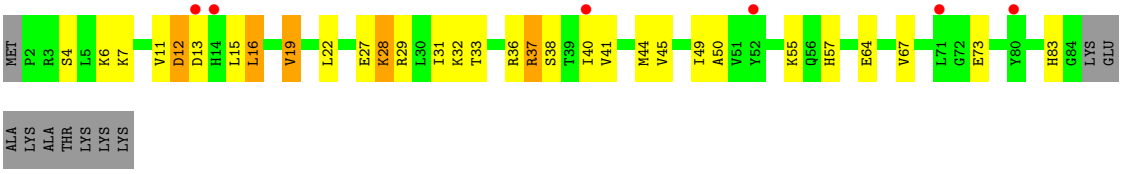
Chain 2r:





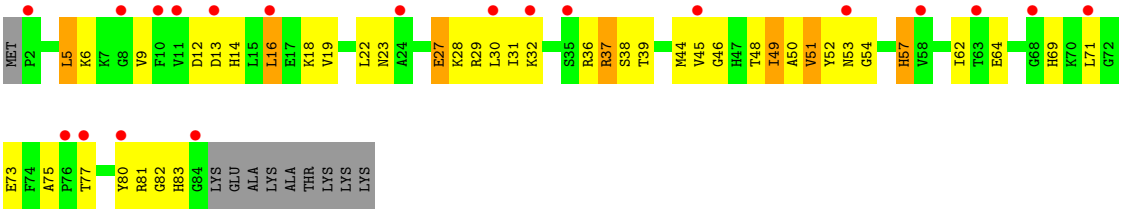
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



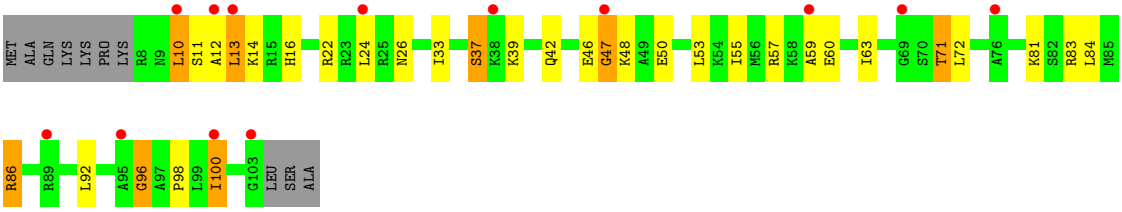
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



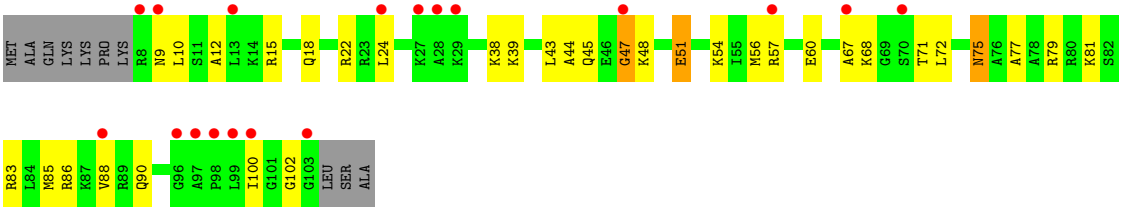
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



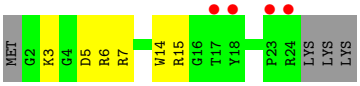
• Molecule 51: 30S ribosomal protein S20

Chain 2t:

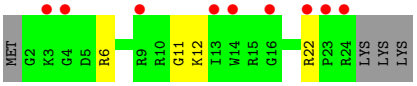


• Molecule 52: 30S ribosomal protein Thx

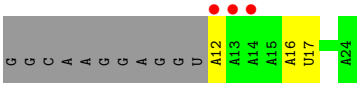
Chain 1u:



• Molecule 52: 30S ribosomal protein Thx

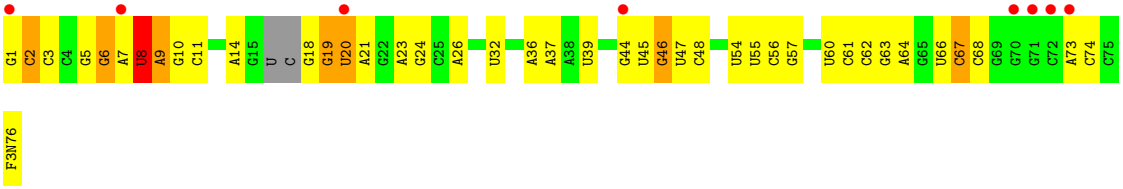


• Molecule 53: MF-mRNA

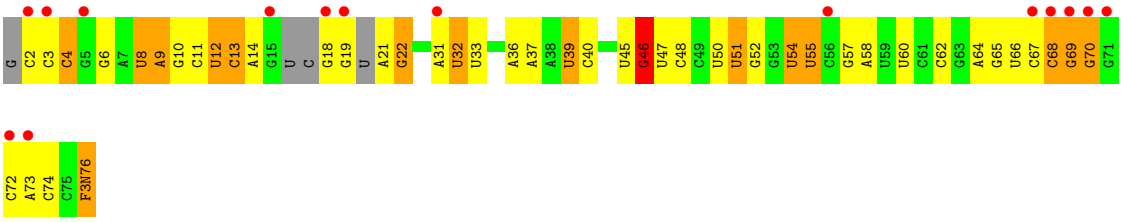


• Molecule 53: MF-mRNA

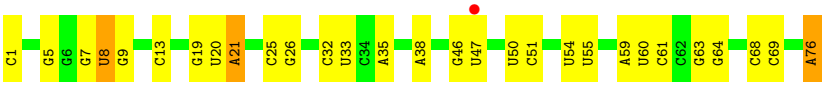
• Molecule 54: A-site Aminoacyl-tRNA Phe-NH-tRNAphe



• Molecule 54: A-site Aminoacyl-tRNA Phe-NH-tRNAphe

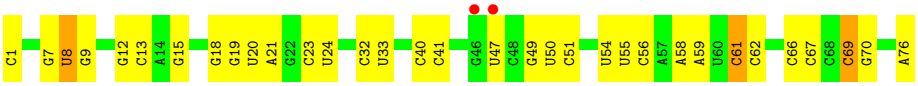


• Molecule 55: P-site Peptidyl-tRNA fMSEAC-NH-tRNAmet RNA-part



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

Chain 2x:

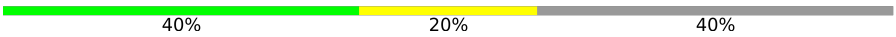


• Molecule 56: P-site Peptidyl-tRNA fMSEAC-NH-tRNAmet Peptide-part

Chain 1z:

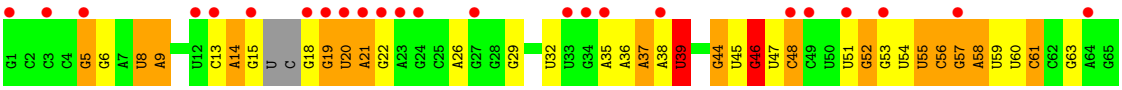
• Molecule 56: P-site Peptidyl-tRNA fMSEAC-NH-tRNAmet Peptide-part

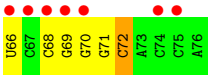
Chain 2z:



• Molecule 57: E-site Deacylated tRNAphe

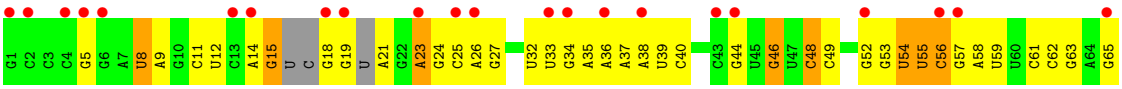
Chain 1y:

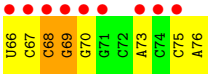




• Molecule 57: E-site Deacylated tRNAphe

Chain 2y:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.47Å 451.32Å 627.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.89 – 2.40 109.89 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (109.89-2.40) 98.1 (109.89-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.246 , 0.295 0.247 , 0.295	Depositor DCC
R_{free} test set	112777 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	42.3	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.34$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	299959	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, MG, UR3, 0TD, OMU, ZN, MA6, K, PSU, OMC, 4OC, 2MG, 2MA, 8AN, MIA, F3N, 4SU, SF4, 5MU, G7M, M2G, 5MC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1A	0.28	0/69011	0.48	1/107720 (0.0%)
1	2A	0.21	0/67295	0.41	1/105042 (0.0%)
2	1B	0.22	0/2882	0.41	0/4494
2	2B	0.19	0/2879	0.38	0/4487
3	1D	0.26	0/2186	0.50	0/2944
3	2D	0.23	0/2186	0.46	0/2944
4	1E	0.28	0/1592	0.50	0/2149
4	2E	0.21	0/1592	0.49	1/2149 (0.0%)
5	1F	0.27	0/1618	0.50	0/2191
5	2F	0.22	0/1614	0.48	2/2186 (0.1%)
6	1G	0.22	0/1448	0.46	0/1957
6	2G	0.18	0/1453	0.46	1/1963 (0.1%)
7	1H	0.23	0/1356	0.44	0/1834
7	2H	0.18	0/1356	0.37	0/1834
8	1I	0.20	0/1112	0.43	0/1514
8	2I	0.21	0/1079	0.46	0/1475
9	1N	0.28	0/1144	0.49	0/1543
9	2N	0.20	0/1144	0.40	0/1543
10	1O	0.25	0/943	0.48	0/1269
10	2O	0.22	0/943	0.42	0/1269
11	1P	0.26	0/1152	0.54	0/1533
11	2P	0.21	0/1152	0.51	0/1533
12	1Q	0.26	0/1143	0.48	0/1527
12	2Q	0.22	0/1143	0.46	0/1527
13	1R	0.30	0/982	0.54	0/1312
13	2R	0.22	0/982	0.44	0/1312
14	1S	0.23	0/883	0.50	0/1176
14	2S	0.21	0/880	0.45	0/1172
15	1T	0.23	0/1105	0.50	0/1477
15	2T	0.21	0/1097	0.46	0/1468
16	1U	0.28	0/977	0.50	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	2U	0.20	0/977	0.42	0/1301
17	1V	0.26	0/782	0.50	0/1049
17	2V	0.19	0/782	0.42	0/1049
18	1W	0.28	0/897	0.48	0/1205
18	2W	0.21	0/897	0.41	0/1205
19	1X	0.26	0/764	0.52	2/1025 (0.2%)
19	2X	0.22	0/764	0.55	2/1025 (0.2%)
20	1Y	0.23	0/819	0.47	0/1095
20	2Y	0.20	0/819	0.43	0/1095
21	1Z	0.23	0/1267	0.47	0/1717
21	2Z	0.22	0/1299	0.48	0/1763
22	10	0.26	0/662	0.50	0/881
22	20	0.19	0/662	0.44	0/881
23	11	0.24	0/762	0.44	0/1014
23	21	0.20	0/762	0.42	0/1014
24	12	0.24	0/590	0.42	0/781
24	22	0.21	0/590	0.41	0/781
25	13	0.29	0/474	0.49	0/635
25	23	0.19	0/469	0.43	0/630
26	14	0.25	0/565	0.57	0/761
26	24	0.23	0/545	0.50	0/737
27	15	0.30	0/469	0.58	0/635
27	25	0.22	0/469	0.45	0/635
28	16	0.25	0/460	0.45	0/613
28	26	0.20	0/456	0.44	0/608
29	17	0.31	0/426	0.57	0/561
29	27	0.25	0/426	0.46	0/561
30	18	0.26	0/525	0.49	0/691
30	28	0.20	0/525	0.40	0/691
31	19	0.28	0/310	0.50	0/407
31	29	0.20	0/310	0.43	0/407
32	1a	0.20	0/35795	0.40	2/55864 (0.0%)
32	2a	0.20	1/35886 (0.0%)	0.38	0/56005
33	1b	0.21	0/1881	0.49	1/2542 (0.0%)
33	2b	0.20	0/1860	0.46	0/2518
34	1c	0.20	0/1572	0.41	0/2126
34	2c	0.20	0/1566	0.42	0/2119
35	1d	0.20	0/1685	0.45	0/2262
35	2d	0.19	0/1704	0.43	0/2284
36	1e	0.21	0/1145	0.47	0/1543
36	2e	0.20	0/1149	0.51	2/1548 (0.1%)
37	1f	0.20	0/823	0.44	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	0.19	0/1250	0.43	0/1679
38	2g	0.19	0/1254	0.42	0/1683
39	1h	0.20	0/1108	0.41	0/1494
39	2h	0.20	0/1108	0.41	0/1494
40	1i	0.20	0/1002	0.50	0/1346
40	2i	0.23	0/997	0.51	0/1343
41	1j	0.20	0/722	0.45	0/982
41	2j	0.22	0/727	0.44	0/988
42	1k	0.19	0/844	0.42	0/1145
42	2k	0.19	0/848	0.40	0/1149
43	1l	0.23	0/937	0.46	0/1260
43	2l	0.20	0/937	0.42	0/1260
44	1m	0.20	0/969	0.50	0/1302
44	2m	0.20	0/961	0.47	0/1291
45	1n	0.21	0/501	0.44	0/664
45	2n	0.21	0/501	0.46	0/664
46	1o	0.19	0/739	0.39	0/985
46	2o	0.18	0/739	0.40	0/985
47	1p	0.19	0/697	0.45	0/939
47	2p	0.20	0/693	0.46	0/935
48	1q	0.20	0/836	0.44	0/1117
48	2q	0.20	0/836	0.44	0/1117
49	1r	0.20	0/560	0.41	0/746
49	2r	0.19	0/560	0.44	0/746
50	1s	0.21	0/667	0.49	0/900
50	2s	0.26	0/661	0.61	1/893 (0.1%)
51	1t	0.20	0/730	0.50	0/965
51	2t	0.21	0/729	0.45	0/965
52	1u	0.21	0/203	0.51	0/266
52	2u	0.21	0/203	0.49	0/266
53	1v	0.20	0/310	0.32	0/480
53	2v	0.20	0/310	0.34	0/480
54	1w	0.30	1/1581 (0.1%)	0.46	0/2458
54	2w	0.30	2/1531 (0.1%)	0.42	0/2379
55	1x	0.28	0/1723	0.42	0/2684
55	2x	0.25	1/1723 (0.1%)	0.40	0/2684
56	1z	0.43	0/25	0.64	0/32
56	2z	0.22	0/19	0.36	0/24
57	1y	0.32	1/1606 (0.1%)	0.43	0/2497
57	2y	0.32	2/1583 (0.1%)	0.43	0/2459
All	All	0.23	8/316678 (0.0%)	0.44	16/474093 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
33	1b	0	1
44	2m	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	46	G7M	O3'-P	5.48	1.61	1.56
57	2y	46	G7M	O3'-P	5.43	1.61	1.56
57	2y	8	4SU	O3'-P	5.29	1.61	1.56
55	2x	8	4SU	O3'-P	5.25	1.61	1.56
57	1y	46	G7M	O3'-P	5.24	1.61	1.56
54	1w	46	G7M	O3'-P	5.17	1.61	1.56
54	2w	8	4SU	O3'-P	5.09	1.61	1.56
32	2a	1498	UR3	O3'-P	5.04	1.61	1.56

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	2E	34	VAL	N-CA-C	-9.41	103.55	112.96
1	1A	1992	G	C2'-C3'-O3'	6.64	119.47	109.50
33	1b	18	GLY	N-CA-C	5.93	119.49	111.72
19	2X	94	GLY	CA-C-N	5.70	131.96	121.70
19	2X	94	GLY	C-N-CA	5.70	131.96	121.70
5	2F	21	ALA	CA-C-N	5.63	131.83	121.70
5	2F	21	ALA	C-N-CA	5.63	131.83	121.70
32	1a	266	G	C2'-C3'-O3'	5.37	117.55	109.50
50	2s	44	MET	N-CA-C	-5.36	107.29	112.97
19	1X	94	GLY	CA-C-N	5.29	131.21	121.70
19	1X	94	GLY	C-N-CA	5.29	131.21	121.70
36	2e	50	GLU	CA-C-N	5.27	124.55	120.33
36	2e	50	GLU	C-N-CA	5.27	124.55	120.33
6	2G	44	GLY	N-CA-C	-5.27	108.73	115.42
32	1a	266	G	P-O3'-C3'	5.15	127.93	120.20
1	2A	1992	G	C2'-C3'-O3'	5.01	117.01	109.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	125	PRO	Peptide
44	2m	106	ASN	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	31193	557	0
1	2A	60322	0	30424	662	0
2	1B	2577	0	1305	17	0
2	2B	2575	0	1303	34	0
3	1D	2136	0	2218	42	0
3	2D	2136	0	2218	37	0
4	1E	1559	0	1617	23	0
4	2E	1559	0	1618	25	0
5	1F	1583	0	1625	31	0
5	2F	1579	0	1619	54	0
6	1G	1423	0	1436	32	0
6	2G	1428	0	1438	61	0
7	1H	1330	0	1407	23	0
7	2H	1330	0	1407	33	0
8	1I	1097	0	1140	25	0
8	2I	1064	0	1082	39	0
9	1N	1117	0	1184	16	0
9	2N	1117	0	1184	24	0
10	1O	933	0	996	20	0
10	2O	933	0	996	19	0
11	1P	1135	0	1212	21	0
11	2P	1135	0	1212	36	0
12	1Q	1122	0	1179	11	0
12	2Q	1122	0	1179	27	0
13	1R	968	0	1033	19	0
13	2R	968	0	1033	17	0
14	1S	873	0	927	14	0
14	2S	870	0	923	41	0
15	1T	1091	0	1151	18	0
15	2T	1083	0	1136	36	0
16	1U	959	0	1019	9	0
16	2U	959	0	1019	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	1V	771	0	830	4	0
17	2V	771	0	830	15	0
18	1W	886	0	939	17	0
18	2W	886	0	940	12	0
19	1X	750	0	814	11	0
19	2X	750	0	813	24	0
20	1Y	806	0	881	17	0
20	2Y	806	0	881	16	0
21	1Z	1240	0	1240	25	0
21	2Z	1271	0	1273	42	0
22	10	653	0	674	9	0
22	20	653	0	674	14	0
23	11	755	0	826	11	0
23	21	755	0	826	21	0
24	12	588	0	643	3	0
24	22	588	0	643	16	0
25	13	469	0	518	11	0
25	23	464	0	514	9	0
26	14	552	0	533	26	0
26	24	532	0	503	25	0
27	15	455	0	465	7	0
27	25	455	0	465	4	0
28	16	453	0	473	10	0
28	26	449	0	469	11	0
29	17	418	0	467	4	0
29	27	418	0	467	9	0
30	18	517	0	582	10	0
30	28	517	0	582	16	0
31	19	307	0	335	3	0
31	29	307	0	335	6	0
32	1a	32246	0	16294	380	0
32	2a	32327	0	16338	483	0
33	1b	1846	0	1867	60	0
33	2b	1825	0	1828	69	0
34	1c	1548	0	1535	42	0
34	2c	1542	0	1517	45	0
35	1d	1655	0	1672	56	0
35	2d	1674	0	1714	57	0
36	1e	1129	0	1185	30	0
36	2e	1133	0	1191	32	0
37	1f	810	0	804	19	0
37	2f	816	0	808	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	1g	1231	0	1238	22	0
38	2g	1235	0	1248	41	0
39	1h	1088	0	1126	29	0
39	2h	1088	0	1126	27	0
40	1i	983	0	986	35	0
40	2i	978	0	966	37	0
41	1j	709	0	650	21	0
41	2j	714	0	672	39	0
42	1k	829	0	825	14	0
42	2k	833	0	834	11	0
43	1l	932	0	981	13	0
43	2l	932	0	981	19	0
44	1m	958	0	1002	28	0
44	2m	950	0	988	33	0
45	1n	492	0	529	11	0
45	2n	492	0	529	19	0
46	1o	728	0	760	16	0
46	2o	728	0	760	21	0
47	1p	681	0	697	20	0
47	2p	677	0	686	20	0
48	1q	823	0	891	13	0
48	2q	823	0	891	13	0
49	1r	555	0	618	10	0
49	2r	555	0	618	26	0
50	1s	652	0	662	20	0
50	2s	646	0	644	34	0
51	1t	728	0	798	26	0
51	2t	727	0	796	25	0
52	1u	199	0	208	5	0
52	2u	199	0	208	2	0
53	1v	277	0	140	3	0
53	2v	277	0	140	3	0
54	1w	1603	0	828	20	0
54	2w	1555	0	797	27	0
55	1x	1646	0	838	19	0
55	2x	1646	0	838	16	0
56	1z	26	0	20	0	0
56	2z	20	0	15	1	0
57	1y	1585	0	803	32	0
57	2y	1565	0	793	39	0
58	10	7	0	0	0	0
58	11	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	12	2	0	0	0	0
58	13	6	0	0	0	0
58	14	1	0	0	0	0
58	15	7	0	0	0	0
58	16	2	0	0	0	0
58	17	5	0	0	0	0
58	18	5	0	0	0	0
58	19	1	0	0	0	0
58	1A	1108	0	0	0	0
58	1B	38	0	0	0	0
58	1D	10	0	0	0	0
58	1E	14	0	0	0	0
58	1F	14	0	0	0	0
58	1G	5	0	0	0	0
58	1H	1	0	0	0	0
58	1I	1	0	0	0	0
58	1N	5	0	0	0	0
58	1O	5	0	0	0	0
58	1P	4	0	0	0	0
58	1Q	8	0	0	0	0
58	1R	3	0	0	0	0
58	1S	3	0	0	0	0
58	1T	3	0	0	0	0
58	1U	11	0	0	0	0
58	1V	6	0	0	0	0
58	1W	4	0	0	0	0
58	1X	6	0	0	0	0
58	1Y	3	0	0	0	0
58	1Z	3	0	0	0	0
58	1a	213	0	0	0	0
58	1b	1	0	0	0	0
58	1d	1	0	0	0	0
58	1e	2	0	0	0	0
58	1f	2	0	0	0	0
58	1k	1	0	0	0	0
58	1l	2	0	0	0	0
58	1m	1	0	0	0	0
58	1n	2	0	0	0	0
58	1t	1	0	0	0	0
58	1v	1	0	0	0	0
58	1w	9	0	0	0	0
58	1x	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	20	3	0	0	0	0
58	21	1	0	0	0	0
58	23	3	0	0	0	0
58	25	6	0	0	0	0
58	27	3	0	0	0	0
58	28	3	0	0	0	0
58	2A	869	0	0	0	0
58	2B	19	0	0	0	0
58	2D	7	0	0	0	0
58	2E	8	0	0	0	0
58	2F	6	0	0	0	0
58	2G	1	0	0	0	0
58	2O	1	0	0	0	0
58	2P	1	0	0	0	0
58	2Q	2	0	0	0	0
58	2R	2	0	0	0	0
58	2T	3	0	0	0	0
58	2U	2	0	0	0	0
58	2V	2	0	0	0	0
58	2W	2	0	0	0	0
58	2X	2	0	0	0	0
58	2Y	1	0	0	0	0
58	2Z	1	0	0	0	0
58	2a	235	0	0	0	0
58	2d	2	0	0	0	0
58	2e	1	0	0	0	0
58	2f	2	0	0	0	0
58	2g	1	0	0	0	0
58	2i	1	0	0	0	0
58	2j	1	0	0	0	0
58	2k	1	0	0	0	0
58	2l	4	0	0	0	0
58	2n	1	0	0	0	0
58	2p	1	0	0	0	0
58	2q	2	0	0	0	0
58	2r	1	0	0	0	0
58	2t	1	0	0	0	0
58	2v	4	0	0	0	0
58	2w	4	0	0	0	0
58	2x	6	0	0	0	0
58	2y	1	0	0	0	0
59	1A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	2x	1	0	0	0	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0
60	25	1	0	0	0	0
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	2	0
61	2d	8	0	0	0	0
62	10	13	0	0	1	0
62	11	12	0	0	0	0
62	12	3	0	0	0	0
62	13	4	0	0	0	0
62	14	1	0	0	0	0
62	15	6	0	0	0	0
62	16	2	0	0	0	0
62	17	10	0	0	1	0
62	18	8	0	0	0	0
62	1A	1956	0	0	90	0
62	1B	62	0	0	1	0
62	1D	27	0	0	0	0
62	1E	28	0	0	1	0
62	1F	22	0	0	0	0
62	1G	3	0	0	1	0
62	1H	2	0	0	0	0
62	1N	4	0	0	1	0
62	1O	5	0	0	0	0
62	1P	21	0	0	1	0
62	1Q	6	0	0	0	0
62	1R	11	0	0	1	0
62	1S	4	0	0	0	0
62	1T	7	0	0	0	0
62	1U	11	0	0	0	0
62	1V	8	0	0	0	0
62	1W	8	0	0	0	0
62	1X	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	1Y	3	0	0	1	0
62	1Z	1	0	0	0	0
62	1a	326	0	0	21	0
62	1b	1	0	0	0	0
62	1e	1	0	0	0	0
62	1f	1	0	0	0	0
62	1g	1	0	0	0	0
62	1i	1	0	0	0	0
62	1l	4	0	0	0	0
62	1m	1	0	0	0	0
62	1o	1	0	0	0	0
62	1p	1	0	0	0	0
62	1q	2	0	0	0	0
62	1u	1	0	0	1	0
62	1v	5	0	0	0	0
62	1w	8	0	0	0	0
62	1x	9	0	0	1	0
62	1y	1	0	0	0	0
62	1z	1	0	0	0	0
62	20	3	0	0	0	0
62	21	10	0	0	1	0
62	22	1	0	0	0	0
62	23	1	0	0	0	0
62	25	2	0	0	0	0
62	27	4	0	0	0	0
62	28	3	0	0	0	0
62	29	1	0	0	0	0
62	2A	1067	0	0	68	0
62	2B	22	0	0	1	0
62	2D	26	0	0	2	0
62	2E	17	0	0	1	0
62	2F	13	0	0	0	0
62	2N	1	0	0	0	0
62	2O	1	0	0	0	0
62	2P	10	0	0	1	0
62	2Q	2	0	0	0	0
62	2R	4	0	0	0	0
62	2T	4	0	0	0	0
62	2U	2	0	0	0	0
62	2W	2	0	0	0	0
62	2X	4	0	0	0	0
62	2Y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	2Z	1	0	0	0	0
62	2a	225	0	0	20	0
62	2c	1	0	0	0	0
62	2d	1	0	0	0	0
62	2e	2	0	0	0	0
62	2i	1	0	0	0	0
62	2j	3	0	0	2	0
62	2l	6	0	0	0	0
62	2p	2	0	0	0	0
62	2r	1	0	0	0	0
62	2t	2	0	0	0	0
62	2v	1	0	0	0	0
62	2w	5	0	0	0	0
62	2x	3	0	0	0	0
62	2z	1	0	0	1	0
All	All	299959	0	196751	3987	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 8.

All (3987) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.27	1.30
1:2A:2143:C:N4	1:2A:2148:G:H1	1.35	1.22
1:1A:1082:U:O4	1:1A:1086:A:N1	1.87	1.05
1:2A:2137:C:H42	1:2A:2154:G:H1	1.04	1.00
32:2a:1025:U:H3	32:2a:1036:G:H1	1.06	0.99
1:1A:2100:G:H1	1:1A:2189:U:H3	1.03	0.98
1:1A:2319:G:H22	14:1S:3:ARG:HD3	1.30	0.96
5:1F:53:THR:HG22	5:1F:55:GLY:H	1.29	0.96
29:17:24:THR:HG22	29:17:27:GLY:H	1.28	0.95
1:1A:2499:C:OP1	62:1A:4202:HOH:O	1.82	0.95
1:1A:1603:A:OP1	62:1A:4203:HOH:O	1.85	0.94
1:2A:2138:C:H42	1:2A:2153:G:H1	1.14	0.94
1:1A:2121:G:H1	1:1A:2177:C:H42	1.13	0.93
1:2A:2137:C:N4	1:2A:2154:G:H1	1.67	0.92
1:2A:2099:U:H3	1:2A:2190:G:H1	1.18	0.91
1:2A:2143:C:N3	1:2A:2148:G:N2	2.18	0.91
32:1a:1027:C:C2	32:1a:1034:G:N2	2.38	0.89
1:1A:2099:U:H3	1:1A:2190:G:H1	0.90	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2O:48:PRO:HB3	32:2a:1422:G:H5”	1.54	0.89
1:1A:2136:C:N3	1:1A:2155:G:C2	2.41	0.88
1:1A:1054:A:H61	1:1A:1105:U:H3	1.22	0.88
1:2A:2110:G:OP1	1:2A:2118:U:N3	2.06	0.88
1:1A:2849:U:OP2	15:1T:95:ARG:NH1	2.07	0.87
57:2y:14:A:H61	57:2y:21:A:H2	1.20	0.87
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.20	0.86
32:2a:64:G:H4’	32:2a:65:U:H3’	1.58	0.86
54:2w:18:G:O2’	54:2w:57:G:N2	2.09	0.85
1:2A:2138:C:N4	1:2A:2153:G:H1	1.73	0.85
57:2y:26:A:N1	57:2y:44:G:O6	2.09	0.84
26:14:16:CYS:SG	26:14:17:GLY:N	2.50	0.84
32:2a:1310:G:H5’	44:2m:77:ASN:HD21	1.43	0.84
32:1a:975:A:H4’	32:1a:976:G:H5”	1.60	0.84
1:1A:2615:U:OP1	62:1A:4204:HOH:O	1.96	0.84
32:2a:662:G:O2’	32:2a:836:G:OP1	1.96	0.83
50:2s:28:LYS:HB3	50:2s:29:ARG:HA	1.60	0.83
32:2a:1055:A:N7	32:2a:1200:C:N4	2.26	0.83
1:2A:943:U:OP2	62:2A:3903:HOH:O	1.95	0.82
1:1A:1602:U:O4	62:1A:4205:HOH:O	1.97	0.82
1:2A:1568:G:N7	62:2D:401:HOH:O	2.11	0.82
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.62	0.82
34:2c:58:GLU:HB3	41:2j:92:THR:HG21	1.61	0.82
32:2a:1029:C:N3	32:2a:1032:G:N2	2.27	0.82
8:2I:82:ARG:HB2	8:2I:89:TYR:HE2	1.43	0.82
1:1A:1183:G:O2’	25:13:29:ARG:NH2	2.12	0.81
1:1A:881:G:N2	1:1A:897:C:O2	2.13	0.81
21:2Z:106:GLY:HA3	21:2Z:141:VAL:HB	1.62	0.81
32:2a:1029:C:N4	32:2a:1032:G:N1	2.29	0.81
26:24:24:THR:OG1	26:24:25:TYR:N	2.13	0.81
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.13	0.81
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.63	0.81
1:1A:1693:U:O2’	3:1D:14:ARG:NH2	2.13	0.80
1:2A:1647:G:OP1	62:2A:3904:HOH:O	2.00	0.80
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.63	0.80
1:1A:1315:C:OP2	62:1A:4207:HOH:O	1.99	0.80
1:1A:802:A:OP1	62:1A:4208:HOH:O	1.99	0.80
32:1a:376:G:H5”	47:1p:5:ARG:HG2	1.63	0.80
32:1a:574:A:OP2	62:1a:1903:HOH:O	1.99	0.80
1:1A:279:C:H42	1:1A:361:G:H1	1.29	0.80
32:2a:1274:G:N2	32:2a:1275:A:N7	2.29	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:192:C:OP1	62:1A:4206:HOH:O	1.99	0.79
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.64	0.79
1:1A:2427:C:OP1	62:1A:4210:HOH:O	2.01	0.79
6:2G:113:ARG:NH2	6:2G:139:LEU:O	2.16	0.79
1:1A:2142:C:O2	1:1A:2149:G:N1	2.15	0.79
1:1A:2142:C:N3	1:1A:2149:G:O6	2.16	0.79
1:1A:2448:A:OP1	62:1A:4202:HOH:O	1.99	0.79
38:2g:16:LEU:HD22	40:2i:42:ARG:HA	1.63	0.79
32:1a:78:G:N2	32:1a:91:C:N3	2.31	0.79
1:2A:711:G:N2	1:2A:720:C:O2	2.15	0.79
1:2A:2808:U:O2	1:2A:2892:A:N6	2.15	0.79
28:26:12:GLU:OE1	28:26:19:ARG:NH1	2.15	0.79
1:2A:570:G:O6	62:2A:3905:HOH:O	2.00	0.78
21:2Z:154:ASP:OD1	21:2Z:154:ASP:N	2.15	0.78
32:2a:407:G:H5"	35:2d:115:ARG:HB3	1.64	0.78
32:1a:1314:C:OP2	50:1s:4:SER:OG	2.02	0.78
1:1A:1023:U:OP2	62:1A:4209:HOH:O	2.00	0.78
40:2i:3:GLN:HE21	40:2i:20:ARG:HE	1.30	0.78
33:1b:77:ALA:HB2	33:1b:211:ILE:HD13	1.66	0.78
32:1a:78:G:N1	32:1a:91:C:N4	2.32	0.78
32:1a:134:A:H61	47:1p:25:ARG:HH12	1.29	0.78
1:1A:2789:C:O2	1:1A:2894:G:N1	2.17	0.78
33:1b:178:ARG:HH22	39:1h:74:PRO:HB3	1.47	0.78
1:2A:2127:G:N1	1:2A:2161:C:N4	2.31	0.78
44:2m:58:GLU:O	44:2m:62:ASN:ND2	2.17	0.78
32:1a:1402:4OC:HM22	32:1a:1403:C:H5'	1.66	0.77
32:1a:1500:A:OP2	62:1a:1904:HOH:O	2.01	0.77
40:2i:121:ARG:NH1	40:2i:122:ALA:O	2.17	0.77
32:2a:588:G:OP2	62:2a:1903:HOH:O	2.01	0.77
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.17	0.77
57:2y:55:PSU:HN1	57:2y:57:G:H5"	1.48	0.77
1:2A:2218:U:O2	23:21:52:ARG:NH1	2.18	0.77
15:2T:105:LEU:HB2	15:2T:110:ILE:HG13	1.65	0.77
55:1x:76:8AN:O2P	62:1x:201:HOH:O	2.01	0.77
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.18	0.76
34:2c:125:GLU:HB2	34:2c:190:ARG:HH21	1.50	0.76
40:2i:16:ARG:HB2	40:2i:64:THR:HG22	1.65	0.76
32:1a:330:C:O2	62:1a:1905:HOH:O	2.03	0.76
1:2A:2759:G:OP2	62:2A:3906:HOH:O	2.03	0.76
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.66	0.76
1:1A:826:U:OP1	62:1A:4210:HOH:O	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:16:13:CYS:SG	28:16:47:THR:HG21	2.26	0.76
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.20	0.76
32:2a:401:C:OP2	35:2d:73:ARG:NH2	2.18	0.76
1:1A:307:G:N7	62:1A:4250:HOH:O	2.18	0.76
1:1A:2121:G:H1	1:1A:2177:C:N4	1.83	0.76
1:2A:1670:C:OP1	62:2A:3907:HOH:O	2.04	0.76
50:2s:18:LYS:HB3	50:2s:31:ILE:HD13	1.67	0.76
32:1a:276:G:O2'	48:1q:68:ARG:NH1	2.18	0.76
1:1A:2550:G:OP1	62:1A:4211:HOH:O	2.04	0.75
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.67	0.75
1:1A:110:G:N7	62:1A:4255:HOH:O	2.19	0.75
1:2A:2677:G:N3	62:2A:3940:HOH:O	2.18	0.75
32:2a:1029:C:C4	32:2a:1032:G:N1	2.54	0.75
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.19	0.75
4:2E:77:ILE:HD13	4:2E:195:LEU:HD22	1.68	0.75
32:2a:617:G:OP2	62:2a:1904:HOH:O	2.04	0.75
1:1A:1265:A:OP2	62:1A:4204:HOH:O	2.04	0.75
1:2A:2807:G:N2	1:2A:2893:G:O6	2.20	0.75
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.17	0.75
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.20	0.74
32:2a:953:G:H5'	32:2a:965:A:H61	1.50	0.74
1:1A:1014:U:OP2	62:1A:4212:HOH:O	2.05	0.74
32:1a:1108:G:O6	62:1a:1906:HOH:O	2.04	0.74
1:1A:2134:A:O2'	1:1A:2135:A:OP1	2.05	0.74
5:1F:184:TYR:O	5:1F:188:ARG:HG3	1.87	0.74
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.19	0.74
1:2A:2127:G:C6	1:2A:2161:C:N4	2.56	0.74
1:2A:2127:G:N2	1:2A:2161:C:N3	2.34	0.74
1:1A:1054:A:N6	1:1A:1105:U:H3	1.86	0.74
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.20	0.74
32:1a:1009:G:O6	32:1a:1020:U:O2	2.06	0.74
46:2o:39:LEU:HB3	46:2o:56:LEU:HD12	1.69	0.74
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.21	0.74
8:2I:40:THR:OG1	8:2I:41:GLU:N	2.18	0.74
32:1a:557:G:OP1	62:1a:1907:HOH:O	2.04	0.73
40:2i:4:TYR:HB2	40:2i:19:LEU:HB2	1.69	0.73
1:1A:2702:U:OP2	62:1A:4213:HOH:O	2.06	0.73
4:1E:110:GLY:O	62:1R:301:HOH:O	2.07	0.73
28:16:6:ARG:HH12	28:16:26:ASN:HB2	1.52	0.73
32:1a:892:A:OP2	62:1a:1908:HOH:O	2.06	0.73
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.06	0.73
1:1A:1064:C:N3	1:1A:1074:G:O6	2.20	0.73
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.21	0.73
57:1y:19:G:N2	57:1y:56:C:N3	2.37	0.73
32:2a:394:G:O6	62:2a:1906:HOH:O	2.06	0.73
1:2A:307:G:N7	62:2A:3956:HOH:O	2.22	0.73
1:2A:2690:C:OP1	13:2R:17:ARG:NH2	2.21	0.73
1:1A:668:G:OP2	62:1A:4214:HOH:O	2.06	0.73
32:1a:573:A:OP2	62:1a:1903:HOH:O	2.06	0.73
32:1a:664:G:H22	32:1a:741:G:H1	1.34	0.73
1:1A:2285:C:OP2	28:16:6:ARG:NH1	2.22	0.73
32:2a:117:G:OP2	62:2a:1905:HOH:O	2.05	0.73
51:2t:79:ARG:HD2	51:2t:83:ARG:HH21	1.54	0.73
1:1A:1670:C:OP1	62:1A:4215:HOH:O	2.06	0.73
54:2w:4:C:H42	54:2w:69:G:H1	1.37	0.73
1:1A:2141:G:O6	1:1A:2150:U:O2	2.07	0.73
1:2A:2879:C:OP2	62:2A:3908:HOH:O	2.05	0.72
45:2n:26:ARG:HD3	45:2n:43:CYS:HB3	1.71	0.72
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.71	0.72
17:2V:10:LYS:NZ	17:2V:23:GLU:OE2	2.22	0.72
32:2a:363:A:OP2	43:2l:34:ARG:NH2	2.21	0.72
1:1A:2111:C:N4	1:1A:2144:U:O2'	2.23	0.72
32:1a:410:G:OP1	35:1d:30:LYS:NZ	2.23	0.72
1:2A:10:G:O2'	1:2A:2801(A):A:N7	2.22	0.72
36:1e:35:GLY:HA3	36:1e:112:LEU:HB3	1.70	0.72
1:1A:1664:A:OP1	62:1A:4217:HOH:O	2.08	0.72
38:1g:64:GLN:HE21	38:1g:68:ASN:HD21	1.35	0.72
1:2A:582:G:OP2	62:2A:3909:HOH:O	2.07	0.72
1:2A:2207:G:H3'	1:2A:2208:A:H5"	1.71	0.72
38:2g:113:GLU:HG2	38:2g:119:ARG:HG2	1.72	0.72
54:1w:26:A:H61	54:1w:44:G:H1	1.37	0.72
1:2A:2138:C:N3	1:2A:2153:G:N2	2.33	0.72
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.07	0.72
1:1A:1062:G:H8	1:1A:1070:A:H4'	1.55	0.71
32:2a:1033:G:H2'	32:2a:1034:G:H8	1.54	0.71
32:2a:1225:A:OP1	44:2m:103:THR:OG1	2.08	0.71
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.22	0.71
7:2H:88:LEU:HD11	7:2H:165:ALA:HA	1.71	0.71
27:15:40:LYS:NZ	27:15:44:THR:O	2.23	0.71
8:2I:59:ALA:HA	8:2I:62:LYS:HB2	1.72	0.71
1:1A:279:C:N3	1:1A:361:G:N2	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2344:U:OP1	28:16:37:ARG:NH1	2.23	0.71
20:1Y:34:LYS:NZ	62:1Y:5101:HOH:O	2.15	0.71
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.26	0.71
1:1A:818:G:O6	62:1A:4218:HOH:O	2.09	0.71
1:2A:1604:C:OP1	62:2A:3912:HOH:O	2.09	0.71
1:2A:963:U:OP2	62:2A:3911:HOH:O	2.08	0.71
1:2A:2319:G:H22	14:2S:3:ARG:HH11	1.37	0.71
4:2E:34:VAL:HG21	4:2E:78:LEU:HD11	1.73	0.71
49:2r:53:ARG:HG2	49:2r:63:GLN:HE21	1.54	0.71
1:1A:1418:G:OP2	62:1A:4216:HOH:O	2.07	0.71
1:2A:217:G:OP2	62:2A:3910:HOH:O	2.08	0.71
5:1F:164:ARG:HD2	5:1F:175:THR:HG23	1.73	0.70
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.39	0.70
32:1a:1381:U:H1'	38:1g:79:ARG:HG2	1.73	0.70
10:2O:20:MET:HE3	10:2O:44:LYS:HE3	1.73	0.70
32:2a:653:A:OP1	39:2h:56:LYS:NZ	2.21	0.70
32:1a:1030(D):A:H2'	32:1a:1031:G:H4'	1.72	0.70
14:2S:71:ARG:NH1	14:2S:107:GLU:OE1	2.22	0.70
1:1A:1265:A:H3'	27:15:19:ARG:HH21	1.54	0.70
10:1O:49:ARG:NH2	32:1a:1423:G:OP1	2.22	0.70
1:2A:2576:G:OP1	62:2A:3915:HOH:O	2.10	0.70
1:1A:2136:C:N4	1:1A:2155:G:C6	2.59	0.70
33:2b:189:ASP:N	33:2b:189:ASP:OD1	2.24	0.70
44:2m:86:CYS:HB2	50:2s:73:GLU:HG2	1.73	0.70
44:2m:5:ALA:HB3	44:2m:22:ILE:HD12	1.72	0.70
1:1A:732:C:OP1	62:1A:4219:HOH:O	2.09	0.70
1:2A:245:G:O6	30:28:8:LYS:NZ	2.25	0.70
1:2A:1711:C:H2'	1:2A:1712:C:H6	1.57	0.70
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.74	0.70
1:2A:1604:C:OP2	62:2A:3913:HOH:O	2.09	0.70
1:1A:2428:G:OP1	62:1A:4210:HOH:O	2.08	0.70
21:1Z:138:GLU:H	21:1Z:156:LYS:HE3	1.57	0.70
52:1u:5:ASP:OD2	62:1u:101:HOH:O	2.10	0.70
1:1A:2350:C:OP2	62:1A:4221:HOH:O	2.10	0.69
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.27	0.69
1:1A:271(I):G:N2	1:1A:271(O):C:O2	2.24	0.69
1:1A:2128:C:N3	1:1A:2160:G:N2	2.39	0.69
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.74	0.69
45:2n:23:ARG:NH1	45:2n:28:GLY:O	2.25	0.69
39:1h:86:ILE:HD12	39:1h:133:LEU:HD22	1.73	0.69
1:2A:1812:A:OP2	62:2A:3914:HOH:O	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2682:U:OP2	62:2A:3917:HOH:O	2.11	0.69
15:1T:84:GLN:HG2	15:1T:85:LYS:HG2	1.72	0.69
50:1s:31:ILE:O	50:1s:50:ALA:N	2.24	0.69
1:2A:2218:U:N3	23:21:55:GLY:O	2.25	0.69
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.41	0.69
1:2A:882:G:H22	1:2A:894:C:H42	1.41	0.69
1:1A:2108:C:H2'	1:1A:2109:U:H6	1.58	0.69
26:14:54:GLY:N	26:14:55:ARG:HA	2.07	0.69
33:1b:30:ARG:HH21	33:1b:194:PRO:HB2	1.57	0.69
1:2A:1345:C:OP2	62:2A:3918:HOH:O	2.11	0.69
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.75	0.69
7:2H:86:GLU:OE2	7:2H:132:ARG:NH2	2.26	0.69
32:2a:142:G:H2'	32:2a:143:A:H8	1.58	0.69
40:2i:86:VAL:HG11	40:2i:93:ARG:HE	1.57	0.69
40:2i:105:ASP:HB2	40:2i:107:ARG:HG3	1.75	0.69
1:1A:1245:G:OP1	11:1P:13:ASN:ND2	2.23	0.69
32:2a:1244:C:H42	32:2a:1293:G:H1	1.39	0.69
1:1A:249:C:O2	30:18:12:LYS:NZ	2.23	0.69
32:1a:812:C:N3	62:1a:1928:HOH:O	2.26	0.69
26:24:53:GLU:HG2	26:24:55:ARG:H	1.58	0.69
1:1A:1669:A:OP2	62:1A:4211:HOH:O	2.11	0.68
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.07	0.68
3:2D:28:GLU:OE2	62:2D:401:HOH:O	2.11	0.68
32:2a:406:G:H21	35:2d:119:GLN:HE22	1.41	0.68
1:2A:1242:A:N1	11:2P:2:LYS:NZ	2.42	0.68
4:2E:119:ARG:HD2	4:2E:160:TYR:HB2	1.75	0.68
32:2a:157:G:H1	32:2a:164:U:H3	1.39	0.68
41:2j:6:ILE:HB	41:2j:72:VAL:HB	1.74	0.68
32:1a:324:G:N7	62:1a:1926:HOH:O	2.26	0.68
51:1t:10:LEU:HD12	51:1t:11:SER:H	1.58	0.68
1:2A:2299:G:H2'	1:2A:2300:G:H8	1.58	0.68
2:2B:43:C:H5"	26:24:1:MET:HG2	1.75	0.68
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	1.75	0.68
57:2y:18:G:N2	57:2y:55:PSU:N3	2.40	0.68
1:1A:72:U:OP1	62:1A:4224:HOH:O	2.12	0.68
1:1A:2128:C:N4	1:1A:2160:G:N1	2.41	0.68
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.41	0.68
32:1a:972:C:OP2	41:1j:57:LYS:NZ	2.23	0.68
40:1i:20:ARG:O	40:1i:60:ASP:N	2.22	0.68
18:2W:34:ASN:OD1	18:2W:37:ARG:NH2	2.26	0.68
32:2a:393:A:OP1	62:2a:1907:HOH:O	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:13:LYS:O	44:2m:45:VAL:N	2.24	0.68
1:1A:1332:G:OP1	62:1A:4207:HOH:O	2.10	0.68
1:1A:2612:C:OP2	27:15:2:ALA:N	2.27	0.68
2:1B:21:G:N7	62:1B:302:HOH:O	2.27	0.68
26:14:55:ARG:N	26:14:56:VAL:HA	2.08	0.68
1:2A:307:G:N1	1:2A:310:A:OP2	2.27	0.68
6:2G:165:THR:OG1	6:2G:167:GLU:OE1	2.10	0.68
32:2a:1027:C:O2'	32:2a:1034:G:N2	2.27	0.68
7:1H:124:GLU:HG3	7:1H:132:ARG:HB3	1.76	0.68
23:21:3:LYS:HB2	23:21:61:ARG:HH22	1.58	0.68
1:1A:2070:G:OP2	62:1A:4226:HOH:O	2.12	0.67
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.29	0.67
1:2A:1346:G:OP2	62:2A:3919:HOH:O	2.11	0.67
15:1T:16:ARG:NH2	15:1T:18:ASP:OD2	2.27	0.67
1:2A:995:C:OP2	16:2U:54:LYS:NZ	2.27	0.67
1:2A:2343:C:HO2'	1:2A:2373:G:HO2'	1.36	0.67
1:2A:2183:C:H2'	1:2A:2184:G:C8	2.30	0.67
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.59	0.67
43:2l:57:LYS:NZ	43:2l:65:GLU:OE2	2.27	0.67
1:1A:1993:U:OP2	62:1A:4223:HOH:O	2.11	0.67
1:1A:2136:C:N4	1:1A:2155:G:N1	2.43	0.67
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.26	0.67
36:1e:78:HIS:HE1	36:1e:143:ARG:H	1.41	0.67
2:2B:87:G:N2	2:2B:90:A:OP2	2.27	0.67
35:2d:193:ASP:OD1	35:2d:193:ASP:N	2.25	0.67
1:1A:1013:C:OP2	62:1A:4212:HOH:O	2.12	0.67
1:1A:1938:A:OP2	62:1A:4225:HOH:O	2.12	0.67
32:1a:1334:G:OP2	62:1a:1909:HOH:O	2.11	0.67
6:1G:145:THR:OG1	6:1G:148:MET:SD	2.49	0.67
1:2A:106:C:H1'	20:2Y:1:MET:HE2	1.75	0.67
1:1A:602:G:O6	62:1A:4220:HOH:O	2.10	0.67
6:1G:18:GLU:HG3	6:1G:22:ARG:HD2	1.76	0.67
28:16:12:GLU:OE1	28:16:19:ARG:NH1	2.27	0.67
32:2a:259:G:OP2	51:2t:83:ARG:NH1	2.26	0.67
32:1a:836:G:OP1	49:1r:61:LYS:NZ	2.28	0.67
1:2A:200:U:O2	1:2A:386:G:N2	2.28	0.67
40:2i:55:ALA:HA	40:2i:58:HIS:HD2	1.60	0.67
1:1A:2156:G:H2'	1:1A:2157:G:C2	2.29	0.67
8:1I:4:ILE:HG12	8:1I:18:VAL:HG22	1.76	0.67
2:2B:118:G:OP2	62:2B:301:HOH:O	2.12	0.67
32:2a:1193:G:O2'	36:2e:25:ARG:NH2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:467:G:OP1	29:17:33:ARG:NH1	2.28	0.67
1:1A:2038:G:O6	62:1A:4222:HOH:O	2.10	0.67
7:1H:3:ARG:HG3	7:1H:6:ARG:HE	1.59	0.67
36:1e:137:GLU:HG3	36:1e:141:GLN:HE21	1.60	0.67
8:2I:82:ARG:HB2	8:2I:89:TYR:CE2	2.29	0.67
33:2b:78:GLN:O	33:2b:94:ASN:ND2	2.27	0.67
8:2I:66:GLU:HA	8:2I:69:LYS:HB3	1.77	0.66
11:2P:36:LYS:O	62:2P:301:HOH:O	2.11	0.66
32:2a:196:A:OP1	51:2t:68:LYS:NZ	2.28	0.66
1:1A:884:C:H42	1:1A:892:G:H1	1.41	0.66
1:1A:2136:C:C2	1:1A:2155:G:N2	2.63	0.66
50:1s:27:GLU:HG3	50:1s:28:LYS:HE3	1.76	0.66
1:2A:586:A:OP2	62:2A:3922:HOH:O	2.13	0.66
1:2A:948:G:OP1	62:2A:3911:HOH:O	2.12	0.66
1:2A:1693:U:O2'	3:2D:14:ARG:NH2	2.28	0.66
3:2D:183:ARG:HG3	3:2D:270:ILE:HD13	1.74	0.66
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.76	0.66
17:2V:40:LEU:HB2	17:2V:46:VAL:HG23	1.76	0.66
32:2a:944:G:OP1	62:2a:1909:HOH:O	2.14	0.66
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.28	0.66
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.27	0.66
1:1A:1452:A:OP2	62:1A:4227:HOH:O	2.12	0.66
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.77	0.66
39:2h:86:ILE:HD12	39:2h:133:LEU:HD22	1.76	0.66
1:2A:301:G:N7	62:2A:3987:HOH:O	2.27	0.66
1:2A:2579:C:OP1	62:2A:3926:HOH:O	2.14	0.66
28:26:9:LEU:HD13	28:26:51:GLU:HG3	1.76	0.66
1:1A:2337:G:OP1	62:1A:4235:HOH:O	2.14	0.66
1:2A:1673:U:OP1	62:2A:3925:HOH:O	2.14	0.66
1:2A:2151:G:H2'	1:2A:2152:G:H8	1.60	0.66
36:2e:102:ALA:O	36:2e:107:ARG:NH2	2.28	0.66
44:2m:23:TYR:HB3	44:2m:67:GLU:HA	1.78	0.66
32:1a:1136:U:H5"	32:1a:1137:C:C4	2.30	0.66
57:1y:55:PSU:C4	57:1y:57:G:H5'	2.30	0.66
46:2o:87:ILE:HG22	46:2o:88:ARG:H	1.59	0.66
1:1A:1890:A:OP2	62:1A:4230:HOH:O	2.13	0.66
32:1a:545:C:OP1	35:1d:61:LYS:NZ	2.29	0.66
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.27	0.66
1:2A:89:G:H3'	1:2A:90:U:H5"	1.76	0.66
1:2A:993:G:OP1	16:2U:50:ARG:NH2	2.28	0.66
1:2A:2127:G:C2	1:2A:2161:C:N3	2.64	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2137:C:N3	1:2A:2154:G:N2	2.37	0.66
1:2A:2502:G:OP1	62:2A:3927:HOH:O	2.14	0.66
27:25:33:CYS:HB2	27:25:40:LYS:HD3	1.76	0.66
33:2b:27:LYS:HB3	33:2b:194:PRO:HD2	1.77	0.66
35:2d:110:PHE:HA	35:2d:162:LEU:HD21	1.76	0.66
41:2j:21:GLN:HE22	41:2j:25:GLU:HG2	1.60	0.66
1:1A:1466:G:O2'	1:1A:1546:C:O2'	2.12	0.66
1:1A:2136:C:N3	1:1A:2155:G:N2	2.43	0.66
1:1A:2438:U:OP1	62:1A:4228:HOH:O	2.13	0.66
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.11	0.66
23:21:73:LEU:HB3	23:21:94:LEU:HD22	1.77	0.66
1:1A:2059:A:OP2	62:1A:4239:HOH:O	2.14	0.66
35:1d:98:GLU:OE1	35:1d:103:ASN:ND2	2.29	0.66
1:2A:912:C:OP1	12:2Q:8:LYS:NZ	2.28	0.66
1:2A:1021:A:H62	1:2A:1141:U:H3	1.44	0.66
1:2A:1204:A:H2	1:2A:1241:A:H62	1.42	0.66
6:2G:114:ILE:HA	6:2G:140:ILE:HD11	1.77	0.66
38:2g:22:LEU:HD21	38:2g:66:VAL:HG11	1.77	0.66
57:2y:18:G:H22	57:2y:55:PSU:HN3	1.44	0.66
24:12:64:LEU:HD11	24:12:68:ARG:HE	1.60	0.65
34:1c:156:ARG:H	34:1c:196:LEU:HD22	1.61	0.65
1:2A:1313:U:OP1	62:2A:3921:HOH:O	2.13	0.65
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.29	0.65
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.76	0.65
21:2Z:171:ILE:HD12	21:2Z:172:ALA:H	1.60	0.65
32:2a:407:G:OP1	35:2d:115:ARG:NH2	2.28	0.65
1:1A:249:C:O2'	11:1P:64:LYS:NZ	2.27	0.65
1:1A:1069:A:H1'	1:1A:1096:A:H4'	1.78	0.65
1:1A:1779:U:OP2	62:1A:4237:HOH:O	2.14	0.65
32:2a:1004:A:N6	32:2a:1037:C:H1'	2.11	0.65
40:2i:8:GLY:HA2	40:2i:79:LEU:HD23	1.78	0.65
21:1Z:156:LYS:HD2	21:1Z:158:PRO:HD3	1.78	0.65
32:1a:1224:G:OP1	62:1a:1910:HOH:O	2.14	0.65
1:1A:530:G:N1	1:1A:2023:G:OP1	2.24	0.65
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.14	0.65
1:2A:2102:U:O2	1:2A:2187:G:O6	2.15	0.65
32:2a:1301:U:O2'	32:2a:1302:U:H5'	1.97	0.65
1:1A:2303:G:O2'	6:1G:132:ASN:ND2	2.29	0.65
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.78	0.65
32:1a:809:G:OP2	46:1o:48:LYS:NZ	2.26	0.65
1:2A:2042:A:OP1	62:2A:3928:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:115:G:OP2	62:2a:1908:HOH:O	2.13	0.65
13:2R:103:ARG:NH1	13:2R:108:GLY:O	2.30	0.65
32:2a:909:A:N3	32:2a:1413:A:O2'	2.29	0.65
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.32	0.65
44:2m:3:ARG:NH2	44:2m:9:ILE:O	2.28	0.65
1:1A:2124:G:H1	1:1A:2174:C:H42	1.45	0.65
19:2X:60:ARG:HH22	29:27:47:ARG:HH22	1.45	0.65
32:2a:328:C:H4'	32:2a:329:A:H5'	1.79	0.65
32:2a:1257:U:O4	45:2n:17:LYS:NZ	2.30	0.65
1:1A:2128:C:H1'	1:1A:2174:C:H4'	1.79	0.65
32:1a:875:C:H1'	39:1h:15:ASN:HD21	1.62	0.65
39:1h:120:THR:H	39:1h:123:GLU:HB2	1.61	0.65
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.79	0.65
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.79	0.65
32:2a:1086:U:H3	32:2a:1099:G:H22	1.45	0.65
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	1.76	0.65
46:2o:82:ILE:HB	46:2o:87:ILE:HB	1.78	0.65
32:1a:504:C:OP1	62:1a:1912:HOH:O	2.15	0.65
8:2I:80:PRO:HA	8:2I:145:VAL:HG12	1.79	0.65
8:2I:123:LEU:HD21	8:2I:145:VAL:HA	1.79	0.65
1:1A:762:U:OP1	62:1A:4234:HOH:O	2.14	0.64
32:2a:504:C:OP1	62:2a:1910:HOH:O	2.14	0.64
57:2y:14:A:O2'	57:2y:15:G:OP1	2.14	0.64
1:1A:2714:G:OP1	62:1A:4233:HOH:O	2.14	0.64
11:1P:42:SER:O	62:1P:301:HOH:O	2.14	0.64
26:14:56:VAL:HB	26:14:60:GLN:HG3	1.79	0.64
32:1a:903:G:OP1	62:1a:1911:HOH:O	2.14	0.64
50:1s:12:ASP:OD1	50:1s:37:ARG:NH2	2.30	0.64
1:2A:271(R):G:OP1	23:21:76:ARG:NE	2.28	0.64
32:2a:473:G:H2'	32:2a:474:G:H8	1.62	0.64
25:13:26:LEU:O	25:13:35:ARG:NE	2.23	0.64
5:2F:123:LEU:HD13	5:2F:192:LEU:HD23	1.79	0.64
50:2s:28:LYS:NZ	50:2s:46:GLY:O	2.29	0.64
57:2y:26:A:N1	57:2y:44:G:C6	2.65	0.64
1:1A:2134:A:HO2'	1:1A:2135:A:P	2.20	0.64
1:2A:1271:G:OP2	62:2A:3904:HOH:O	2.15	0.64
48:2q:41:LYS:NZ	48:2q:88:TYR:OH	2.31	0.64
54:2w:68:C:H2'	54:2w:69:G:H8	1.60	0.64
1:1A:1637:A:OP2	62:1A:4240:HOH:O	2.15	0.64
32:1a:948:C:OP1	44:1m:109:THR:OG1	2.15	0.64
33:1b:12:GLU:HB2	33:1b:213:LEU:HD21	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:23:ASN:HD21	40:2i:25:LYS:HE2	1.62	0.64
1:1A:11:G:H2'	1:1A:12:U:H5'	1.80	0.64
1:1A:422:A:OP2	62:1A:4229:HOH:O	2.13	0.64
1:1A:2790:A:H3'	1:1A:2790:A:N3	2.13	0.64
32:1a:1320:C:O2	50:1s:36:ARG:NH2	2.31	0.64
5:2F:143:ALA:HB1	5:2F:148:LEU:HB2	1.80	0.64
32:2a:1105:A:H2'	32:2a:1106:G:H8	1.62	0.64
21:1Z:52:SER:O	21:1Z:54:HIS:N	2.30	0.64
26:14:55:ARG:H	26:14:56:VAL:HA	1.62	0.64
32:1a:92:C:H2'	32:1a:93:G:C8	2.33	0.64
32:1a:636:U:H2'	32:1a:637:G:H8	1.62	0.64
32:1a:677:U:H3	32:1a:713:G:H22	1.46	0.64
1:2A:586:A:N1	1:2A:809:G:O2'	2.27	0.64
26:24:46:GLN:C	26:24:48:ARG:H	2.06	0.64
32:2a:403:C:O2'	35:2d:122:ARG:NH2	2.31	0.64
38:2g:78:ARG:HE	38:2g:79:ARG:HE	1.45	0.64
51:1t:42:GLN:NE2	51:1t:46:GLU:OE2	2.31	0.64
1:2A:1973:G:OP1	62:2A:3930:HOH:O	2.15	0.64
1:2A:2306:C:N4	6:2G:42:GLY:O	2.30	0.64
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.80	0.64
1:2A:2394:C:N3	57:2y:76:A:O2'	2.28	0.64
50:2s:32:LYS:HA	50:2s:50:ALA:HB3	1.80	0.64
7:1H:90:LYS:HD2	7:1H:159:GLU:HG2	1.80	0.64
32:1a:79:G:O6	32:1a:90:U:O2	2.15	0.64
41:1j:49:VAL:HG22	45:1n:41:ARG:HB2	1.79	0.64
1:2A:2637:U:H5"	4:2E:82:ARG:HH12	1.63	0.64
1:2A:2448:A:OP1	62:2A:3905:HOH:O	2.15	0.63
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.32	0.63
33:2b:15:VAL:HG13	33:2b:209:ARG:HB3	1.80	0.63
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.62	0.63
32:2a:43:C:OP2	47:2p:12:LYS:NZ	2.28	0.63
32:2a:876:G:O5'	39:2h:14:ARG:NH1	2.31	0.63
1:1A:2384:G:O6	62:1A:4232:HOH:O	2.14	0.63
2:1B:103:G:H21	21:1Z:73:GLN:HE22	1.47	0.63
40:2i:31:GLN:HE21	40:2i:36:TYR:HD1	1.46	0.63
1:1A:2222:G:OP2	62:1A:4241:HOH:O	2.15	0.63
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.33	0.63
1:2A:2819:G:N7	62:2A:4001:HOH:O	2.30	0.63
32:2a:544:G:OP1	35:2d:59:ARG:NH2	2.24	0.63
32:2a:1402:4OC:HM22	32:2a:1403:C:H5'	1.80	0.63
1:1A:453:C:O2	1:1A:457:A:O2'	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:96:LEU:HD13	40:1i:101:PHE:HD2	1.61	0.63
7:2H:103:LEU:HB3	7:2H:115:VAL:HB	1.80	0.63
26:24:44:THR:O	26:24:46:GLN:N	2.30	0.63
42:2k:98:LEU:O	42:2k:101:SER:OG	2.14	0.63
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	1.81	0.63
1:2A:2064:C:OP2	62:2A:3929:HOH:O	2.15	0.63
1:1A:763:G:OP1	62:1A:4243:HOH:O	2.16	0.63
6:1G:3:LEU:O	6:1G:8:LYS:NZ	2.32	0.63
37:1f:82:ARG:HB2	37:1f:85:VAL:HG23	1.80	0.63
1:2A:652(B):A:H61	1:2A:655:A:H1'	1.64	0.63
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.16	0.63
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.30	0.63
6:2G:11:TYR:HB2	6:2G:176:LEU:HD21	1.80	0.63
12:2Q:77:LYS:NZ	12:2Q:86:GLY:O	2.31	0.63
26:24:16:CYS:SG	26:24:17:GLY:N	2.70	0.63
32:2a:142:G:H2'	32:2a:143:A:C8	2.33	0.63
26:14:34:GLU:HG2	26:14:35:VAL:HG12	1.81	0.63
2:2B:14:U:O4'	2:2B:107:G:N2	2.32	0.63
32:2a:562:C:H1'	43:2l:15:ARG:HB3	1.79	0.63
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.64	0.63
15:2T:17:THR:O	15:2T:17:THR:OG1	2.14	0.63
21:2Z:4:ARG:HH21	21:2Z:60:GLU:HG2	1.64	0.63
57:2y:9:A:O2'	57:2y:11:C:N4	2.22	0.63
1:2A:2518:A:OP2	62:2A:3931:HOH:O	2.15	0.62
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.32	0.62
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.81	0.62
38:1g:113:GLU:HB2	38:1g:119:ARG:HG2	1.81	0.62
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.32	0.62
9:2N:1:MET:HE1	16:2U:94:ASN:ND2	2.13	0.62
32:2a:1521:G:N3	62:2a:1937:HOH:O	2.31	0.62
1:1A:2706:G:N7	62:1A:4307:HOH:O	2.30	0.62
32:1a:430:A:H4'	35:1d:7:PRO:HG3	1.82	0.62
15:2T:31:SER:OG	15:2T:85:LYS:NZ	2.29	0.62
32:2a:352:C:O2'	32:2a:354:G:OP1	2.16	0.62
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.80	0.62
34:2c:63:ASN:HB3	34:2c:98:ASN:HD22	1.64	0.62
40:2i:50:LEU:HD13	40:2i:56:LEU:HA	1.80	0.62
32:1a:1531:A:H8	32:1a:1531:A:O5'	1.82	0.62
57:1y:57:G:H2'	57:1y:58:A:H5'	1.81	0.62
1:2A:441:U:O2	5:2F:46:ARG:NH2	2.33	0.62
12:2Q:67:ARG:NH1	12:2Q:105:GLU:OE2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:2p:18:ARG:HD3	47:2p:35:LYS:HD2	1.82	0.62
1:1A:2431:U:O4	62:1A:4238:HOH:O	2.14	0.62
1:1A:2629:A:O2'	1:1A:2630:G:OP2	2.16	0.62
3:1D:37:LEU:HD12	3:1D:62:TYR:HB2	1.82	0.62
1:2A:2134:A:OP2	1:2A:2157:G:N2	2.33	0.62
33:2b:98:LEU:HB2	33:2b:101:MET:HE3	1.82	0.62
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.14	0.62
1:1A:2128:C:N4	1:1A:2160:G:H1	1.96	0.62
1:2A:2875:C:O2'	15:2T:2:ASN:OD1	2.16	0.62
32:2a:976:G:OP2	32:2a:1358:U:O2'	2.18	0.62
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.80	0.62
49:2r:52:PRO:O	49:2r:56:THR:OG1	2.18	0.62
1:1A:1466:G:HO2'	1:1A:1546:C:HO2'	1.47	0.62
1:2A:307:G:H21	1:2A:330:A:H62	1.45	0.62
33:2b:7:VAL:O	33:2b:217:ARG:NE	2.27	0.62
32:1a:399:G:H2'	32:1a:400:C:C6	2.35	0.62
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.30	0.62
1:2A:1785:A:N6	62:2A:3933:HOH:O	2.32	0.62
1:2A:2506:U:H1'	54:2w:76:F3N:HD2	1.82	0.62
5:2F:116:ASP:OD1	5:2F:119:ARG:NH2	2.33	0.62
32:2a:1373:G:H5"	38:2g:36:LYS:HE2	1.82	0.62
34:2c:162:GLN:NE2	53:2v:24:A:O3'	2.33	0.62
33:1b:37:ASN:C	33:1b:39:ILE:H	2.08	0.62
15:2T:19:LEU:HD13	15:2T:86:ILE:HD12	1.82	0.62
18:2W:12:ILE:HD13	18:2W:17:VAL:HG13	1.81	0.62
32:2a:1137:C:O2	32:2a:1138:G:N2	2.31	0.62
37:2f:1:MET:N	37:2f:69:GLU:OE2	2.32	0.62
1:1A:184:C:H2'	1:1A:185:U:C6	2.35	0.61
32:1a:79:G:O6	32:1a:90:U:C2	2.53	0.61
51:1t:33:ILE:O	51:1t:37:SER:OG	2.14	0.61
32:2a:1102:A:O3'	33:2b:96:ARG:NH2	2.33	0.61
38:2g:78:ARG:HE	38:2g:79:ARG:NE	1.98	0.61
32:1a:1025:U:O2	32:1a:1036:G:O6	2.17	0.61
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.32	0.61
1:2A:2316:C:O2'	6:2G:128:ARG:NH2	2.32	0.61
7:2H:124:GLU:HG3	7:2H:132:ARG:HB3	1.82	0.61
32:2a:1302:U:OP2	44:2m:21:TYR:OH	2.18	0.61
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.32	0.61
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.00	0.61
1:2A:1129:A:N6	1:2A:2491:U:OP1	2.32	0.61
34:2c:16:ARG:HD2	34:2c:17:ASP:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:78:LYS:HE2	40:2i:101:PHE:HE1	1.65	0.61
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.36	0.61
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.81	0.61
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.15	0.61
51:1t:50:GLU:HA	51:1t:100:ILE:HG12	1.81	0.61
54:1w:18:G:H4'	54:1w:60:U:C5	2.35	0.61
57:1y:18:G:O2'	57:1y:57:G:O6	2.16	0.61
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.64	0.61
12:2Q:89:ASN:HB2	55:2x:1:C:C4	2.35	0.61
54:2w:51:U:H2'	54:2w:52:G:C8	2.34	0.61
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.36	0.61
33:2b:16:HIS:O	33:2b:18:GLY:N	2.33	0.61
33:2b:81:VAL:HB	33:2b:94:ASN:HD21	1.66	0.61
38:2g:65:ALA:HB1	38:2g:127:ALA:HB3	1.82	0.61
1:2A:880:G:N2	1:2A:898:C:O2	2.34	0.61
8:2I:77:LEU:HD23	8:2I:142:VAL:HG13	1.82	0.61
9:1N:137:LYS:NZ	9:1N:139:GLU:OE2	2.34	0.61
39:1h:34:GLU:OE1	39:1h:37:ARG:NH1	2.33	0.61
54:1w:60:U:H5"	54:1w:61:C:H5	1.65	0.61
1:2A:72:U:OP1	62:2A:3932:HOH:O	2.16	0.61
1:2A:2049:G:N7	62:2A:4005:HOH:O	2.31	0.61
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.29	0.61
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.70	0.61
32:2a:1095:U:OP2	62:2a:1911:HOH:O	2.16	0.61
39:2h:64:LYS:HG2	39:2h:79:VAL:HG21	1.83	0.61
57:2y:18:G:O6	57:2y:56:C:N4	2.34	0.61
1:1A:2239:G:OP2	62:1A:4244:HOH:O	2.16	0.61
28:16:9:LEU:HD13	28:16:51:GLU:HG3	1.82	0.61
32:1a:78:G:C6	32:1a:91:C:N4	2.69	0.61
32:1a:922:G:H4'	36:1e:20:GLN:HA	1.83	0.61
32:2a:770:C:OP1	62:2a:1912:HOH:O	2.16	0.61
1:1A:1365:A:O2'	23:11:11:ARG:NH1	2.34	0.61
1:1A:2552:OMU:O5'	1:1A:2552:OMU:H6	2.00	0.61
11:1P:39:LYS:HB2	11:1P:45:LEU:HD13	1.83	0.61
23:11:8:SER:HB3	23:11:66:HIS:CD2	2.36	0.61
33:1b:162:ILE:O	33:1b:185:ILE:HG12	2.01	0.61
50:2s:19:VAL:O	50:2s:23:ASN:ND2	2.34	0.61
1:1A:2379:G:O2'	14:1S:17:ARG:NH2	2.34	0.60
25:13:55:ARG:HH22	25:13:57:GLU:HB2	1.65	0.60
32:1a:1179:A:O3'	40:1i:103:THR:HB	2.00	0.60
1:2A:300:A:P	20:2Y:86:ARG:HH12	2.23	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:90:LYS:HD2	7:2H:159:GLU:HG2	1.82	0.60
32:2a:973:G:H3'	32:2a:974:A:H5"	1.81	0.60
15:1T:108:ARG:HA	15:1T:111:ARG:HD3	1.83	0.60
20:1Y:82:PRO:O	20:1Y:101:LYS:NZ	2.29	0.60
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.19	0.60
40:1i:53:VAL:O	40:1i:55:ALA:N	2.34	0.60
1:2A:800:A:H8	1:2A:800:A:OP1	1.84	0.60
8:2I:37:VAL:HG12	8:2I:38:LEU:HD12	1.81	0.60
32:2a:45:U:H2'	32:2a:46:G:C8	2.36	0.60
8:2I:69:LYS:HA	8:2I:138:ILE:HD11	1.82	0.60
32:2a:427:U:OP1	35:2d:13:ARG:NH1	2.34	0.60
38:2g:138:LYS:NZ	38:2g:142:GLU:OE1	2.34	0.60
45:2n:48:ALA:HB2	45:2n:53:LEU:HD12	1.82	0.60
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.01	0.60
32:1a:742:G:OP2	46:1o:35:ARG:NH2	2.32	0.60
44:1m:11:ARG:HA	44:1m:45:VAL:HB	1.82	0.60
5:2F:24:LEU:HD21	5:2F:114:VAL:HG12	1.84	0.60
8:2I:123:LEU:HG	8:2I:144:VAL:HB	1.83	0.60
21:2Z:121:HIS:N	21:2Z:171:ILE:O	2.35	0.60
23:21:17:SER:OG	62:21:201:HOH:O	2.16	0.60
32:2a:953:G:H5'	32:2a:965:A:N6	2.16	0.60
32:2a:1366:C:O2'	41:2j:60:ARG:NH2	2.33	0.60
1:1A:2218:U:O4'	23:11:52:ARG:NH2	2.35	0.60
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.82	0.60
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.75	0.60
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.35	0.60
30:18:23:VAL:HG13	30:18:47:LYS:HB3	1.83	0.60
32:1a:559:A:H4'	32:1a:560:U:H3'	1.83	0.60
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.82	0.60
15:2T:102:ILE:HA	15:2T:105:LEU:HG	1.83	0.60
32:2a:1009:G:O6	32:2a:1020:U:O2	2.20	0.60
1:1A:1494:A:OP1	62:1A:4242:HOH:O	2.15	0.60
1:1A:1753:G:N1	1:1A:1756:G:OP2	2.33	0.60
12:1Q:16:ARG:HG2	12:1Q:18:LYS:HE3	1.82	0.60
1:2A:686:G:N2	1:2A:788:A:H61	2.00	0.60
3:2D:66:ASP:OD2	3:2D:103:ARG:NH1	2.34	0.60
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.83	0.60
19:2X:53:LYS:NZ	19:2X:55:ASN:OD1	2.24	0.60
32:2a:7:G:H5'	32:2a:298:A:O4'	2.01	0.60
33:2b:104:ASN:OD1	33:2b:107:THR:OG1	2.18	0.60
1:1A:784:A:N6	3:1D:229:VAL:HG11	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1h:96:GLY:N	39:1h:99:GLU:OE1	2.35	0.60
32:2a:1005:A:H3'	32:2a:1006:C:C6	2.36	0.60
1:1A:1851:U:H4'	57:1y:71:G:H4'	1.82	0.60
32:1a:44:G:O6	62:1a:1913:HOH:O	2.16	0.60
32:1a:642:A:N3	39:1h:113:SER:OG	2.30	0.60
1:2A:324:A:N6	1:2A:338:G:O2'	2.35	0.60
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.37	0.60
32:1a:737:A:H5"	37:1f:92:LYS:HG3	1.82	0.60
40:1i:9:ARG:HG3	40:1i:14:VAL:HG12	1.84	0.60
1:2A:84:A:H5'	20:2Y:8:LYS:HG2	1.83	0.60
1:2A:2166:G:O6	1:2A:2171:A:N6	2.34	0.60
11:2P:85:LEU:HA	11:2P:88:LEU:HD12	1.83	0.60
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.67	0.60
1:2A:450:G:OP1	62:2A:3935:HOH:O	2.17	0.60
1:2A:894:C:O2'	1:2A:895:U:H5"	2.01	0.60
9:2N:123:TYR:OH	9:2N:130:HIS:NE2	2.34	0.60
30:28:28:GLY:O	30:28:36:LYS:NZ	2.34	0.60
41:2j:33:GLN:HG2	41:2j:34:VAL:H	1.66	0.60
32:1a:96:U:H2'	32:1a:97:G:C8	2.37	0.59
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.03	0.59
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.35	0.59
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.83	0.59
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.67	0.59
1:2A:2118:U:OP1	1:2A:2148:G:H4'	2.02	0.59
10:1O:48:PRO:HB3	32:1a:1422:G:H5"	1.83	0.59
1:2A:922:U:H2'	1:2A:923:C:C6	2.38	0.59
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.83	0.59
12:2Q:78:PRO:HG2	12:2Q:81:VAL:HG11	1.82	0.59
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.29	0.59
21:2Z:4:ARG:NH2	21:2Z:66:SER:OG	2.35	0.59
24:22:22:GLU:OE2	24:22:68:ARG:NH2	2.35	0.59
32:2a:1263:C:N3	32:2a:1272:G:O6	2.35	0.59
34:2c:179:ARG:NH1	34:2c:206:GLU:OE1	2.28	0.59
33:1b:163:PHE:HD1	33:1b:185:ILE:HG13	1.66	0.59
5:2F:117:ARG:NH2	5:2F:189:THR:O	2.33	0.59
33:2b:187:LEU:HA	33:2b:201:ILE:HB	1.83	0.59
34:1c:15:THR:HG21	34:1c:181:ASN:HA	1.83	0.59
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.35	0.59
54:1w:5:G:H2'	54:1w:6:G:H8	1.66	0.59
1:2A:643:A:N1	1:2A:2369:A:O2'	2.33	0.59
8:2I:2:LYS:HA	8:2I:20:ASP:HA	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:8:LEU:HB3	41:2j:96:ILE:HG23	1.84	0.59
1:1A:1025:G:O2'	62:1A:4209:HOH:O	2.06	0.59
8:1I:87:LYS:NZ	8:1I:88:ILE:O	2.35	0.59
41:1j:9:ARG:NH2	41:1j:97:GLU:OE1	2.36	0.59
30:28:62:LEU:HB3	30:28:65:GLU:HG3	1.85	0.59
32:2a:1272:G:N2	32:2a:1273:G:C5	2.70	0.59
33:2b:91:PRO:HG3	33:2b:154:LEU:HB2	1.83	0.59
35:2d:72:GLU:OE2	35:2d:207:TYR:OH	2.20	0.59
39:2h:64:LYS:HD2	39:2h:79:VAL:HG11	1.83	0.59
42:2k:79:SER:HB3	42:2k:104:GLN:HE21	1.67	0.59
50:2s:64:GLU:CD	50:2s:64:GLU:H	2.09	0.59
1:1A:2765:A:OP2	62:1A:4247:HOH:O	2.17	0.59
39:1h:2:LEU:HD21	39:1h:8:ASP:HB2	1.85	0.59
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.11	0.59
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.38	0.59
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.38	0.59
34:2c:58:GLU:HB2	34:2c:65:ALA:HB3	1.84	0.59
1:1A:2105:C:H2'	1:1A:2106:G:C8	2.38	0.59
1:1A:2108:C:H2'	1:1A:2109:U:C6	2.36	0.59
3:1D:71:ASP:HB2	3:1D:103:ARG:HH12	1.67	0.59
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.38	0.59
9:1N:67:LEU:HA	9:1N:87:LEU:HD23	1.85	0.59
44:1m:49:THR:HG22	44:1m:51:ALA:H	1.68	0.59
47:1p:3:LYS:NZ	47:1p:65:GLN:O	2.32	0.59
2:2B:7:G:N2	14:2S:38:GLN:HE22	1.97	0.59
32:2a:473:G:H2'	32:2a:474:G:C8	2.38	0.59
32:2a:1280:A:H5'	41:2j:40:LEU:HD22	1.85	0.59
34:2c:37:GLN:NE2	45:2n:52:GLN:OE1	2.34	0.59
1:1A:1359:A:H2'	1:1A:1360:A:H5'	1.84	0.59
10:1O:104:ARG:NE	15:1T:36:GLU:OE2	2.27	0.59
32:1a:197:A:C6	32:1a:221:C:H4'	2.38	0.59
33:1b:16:HIS:CD2	33:1b:204:ASN:H	2.20	0.59
48:1q:12:SER:HB3	48:1q:20:THR:HB	1.85	0.59
2:2B:13:A:N1	2:2B:69:G:O2'	2.36	0.59
14:2S:38:GLN:HB3	14:2S:40:ILE:HD11	1.83	0.59
32:2a:1060:C:H5'	45:2n:45:ARG:HH12	1.68	0.59
1:1A:1039:G:H1	1:1A:1116:C:H42	1.49	0.59
2:1B:66:A:H61	2:1B:109:C:H5'	1.68	0.59
32:1a:865:A:H2	32:1a:918:A:H4'	1.68	0.59
1:2A:2419:U:H2'	1:2A:2420:C:H6	1.67	0.59
1:2A:2755:C:OP1	62:2A:3934:HOH:O	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:181:G:H4'	32:2a:182:U:H5'	1.83	0.59
3:1D:206:LEU:HA	3:1D:211:ARG:NH1	2.18	0.59
35:1d:11:LEU:HG	35:1d:66:ARG:HD3	1.85	0.59
44:1m:40:ASN:O	44:1m:43:THR:OG1	2.21	0.59
1:2A:2262:U:OP2	22:20:16:SER:OG	2.18	0.59
57:1y:19:G:N1	57:1y:56:C:N4	2.51	0.58
32:2a:673:G:H2'	32:2a:674:G:C8	2.38	0.58
51:2t:56:MET:HE3	51:2t:85:MET:HG2	1.85	0.58
1:1A:2365:G:OP1	62:1A:4245:HOH:O	2.16	0.58
32:1a:67:C:H2'	32:1a:68:G:C8	2.38	0.58
32:1a:473:G:OP2	47:1p:75:ARG:NH1	2.36	0.58
32:1a:1179:A:H4'	40:1i:103:THR:HA	1.85	0.58
1:2A:1527:G:O2'	1:2A:1544:A:N6	2.30	0.58
1:2A:2127:G:N1	1:2A:2161:C:C4	2.71	0.58
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.21	0.58
32:2a:1203:C:H2'	32:2a:1204:A:H8	1.67	0.58
51:2t:60:GLU:HG3	51:2t:81:LYS:HD2	1.84	0.58
35:1d:134:ASP:N	35:1d:134:ASP:OD1	2.36	0.58
1:2A:133:C:H42	1:2A:146:G:H1	1.50	0.58
1:2A:468:G:N7	29:27:39:ARG:NH2	2.48	0.58
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.35	0.58
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.38	0.58
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.85	0.58
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.37	0.58
51:1t:22:ARG:O	51:1t:26:ASN:ND2	2.36	0.58
29:27:12:ARG:NH2	29:27:44:PRO:HB3	2.18	0.58
50:2s:36:ARG:HG2	50:2s:51:VAL:HG12	1.84	0.58
32:1a:729:A:H2'	32:1a:730:G:H8	1.69	0.58
32:1a:1264:C:H42	32:1a:1271:G:H1	1.51	0.58
40:1i:27:THR:HG23	40:1i:62:TYR:HA	1.85	0.58
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.85	0.58
1:1A:2136:C:C4	1:1A:2155:G:C2	2.92	0.58
3:1D:183:ARG:HG3	3:1D:270:ILE:HD13	1.86	0.58
32:1a:23:C:OP2	32:1a:561:U:N3	2.35	0.58
33:1b:33:TYR:HB2	33:1b:43:ASP:HB2	1.86	0.58
1:2A:1225:G:H4'	17:2V:84:LYS:HG2	1.86	0.58
11:2P:121:LYS:O	11:2P:123:LEU:N	2.35	0.58
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.86	0.58
32:2a:701:C:OP1	32:2a:702:A:O2'	2.19	0.58
38:2g:27:ILE:HG22	38:2g:39:ALA:HB1	1.85	0.58
1:1A:278:A:H2'	1:1A:279:C:C6	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.38	0.58
2:1B:42:C:OP1	6:1G:67:LYS:NZ	2.36	0.58
32:1a:79:G:C6	32:1a:90:U:O2	2.57	0.58
32:1a:1198:G:N7	62:1a:1938:HOH:O	2.32	0.58
33:1b:185:ILE:HG22	33:1b:199:TYR:HD2	1.69	0.58
39:1h:43:GLY:O	39:1h:64:LYS:NZ	2.26	0.58
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.02	0.58
14:2S:10:ARG:NE	14:2S:91:PRO:O	2.37	0.58
32:1a:1036:G:H5"	32:1a:1037:C:C5	2.39	0.58
44:1m:2:ALA:N	44:1m:8:GLU:OE1	2.37	0.58
1:2A:247:G:H4'	1:2A:386:G:C5	2.39	0.58
5:2F:18:ARG:NH1	5:2F:127:GLU:OE2	2.37	0.58
5:2F:178:PRO:HB2	5:2F:201:VAL:HG21	1.86	0.58
33:2b:126:GLU:CD	33:2b:126:GLU:H	2.12	0.58
1:1A:2110:G:OP2	1:1A:2118:U:N3	2.36	0.58
32:1a:954:G:H5"	44:1m:120:LYS:HD3	1.85	0.58
32:1a:1239:A:H62	32:1a:1299:A:N6	2.01	0.58
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.03	0.58
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.85	0.58
26:24:67:TYR:HD2	50:2s:9:VAL:HB	1.68	0.58
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.18	0.58
28:16:47:THR:HG22	28:16:49:HIS:CE1	2.38	0.57
48:1q:67:LYS:O	48:1q:68:ARG:HB2	2.02	0.57
51:1t:71:THR:HG22	51:1t:72:LEU:HG	1.86	0.57
11:2P:38:GLN:O	11:2P:40:SER:N	2.34	0.57
12:2Q:45:GLN:N	12:2Q:45:GLN:OE1	2.37	0.57
32:2a:1176:A:H2'	32:2a:1177:G:C8	2.38	0.57
33:2b:16:HIS:HB2	33:2b:204:ASN:HD22	1.69	0.57
54:2w:68:C:H2'	54:2w:69:G:C8	2.39	0.57
32:1a:57:G:H2'	32:1a:58:C:C6	2.39	0.57
32:1a:316:G:OP2	32:1a:351:G:O2'	2.22	0.57
32:1a:714:G:H2'	32:1a:715:A:C8	2.39	0.57
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.18	0.57
32:1a:1027:C:C4	32:1a:1034:G:N1	2.72	0.57
36:1e:84:PHE:HB2	36:1e:134:ALA:HB2	1.84	0.57
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.69	0.57
1:2A:1689:A:H62	1:2A:1698:A:H2	1.51	0.57
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.37	0.57
14:2S:83:LYS:HB2	14:2S:111:GLU:HG3	1.84	0.57
32:2a:560:U:H5'	32:2a:566:G:N2	2.19	0.57
1:1A:1568:G:H5"	3:1D:61:LEU:HD13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:1l:77:LEU:HD21	43:1l:107:ALA:HB2	1.86	0.57
32:2a:1239:A:H62	32:2a:1299:A:H61	1.52	0.57
54:2w:10:G:H2'	54:2w:11:C:H6	1.70	0.57
32:1a:693:G:OP2	62:1a:1914:HOH:O	2.18	0.57
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	1.85	0.57
1:2A:531:C:OP1	1:2A:561:G:N1	2.37	0.57
1:2A:563:G:OP2	62:2A:3937:HOH:O	2.17	0.57
1:2A:994:C:O2'	1:2A:996:A:OP1	2.21	0.57
32:2a:157:G:N2	32:2a:164:U:O2	2.29	0.57
32:2a:547:A:OP1	62:2a:1913:HOH:O	2.17	0.57
32:2a:1239:A:H62	32:2a:1299:A:N6	2.01	0.57
33:2b:54:THR:HG21	33:2b:201:ILE:HD11	1.86	0.57
33:2b:71:VAL:HG12	33:2b:170:GLU:HG2	1.86	0.57
54:2w:33:U:N3	54:2w:36:A:OP2	2.34	0.57
57:2y:66:U:H2'	57:2y:67:C:O4'	2.04	0.57
12:1Q:31:ASP:OD1	12:1Q:134:ARG:NH1	2.33	0.57
54:1w:9:A:O2'	54:1w:10:G:N7	2.37	0.57
32:2a:1005:A:H5"	32:2a:1006:C:C5	2.40	0.57
1:1A:1076:C:O2'	1:1A:1077:A:N7	2.37	0.57
5:1F:132:VAL:HA	5:1F:138:GLU:HB3	1.86	0.57
21:1Z:93:ASP:HB3	21:1Z:131:ARG:HH22	1.69	0.57
2:2B:7:G:H21	14:2S:38:GLN:NE2	1.97	0.57
5:2F:33:LEU:HB3	11:2P:6:LEU:HD21	1.86	0.57
32:2a:1128:C:O2'	32:2a:1129:C:OP1	2.21	0.57
57:2y:5:G:H1	57:2y:68:C:H42	1.51	0.57
1:1A:1192:G:OP2	62:1A:4248:HOH:O	2.18	0.57
1:2A:1297:C:OP2	62:2A:3936:HOH:O	2.17	0.57
1:2A:2105:C:H2'	1:2A:2106:G:H8	1.69	0.57
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.67	0.57
3:2D:164:GLN:OE1	3:2D:176:ARG:NH1	2.32	0.57
8:2I:78:THR:HA	8:2I:143:SER:HB2	1.86	0.57
34:2c:35:GLU:O	34:2c:39:ILE:HG13	2.05	0.57
1:1A:2630:G:H2'	1:1A:2631:G:C8	2.39	0.57
4:1E:101:ARG:CZ	4:1E:171:GLU:HB2	2.35	0.57
7:1H:68:THR:O	7:1H:72:ILE:HG12	2.05	0.57
31:19:25:VAL:HB	31:19:34:GLN:HB2	1.87	0.57
1:2A:882:G:H22	1:2A:894:C:N4	2.02	0.57
6:2G:115:ARG:HB2	6:2G:115:ARG:HH11	1.70	0.57
1:1A:1243:G:O2'	11:1P:7:ARG:NH2	2.38	0.57
8:1I:87:LYS:HZ3	8:1I:121:LYS:HE3	1.70	0.57
36:1e:144:THR:H	36:1e:147:ASP:HB2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:1w:5:G:H2'	54:1w:6:G:C8	2.40	0.57
21:2Z:4:ARG:HG2	21:2Z:58:VAL:HB	1.86	0.57
38:2g:78:ARG:HG3	38:2g:156:TRP:CZ3	2.40	0.57
1:1A:922:U:H2'	1:1A:923:C:C6	2.40	0.57
1:1A:1068:G:H2'	1:1A:1096:A:H1'	1.86	0.57
8:1I:38:LEU:HD23	8:1I:38:LEU:H	1.68	0.57
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.38	0.57
1:2A:2817:G:O2'	1:2A:2836:U:O2	2.18	0.57
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.40	0.57
32:2a:1317:C:O2	50:2s:37:ARG:NH2	2.38	0.57
38:2g:69:VAL:HG12	38:2g:103:TRP:HE3	1.70	0.57
54:2w:10:G:H2'	54:2w:11:C:C6	2.40	0.57
1:1A:271(B):C:H42	1:1A:271(V):G:H1	1.51	0.56
1:1A:271(I):G:N7	1:1A:271(J):C:N4	2.53	0.56
1:1A:579:G:H2'	1:1A:580:C:C6	2.40	0.56
1:1A:880:G:H2'	1:1A:881:G:C8	2.40	0.56
1:1A:899:A:H2'	1:1A:899:A:N3	2.20	0.56
1:1A:2105:C:H2'	1:1A:2106:G:H8	1.69	0.56
1:1A:2754:U:OP1	62:1A:4246:HOH:O	2.17	0.56
4:1E:122:PHE:O	62:1E:401:HOH:O	2.17	0.56
41:1j:38:ILE:HD11	41:1j:71:LEU:HD23	1.86	0.56
1:2A:2166:G:H3'	1:2A:2167:U:H5"	1.87	0.56
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.37	0.56
32:2a:1134:G:C2	32:2a:1135:U:H1'	2.39	0.56
33:2b:185:ILE:HB	33:2b:199:TYR:HB2	1.87	0.56
1:1A:2169:A:H1'	57:1y:56:C:H5'	1.86	0.56
32:1a:92:C:H2'	32:1a:93:G:H8	1.68	0.56
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.38	0.56
32:1a:1003:G:C4	32:1a:1004:A:H2	2.22	0.56
32:1a:1036:G:H5"	32:1a:1037:C:H5	1.69	0.56
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.40	0.56
1:2A:2431:U:OP2	62:2A:3938:HOH:O	2.18	0.56
28:26:14:THR:OG1	28:26:48:VAL:O	2.23	0.56
39:2h:39:LEU:HG	39:2h:44:PHE:HB2	1.87	0.56
46:2o:16:ALA:HB1	46:2o:21:ASP:HB3	1.86	0.56
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.40	0.56
1:1A:1062:G:C8	1:1A:1070:A:H4'	2.37	0.56
1:1A:2849:U:P	15:1T:95:ARG:HH12	2.29	0.56
10:1O:68:GLU:HB3	10:1O:78:ARG:HB2	1.87	0.56
32:1a:7:G:H5'	32:1a:298:A:O4'	2.06	0.56
32:1a:45:U:H2'	32:1a:46:G:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:748:C:H4'	32:1a:749:C:O5'	2.05	0.56
32:1a:1033:G:H3'	32:1a:1034:G:H8	1.70	0.56
32:1a:1040:U:H2'	32:1a:1041:A:H8	1.70	0.56
55:1x:19:G:H3'	55:1x:20:U:C5	2.40	0.56
3:2D:97:TYR:C	3:2D:99:ASP:H	2.13	0.56
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	1.86	0.56
15:2T:30:VAL:HG22	15:2T:86:ILE:HG12	1.87	0.56
32:2a:737:A:H1'	37:2f:73:ASN:HD21	1.70	0.56
36:2e:60:TYR:OH	36:2e:64:ARG:NH1	2.38	0.56
57:2y:18:G:N2	57:2y:55:PSU:HN3	2.02	0.56
1:1A:528:A:O2'	1:1A:529:A:H5'	2.05	0.56
32:1a:17:U:H2'	32:1a:18:C:C6	2.40	0.56
32:1a:1095:U:P	32:1a:1108:G:H1	2.27	0.56
33:1b:84:GLU:HB3	33:1b:219:VAL:HG21	1.86	0.56
40:1i:55:ALA:HA	40:1i:58:HIS:CD2	2.40	0.56
7:2H:118:PRO:HD2	7:2H:121:ILE:HB	1.87	0.56
1:1A:1082:U:N3	1:1A:1086:A:N6	2.08	0.56
1:1A:2096:U:H3	1:1A:2193:G:H1	1.53	0.56
4:1E:176:ILE:HB	4:1E:181:LEU:HB2	1.87	0.56
35:1d:111:ALA:HB2	35:1d:120:LEU:HD12	1.87	0.56
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.17	0.56
10:2O:73:ASP:OD2	15:2T:32:TYR:OH	2.19	0.56
50:2s:30:LEU:HD11	50:2s:50:ALA:HB2	1.87	0.56
1:1A:918:A:N3	2:1B:80:U:O2'	2.37	0.56
6:1G:64:THR:HB	6:1G:94:LEU:HD11	1.86	0.56
1:2A:938:G:OP2	30:28:52:LYS:NZ	2.28	0.56
8:2I:72:LEU:HA	8:2I:75:LEU:HD12	1.88	0.56
34:2c:156:ARG:H	34:2c:196:LEU:HD22	1.70	0.56
35:2d:18:LYS:NZ	35:2d:26:CYS:O	2.28	0.56
38:2g:111:ARG:NH2	38:2g:126:ASP:OD2	2.39	0.56
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.86	0.56
6:1G:179:PRO:HG3	26:14:43:TYR:CZ	2.41	0.56
32:1a:447:G:O6	32:1a:485:G:O2'	2.17	0.56
34:1c:71:ALA:O	34:1c:73:PRO:HD3	2.05	0.56
36:1e:78:HIS:CE1	36:1e:143:ARG:H	2.23	0.56
43:1l:38:THR:OG1	43:1l:57:LYS:NZ	2.39	0.56
50:1s:45:VAL:HG11	50:1s:64:GLU:HG3	1.87	0.56
57:1y:60:U:O2'	57:1y:61:C:H5'	2.06	0.56
17:2V:16:PRO:HD3	17:2V:99:ILE:HD11	1.87	0.56
33:2b:144:ARG:NH2	33:2b:148:TYR:OH	2.39	0.56
33:2b:188:ALA:HB1	33:2b:192:SER:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:142:MET:HG3	34:2c:170:GLN:HB3	1.87	0.56
54:2w:39:PSU:H2'	54:2w:40:C:H6	1.71	0.56
1:1A:1906:G:H5"	1:1A:1929:G:O2'	2.05	0.56
33:1b:230:VAL:HG12	33:1b:231:GLU:H	1.70	0.56
1:2A:1783:A:HO2'	1:2A:2607:G:HO2'	1.53	0.56
9:2N:67:LEU:HB3	9:2N:88:GLU:HG3	1.87	0.56
21:2Z:17:ALA:HA	21:2Z:20:ARG:HH11	1.70	0.56
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.39	0.56
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.41	0.56
6:1G:77:ILE:HD12	6:1G:82:LEU:HD23	1.87	0.56
1:2A:900:A:O2'	1:2A:901:A:OP1	2.22	0.56
1:2A:2137:C:N4	1:2A:2154:G:N1	2.45	0.56
1:2A:2148:G:H2'	1:2A:2149:G:C8	2.40	0.56
8:2I:62:LYS:HG2	8:2I:133:HIS:CE1	2.40	0.56
15:2T:127:ALA:C	15:2T:129:ARG:H	2.14	0.56
32:2a:1181:G:O2'	32:2a:1182:G:N7	2.38	0.56
1:1A:363:G:H2'	1:1A:363(A):A:C8	2.40	0.56
32:1a:598:U:H2'	32:1a:599:C:H6	1.70	0.56
55:1x:8:4SU:O2	55:1x:21:A:H2	1.89	0.56
1:2A:1648:C:OP1	62:2A:3904:HOH:O	2.18	0.56
1:2A:2524:G:N7	62:2A:4016:HOH:O	2.33	0.56
21:2Z:70:LEU:HD12	21:2Z:71:VAL:H	1.71	0.56
32:2a:839:U:H3'	32:2a:840:C:H5'	1.86	0.56
32:2a:1151:A:O2'	32:2a:1152:A:O5'	2.22	0.56
35:2d:78:LEU:HB3	35:2d:93:PHE:HE1	1.71	0.56
35:1d:100:ARG:NH2	35:1d:102:ASP:OD2	2.39	0.55
48:1q:9:VAL:HG23	48:1q:56:VAL:HG22	1.88	0.55
1:2A:81:G:N7	62:2A:4017:HOH:O	2.33	0.55
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.38	0.55
1:2A:2120:G:H2'	1:2A:2121:G:C8	2.41	0.55
1:2A:2151:G:H2'	1:2A:2152:G:C8	2.40	0.55
6:2G:152:LEU:H	6:2G:152:LEU:HD12	1.71	0.55
32:2a:975:A:H4'	32:2a:976:G:H5"	1.87	0.55
32:2a:1004:A:H61	32:2a:1037:C:H1'	1.71	0.55
32:2a:1077:G:N1	32:2a:1080:A:OP2	2.39	0.55
33:2b:219:VAL:HA	33:2b:222:ILE:HG12	1.88	0.55
10:1O:20:MET:HE3	10:1O:44:LYS:HE3	1.87	0.55
46:1o:74:ASP:HB3	46:1o:77:ARG:HB2	1.87	0.55
6:2G:138:GLN:HE22	6:2G:152:LEU:HA	1.71	0.55
32:2a:1130:A:H5"	40:2i:18:PHE:CE2	2.40	0.55
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:70:PHE:HE2	33:2b:90:MET:HB2	1.71	0.55
36:2e:83:GLU:HA	36:2e:88:LYS:HA	1.88	0.55
1:1A:1095:A:N6	1:1A:1097:U:O2	2.38	0.55
7:1H:124:GLU:OE2	7:1H:134:SER:OG	2.23	0.55
10:1O:104:ARG:CZ	15:1T:34:VAL:HG11	2.36	0.55
32:1a:848:C:H2'	32:1a:849:C:C6	2.41	0.55
32:1a:1027:C:N4	32:1a:1034:G:H1	2.04	0.55
1:2A:2298:A:H62	1:2A:2318:G:H8	1.55	0.55
2:2B:9:G:OP1	14:2S:15:ARG:HD3	2.06	0.55
18:2W:57:ASN:HA	18:2W:61:ASN:HD22	1.70	0.55
32:2a:165:C:H2'	32:2a:166:G:H8	1.70	0.55
32:2a:1129:C:H5'	40:2i:16:ARG:HH22	1.71	0.55
44:2m:13:LYS:HA	44:2m:44:ARG:HH11	1.72	0.55
57:2y:15:G:N2	57:2y:48:C:H42	2.03	0.55
1:1A:2165:G:H1	1:1A:2171:A:H2'	1.71	0.55
28:16:28:ARG:NH1	28:16:29:ASN:OD1	2.39	0.55
32:1a:404:U:OP1	35:1d:118:ARG:NH1	2.39	0.55
32:1a:1498:UR3:O2'	53:1v:17:U:OP1	2.22	0.55
14:2S:34:HIS:O	14:2S:97:ARG:NH2	2.39	0.55
32:2a:1427:U:H2'	32:2a:1428:A:C8	2.41	0.55
1:1A:2136:C:C4	1:1A:2155:G:N1	2.75	0.55
42:1k:20:TYR:HB2	42:1k:31:THR:HG23	1.88	0.55
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.41	0.55
16:2U:49:HIS:HA	16:2U:52:ARG:HB2	1.87	0.55
26:24:26:SER:OG	26:24:27:THR:N	2.35	0.55
32:2a:1029:C:N4	32:2a:1032:G:C6	2.75	0.55
32:2a:1130:A:H5"	40:2i:18:PHE:HE2	1.71	0.55
32:2a:1226:C:OP2	44:2m:91:ARG:NH1	2.37	0.55
1:1A:2228:G:OP1	3:1D:261:LYS:NZ	2.39	0.55
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.42	0.55
5:1F:133:ASN:N	5:1F:138:GLU:OE1	2.37	0.55
21:1Z:8:TYR:HB2	21:1Z:38:TYR:CE2	2.41	0.55
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.06	0.55
47:1p:53:VAL:HG13	47:1p:79:VAL:HG22	1.89	0.55
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.39	0.55
32:2a:1027:C:C2	32:2a:1034:G:N1	2.70	0.55
32:2a:1030(A):G:N2	32:2a:1030(D):A:OP2	2.39	0.55
28:16:35:GLU:OE2	28:16:50:ARG:NH1	2.40	0.55
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.89	0.55
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	1.89	0.55
21:2Z:105:VAL:O	21:2Z:141:VAL:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:759:G:OP1	62:1A:4251:HOH:O	2.18	0.55
32:2a:7:G:O2'	36:2e:120:THR:O	2.24	0.55
44:2m:40:ASN:HD22	44:2m:43:THR:HG23	1.72	0.55
1:1A:84:A:H5"	20:1Y:8:LYS:HE3	1.89	0.55
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.36	0.55
8:1I:3:VAL:HG12	8:1I:38:LEU:HA	1.89	0.55
43:1l:117:ARG:HB3	43:1l:122:THR:HB	1.88	0.55
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.42	0.55
1:2A:2821:A:H2'	1:2A:2822:G:C8	2.42	0.55
8:2I:58:LEU:O	8:2I:62:LYS:N	2.40	0.55
17:2V:58:VAL:HB	17:2V:98:GLU:HG3	1.89	0.55
24:22:38:GLN:HG2	24:22:43:GLN:HB2	1.89	0.55
32:2a:1263:C:C4	32:2a:1272:G:O6	2.59	0.55
1:1A:602:G:O2'	1:1A:655:A:N6	2.39	0.55
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.42	0.55
18:1W:67:ASP:OD1	18:1W:67:ASP:N	2.37	0.55
32:1a:973:G:H3'	32:1a:974:A:H5"	1.89	0.55
39:1h:13:ILE:HD11	39:1h:61:VAL:HG11	1.88	0.55
47:1p:15:PRO:O	47:1p:16:HIS:ND1	2.40	0.55
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.06	0.55
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.42	0.55
6:2G:25:TYR:CD1	6:2G:30:GLU:HB3	2.41	0.55
54:2w:4:C:N4	54:2w:69:G:H1	2.04	0.55
32:1a:1030(B):C:H2'	32:1a:1030(C):G:H5'	1.89	0.54
47:1p:11:SER:H	47:1p:14:ASN:HB3	1.71	0.54
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.88	0.54
13:2R:44:LEU:HD22	13:2R:48:VAL:HG23	1.89	0.54
19:2X:65:ARG:HH11	19:2X:70:LEU:HD21	1.71	0.54
32:2a:972:C:O2'	41:2j:55:LYS:O	2.26	0.54
32:2a:1051:C:H42	32:2a:1207:2MG:HN1	1.53	0.54
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.71	0.54
32:2a:1446:U:O4	62:2a:1914:HOH:O	2.18	0.54
33:2b:16:HIS:C	33:2b:18:GLY:H	2.15	0.54
38:2g:15:ASP:OD1	38:2g:19:GLY:N	2.41	0.54
57:2y:9:A:H4'	57:2y:46:G7M:H5'	1.88	0.54
57:2y:15:G:N1	57:2y:48:C:N3	2.53	0.54
1:1A:1062:G:H22	1:1A:1077:A:H61	1.56	0.54
32:1a:1064:G:O2'	32:1a:1190:G:N2	2.41	0.54
34:1c:79:ARG:O	34:1c:82:GLU:HG2	2.06	0.54
54:1w:63:G:H2'	54:1w:64:A:C8	2.43	0.54
1:2A:242:G:C8	30:28:5:LYS:HG2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2Y:28:LYS:HD2	20:2Y:40:GLU:HG3	1.89	0.54
34:2c:82:GLU:O	34:2c:86:VAL:N	2.40	0.54
41:2j:44:VAL:HG13	41:2j:66:ARG:HG2	1.89	0.54
57:2y:61:C:H2'	57:2y:62:C:C6	2.42	0.54
1:1A:1064:C:H2'	1:1A:1065:U:H5'	1.90	0.54
1:1A:1339:G:H5"	19:1X:16:LYS:HD3	1.89	0.54
1:1A:1683:C:H2'	1:1A:1684:C:C6	2.43	0.54
6:1G:73:ALA:HB3	6:1G:85:GLY:H	1.72	0.54
14:1S:20:ARG:NH2	22:10:51:VAL:O	2.41	0.54
32:1a:940:C:OP1	38:1g:29:LYS:NZ	2.40	0.54
34:1c:57:ILE:HG12	34:1c:66:VAL:HG12	1.89	0.54
36:1e:77:PRO:HD2	36:1e:142:LEU:HD22	1.89	0.54
1:2A:1599:C:OP1	62:2A:3939:HOH:O	2.18	0.54
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.42	0.54
11:2P:29:LYS:HG3	11:2P:30:THR:N	2.22	0.54
32:2a:56:U:H2'	32:2a:57:G:C8	2.43	0.54
32:2a:792:A:H4'	32:2a:793:U:H5"	1.89	0.54
32:2a:1097:C:O2'	32:2a:1169:A:N3	2.34	0.54
32:2a:1381:U:H1'	38:2g:79:ARG:HD2	1.89	0.54
44:2m:19:LEU:HD11	44:2m:56:LEU:HD21	1.87	0.54
20:1Y:92:ASN:OD1	20:1Y:94:LYS:HG2	2.08	0.54
32:1a:750:G:O2'	46:1o:21:ASP:OD1	2.25	0.54
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.43	0.54
32:2a:1139:G:N2	32:2a:1142:G:O6	2.27	0.54
39:2h:14:ARG:O	39:2h:18:ARG:HD2	2.07	0.54
6:1G:67:LYS:H	26:14:6:HIS:CE1	2.24	0.54
11:1P:29:LYS:HG3	11:1P:30:THR:H	1.73	0.54
37:1f:100:ASN:HB2	49:1r:28:GLU:HA	1.89	0.54
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.89	0.54
1:2A:300:A:OP2	20:2Y:86:ARG:NH1	2.41	0.54
12:2Q:12:GLN:NE2	12:2Q:72:LYS:HG3	2.22	0.54
32:2a:134:A:H61	47:2p:25:ARG:NH1	2.05	0.54
32:2a:263:A:OP1	51:2t:79:ARG:NH1	2.41	0.54
1:1A:484:C:H2'	1:1A:485:C:C6	2.43	0.54
1:1A:639:U:H2'	1:1A:640:C:C6	2.42	0.54
1:1A:1670:C:OP2	62:1A:4211:HOH:O	2.18	0.54
34:1c:52:LEU:HD13	34:1c:68:VAL:HG13	1.90	0.54
40:1i:49:PRO:HG2	40:1i:81:ILE:HG23	1.90	0.54
1:2A:1899:G:O2'	1:2A:1900:A:OP2	2.24	0.54
32:2a:1118:C:OP1	40:2i:104:ARG:NH1	2.39	0.54
33:2b:18:GLY:HA2	33:2b:42:ILE:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2614:A:N7	62:1A:4326:HOH:O	2.33	0.54
12:1Q:78:PRO:HG2	12:1Q:81:VAL:HG11	1.90	0.54
33:1b:15:VAL:HB	33:1b:209:ARG:HG3	1.90	0.54
21:2Z:126:VAL:HB	21:2Z:161:VAL:HG23	1.90	0.54
32:2a:406:G:O2'	35:2d:3:ARG:NH2	2.41	0.54
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	1.90	0.54
33:2b:71:VAL:HB	33:2b:164:VAL:HG13	1.90	0.54
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.43	0.54
1:1A:120:U:OP2	62:1A:4249:HOH:O	2.18	0.54
1:1A:2690:C:OP1	13:1R:17:ARG:NH2	2.41	0.54
1:1A:2698:U:H2'	1:1A:2699:C:C6	2.42	0.54
32:1a:1469:G:H2'	32:1a:1470:G:C8	2.43	0.54
33:1b:224:GLN:HG2	33:1b:229:VAL:HG22	1.90	0.54
1:2A:1011:G:OP1	16:2U:77:SER:OG	2.26	0.54
1:2A:2134:A:H1'	1:2A:2158:A:C6	2.43	0.54
1:2A:2611:U:H6	1:2A:2611:U:H5'	1.72	0.54
5:2F:133:ASN:N	5:2F:138:GLU:OE1	2.41	0.54
32:2a:88:A:H5"	32:2a:89:C:C6	2.42	0.54
41:2j:12:ASP:O	41:2j:15:THR:OG1	2.24	0.54
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.05	0.54
6:1G:45:GLU:OE2	62:1G:301:HOH:O	2.19	0.54
6:1G:126:ASP:HB2	6:1G:130:ASN:O	2.08	0.54
32:1a:222:U:H2'	32:1a:223:U:C6	2.43	0.54
32:1a:1318:A:OP1	50:1s:7:LYS:NZ	2.37	0.54
1:2A:1756:G:H4'	1:2A:1758:G:O4'	2.08	0.54
5:2F:13:SER:OG	5:2F:16:GLY:N	2.41	0.54
5:2F:196:LEU:HA	5:2F:199:TRP:HB3	1.90	0.54
6:2G:138:GLN:OE1	6:2G:138:GLN:N	2.41	0.54
24:22:25:VAL:HG22	24:22:60:LEU:HB3	1.89	0.54
28:26:40:CYS:O	28:26:44:ARG:N	2.40	0.54
37:2f:50:TYR:CE2	49:2r:77:GLY:HA2	2.43	0.54
1:1A:272(G):C:H42	1:1A:363(C):G:H1	1.56	0.54
32:1a:653:A:OP1	39:1h:56:LYS:NZ	2.41	0.54
1:2A:8:A:H2'	1:2A:9:U:C6	2.43	0.54
1:2A:686:G:H21	1:2A:788:A:H61	1.54	0.54
1:2A:1641:A:H2'	1:2A:1642:G:O4'	2.08	0.54
1:2A:2889:C:H2'	1:2A:2891:G:O4'	2.08	0.54
6:2G:63:ILE:HD11	6:2G:144:ILE:HG13	1.90	0.54
7:2H:143:GLN:NE2	7:2H:147:ASN:OD1	2.41	0.54
21:2Z:6:LYS:HE3	21:2Z:8:TYR:HE2	1.74	0.54
32:2a:1026:G:H5'	32:2a:1027:C:O5'	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1255:G:H5”	34:2c:26:LYS:HE2	1.89	0.54
32:2a:1442:G:H2’	32:2a:1442:G:N3	2.23	0.54
47:2p:1:MET:O	47:2p:24:ALA:N	2.33	0.54
1:1A:1379:A:H4’	1:1A:1380:G:OP2	2.09	0.53
1:1A:1798:U:H5’	3:1D:259:THR:HG22	1.89	0.53
1:1A:2591:C:H2’	1:1A:2592:G:C8	2.42	0.53
6:1G:11:TYR:OH	6:1G:32:PRO:O	2.23	0.53
38:1g:38:LEU:HA	38:1g:41:ARG:HD3	1.90	0.53
42:1k:48:ILE:O	42:1k:50:TYR:N	2.31	0.53
1:2A:392:C:H5”	1:2A:409:C:H5”	1.90	0.53
1:2A:1507:A:O2’	1:2A:1508:A:O5’	2.26	0.53
1:2A:2461:C:H2’	1:2A:2462:U:C6	2.43	0.53
2:2B:66:A:N6	2:2B:108:U:H3’	2.23	0.53
7:2H:149:ARG:NH1	7:2H:167:GLU:OE1	2.40	0.53
12:2Q:78:PRO:HD3	55:2x:1:C:N3	2.23	0.53
19:2X:35:THR:OG1	19:2X:38:GLU:HB2	2.08	0.53
32:2a:1053:G:N7	32:2a:1200:C:H5”	2.23	0.53
38:2g:152:ALA:O	38:2g:155:ARG:HD3	2.08	0.53
50:2s:12:ASP:HB3	50:2s:14:HIS:CD2	2.43	0.53
51:2t:43:LEU:HD13	51:2t:51:GLU:HG2	1.90	0.53
54:2w:72:C:H2’	54:2w:73:A:C8	2.42	0.53
1:1A:264:C:O2’	1:1A:265:A:H2’	2.08	0.53
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.07	0.53
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	1.91	0.53
32:1a:619:U:C2	35:1d:135:LEU:HD22	2.44	0.53
33:1b:103:THR:HG23	33:1b:176:GLU:HB3	1.90	0.53
1:2A:131:G:OP1	62:2A:3943:HOH:O	2.19	0.53
1:2A:668:G:H5’	1:2A:669:G:OP2	2.08	0.53
1:2A:2127:G:N2	1:2A:2161:C:C2	2.76	0.53
32:2a:1510:U:H2’	32:2a:1511:G:C8	2.43	0.53
36:2e:76:ILE:HD13	36:2e:118:ILE:HD11	1.91	0.53
8:1I:12:LEU:HD22	8:1I:19:VAL:HG21	1.90	0.53
32:1a:1036:G:H3’	32:1a:1037:C:C6	2.43	0.53
57:1y:9:A:H4’	57:1y:46:G7M:OP2	2.08	0.53
1:2A:1671:U:OP2	62:2A:3907:HOH:O	2.18	0.53
1:2A:2577:A:OP1	62:2A:3915:HOH:O	2.17	0.53
6:2G:3:LEU:O	6:2G:8:LYS:NZ	2.33	0.53
10:2O:2:ILE:O	10:2O:33:ALA:N	2.41	0.53
1:1A:363:G:H2’	1:1A:363(A):A:H8	1.74	0.53
1:1A:376:C:OP1	62:1A:4253:HOH:O	2.19	0.53
1:1A:2000:G:OP1	13:1R:5:LYS:NZ	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2114:A:H2	1:1A:2168:G:HO2'	1.57	0.53
7:1H:116:GLU:HG3	7:1H:117:PRO:HD2	1.89	0.53
1:2A:212:G:H2'	1:2A:213:A:O4'	2.09	0.53
1:2A:2419:U:H2'	1:2A:2420:C:C6	2.43	0.53
5:2F:137:LYS:HA	5:2F:140:LEU:HD12	1.90	0.53
32:2a:1252:A:H2'	32:2a:1253:G:O4'	2.08	0.53
32:2a:1320:C:N3	50:2s:36:ARG:NH2	2.56	0.53
33:2b:96:ARG:HG2	33:2b:98:LEU:HD12	1.90	0.53
39:2h:20:TYR:CE1	39:2h:76:PRO:HG2	2.43	0.53
1:1A:1352:U:OP1	62:1A:4254:HOH:O	2.19	0.53
1:1A:1506:C:H2'	1:1A:1507:A:H8	1.72	0.53
1:2A:675:A:OP1	5:2F:63:LYS:NZ	2.35	0.53
1:2A:893:C:H2'	1:2A:894:C:C4	2.44	0.53
1:2A:956:G:H5"	12:2Q:77:LYS:HE2	1.90	0.53
29:27:26:GLY:O	29:27:30:VAL:HG23	2.08	0.53
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.23	0.53
37:2f:2:ARG:NE	37:2f:69:GLU:HG2	2.23	0.53
1:1A:528:A:OP2	9:1N:114:ARG:NH1	2.42	0.53
32:1a:920:U:H2'	32:1a:921:U:C6	2.44	0.53
1:2A:27:G:O2'	1:2A:28:A:OP2	2.22	0.53
1:2A:852:G:H2'	1:2A:853:G:H8	1.72	0.53
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.89	0.53
37:2f:33:TYR:HE2	37:2f:78:GLU:HG2	1.73	0.53
41:2j:98:ILE:O	62:2j:301:HOH:O	2.18	0.53
43:2l:89:ARG:HH21	43:2l:91:LYS:HA	1.74	0.53
1:1A:652(F):G:H1	1:1A:652(S):C:H42	1.55	0.53
7:1H:20:ALA:HB3	7:1H:23:ARG:HB2	1.91	0.53
21:1Z:61:LEU:HD21	21:1Z:67:LEU:HG	1.89	0.53
32:1a:1025:U:C2	32:1a:1036:G:O6	2.62	0.53
34:1c:62:ASP:HA	34:1c:97:LYS:HG2	1.91	0.53
57:1y:8:4SU:H4'	57:1y:48:C:H4'	1.91	0.53
1:2A:2079:U:OP1	23:21:21:ARG:NH2	2.42	0.53
7:2H:5:GLY:HA2	7:2H:69:ARG:HB2	1.90	0.53
11:2P:124:LYS:HG3	11:2P:144:GLU:HB3	1.91	0.53
1:1A:897:C:N3	1:1A:898:C:N4	2.57	0.53
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.91	0.53
36:1e:78:HIS:CD2	39:1h:104:ARG:HD2	2.43	0.53
32:2a:1299:A:H2'	32:2a:1299:A:N3	2.24	0.53
56:2z:5:CYS:O	62:2z:101:HOH:O	2.18	0.53
32:1a:130:A:O2'	32:1a:131:C:O5'	2.24	0.53
32:1a:266:G:O2'	32:1a:267:C:OP2	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:187:LEU:HD12	33:1b:201:ILE:O	2.09	0.53
51:1t:83:ARG:HA	51:1t:86:ARG:HH11	1.73	0.53
4:2E:119:ARG:HG2	4:2E:120:TRP:NE1	2.23	0.53
7:2H:24:VAL:HG21	7:2H:72:ILE:HD12	1.90	0.53
24:22:29:LYS:HG2	24:22:57:ILE:HD13	1.90	0.53
1:1A:2140:C:N3	1:1A:2151:G:O6	2.41	0.53
1:1A:2161:C:O2'	1:1A:2162:G:H8	1.92	0.53
32:1a:1006:C:H2'	32:1a:1007:C:C6	2.44	0.53
32:1a:1255:G:O2'	32:1a:1258:G:N3	2.40	0.53
33:1b:116:GLU:HA	33:1b:119:GLU:HB2	1.91	0.53
33:1b:195:ASP:O	39:1h:68:ARG:NH2	2.42	0.53
35:1d:3:ARG:HD3	35:1d:118:ARG:HD3	1.89	0.53
2:2B:3:C:H2'	2:2B:4:C:C6	2.44	0.53
6:2G:105:LYS:NZ	26:24:25:TYR:O	2.38	0.53
32:2a:17:U:H2'	32:2a:18:C:C6	2.43	0.53
34:2c:6:HIS:HD2	34:2c:7:PRO:HD2	1.74	0.53
35:2d:173:TRP:CD2	35:2d:189:PRO:HB3	2.43	0.53
40:2i:28:VAL:HG22	40:2i:63:ILE:HD12	1.90	0.53
41:2j:78:ASN:O	41:2j:80:LYS:N	2.42	0.53
1:1A:272(I):U:H2'	1:1A:272(J):C:O4'	2.10	0.52
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.09	0.52
15:1T:127:ALA:C	15:1T:129:ARG:H	2.17	0.52
32:1a:562:C:H1'	43:1l:15:ARG:HB3	1.90	0.52
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.74	0.52
32:1a:1411:C:N4	62:1a:1946:HOH:O	2.34	0.52
46:1o:61:GLY:O	46:1o:65:ARG:HG3	2.09	0.52
1:2A:321:G:OP1	5:2F:135:LYS:NZ	2.31	0.52
1:2A:2478:A:OP2	31:29:2:LYS:NZ	2.38	0.52
3:2D:180:GLY:HA3	3:2D:275:LYS:HD3	1.91	0.52
23:21:2:SER:HB3	23:21:46:LEU:HD12	1.92	0.52
32:2a:1366:C:H2'	32:2a:1367:C:C6	2.44	0.52
1:1A:2361:A:OP1	30:18:27:THR:OG1	2.27	0.52
32:1a:421:U:O4	34:1c:127:ARG:NH2	2.40	0.52
40:1i:77:ILE:O	40:1i:81:ILE:HG22	2.08	0.52
47:1p:69:THR:O	47:1p:72:ARG:HG2	2.08	0.52
1:2A:310:A:H1'	1:2A:311:A:H2'	1.91	0.52
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.09	0.52
3:2D:275:LYS:HG3	3:2D:276:LYS:HB2	1.90	0.52
18:2W:2:GLU:OE2	18:2W:72:LYS:NZ	2.28	0.52
26:24:58:ARG:HH21	50:2s:69:HIS:CE1	2.26	0.52
32:2a:1077:G:N2	32:2a:1080:A:OP2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.44	0.52
32:1a:421:U:OP2	32:1a:422:C:N4	2.32	0.52
1:2A:492:A:H2'	1:2A:493:G:O4'	2.10	0.52
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.45	0.52
9:2N:12:ARG:NH2	9:2N:50:ASP:OD2	2.38	0.52
15:2T:16:ARG:NH2	15:2T:18:ASP:OD2	2.42	0.52
26:24:46:GLN:HG2	26:24:48:ARG:HD2	1.91	0.52
34:2c:179:ARG:NH1	34:2c:206:GLU:HB2	2.25	0.52
38:2g:9:VAL:O	38:2g:11:GLN:NE2	2.42	0.52
1:1A:1075:C:H2'	1:1A:1076:C:H5'	1.91	0.52
1:1A:2135:A:N6	1:1A:2156:G:O2'	2.43	0.52
1:1A:2306:C:N4	6:1G:42:GLY:O	2.32	0.52
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.44	0.52
2:1B:108:U:H2'	2:1B:109:C:H5"	1.91	0.52
4:1E:179:GLU:HB2	4:1E:181:LEU:HG	1.91	0.52
23:11:89:GLU:O	23:11:93:GLU:HG2	2.10	0.52
32:1a:123:C:OP1	32:1a:311:C:O2'	2.27	0.52
51:1t:83:ARG:HA	51:1t:86:ARG:NH1	2.24	0.52
1:2A:1790:C:H5"	1:2A:1791:A:OP1	2.09	0.52
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.91	0.52
1:2A:2125:G:N1	1:2A:2172:U:OP1	2.40	0.52
6:2G:7:LEU:HB2	6:2G:104:GLU:HB2	1.92	0.52
32:2a:6:G:O6	36:2e:95:ALA:N	2.42	0.52
32:2a:237:C:H5"	48:2q:25:ARG:CZ	2.40	0.52
32:2a:1206:G:O2'	34:2c:193:TYR:HA	2.10	0.52
37:2f:95:GLU:O	49:2r:32:ARG:NH1	2.42	0.52
50:2s:80:TYR:O	50:2s:82:GLY:N	2.32	0.52
51:2t:86:ARG:O	51:2t:90:GLN:HB2	2.09	0.52
1:1A:1846:G:H5"	1:1A:1847:A:OP2	2.09	0.52
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.10	0.52
7:1H:5:GLY:HA2	7:1H:69:ARG:HB2	1.92	0.52
35:1d:101:LEU:HB2	35:1d:138:TYR:HB3	1.90	0.52
48:1q:83:ASP:OD1	48:1q:83:ASP:N	2.37	0.52
54:1w:1:G:H2'	54:1w:2:C:C6	2.44	0.52
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.45	0.52
1:2A:2461:C:H2'	1:2A:2462:U:H6	1.75	0.52
32:2a:1002:G:C2	32:2a:1003:G:H1'	2.44	0.52
33:2b:81:VAL:HB	33:2b:94:ASN:ND2	2.25	0.52
38:2g:93:PRO:HA	38:2g:96:GLN:HB2	1.91	0.52
50:2s:13:ASP:HA	50:2s:16:LEU:HB3	1.92	0.52
54:2w:45:U:H5"	54:2w:46:G7M:OP2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:687:C:H5"	29:17:2:LYS:HE2	1.91	0.52
62:1A:5484:HOH:O	11:1P:44:GLY:HA2	2.08	0.52
6:1G:149:VAL:HG22	6:1G:150:ASP:H	1.75	0.52
18:1W:62:HIS:O	18:1W:64:MET:HG3	2.10	0.52
32:1a:335:C:H2'	32:1a:336:C:C6	2.44	0.52
33:1b:101:MET:HA	33:1b:108:ILE:HD12	1.91	0.52
1:2A:857:C:H1'	22:20:26:TYR:HE1	1.73	0.52
1:2A:1782:C:O2	1:2A:2608:G:O2'	2.26	0.52
1:2A:2124:G:O6	1:2A:2125:G:N2	2.42	0.52
19:2X:88:LYS:NZ	19:2X:90:GLU:OE1	2.33	0.52
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.08	0.52
32:2a:1275:A:H2'	32:2a:1276:G:O4'	2.09	0.52
42:2k:81:ASP:OD1	42:2k:106:LYS:HB2	2.09	0.52
1:1A:897:C:H5'	54:1w:56:C:OP1	2.09	0.52
1:1A:898:C:N4	1:1A:899:A:H62	2.08	0.52
1:1A:2155:G:H2'	1:1A:2155:G:N3	2.25	0.52
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.10	0.52
12:1Q:78:PRO:HD3	55:1x:1:C:N3	2.25	0.52
1:2A:2120:G:H2'	1:2A:2121:G:H8	1.75	0.52
5:2F:196:LEU:O	5:2F:200:GLU:N	2.40	0.52
32:2a:1272:G:N2	32:2a:1273:G:N7	2.57	0.52
42:2k:87:THR:O	42:2k:87:THR:OG1	2.28	0.52
52:2u:6:ARG:HA	52:2u:11:GLY:HA3	1.92	0.52
1:1A:271(B):C:N4	1:1A:271(V):G:H1	2.08	0.52
35:1d:65:ARG:NH1	35:1d:72:GLU:HB2	2.24	0.52
38:1g:14:PRO:HG3	38:1g:21:VAL:HG13	1.91	0.52
38:1g:136:LYS:O	38:1g:140:ASP:HB2	2.09	0.52
51:1t:83:ARG:HG2	51:1t:86:ARG:HH12	1.75	0.52
1:2A:744:G:OP1	62:2A:3942:HOH:O	2.18	0.52
1:2A:921:G:O6	62:2A:3916:HOH:O	2.10	0.52
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.09	0.52
1:2A:2061:G:OP2	62:2A:3941:HOH:O	2.18	0.52
1:2A:2815:C:H2'	1:2A:2816:C:C6	2.45	0.52
19:2X:94:GLY:CA	19:2X:95:LEU:HB2	2.40	0.52
32:2a:79:G:H1	32:2a:90:U:H3	1.58	0.52
34:2c:156:ARG:N	34:2c:196:LEU:HD22	2.25	0.52
47:2p:53:VAL:HG22	47:2p:79:VAL:HG22	1.92	0.52
10:1O:59:LYS:NZ	10:1O:89:ASN:OD1	2.42	0.52
32:1a:68:G:H1	32:1a:101:A:H61	1.57	0.52
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.44	0.52
1:2A:616:G:H4'	5:2F:205:ARG:HH21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:796:C:H2'	1:2A:797:C:C6	2.44	0.52
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.91	0.52
32:2a:276:G:O2'	48:2q:68:ARG:NH1	2.43	0.52
1:1A:414:C:H2'	1:1A:415:A:C8	2.45	0.52
3:1D:18:VAL:HG12	3:1D:211:ARG:NH2	2.25	0.52
33:1b:60:ASP:HA	33:1b:63:MET:HE3	1.91	0.52
35:1d:7:PRO:HB2	35:1d:10:ARG:HD2	1.92	0.52
1:2A:1287:A:H8	13:2R:104:ARG:HD3	1.75	0.52
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.75	0.52
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.92	0.52
1:2A:2319:G:N2	14:2S:3:ARG:HA	2.25	0.52
1:2A:2390:U:P	30:28:35:GLN:HE22	2.33	0.52
1:2A:2506:U:O2'	54:2w:76:F3N:H4'	2.10	0.52
15:2T:51:ARG:HG3	15:2T:98:LYS:HD2	1.92	0.52
32:2a:34:C:H2'	32:2a:35:G:H8	1.75	0.52
32:2a:678:U:H2'	32:2a:679:C:C6	2.45	0.52
32:2a:755:G:OP2	46:2o:65:ARG:HD2	2.10	0.52
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.92	0.52
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.44	0.52
39:2h:6:ILE:O	39:2h:10:LEU:HG	2.10	0.52
40:2i:28:VAL:HG13	40:2i:63:ILE:HB	1.90	0.52
54:2w:51:U:H2'	54:2w:52:G:H8	1.74	0.52
1:1A:796:C:H2'	1:1A:797:C:C6	2.44	0.51
1:1A:1087:G:H2'	1:1A:1089:G:C8	2.45	0.51
1:1A:1670:C:O2	4:1E:129:HIS:NE2	2.41	0.51
9:1N:29:LYS:O	9:1N:33:LEU:HD12	2.10	0.51
32:1a:848:C:H2'	32:1a:849:C:H6	1.74	0.51
32:1a:1060:C:H5"	41:1j:51:ARG:HG2	1.92	0.51
43:1l:70:ILE:HG12	43:1l:100:ILE:HD12	1.92	0.51
1:2A:2100:G:H2'	1:2A:2101:G:H8	1.75	0.51
15:2T:23:ARG:HD3	15:2T:120:ARG:CZ	2.40	0.51
32:2a:15:G:H21	36:2e:18:ARG:HA	1.75	0.51
32:2a:1189:C:OP1	41:2j:51:ARG:NH2	2.43	0.51
32:2a:1271:G:C2	32:2a:1272:G:N7	2.78	0.51
35:2d:103:ASN:OD1	35:2d:114:ARG:NE	2.40	0.51
1:1A:1060:U:H3	1:1A:1088:A:H8	1.57	0.51
1:1A:1551:C:OP2	62:1A:4256:HOH:O	2.19	0.51
51:1t:57:ARG:HH12	51:1t:100:ILE:HD12	1.74	0.51
1:2A:1919:A:O2'	32:2a:1517:G:N3	2.41	0.51
3:2D:182:LEU:HB2	3:2D:272:ALA:HB3	1.91	0.51
4:2E:49:LEU:N	4:2E:79:ARG:O	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:10:ARG:HG2	14:2S:91:PRO:HA	1.91	0.51
32:2a:148:G:H2'	32:2a:149:A:H8	1.74	0.51
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.27	0.51
32:2a:573:A:N3	32:2a:883:C:O2'	2.43	0.51
39:2h:103:VAL:HG21	39:2h:109:ILE:C	2.35	0.51
40:2i:79:LEU:HG	40:2i:83:ARG:HD2	1.92	0.51
46:2o:24:SER:OG	46:2o:25:THR:N	2.42	0.51
1:1A:1252:G:N3	16:1U:33:ARG:HG2	2.26	0.51
5:1F:197:ASP:N	5:1F:197:ASP:OD1	2.43	0.51
23:11:50:ARG:HG2	23:11:59:THR:HG23	1.91	0.51
30:18:23:VAL:HG11	30:18:47:LYS:HD3	1.91	0.51
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.93	0.51
54:1w:26:A:N6	54:1w:44:G:H1	2.04	0.51
1:2A:1645:G:H5"	1:2A:1646:C:H5'	1.93	0.51
1:2A:2081:C:O2'	62:2A:3924:HOH:O	2.13	0.51
1:2A:2540:C:O2'	1:2A:2740:A:N3	2.40	0.51
32:2a:450:G:OP1	47:2p:43:LYS:NZ	2.42	0.51
32:2a:1397:C:OP2	36:2e:24:ARG:NH2	2.44	0.51
33:2b:92:TYR:CE2	33:2b:151:GLY:HA3	2.46	0.51
1:1A:1058:G:H1	1:1A:1080:C:H42	1.58	0.51
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.92	0.51
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	1.92	0.51
21:1Z:98:MET:HE2	21:1Z:100:VAL:HG22	1.91	0.51
32:1a:532:A:N6	32:1a:1206:G:O2'	2.43	0.51
35:1d:107:ARG:NH2	35:1d:194:LEU:HD11	2.25	0.51
47:1p:47:ASP:OD1	47:1p:47:ASP:N	2.39	0.51
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.46	0.51
8:2I:140:LEU:HD23	8:2I:142:VAL:HG22	1.91	0.51
1:2A:330:A:HO2'	1:2A:331:A:H8	1.57	0.51
1:2A:1358:G:O2'	1:2A:1373:A:N6	2.43	0.51
1:2A:1886:C:H2'	1:2A:1887:C:H6	1.75	0.51
21:2Z:47:VAL:HA	21:2Z:50:GLN:HE22	1.76	0.51
32:2a:266:G:H5"	32:2a:268:C:H41	1.75	0.51
32:2a:1239:A:H4'	32:2a:1240:U:H5"	1.92	0.51
34:2c:150:LYS:HG3	34:2c:169:ALA:HB2	1.91	0.51
39:2h:39:LEU:HB3	39:2h:45:ILE:HD11	1.93	0.51
44:2m:107:ALA:O	44:2m:111:LYS:N	2.33	0.51
50:2s:49:ILE:HG22	50:2s:62:ILE:HD11	1.92	0.51
32:1a:6:G:H1	36:1e:98:THR:HG21	1.76	0.51
32:1a:96:U:H2'	32:1a:97:G:H8	1.75	0.51
33:1b:59:GLU:HG3	33:1b:225:ALA:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1502:C:H2'	1:2A:1503:U:H6	1.76	0.51
1:2A:2637:U:OP1	4:2E:82:ARG:NH1	2.41	0.51
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.10	0.51
25:23:59:VAL:HG12	25:23:60:GLU:H	1.76	0.51
32:2a:743:U:H2'	32:2a:744:C:C6	2.45	0.51
46:2o:4:THR:N	46:2o:7:GLU:OE2	2.40	0.51
54:2w:54:5MU:H2'	54:2w:55:PSU:O4'	2.11	0.51
1:1A:1078:U:HO2'	1:1A:1088:A:H2	1.57	0.51
6:1G:34:LEU:HD23	6:1G:161:THR:HG22	1.92	0.51
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.92	0.51
9:1N:108:PRO:O	9:1N:113:GLY:HA3	2.11	0.51
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.92	0.51
32:1a:7:G:H2'	36:1e:119:LEU:HD22	1.91	0.51
32:1a:963:G:H5'	62:1a:1919:HOH:O	2.11	0.51
39:1h:111:ILE:HB	39:1h:135:CYS:SG	2.51	0.51
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.46	0.51
1:2A:1445(A):C:H42	1:2A:1466:G:H1	1.58	0.51
1:2A:2379:G:HO2'	14:2S:17:ARG:HH12	1.54	0.51
1:2A:2564:A:C2	1:2A:2647:U:H4'	2.46	0.51
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.26	0.51
32:2a:123:C:OP1	32:2a:311:C:O2'	2.28	0.51
32:2a:1010:G:H2'	32:2a:1011:G:H8	1.75	0.51
44:2m:4:ILE:HG23	44:2m:5:ALA:H	1.75	0.51
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	1.93	0.51
7:1H:84:SER:HA	7:1H:133:VAL:O	2.10	0.51
32:1a:332:G:OP2	51:1t:10:LEU:HD23	2.11	0.51
32:2a:297:G:N2	32:2a:300:A:OP2	2.44	0.51
32:2a:620:C:C2	35:2d:135:LEU:HG	2.46	0.51
32:2a:1004:A:C8	32:2a:1005:A:H4'	2.45	0.51
34:2c:134:ILE:HG23	34:2c:151:VAL:HB	1.91	0.51
39:2h:12:ARG:HD3	39:2h:26:VAL:HG12	1.92	0.51
41:2j:5:ARG:HA	41:2j:73:ASP:OD1	2.11	0.51
43:2l:102:ARG:NE	43:2l:108:ALA:O	2.32	0.51
1:1A:536:A:H2'	1:1A:537:C:C6	2.46	0.51
1:1A:548:A:H61	17:1V:18:LEU:HA	1.76	0.51
1:1A:686:G:N2	1:1A:788:A:H61	2.09	0.51
1:1A:1074:G:C6	1:1A:1075:C:H1'	2.46	0.51
1:1A:1125:G:H5'	31:19:37:GLY:HA2	1.92	0.51
8:1I:77:LEU:HB3	8:1I:142:VAL:HG12	1.93	0.51
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.18	0.51
39:1h:100:ILE:HB	39:1h:125:ARG:NH1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:1y:38:A:H2'	57:1y:39:PSU:O4'	2.11	0.51
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.11	0.51
1:2A:652(A):A:H3'	1:2A:652(B):A:H5"	1.92	0.51
32:2a:499:A:H4'	32:2a:500:G:OP1	2.10	0.51
32:2a:986:A:H2'	32:2a:987:G:C8	2.46	0.51
32:2a:1343:G:H4'	40:2i:122:ALA:HB3	1.93	0.51
49:2r:38:GLU:OE1	49:2r:41:LYS:NZ	2.44	0.51
51:2t:9:ASN:O	51:2t:10:LEU:HB2	2.10	0.51
1:1A:2681:C:OP2	4:1E:109:LYS:NZ	2.42	0.51
7:1H:97:ARG:NE	7:1H:104:GLU:OE1	2.36	0.51
21:1Z:153:SER:HB3	21:1Z:167:PRO:HB3	1.93	0.51
32:1a:407:G:OP1	35:1d:115:ARG:NH2	2.44	0.51
33:1b:59:GLU:HB2	33:1b:221:LEU:HD11	1.93	0.51
39:1h:112:LEU:HA	39:1h:134:ILE:HG12	1.93	0.51
1:2A:893:C:H5'	1:2A:894:C:C5	2.46	0.51
1:2A:1952:A:OP1	10:2O:42:SER:OG	2.29	0.51
5:2F:117:ARG:NH2	5:2F:186:ILE:O	2.44	0.51
32:2a:424:G:H2'	32:2a:425:G:H8	1.76	0.51
32:2a:1161:C:H2'	32:2a:1162:C:H6	1.76	0.51
32:2a:1244:C:N4	32:2a:1293:G:H1	2.07	0.51
48:2q:58:GLU:OE2	48:2q:75:ARG:NH2	2.44	0.51
55:2x:7:G:O2'	55:2x:49:G:OP2	2.25	0.51
2:1B:88:C:H2'	2:1B:89:G:O4'	2.11	0.50
11:1P:38:GLN:O	11:1P:39:LYS:HB3	2.10	0.50
32:1a:418:C:H2'	32:1a:419:C:C6	2.46	0.50
32:1a:445:G:H2'	32:1a:446:G:O4'	2.11	0.50
35:1d:178:VAL:C	35:1d:180:GLY:H	2.19	0.50
43:1l:39:VAL:HG11	43:1l:41:ARG:HH11	1.76	0.50
1:2A:641:C:H42	1:2A:647:G:H1	1.59	0.50
3:2D:146:GLU:HB2	3:2D:189:CYS:HB3	1.92	0.50
4:2E:27:LEU:HD22	15:2T:1:MET:SD	2.50	0.50
1:1A:2144:U:H3'	1:1A:2146:C:N4	2.26	0.50
18:1W:46:PHE:O	18:1W:50:VAL:HG23	2.11	0.50
35:1d:144:ASP:HB2	35:1d:146:ILE:HD11	1.92	0.50
42:1k:16:SER:HB2	42:1k:79:SER:HB3	1.92	0.50
1:2A:1478:G:O2'	1:2A:1558:A:N1	2.43	0.50
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.45	0.50
6:2G:39:ILE:HG21	6:2G:60:LEU:HD21	1.93	0.50
12:2Q:35:VAL:HG22	12:2Q:102:VAL:HG22	1.92	0.50
21:2Z:23:LYS:HB3	21:2Z:38:TYR:CD1	2.45	0.50
22:20:11:ARG:O	22:20:14:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:26:33:LYS:HA	28:26:51:GLU:OE1	2.11	0.50
32:2a:1124:G:N7	32:2a:1145:C:O2'	2.44	0.50
35:2d:98:GLU:OE1	35:2d:103:ASN:ND2	2.45	0.50
37:2f:76:ALA:HB1	37:2f:80:ARG:HH22	1.76	0.50
40:2i:71:SER:HA	40:2i:74:ILE:HD12	1.92	0.50
32:1a:339:C:H2'	32:1a:340:U:H6	1.77	0.50
32:1a:582:U:OP1	46:1o:68:ARG:NH2	2.36	0.50
33:1b:98:LEU:HB2	33:1b:101:MET:HG3	1.94	0.50
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.93	0.50
1:2A:658:C:H2'	1:2A:659:C:C6	2.45	0.50
5:2F:13:SER:OG	5:2F:16:GLY:O	2.26	0.50
6:2G:114:ILE:HB	6:2G:117:PHE:HD1	1.76	0.50
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.94	0.50
29:27:24:THR:HG22	29:27:26:GLY:N	2.26	0.50
34:2c:39:ILE:O	34:2c:43:LEU:HG	2.11	0.50
51:2t:44:ALA:HB2	51:2t:88:VAL:HG13	1.93	0.50
1:1A:2110:G:C2	1:1A:2120:G:H1'	2.47	0.50
1:1A:2805:G:H2'	1:1A:2807:G:H8	1.76	0.50
32:1a:62:U:OP1	32:1a:385:C:O2'	2.27	0.50
32:1a:362:G:N1	32:1a:365:U:OP2	2.42	0.50
32:1a:551:U:H2'	32:1a:552:U:C6	2.47	0.50
1:2A:340:A:H2'	1:2A:341:G:O4'	2.12	0.50
1:2A:1009:A:O4'	16:2U:59:ARG:HD2	2.11	0.50
1:2A:2875:C:OP1	15:2T:3:ARG:NH1	2.44	0.50
8:2I:45:LYS:O	8:2I:49:ALA:N	2.43	0.50
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	1.92	0.50
32:2a:757:U:H2'	32:2a:758:G:O4'	2.11	0.50
32:2a:1373:G:H5"	38:2g:36:LYS:HB2	1.94	0.50
41:2j:11:PHE:HE1	41:2j:67:THR:HG22	1.76	0.50
46:2o:39:LEU:HD13	46:2o:56:LEU:HB2	1.93	0.50
57:2y:34:G:H2'	57:2y:35:A:C8	2.46	0.50
1:1A:586:A:N1	1:1A:809:G:O2'	2.40	0.50
1:1A:674:G:O2'	5:1F:74:ARG:HD3	2.12	0.50
1:1A:1069:A:H4'	1:1A:1070:A:H5"	1.93	0.50
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.12	0.50
26:14:15:ILE:O	26:14:33:VAL:N	2.38	0.50
32:1a:1039:C:H2'	32:1a:1040:U:C6	2.46	0.50
32:1a:1364:U:C6	52:1u:14:TRP:HH2	2.30	0.50
34:1c:150:LYS:HB2	34:1c:173:VAL:HG21	1.93	0.50
36:1e:57:LYS:HG2	36:1e:61:TYR:CE2	2.47	0.50
42:1k:33:THR:HA	42:1k:39:PRO:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:918:A:N3	2:2B:80:U:H4'	2.26	0.50
1:2A:1405:U:H2'	1:2A:1406:U:H6	1.76	0.50
14:2S:23:ARG:HG2	14:2S:24:LEU:H	1.77	0.50
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.11	0.50
26:24:64:GLY:C	26:24:66:SER:H	2.20	0.50
32:2a:448:A:P	32:2a:485:G:H22	2.33	0.50
38:2g:70:LYS:O	38:2g:138:LYS:HD2	2.11	0.50
1:1A:1427:A:H4'	1:1A:1428:C:O4'	2.12	0.50
21:1Z:61:LEU:HD23	21:1Z:65:GLN:HB2	1.94	0.50
32:1a:657:G:H4'	46:1o:28:GLN:HG2	1.92	0.50
47:1p:4:ILE:HB	47:1p:66:PRO:HA	1.92	0.50
1:2A:700:G:O2'	1:2A:1632:A:N3	2.37	0.50
14:2S:64:GLU:O	14:2S:68:GLN:HG2	2.11	0.50
19:2X:2:LYS:NZ	19:2X:38:GLU:OE2	2.43	0.50
39:2h:120:THR:H	39:2h:123:GLU:HB2	1.76	0.50
54:2w:39:PSU:H2'	54:2w:40:C:C6	2.46	0.50
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.26	0.50
32:1a:1004:A:H5"	32:1a:1025:U:C5	2.47	0.50
32:1a:1503:A:N1	53:1v:12:A:H2	2.08	0.50
33:1b:204:ASN:OD1	33:1b:205:ASP:N	2.44	0.50
51:1t:60:GLU:HG3	51:1t:81:LYS:HD2	1.94	0.50
1:2A:1125:G:H5'	31:29:37:GLY:HA2	1.94	0.50
1:2A:2502:G:H5"	1:2A:2503:2MA:H5"	1.93	0.50
32:2a:664:G:H22	32:2a:741:G:H1	1.59	0.50
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.47	0.50
33:2b:178:ARG:HH22	39:2h:68:ARG:HH12	1.58	0.50
1:1A:1048:A:N1	1:1A:1112:G:O2'	2.40	0.50
1:1A:2235:G:N7	62:1A:4327:HOH:O	2.33	0.50
4:1E:36:ARG:NH1	4:1E:85:ASN:OD1	2.45	0.50
6:2G:173:LEU:HA	6:2G:176:LEU:HB2	1.93	0.50
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.45	0.50
32:2a:537:G:H5"	43:2l:113:ARG:NH1	2.27	0.50
32:2a:1187:G:OP1	40:2i:113:LYS:NZ	2.45	0.50
1:1A:214:G:O2'	1:1A:215:G:O4'	2.30	0.50
1:1A:1057:A:H61	1:1A:1081:U:H3	1.58	0.50
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.27	0.50
33:1b:163:PHE:CD1	33:1b:185:ILE:HG13	2.47	0.50
34:1c:52:LEU:HD12	34:1c:53:ALA:H	1.77	0.50
35:1d:68:TYR:HB2	35:1d:70:ILE:HG22	1.94	0.50
41:1j:78:ASN:O	41:1j:80:LYS:N	2.45	0.50
1:2A:1927:A:H2'	1:2A:1928:A:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2114:A:H2	1:2A:2167:U:H3	1.58	0.50
1:2A:2396:G:OP1	23:21:25:LYS:NZ	2.30	0.50
1:2A:2831:G:OP1	1:2A:2834:G:H4'	2.11	0.50
4:2E:12:THR:HG21	15:2T:11:GLU:OE2	2.12	0.50
15:2T:118:ARG:HG2	32:2a:1442(A):G:C8	2.47	0.50
17:2V:1:MET:HB3	17:2V:99:ILE:HD12	1.93	0.50
19:2X:60:ARG:NH2	29:27:47:ARG:HH22	2.08	0.50
32:2a:114:U:H2'	32:2a:115:G:C8	2.47	0.50
32:2a:674:G:N2	32:2a:717:C:O2	2.45	0.50
32:2a:921:U:O2'	36:2e:19:MET:O	2.27	0.50
41:2j:25:GLU:O	41:2j:29:ARG:HG2	2.12	0.50
1:1A:1041:C:H42	1:1A:1114:G:H1	1.60	0.49
1:1A:1047:G:H2'	1:1A:1110:G:N2	2.27	0.49
1:1A:2099:U:O2	1:1A:2190:G:N2	2.35	0.49
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.94	0.49
47:1p:19:ILE:HG22	47:1p:36:ILE:HG13	1.93	0.49
57:1y:5:G:H1'	57:1y:69:G:N2	2.26	0.49
1:2A:38:A:H2'	1:2A:39:C:C6	2.47	0.49
8:2I:123:LEU:HD11	8:2I:145:VAL:C	2.37	0.49
11:2P:118:GLY:O	11:2P:137:LYS:NZ	2.38	0.49
25:23:8:LEU:HB2	25:23:28:LEU:HD22	1.94	0.49
32:2a:1373:G:O3'	38:2g:36:LYS:NZ	2.43	0.49
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.46	0.49
1:1A:1937:A:H1'	1:1A:1939:5MU:H72	1.94	0.49
1:1A:2010:G:H5"	18:1W:42:ARG:HB2	1.93	0.49
1:1A:2123:G:H2'	1:1A:2124:G:C8	2.47	0.49
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.47	0.49
5:1F:24:LEU:HB3	5:1F:115:ALA:HB2	1.94	0.49
32:1a:178:C:H2'	32:1a:179:A:H8	1.77	0.49
32:1a:767:A:H2'	32:1a:768:A:O4'	2.12	0.49
40:1i:32:ASP:OD1	40:1i:33:PHE:N	2.44	0.49
41:1j:5:ARG:NE	41:1j:73:ASP:OD1	2.40	0.49
1:2A:30:G:H2'	1:2A:31:C:C6	2.47	0.49
1:2A:724:U:H2'	1:2A:725:G:O4'	2.12	0.49
1:2A:1365:A:O2'	23:21:11:ARG:NH1	2.45	0.49
6:2G:51:ARG:H	6:2G:51:ARG:HD2	1.76	0.49
11:2P:50:ARG:HH21	30:28:7:HIS:CD2	2.30	0.49
14:2S:67:ARG:O	14:2S:71:ARG:HG3	2.11	0.49
32:2a:921:U:O2	36:2e:19:MET:HB2	2.12	0.49
32:2a:936:C:H2'	32:2a:937:A:O4'	2.12	0.49
46:2o:56:LEU:O	46:2o:60:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:2r:52:PRO:HB2	49:2r:54:ARG:HG2	1.94	0.49
32:1a:265:G:H2'	32:1a:267:C:H5	1.78	0.49
36:1e:78:HIS:HD2	39:1h:104:ARG:HD2	1.76	0.49
36:1e:81:GLU:HG2	36:1e:90:VAL:HG22	1.95	0.49
1:2A:1426:G:O2'	1:2A:1572:A:N6	2.39	0.49
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.45	0.49
16:2U:8:VAL:HG23	16:2U:11:ARG:NH2	2.27	0.49
19:2X:92:LEU:O	19:2X:94:GLY:N	2.46	0.49
23:21:83:GLU:OE1	23:21:83:GLU:N	2.46	0.49
25:23:12:PRO:HB2	25:23:20:LYS:HG2	1.94	0.49
33:2b:113:HIS:O	33:2b:117:GLU:HB2	2.12	0.49
35:2d:60:GLU:HG3	35:2d:202:LEU:HD12	1.93	0.49
38:2g:51:GLN:O	38:2g:55:GLY:HA2	2.11	0.49
40:2i:128:ARG:NH2	55:2x:33:U:OP2	2.44	0.49
49:2r:22:VAL:HG23	49:2r:55:ARG:O	2.12	0.49
7:1H:101:ARG:HH12	7:1H:122:THR:HA	1.78	0.49
8:1I:79:ILE:HB	8:1I:144:VAL:HG12	1.94	0.49
32:1a:1329:A:N7	52:1u:7:ARG:NH2	2.61	0.49
38:1g:78:ARG:HG3	38:1g:79:ARG:H	1.78	0.49
1:2A:900:A:H2'	1:2A:901:A:H8	1.76	0.49
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.46	0.49
26:24:45:GLY:C	26:24:47:GLN:H	2.20	0.49
32:2a:523:A:H61	43:2l:92:0TD:CG	2.26	0.49
32:2a:979:C:H42	45:2n:18:VAL:HG22	1.77	0.49
32:2a:1161:C:H2'	32:2a:1162:C:C6	2.47	0.49
33:2b:74:LYS:HD2	33:2b:166:ASP:HB3	1.93	0.49
33:2b:162:ILE:HD11	33:2b:184:VAL:HG22	1.95	0.49
1:1A:483:A:O2'	20:1Y:49:VAL:O	2.28	0.49
2:1B:11:C:OP2	22:10:72:ARG:NH2	2.42	0.49
4:1E:119:ARG:HG2	4:1E:120:TRP:NE1	2.28	0.49
20:1Y:6:HIS:HE1	20:1Y:72:VAL:O	1.94	0.49
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.95	0.49
32:1a:1101:A:H4'	32:1a:1102:A:O5'	2.13	0.49
32:1a:1513:A:H2'	32:1a:1514:C:C6	2.47	0.49
1:2A:1364:G:P	23:21:3:LYS:HG3	2.53	0.49
5:2F:197:ASP:O	5:2F:200:GLU:HB3	2.13	0.49
7:2H:159:GLU:HG3	7:2H:169:VAL:HG11	1.95	0.49
11:2P:86:LYS:HG2	11:2P:87:ASP:N	2.27	0.49
35:2d:196:LEU:O	35:2d:198:VAL:N	2.41	0.49
40:2i:21:PRO:HA	40:2i:59:PHE:HA	1.93	0.49
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:453:A:O2'	47:1p:68:ASP:O	2.29	0.49
32:1a:946:A:H2'	32:1a:947:G:C8	2.48	0.49
55:1x:68:C:H2'	55:1x:69:C:C6	2.47	0.49
1:2A:479:A:N3	1:2A:481:G:H5"	2.28	0.49
1:2A:1015:G:H2'	1:2A:1016:G:C8	2.47	0.49
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.47	0.49
1:2A:1263:U:C4	1:2A:1264:G:C6	3.00	0.49
2:2B:44:G:N3	2:2B:47:C:N4	2.57	0.49
21:2Z:158:PRO:O	21:2Z:161:VAL:HG12	2.12	0.49
32:2a:163:C:H2'	32:2a:164:U:C6	2.48	0.49
32:2a:222:U:H2'	32:2a:223:U:C6	2.48	0.49
32:2a:537:G:H5"	43:2l:113:ARG:HH12	1.78	0.49
32:2a:609:A:H5'	47:2p:18:ARG:HH22	1.75	0.49
1:1A:1784:A:OP2	62:1A:4258:HOH:O	2.19	0.49
1:1A:2801(A):A:H1'	1:1A:2895:U:H1'	1.95	0.49
32:1a:933:G:O6	38:1g:3:ARG:NH2	2.46	0.49
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.47	0.49
33:1b:163:PHE:HA	33:1b:185:ILE:O	2.12	0.49
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.95	0.49
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.12	0.49
8:2I:40:THR:HG1	8:2I:41:GLU:H	1.57	0.49
32:2a:1184:G:H2'	32:2a:1185:G:C8	2.48	0.49
33:2b:87:ARG:HH21	33:2b:230:VAL:HG12	1.78	0.49
47:2p:21:VAL:HG22	47:2p:33:ILE:HB	1.94	0.49
1:1A:2378:A:H2'	14:1S:21:THR:HG21	1.95	0.49
1:1A:2786:U:O2'	4:1E:62:PRO:O	2.26	0.49
6:1G:75:LYS:HE3	6:1G:77:ILE:HG12	1.95	0.49
9:1N:1:MET:HE1	16:1U:94:ASN:ND2	2.28	0.49
1:2A:2378:A:O3'	14:2S:23:ARG:NH2	2.46	0.49
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.43	0.49
9:2N:108:PRO:O	9:2N:113:GLY:HA3	2.13	0.49
32:2a:67:C:H2'	32:2a:68:G:C8	2.48	0.49
35:2d:10:ARG:HG3	35:2d:11:LEU:HD12	1.94	0.49
55:2x:61:C:H2'	55:2x:62:C:H6	1.78	0.49
1:1A:592:G:N7	62:1A:4335:HOH:O	2.35	0.49
1:1A:700:G:O2'	1:1A:1632:A:N3	2.42	0.49
1:1A:1184:G:H5'	25:13:29:ARG:HH21	1.77	0.49
1:1A:1649:G:O2'	13:1R:107:ASP:OD2	2.24	0.49
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.45	0.49
1:2A:2162:G:H2'	1:2A:2163:C:O4'	2.12	0.49
1:2A:2270:G:H2'	1:2A:2271:G:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:27:9:ARG:NH2	29:27:47:ARG:HD3	2.28	0.49
32:2a:179:A:H2'	32:2a:180:U:C6	2.47	0.49
32:2a:737:A:H2'	32:2a:738:C:C6	2.48	0.49
1:1A:1607:C:H4'	1:1A:1608:A:O5'	2.13	0.49
3:1D:8:PRO:HB3	3:1D:14:ARG:HG2	1.95	0.49
21:1Z:61:LEU:HD22	21:1Z:61:LEU:H	1.78	0.49
32:1a:106:C:O2'	32:1a:379:C:H5"	2.12	0.49
32:1a:562:C:O2	43:1l:16:GLU:N	2.43	0.49
32:1a:811:C:O2'	32:1a:901:A:N1	2.41	0.49
32:1a:1346:A:OP1	40:1i:120:ARG:NH1	2.31	0.49
37:1f:37:VAL:HA	37:1f:65:VAL:HG12	1.94	0.49
39:1h:83:ILE:HG13	39:1h:137:VAL:HG22	1.94	0.49
50:1s:32:LYS:HA	50:1s:50:ALA:HB3	1.94	0.49
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.38	0.49
57:1y:15:G:H22	57:1y:48:C:H42	1.61	0.49
15:2T:107:ASP:O	15:2T:111:ARG:HG3	2.13	0.49
21:2Z:31:ARG:HG3	21:2Z:32:HIS:CD2	2.48	0.49
28:26:35:GLU:HG3	28:26:50:ARG:HD3	1.94	0.49
32:2a:64:G:C4'	32:2a:65:U:H3'	2.38	0.49
32:2a:1051:C:N4	32:2a:1207:2MG:HN1	2.11	0.49
1:1A:1804:C:OP1	3:1D:259:THR:OG1	2.31	0.48
30:18:26:LYS:HG2	30:18:46:ARG:O	2.13	0.48
32:1a:60:A:H4'	32:1a:61:G:H5'	1.94	0.48
32:1a:890:G:O2'	32:1a:906:G:O6	2.25	0.48
35:1d:107:ARG:HH21	35:1d:194:LEU:HD21	1.78	0.48
48:1q:51:TYR:HE1	48:1q:76:LEU:HB2	1.78	0.48
1:2A:458:G:O2'	1:2A:469:G:O6	2.24	0.48
1:2A:856:C:H2'	1:2A:857:C:C6	2.48	0.48
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.38	0.48
2:2B:14:U:OP2	2:2B:70:C:O2'	2.28	0.48
9:2N:15:LEU:HD23	9:2N:137:LYS:HG2	1.94	0.48
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.94	0.48
32:2a:1123:A:O2'	41:2j:36:GLY:O	2.30	0.48
32:2a:1278:U:H5'	32:2a:1279:A:OP1	2.12	0.48
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.49	0.48
38:2g:78:ARG:HG3	38:2g:156:TRP:HZ3	1.77	0.48
40:2i:8:GLY:HA3	40:2i:76:ALA:O	2.13	0.48
1:1A:1063:G:H2'	1:1A:1064:C:C5	2.48	0.48
1:1A:2092:U:H4'	1:1A:2093:G:O5'	2.13	0.48
8:1I:9:LEU:HG	8:1I:10:GLU:HG3	1.95	0.48
12:1Q:12:GLN:NE2	12:1Q:72:LYS:HG3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:44:THR:O	26:14:44:THR:OG1	2.21	0.48
35:1d:100:ARG:HG2	35:1d:137:SER:HA	1.94	0.48
1:2A:118:A:H5'	1:2A:119:A:H8	1.77	0.48
1:2A:271(A):A:H8	1:2A:271(B):C:C6	2.30	0.48
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.49	0.48
2:2B:29:A:H2'	2:2B:30:C:C6	2.49	0.48
7:2H:121:ILE:HG13	7:2H:144:VAL:HG21	1.95	0.48
11:2P:88:LEU:HA	11:2P:91:PHE:HD2	1.78	0.48
29:27:24:THR:HG22	29:27:26:GLY:H	1.78	0.48
32:2a:630:G:H2'	32:2a:631:G:H8	1.78	0.48
34:2c:40:ARG:HE	34:2c:55:VAL:HG13	1.78	0.48
1:1A:2124:G:H1	1:1A:2174:C:N4	2.10	0.48
1:1A:2394:C:O2	62:1A:4257:HOH:O	2.19	0.48
18:1W:13:SER:HB3	18:1W:16:LYS:HD2	1.94	0.48
32:1a:310:G:OP2	47:1p:27:LYS:HE2	2.14	0.48
32:1a:974:A:H8	32:1a:974:A:OP1	1.96	0.48
32:1a:1151:A:O2'	32:1a:1152:A:H8	1.96	0.48
1:2A:884:C:H3'	1:2A:885:C:C6	2.48	0.48
2:2B:11:C:OP2	22:20:72:ARG:NH2	2.46	0.48
3:2D:20:ASP:OD1	3:2D:20:ASP:N	2.32	0.48
32:2a:544:G:P	35:2d:59:ARG:HH22	2.35	0.48
32:2a:995:C:O2	45:2n:4:LYS:NZ	2.33	0.48
32:2a:1018:C:H2'	32:2a:1019:C:O4'	2.13	0.48
32:2a:1184:G:H2'	32:2a:1185:G:H8	1.78	0.48
32:2a:1312:G:H5'	50:2s:5:LEU:HD21	1.95	0.48
33:2b:185:ILE:HG22	33:2b:199:TYR:HD2	1.78	0.48
42:2k:48:ILE:O	42:2k:50:TYR:N	2.38	0.48
1:1A:2114:A:H2'	1:1A:2115:G:O4'	2.14	0.48
1:1A:2147:G:H3'	1:1A:2147:G:N3	2.28	0.48
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.78	0.48
32:1a:56:U:H2'	32:1a:57:G:C8	2.49	0.48
32:1a:711:G:OP1	37:1f:54:LYS:NZ	2.39	0.48
32:1a:1002:G:H3'	32:1a:1003:G:C4'	2.43	0.48
40:1i:17:VAL:HG11	40:1i:80:GLY:C	2.39	0.48
44:1m:3:ARG:HG2	44:1m:8:GLU:HA	1.95	0.48
50:1s:15:LEU:HD22	50:1s:33:THR:HG21	1.94	0.48
1:2A:320:A:O2'	1:2A:322:A:OP2	2.29	0.48
1:2A:1183:G:H5"	25:23:30:ARG:NH2	2.28	0.48
2:2B:55:U:H1'	6:2G:29:TRP:HE1	1.78	0.48
14:2S:62:LYS:HB3	14:2S:97:ARG:HD2	1.95	0.48
25:23:7:LYS:HE3	25:23:32:GLN:HE21	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:26:11:LEU:HB2	28:26:21:TYR:HB2	1.95	0.48
30:28:29:LYS:HD2	30:28:44:LYS:HB3	1.94	0.48
32:2a:728:A:H2'	32:2a:729:A:C8	2.47	0.48
32:2a:804:U:OP1	62:2a:1915:HOH:O	2.19	0.48
32:2a:1391:U:H2'	32:2a:1392:G:C8	2.48	0.48
44:2m:10:PRO:HD2	44:2m:18:ALA:HB1	1.95	0.48
54:2w:21:A:O2'	54:2w:22:G:OP1	2.29	0.48
57:2y:55:PSU:N1	57:2y:57:G:H5"	2.21	0.48
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.14	0.48
22:10:11:ARG:HG3	62:10:206:HOH:O	2.14	0.48
32:1a:189(D):C:H2'	32:1a:189(E):U:O4'	2.14	0.48
32:1a:405:U:H5"	32:1a:495:A:H2	1.78	0.48
32:1a:582:U:H2'	32:1a:583:A:H8	1.79	0.48
32:1a:715:A:H2'	32:1a:716:A:C8	2.48	0.48
1:2A:197:A:O2'	62:2A:3923:HOH:O	2.13	0.48
1:2A:307:G:H21	1:2A:330:A:N6	2.11	0.48
1:2A:639:U:H2'	1:2A:640:C:C6	2.48	0.48
1:2A:1372:U:H2'	1:2A:1373:A:O4'	2.14	0.48
1:2A:2886:G:H2'	1:2A:2887:U:C6	2.49	0.48
6:2G:39:ILE:HD11	6:2G:102:PHE:CZ	2.48	0.48
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.38	0.48
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.50	0.48
15:2T:41:ARG:NH1	32:2a:346:G:OP1	2.42	0.48
32:2a:977:A:O2'	32:2a:979:C:OP2	2.28	0.48
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.81	0.48
34:2c:87:LEU:C	34:2c:89:GLU:H	2.21	0.48
36:2e:41:VAL:O	36:2e:66:MET:HA	2.14	0.48
37:2f:69:GLU:CD	37:2f:69:GLU:H	2.19	0.48
54:2w:2:C:H2'	54:2w:3:C:C6	2.49	0.48
1:1A:26:G:H1'	1:1A:515:A:H61	1.79	0.48
1:1A:1055:G:H1	1:1A:1104:C:H42	1.61	0.48
1:1A:1359:A:N3	1:1A:1359:A:H5'	2.28	0.48
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	1.95	0.48
1:1A:2130:U:O2'	1:1A:2131:G:N2	2.46	0.48
1:1A:2331:G:O2'	22:10:43:THR:HG22	2.13	0.48
5:1F:64:ILE:HD11	5:1F:75:HIS:HB2	1.96	0.48
13:1R:104:ARG:HD2	13:1R:107:ASP:OD1	2.14	0.48
18:1W:68:ARG:NH1	18:1W:112:GLY:H	2.12	0.48
33:1b:88:ALA:O	33:1b:226:ARG:NH1	2.47	0.48
57:1y:26:A:H61	57:1y:44:G:H1	1.58	0.48
1:2A:2029:G:H2'	1:2A:2031:A:OP1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2674:G:H5”	10:2O:26:LYS:HE3	1.95	0.48
13:2R:98:LEU:HB2	13:2R:113:LEU:HD11	1.95	0.48
15:2T:23:ARG:HD3	15:2T:120:ARG:NH1	2.29	0.48
32:2a:22:G:H4’	32:2a:885:G:C8	2.48	0.48
32:2a:197:A:N1	32:2a:220:G:O2’	2.44	0.48
32:2a:1152:A:H5’	41:2j:13:HIS:HD2	1.78	0.48
35:2d:57:ARG:HB3	35:2d:206:PHE:HB2	1.94	0.48
36:2e:57:LYS:HG2	36:2e:61:TYR:HE2	1.77	0.48
44:2m:4:ILE:HG23	44:2m:22:ILE:HD11	1.96	0.48
47:2p:15:PRO:HD2	47:2p:42:ARG:HD3	1.95	0.48
50:2s:27:GLU:H	50:2s:27:GLU:HG3	1.34	0.48
54:2w:18:G:H4’	54:2w:60:U:C5	2.48	0.48
6:1G:7:LEU:HB2	6:1G:104:GLU:HB2	1.96	0.48
8:1I:62:LYS:O	8:1I:66:GLU:HG2	2.13	0.48
21:1Z:93:ASP:HA	21:1Z:131:ARG:HH12	1.78	0.48
32:1a:202:U:H3’	32:1a:203:U:C5	2.48	0.48
32:1a:454:C:H3’	32:1a:455:C:C6	2.48	0.48
32:1a:1498:UR3:OP2	53:1v:16:A:O2’	2.27	0.48
37:1f:3:ARG:O	37:1f:93:SER:HB2	2.13	0.48
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.48	0.48
1:2A:2134:A:H1’	1:2A:2158:A:N1	2.29	0.48
3:2D:123:ALA:HB3	3:2D:131:LEU:HG	1.94	0.48
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.14	0.48
32:2a:148:G:H2’	32:2a:149:A:C8	2.49	0.48
32:2a:920:U:H2’	32:2a:921:U:C6	2.48	0.48
32:2a:1245:A:H2’	32:2a:1246:C:O4’	2.14	0.48
36:2e:146:ALA:O	36:2e:150:ARG:HG2	2.13	0.48
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.49	0.48
1:1A:1071:G:H1’	1:1A:1089:G:H2’	1.96	0.48
1:1A:2142:C:N3	1:1A:2149:G:C6	2.80	0.48
5:1F:143:ALA:HB1	5:1F:148:LEU:HB2	1.95	0.48
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.95	0.48
34:1c:21:ARG:HG3	34:1c:58:GLU:HG2	1.95	0.48
36:1e:91:LEU:HB3	36:1e:118:ILE:HD11	1.94	0.48
49:1r:56:THR:HG22	49:1r:58:LEU:HG	1.96	0.48
1:2A:632:A:H2’	1:2A:633:A:C8	2.48	0.48
1:2A:656:G:H2’	1:2A:657:U:O4’	2.13	0.48
1:2A:987:G:O2’	1:2A:1000:A:N3	2.40	0.48
6:2G:5:VAL:HG23	6:2G:8:LYS:H	1.78	0.48
32:2a:509:A:O2’	32:2a:510:A:OP1	2.25	0.48
32:2a:952:U:H2’	32:2a:953:G:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:8:LYS:HG3	33:2b:51:LEU:HD13	1.95	0.48
35:2d:92:VAL:O	35:2d:96:LEU:HD22	2.14	0.48
36:2e:57:LYS:HG2	36:2e:61:TYR:CE2	2.49	0.48
37:2f:91:VAL:HG11	49:2r:72:ARG:HH12	1.79	0.48
44:2m:90:LEU:HD23	44:2m:93:ARG:HE	1.77	0.48
50:2s:53:ASN:OD1	50:2s:54:GLY:N	2.46	0.48
1:1A:320:A:H4'	1:1A:322:A:N7	2.29	0.48
1:1A:1094:U:N3	1:1A:1097:U:OP2	2.47	0.48
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.48	0.48
1:1A:1508:A:O2'	1:1A:1509:C:H5"	2.14	0.48
1:1A:1680:U:O2'	1:1A:1763:G:N7	2.39	0.48
1:1A:1866:C:H2'	1:1A:1876:A:O4'	2.14	0.48
19:1X:61:GLY:HA3	19:1X:73:ARG:O	2.14	0.48
32:1a:507:C:OP2	32:1a:508:C:O2'	2.26	0.48
32:1a:1136:U:H5"	32:1a:1137:C:N3	2.28	0.48
33:1b:13:ALA:HB2	33:1b:44:LEU:HD13	1.95	0.48
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.82	0.48
35:1d:165:MET:SD	35:1d:168:ARG:HD2	2.54	0.48
39:1h:100:ILE:HB	39:1h:125:ARG:HH12	1.79	0.48
46:1o:7:GLU:O	46:1o:11:VAL:HG23	2.14	0.48
51:1t:92:LEU:O	51:1t:96:GLY:HA2	2.13	0.48
1:2A:99:U:H4'	1:2A:100:G:H5'	1.94	0.48
1:2A:332:A:O2'	1:2A:334:C:OP2	2.26	0.48
1:2A:600:G:H2'	1:2A:601:C:C6	2.49	0.48
1:2A:2632:A:O2'	1:2A:2811:G:O2'	2.23	0.48
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.95	0.48
22:20:38:VAL:HG11	22:20:45:PHE:HD2	1.79	0.48
32:2a:524:G:H2'	32:2a:525:C:C6	2.49	0.48
32:2a:1027:C:C4	32:2a:1034:G:O6	2.67	0.48
32:2a:1314:C:H2'	32:2a:1315:U:C6	2.49	0.48
34:2c:88:ARG:HA	34:2c:91:LEU:HD13	1.94	0.48
37:2f:24:GLU:O	37:2f:28:ARG:N	2.39	0.48
1:1A:1683:C:H2'	1:1A:1684:C:H6	1.77	0.48
1:1A:2131:G:H5'	1:1A:2133:G:C8	2.48	0.48
5:1F:106:ARG:H	5:1F:106:ARG:HG2	1.45	0.48
32:1a:148:G:H2'	32:1a:149:A:C8	2.49	0.48
34:1c:87:LEU:O	34:1c:91:LEU:N	2.39	0.48
34:1c:195:VAL:C	34:1c:196:LEU:HD23	2.39	0.48
35:1d:57:ARG:HD3	35:1d:205:GLU:HB3	1.96	0.48
40:1i:70:LYS:O	40:1i:74:ILE:HG13	2.14	0.48
54:1w:9:A:H8	54:1w:11:C:H41	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:1x:68:C:H2'	55:1x:69:C:H6	1.79	0.48
1:2A:848:G:H2'	1:2A:849:A:C8	2.48	0.48
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.48	0.48
1:2A:1359:A:H2'	1:2A:1360:A:H5'	1.96	0.48
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.48	0.48
32:2a:396:G:O2'	32:2a:398:C:OP1	2.29	0.48
32:2a:881:G:P	43:2l:12:ARG:HH22	2.37	0.48
32:2a:1002:G:N3	32:2a:1003:G:H1'	2.28	0.48
32:2a:1152:A:H5'	41:2j:13:HIS:CD2	2.49	0.48
38:2g:23:VAL:O	38:2g:27:ILE:HG13	2.14	0.48
1:1A:1278:A:OP1	13:1R:36:THR:HG23	2.14	0.47
1:1A:1570:A:H2'	1:1A:1571:A:C8	2.49	0.47
3:1D:2:ALA:N	3:1D:200:ASP:OD2	2.47	0.47
4:1E:55:ASN:HB3	4:1E:58:ARG:HB2	1.96	0.47
9:1N:73:THR:OG1	9:1N:82:LEU:HD11	2.14	0.47
32:1a:103:C:O2'	32:1a:172:A:N1	2.41	0.47
32:1a:502:G:OP1	43:1l:118:SER:HB3	2.14	0.47
32:1a:1004:A:H5'	32:1a:1024:G:H1	1.78	0.47
37:1f:36:ARG:HB2	37:1f:66:GLU:O	2.14	0.47
48:1q:87:LYS:HA	48:1q:87:LYS:HD3	1.63	0.47
51:1t:13:LEU:HD12	51:1t:14:LYS:N	2.29	0.47
1:2A:2495:G:OP1	12:2Q:82:ARG:NE	2.46	0.47
5:2F:20:LEU:HD23	5:2F:22:ALA:HB2	1.95	0.47
25:23:6:VAL:HG22	25:23:56:VAL:HG13	1.95	0.47
32:2a:224:C:H2'	32:2a:225:C:H6	1.79	0.47
32:2a:952:U:H2'	32:2a:953:G:H8	1.79	0.47
32:2a:1346:A:N6	38:2g:10:ARG:HH12	2.12	0.47
35:2d:57:ARG:NH1	35:2d:205:GLU:HB3	2.29	0.47
49:2r:56:THR:H	49:2r:56:THR:HG1	1.40	0.47
57:2y:34:G:H2'	57:2y:35:A:H8	1.79	0.47
1:1A:305:U:H2'	1:1A:306:U:C6	2.49	0.47
1:1A:518:G:H2'	1:1A:519:U:C6	2.49	0.47
1:1A:606:U:OP2	62:1A:4260:HOH:O	2.20	0.47
1:1A:1075:C:C2'	1:1A:1076:C:H5'	2.44	0.47
1:1A:1316:U:H2'	1:1A:1317:A:C8	2.49	0.47
1:1A:2771:C:H2'	1:1A:2772:C:C6	2.49	0.47
62:1A:5464:HOH:O	10:1O:20:MET:HE2	2.14	0.47
3:1D:206:LEU:HA	3:1D:211:ARG:HH11	1.79	0.47
8:1I:61:ARG:HD3	8:1I:61:ARG:HA	1.75	0.47
8:1I:64:GLU:O	8:1I:68:LEU:HD12	2.15	0.47
32:1a:731:G:H5'	32:1a:766:A:H4'	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.49	0.47
33:1b:95:GLN:OE1	33:1b:147:LYS:HG2	2.14	0.47
44:1m:86:CYS:HB2	50:1s:73:GLU:HB3	1.96	0.47
57:1y:51:U:H3	57:1y:63:G:H1	1.62	0.47
1:2A:35:G:H1'	1:2A:454:A:C4	2.49	0.47
1:2A:918:A:C2	2:2B:80:U:H4'	2.48	0.47
1:2A:1164:G:H2'	1:2A:1165:U:C6	2.49	0.47
1:2A:1768:U:OP2	62:2A:3945:HOH:O	2.19	0.47
2:2B:52:A:N6	14:2S:33:LYS:HG2	2.29	0.47
16:2U:50:ARG:HH12	17:2V:72:VAL:HA	1.79	0.47
21:2Z:144:LEU:HG	21:2Z:145:GLU:H	1.78	0.47
35:2d:4:TYR:O	35:2d:115:ARG:NH1	2.47	0.47
35:2d:155:LEU:HA	35:2d:155:LEU:HD23	1.73	0.47
47:2p:58:TYR:O	47:2p:61:SER:OG	2.23	0.47
1:1A:2393:A:H5"	11:1P:63:PRO:HB3	1.97	0.47
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.14	0.47
32:1a:376:G:O3'	47:1p:5:ARG:NH1	2.46	0.47
38:1g:46:ALA:HB2	38:1g:117:ALA:HB1	1.95	0.47
39:1h:116:LYS:HD2	39:1h:129:VAL:HG11	1.96	0.47
50:1s:31:ILE:HB	50:1s:49:ILE:HA	1.95	0.47
51:1t:57:ARG:HH22	51:1t:100:ILE:HD12	1.79	0.47
54:1w:19:G:H4'	54:1w:20:U:OP1	2.15	0.47
1:2A:580:C:H2'	1:2A:581:C:C6	2.49	0.47
1:2A:584:C:H2'	1:2A:585:G:O4'	2.14	0.47
1:2A:1805:U:O2	3:2D:50:THR:HB	2.14	0.47
1:2A:2123:G:H2'	1:2A:2124:G:C8	2.49	0.47
7:2H:104:GLU:HA	7:2H:113:VAL:O	2.14	0.47
11:2P:29:LYS:HG3	11:2P:30:THR:H	1.78	0.47
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.49	0.47
20:2Y:8:LYS:HD3	20:2Y:97:ARG:NH1	2.28	0.47
21:2Z:72:ARG:HH22	21:2Z:97:GLU:HB2	1.78	0.47
21:2Z:130:PRO:HA	21:2Z:133:ILE:HG13	1.96	0.47
32:2a:397:A:H3'	32:2a:397:A:N3	2.29	0.47
32:2a:406:G:H21	35:2d:119:GLN:NE2	2.11	0.47
32:2a:457:C:H2'	32:2a:458:C:C6	2.49	0.47
33:2b:48:MET:HA	33:2b:51:LEU:HB2	1.97	0.47
33:2b:212:GLN:O	33:2b:216:SER:OG	2.29	0.47
1:1A:668:G:H5'	1:1A:669:G:OP2	2.14	0.47
1:1A:1009:A:OP2	9:1N:37:LYS:NZ	2.47	0.47
1:1A:2561:A:H2'	1:1A:2562:U:O4'	2.14	0.47
1:1A:2584:U:O2	1:1A:2585:U:C4	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2629:A:H1'	1:1A:2630:G:O5'	2.14	0.47
2:1B:48:A:H2'	2:1B:49:C:C6	2.49	0.47
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.96	0.47
38:1g:46:ALA:HB1	38:1g:121:ALA:HB2	1.96	0.47
39:1h:44:PHE:HB3	39:1h:80:ILE:HD11	1.96	0.47
46:1o:39:LEU:HD13	46:1o:56:LEU:HB2	1.96	0.47
49:1r:65:ILE:O	49:1r:69:THR:HG23	2.15	0.47
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.50	0.47
1:2A:1253:A:OP1	62:2A:3949:HOH:O	2.20	0.47
1:2A:1423:G:H2'	1:2A:1424:G:H8	1.80	0.47
1:2A:1666:G:HO2'	10:2O:6:THR:HG1	1.61	0.47
1:2A:2474:C:H5"	1:2A:2475:C:OP2	2.15	0.47
6:2G:41:GLN:O	6:2G:43:LEU:N	2.47	0.47
6:2G:73:ALA:HB3	6:2G:85:GLY:H	1.79	0.47
11:2P:29:LYS:HG3	11:2P:30:THR:HG23	1.97	0.47
32:2a:1004:A:N3	32:2a:1038:C:C2	2.82	0.47
32:2a:1310:G:H5'	44:2m:77:ASN:ND2	2.21	0.47
33:2b:76:GLN:HB2	33:2b:208:ILE:HD11	1.95	0.47
34:2c:14:ILE:HG22	34:2c:15:THR:HG23	1.96	0.47
38:2g:27:ILE:HG13	38:2g:27:ILE:H	1.45	0.47
1:1A:1062:G:H2'	1:1A:1063:G:C8	2.50	0.47
1:1A:1184:G:H5'	25:13:29:ARG:NH2	2.30	0.47
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.14	0.47
1:1A:1762:A:H2'	62:1A:5893:HOH:O	2.14	0.47
32:1a:78:G:C2	32:1a:91:C:N3	2.81	0.47
32:1a:335:C:H2'	32:1a:336:C:H6	1.79	0.47
33:1b:19:HIS:HA	33:1b:39:ILE:HG23	1.97	0.47
33:1b:109:SER:O	33:1b:112:VAL:HG22	2.14	0.47
36:1e:8:GLU:OE2	36:1e:63:ARG:NH2	2.48	0.47
37:1f:5:GLU:OE1	49:1r:34:TYR:OH	2.24	0.47
37:1f:68:PRO:HG3	37:1f:71:ARG:NH1	2.30	0.47
44:1m:67:GLU:HG3	44:1m:71:ARG:NH2	2.30	0.47
1:2A:271(N):U:O2'	1:2A:271(O):C:H5'	2.14	0.47
6:2G:35:GLU:HB3	6:2G:160:VAL:HG12	1.95	0.47
26:24:30:GLU:C	26:24:31:ILE:HG13	2.40	0.47
32:2a:997:U:H2'	32:2a:998:G:O4'	2.15	0.47
33:2b:27:LYS:HD3	33:2b:193:ASP:OD1	2.14	0.47
33:2b:27:LYS:HE2	33:2b:195:ASP:OD2	2.14	0.47
34:2c:6:HIS:ND1	45:2n:49:HIS:HB3	2.29	0.47
35:2d:152:SER:O	35:2d:158:ILE:HD11	2.15	0.47
1:1A:1045:A:OP1	1:1A:1046:A:H3'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1667:G:O2'	1:1A:1991:U:O4	2.29	0.47
1:1A:2040:C:H2'	1:1A:2041:U:O4'	2.15	0.47
6:1G:83:ARG:O	6:1G:86:MET:HG3	2.15	0.47
11:1P:95:VAL:HA	11:1P:99:LEU:HD23	1.96	0.47
32:1a:78:G:N1	32:1a:91:C:C4	2.83	0.47
32:1a:339:C:H2'	32:1a:340:U:C6	2.50	0.47
35:1d:108:LEU:HD12	35:1d:174:LEU:HD13	1.96	0.47
42:1k:16:SER:O	42:1k:35:PRO:HD3	2.14	0.47
1:2A:779:U:O4	62:2A:3946:HOH:O	2.19	0.47
1:2A:829:A:N7	1:2A:2248:C:H5'	2.30	0.47
1:2A:1179:C:H2'	1:2A:1180:C:H6	1.79	0.47
1:2A:1240:U:HO2'	1:2A:1241:A:P	2.38	0.47
1:2A:1489:U:O2'	1:2A:1490:A:H8	1.97	0.47
1:2A:2299:G:H2'	1:2A:2300:G:C8	2.46	0.47
1:2A:2331:G:O2'	1:2A:2336:A:N1	2.46	0.47
6:2G:12:TYR:O	6:2G:16:ARG:HB2	2.14	0.47
14:2S:15:ARG:O	14:2S:19:LYS:HG2	2.15	0.47
32:2a:115:G:OP1	62:2a:1918:HOH:O	2.20	0.47
32:2a:324:G:N1	32:2a:327:A:OP2	2.44	0.47
32:2a:410:G:H21	32:2a:432:A:H62	1.62	0.47
32:2a:841:U:H6	32:2a:841:U:P	2.38	0.47
32:2a:979:C:N4	45:2n:18:VAL:HG22	2.30	0.47
32:2a:1023:G:H8	32:2a:1023:G:OP2	1.98	0.47
55:2x:61:C:H2'	55:2x:62:C:C6	2.50	0.47
1:1A:219:G:O6	62:1A:4259:HOH:O	2.20	0.47
1:1A:970:C:H2'	1:1A:971:C:C6	2.50	0.47
1:1A:1007:C:OP2	62:1A:4261:HOH:O	2.20	0.47
1:1A:1072:C:H5"	1:1A:1073:A:OP1	2.14	0.47
1:1A:2123:G:H2'	1:1A:2124:G:H8	1.80	0.47
15:1T:3:ARG:HA	15:1T:6:LEU:HD12	1.96	0.47
25:13:7:LYS:HB2	25:13:34:GLU:HG3	1.95	0.47
32:1a:690:G:H2'	32:1a:691:G:O4'	2.15	0.47
32:1a:755:G:OP2	46:1o:65:ARG:HD2	2.15	0.47
32:1a:1404:5MC:O2	32:1a:1519:MA6:O2'	2.25	0.47
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.28	0.47
35:1d:8:VAL:O	35:1d:11:LEU:HB2	2.14	0.47
1:2A:71:A:H5"	1:2A:73:A:C8	2.49	0.47
1:2A:839:U:H2'	1:2A:840:C:C6	2.49	0.47
1:2A:1034:G:H5'	31:29:18:ARG:HD2	1.97	0.47
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.15	0.47
1:2A:2823:A:OP1	4:2E:159:HIS:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2886:G:H2'	1:2A:2887:U:H6	1.80	0.47
5:2F:11:VAL:HG22	5:2F:125:LEU:HD12	1.97	0.47
6:2G:106:LEU:O	6:2G:110:ALA:HB3	2.15	0.47
6:2G:115:ARG:HB2	6:2G:115:ARG:NH1	2.30	0.47
11:2P:87:ASP:O	11:2P:90:ARG:NH1	2.47	0.47
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.14	0.47
32:2a:266:G:H2'	32:2a:266:G:N3	2.28	0.47
32:2a:532:A:N6	32:2a:1206:G:O2'	2.48	0.47
32:2a:1004:A:C6	32:2a:1037:C:H1'	2.50	0.47
32:2a:1201:A:H4'	32:2a:1202:G:O5'	2.15	0.47
32:2a:1239:A:O2'	38:2g:114:ARG:O	2.24	0.47
32:2a:1242:C:H2'	32:2a:1243:C:H6	1.80	0.47
32:2a:1260:C:P	32:2a:1284:C:H4'	2.55	0.47
32:2a:1427:U:H2'	32:2a:1428:A:H8	1.79	0.47
39:2h:33:GLU:OE2	39:2h:50:ARG:HD2	2.15	0.47
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.50	0.47
1:1A:2165:G:H2'	1:1A:2166:G:C5	2.50	0.47
1:1A:2608:G:N7	62:1A:4333:HOH:O	2.35	0.47
2:1B:14:U:O2	2:1B:108:U:H4'	2.15	0.47
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.50	0.47
13:1R:56:LYS:NZ	13:1R:90:ARG:O	2.47	0.47
26:14:12:ALA:HA	26:14:29:PRO:O	2.15	0.47
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.42	0.47
32:1a:1438:G:H2'	32:1a:1439:C:C6	2.49	0.47
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.50	0.47
42:1k:73:MET:C	42:1k:75:TYR:H	2.21	0.47
1:2A:982:C:N4	62:2A:4112:HOH:O	2.48	0.47
1:2A:1169:G:N2	1:2A:1181:C:N3	2.62	0.47
2:2B:24:G:H4'	2:2B:25:A:C8	2.50	0.47
7:2H:23:ARG:O	7:2H:24:VAL:HG13	2.15	0.47
12:2Q:16:ARG:HG3	12:2Q:18:LYS:HG3	1.97	0.47
19:2X:20:GLY:O	19:2X:25:LYS:N	2.42	0.47
24:22:32:LEU:HA	24:22:53:LEU:HD13	1.97	0.47
32:2a:1309:G:O3'	44:2m:77:ASN:ND2	2.48	0.47
38:2g:79:ARG:HH21	38:2g:79:ARG:HB2	1.79	0.47
41:2j:77:PRO:O	41:2j:81:THR:OG1	2.31	0.47
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.50	0.47
3:1D:35:LYS:HD3	3:1D:62:TYR:HD2	1.80	0.47
3:1D:85:ASP:OD2	3:1D:88:ARG:NH1	2.43	0.47
19:1X:12:VAL:HG22	19:1X:29:TRP:CE2	2.50	0.47
21:1Z:132:ASN:HD22	21:1Z:160:GLY:HA3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:161:A:H2'	32:1a:162:A:C8	2.50	0.47
32:1a:1525:G:P	42:1k:120:ARG:HH22	2.38	0.47
33:1b:80:ILE:O	33:1b:84:GLU:HG2	2.14	0.47
33:1b:131:PRO:O	33:1b:135:GLN:N	2.48	0.47
1:2A:289:A:H61	1:2A:351:G:H1'	1.80	0.47
1:2A:2319:G:N2	14:2S:3:ARG:HH11	2.09	0.47
21:2Z:102:LEU:HB3	21:2Z:139:VAL:HG21	1.96	0.47
21:2Z:171:ILE:H	21:2Z:171:ILE:HG13	1.51	0.47
25:23:10:LYS:HB3	25:23:53:LEU:HA	1.96	0.47
32:2a:34:C:H2'	32:2a:35:G:C8	2.50	0.47
32:2a:41:G:H2'	32:2a:42:G:C8	2.50	0.47
32:2a:1266:G:N2	32:2a:1268:A:H3'	2.30	0.47
35:2d:65:ARG:NH1	35:2d:70:ILE:O	2.48	0.47
40:2i:78:LYS:HE2	40:2i:101:PHE:CE1	2.48	0.47
47:2p:8:ARG:HB3	47:2p:28:ARG:NH1	2.30	0.47
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.49	0.47
13:1R:59:ASP:OD1	13:1R:59:ASP:N	2.43	0.47
32:1a:110:C:O2'	47:1p:25:ARG:O	2.33	0.47
32:1a:404:U:P	35:1d:118:ARG:HH12	2.36	0.47
32:1a:461:A:O2'	32:1a:471:G:N7	2.35	0.47
54:1w:18:G:O2'	54:1w:57:G:N2	2.38	0.47
6:2G:25:TYR:HD1	6:2G:30:GLU:HB3	1.78	0.47
32:2a:1125:U:OP1	41:2j:35:SER:OG	2.31	0.47
33:2b:58:ILE:HA	33:2b:61:LEU:HB3	1.97	0.47
38:2g:54:THR:O	38:2g:56:GLN:N	2.48	0.47
38:2g:130:GLY:O	38:2g:135:VAL:HG11	2.14	0.47
51:2t:67:ALA:HA	51:2t:72:LEU:O	2.14	0.47
1:1A:247:G:H4'	1:1A:386:G:C5	2.49	0.46
1:1A:2811:G:H22	1:1A:2891:G:H1'	1.80	0.46
3:1D:20:ASP:OD1	3:1D:20:ASP:N	2.48	0.46
15:1T:127:ALA:C	15:1T:129:ARG:N	2.73	0.46
18:1W:88:ARG:HB2	18:1W:92:ARG:HG2	1.96	0.46
32:1a:601:C:H2'	32:1a:602:A:H8	1.80	0.46
32:1a:865:A:C2	32:1a:918:A:H4'	2.50	0.46
32:1a:1160:G:H22	32:1a:1176:A:H2	1.61	0.46
33:1b:178:ARG:NH2	39:1h:71:GLY:O	2.25	0.46
41:1j:7:LYS:HG3	41:1j:71:LEU:HD13	1.97	0.46
1:2A:236:C:H2'	1:2A:237:C:H6	1.80	0.46
1:2A:1467:C:C5	1:2A:1546:C:H2'	2.50	0.46
1:2A:2314:C:H2'	1:2A:2315:G:H8	1.80	0.46
2:2B:14:U:H1'	2:2B:108:U:O2'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:146:GLU:HG2	3:2D:152:GLY:C	2.40	0.46
5:2F:32:LEU:HD22	5:2F:112:MET:HE2	1.98	0.46
7:2H:17:VAL:HG11	7:2H:50:VAL:HG21	1.97	0.46
32:2a:376:G:H5"	47:2p:5:ARG:HB2	1.96	0.46
32:2a:1203:C:H2'	32:2a:1204:A:C8	2.49	0.46
50:2s:52:TYR:HB2	50:2s:57:HIS:CE1	2.50	0.46
1:1A:106:C:H1'	20:1Y:1:MET:HE2	1.97	0.46
1:1A:118:A:C8	1:1A:119:A:C8	3.03	0.46
32:1a:116:A:H8	32:1a:116:A:O5'	1.98	0.46
32:1a:1129:C:O2'	32:1a:1139:G:N7	2.38	0.46
32:1a:1131:G:OP1	40:1i:20:ARG:NH2	2.46	0.46
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.98	0.46
41:1j:57:LYS:HE2	41:1j:60:ARG:NH2	2.30	0.46
1:2A:276:A:H5"	1:2A:277:C:H5'	1.96	0.46
1:2A:531:C:H4'	1:2A:532:A:H5"	1.95	0.46
1:2A:2165:G:H2'	1:2A:2166:G:H5"	1.96	0.46
1:2A:2355:C:H4'	22:20:24:LYS:HG3	1.97	0.46
12:2Q:16:ARG:HG2	12:2Q:18:LYS:HE2	1.98	0.46
15:2T:113:LYS:HA	15:2T:113:LYS:HD3	1.61	0.46
23:21:50:ARG:HG2	23:21:59:THR:HG23	1.97	0.46
32:2a:1314:C:OP1	50:2s:6:LYS:NZ	2.33	0.46
32:2a:1507:A:OP2	53:2v:13:A:N6	2.48	0.46
33:2b:80:ILE:HD13	33:2b:211:ILE:HG22	1.96	0.46
50:2s:38:SER:HB2	50:2s:71:LEU:HD12	1.97	0.46
1:1A:1263:U:H2'	1:1A:1264:G:C8	2.51	0.46
1:1A:2753:A:N3	31:19:15:LYS:NZ	2.63	0.46
5:1F:122:LYS:HB3	5:1F:191:ARG:HG2	1.97	0.46
7:1H:3:ARG:HH22	7:1H:66:GLY:N	2.13	0.46
25:13:44:ARG:O	25:13:48:GLU:HG3	2.15	0.46
44:1m:20:THR:C	44:1m:22:ILE:H	2.23	0.46
1:2A:840:C:H2'	1:2A:841:A:H8	1.80	0.46
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.46	0.46
2:2B:22:U:H2'	2:2B:23:G:C8	2.51	0.46
5:2F:178:PRO:HG2	5:2F:179:GLU:OE2	2.15	0.46
14:2S:26:LEU:HD12	14:2S:39:ILE:HG12	1.97	0.46
20:2Y:9:LYS:HE2	20:2Y:28:LYS:O	2.15	0.46
32:2a:347:G:H8	32:2a:347:G:OP2	1.98	0.46
32:2a:376:G:H1	32:2a:387:U:H3	1.63	0.46
39:2h:96:GLY:N	39:2h:99:GLU:OE1	2.47	0.46
47:2p:17:TYR:HE2	47:2p:41:PRO:HG3	1.79	0.46
54:2w:31:A:H2'	54:2w:32:PSU:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1062:G:H22	1:1A:1077:A:N6	2.12	0.46
32:1a:1456:G:C4	51:1t:55:ILE:HD11	2.51	0.46
40:1i:79:LEU:HD22	40:1i:104:ARG:HB2	1.98	0.46
1:2A:597:U:H2'	1:2A:598:G:C8	2.51	0.46
1:2A:2206:G:H3'	1:2A:2207:G:N7	2.29	0.46
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.50	0.46
1:2A:2853:C:H2'	1:2A:2854:G:H8	1.80	0.46
5:2F:10:PRO:HB3	5:2F:17:ARG:NH1	2.31	0.46
21:2Z:152:ALA:O	21:2Z:155:LEU:HG	2.16	0.46
22:20:56:ASP:OD1	22:20:58:THR:OG1	2.30	0.46
28:26:32:ASN:OD1	28:26:32:ASN:N	2.38	0.46
32:2a:826:C:H4'	39:2h:12:ARG:HG2	1.97	0.46
38:2g:65:ALA:O	38:2g:69:VAL:HG23	2.16	0.46
1:1A:588:U:H2'	1:1A:589:C:C6	2.50	0.46
1:1A:793:A:OP2	1:1A:2071:A:O2'	2.31	0.46
1:1A:1805:U:O2	3:1D:50:THR:HB	2.16	0.46
6:1G:33:ARG:N	6:1G:162:THR:OG1	2.46	0.46
7:1H:96:ALA:HB2	7:1H:105:LEU:HD23	1.96	0.46
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.98	0.46
32:1a:664:G:N2	32:1a:741:G:H1	2.07	0.46
32:1a:1192:C:OP2	34:1c:4:LYS:NZ	2.47	0.46
34:1c:66:VAL:HG21	34:1c:91:LEU:HD21	1.97	0.46
50:1s:16:LEU:O	50:1s:19:VAL:HG12	2.15	0.46
1:2A:2125:G:H1'	1:2A:2173:A:H61	1.80	0.46
1:2A:2516:G:O6	1:2A:2517:C:N4	2.48	0.46
1:2A:2645:G:N2	1:2A:2767:C:OP2	2.49	0.46
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.80	0.46
9:2N:62:VAL:HG11	9:2N:66:LYS:HB2	1.97	0.46
11:2P:121:LYS:HE2	11:2P:123:LEU:HD11	1.98	0.46
25:23:35:ARG:HG2	25:23:37:LEU:HD21	1.98	0.46
32:2a:56:U:H2'	32:2a:57:G:H8	1.78	0.46
33:2b:92:TYR:N	33:2b:151:GLY:O	2.32	0.46
35:2d:135:LEU:C	35:2d:137:SER:H	2.22	0.46
40:2i:17:VAL:HG11	40:2i:81:ILE:HG12	1.97	0.46
42:2k:79:SER:HB3	42:2k:104:GLN:NE2	2.29	0.46
48:2q:67:LYS:O	48:2q:68:ARG:HB2	2.15	0.46
1:1A:84:A:H5'	20:1Y:8:LYS:HG2	1.96	0.46
1:1A:185:U:H4'	1:1A:218:A:H4'	1.97	0.46
5:1F:170:LEU:HD13	5:1F:172:TRP:CZ2	2.51	0.46
8:1I:48:GLU:HB3	8:1I:52:ARG:HH12	1.80	0.46
9:1N:67:LEU:HB3	9:1N:88:GLU:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:61:ARG:HD3	50:1s:67:VAL:HG12	1.97	0.46
32:1a:598:U:H2'	32:1a:599:C:C6	2.50	0.46
32:1a:702:A:OP2	62:1a:1915:HOH:O	2.21	0.46
32:1a:953:G:H5'	32:1a:965:A:H61	1.80	0.46
32:1a:1057:G:H2'	32:1a:1058:G:O4'	2.16	0.46
34:1c:181:ASN:ND2	34:1c:204:LEU:HD12	2.30	0.46
35:1d:194:LEU:HA	35:1d:194:LEU:HD13	1.68	0.46
48:1q:22:LEU:HD11	48:1q:39:SER:HB2	1.97	0.46
55:1x:59:A:H2'	55:1x:60:U:H5'	1.97	0.46
1:2A:11:G:O5'	1:2A:11:G:H8	1.98	0.46
1:2A:1564:C:H2'	1:2A:1565:C:C6	2.51	0.46
5:2F:164:ARG:O	5:2F:168:ARG:HB2	2.16	0.46
6:2G:104:GLU:OE2	26:24:24:THR:HB	2.16	0.46
8:2I:69:LYS:NZ	8:2I:138:ILE:HG12	2.30	0.46
9:2N:110:GLY:O	9:2N:114:ARG:HG3	2.16	0.46
10:2O:13:ASN:ND2	10:2O:97:ARG:HB2	2.31	0.46
11:2P:28:GLY:O	11:2P:30:THR:N	2.48	0.46
19:2X:60:ARG:HH12	29:27:47:ARG:NH2	2.14	0.46
26:24:46:GLN:O	26:24:48:ARG:N	2.49	0.46
32:2a:108:G:C6	51:2t:15:ARG:HG2	2.50	0.46
32:2a:1039:C:C2	32:2a:1040:U:H1'	2.50	0.46
38:2g:59:LEU:O	38:2g:63:LYS:HB2	2.15	0.46
38:2g:146:GLU:OE2	38:2g:149:ARG:NE	2.48	0.46
57:2y:8:4SU:C2	57:2y:14:A:H62	2.28	0.46
1:1A:8:A:H2'	1:1A:9:U:C6	2.51	0.46
1:1A:34:C:H5"	1:1A:35:G:OP2	2.16	0.46
1:1A:762:U:H5"	62:1A:5634:HOH:O	2.14	0.46
1:1A:2153:G:H2'	1:1A:2154:G:H8	1.81	0.46
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.97	0.46
32:1a:601:C:H2'	32:1a:602:A:C8	2.51	0.46
34:1c:124:ILE:HG22	34:1c:130:VAL:HG22	1.97	0.46
42:1k:58:PRO:O	42:1k:93:GLN:HG2	2.15	0.46
44:1m:3:ARG:HG3	44:1m:4:ILE:H	1.81	0.46
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.50	0.46
1:2A:1740:G:H2'	1:2A:1740:G:N3	2.31	0.46
1:2A:1830:C:H2'	1:2A:1831:G:H8	1.80	0.46
1:2A:2336:A:H61	22:20:43:THR:HG21	1.80	0.46
1:2A:2701:C:H2'	1:2A:2702:U:H2'	1.98	0.46
6:2G:165:THR:OG1	6:2G:166:ASP:N	2.47	0.46
8:2I:77:LEU:HD12	8:2I:78:THR:H	1.80	0.46
21:2Z:159:PRO:HA	21:2Z:160:GLY:HA2	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:357:G:OP1	32:2a:367:U:H5"	2.16	0.46
34:2c:112:SER:HB3	34:2c:115:LEU:HB2	1.95	0.46
36:2e:53:LEU:O	36:2e:57:LYS:N	2.34	0.46
47:2p:26:ARG:HG3	47:2p:27:LYS:O	2.16	0.46
51:2t:10:LEU:HG	51:2t:12:ALA:H	1.80	0.46
1:1A:910:A:N1	1:1A:2277:G:H1'	2.30	0.46
1:1A:1266:G:O2'	1:1A:2012:G:O6	2.30	0.46
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.59	0.46
32:1a:201:C:N4	32:1a:203:U:H3	2.13	0.46
33:1b:124:SER:HA	33:1b:125:PRO:HA	1.56	0.46
34:1c:6:HIS:HD2	34:1c:8:ILE:N	2.12	0.46
34:1c:134:ILE:O	34:1c:138:VAL:HG23	2.15	0.46
35:1d:36:ARG:HB3	35:1d:38:TYR:CZ	2.51	0.46
40:1i:8:GLY:HA3	40:1i:76:ALA:O	2.16	0.46
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	1.97	0.46
47:1p:14:ASN:HA	47:1p:42:ARG:NH2	2.31	0.46
57:1y:56:C:H2'	57:1y:57:G:O4'	2.15	0.46
1:2A:252:G:OP1	11:2P:50:ARG:NH1	2.41	0.46
1:2A:275:G:H2'	1:2A:276:A:O4'	2.16	0.46
1:2A:287:C:H2'	1:2A:288:C:H6	1.80	0.46
1:2A:676:A:H2	1:2A:2069:G:N3	2.13	0.46
1:2A:2136:C:O2'	1:2A:2137:C:O4'	2.34	0.46
1:2A:2193:G:H2'	1:2A:2194:G:H8	1.81	0.46
19:2X:12:VAL:HG12	19:2X:17:ALA:HB2	1.98	0.46
20:2Y:11:ASP:N	20:2Y:11:ASP:OD1	2.49	0.46
32:2a:141:A:H1'	32:2a:182:U:O2	2.15	0.46
34:2c:47:LEU:HD22	34:2c:68:VAL:HG11	1.96	0.46
37:2f:28:ARG:O	37:2f:32:ASN:ND2	2.48	0.46
41:2j:9:ARG:O	41:2j:16:LEU:HD21	2.16	0.46
48:2q:81:ARG:NH2	48:2q:84:LEU:HD21	2.31	0.46
1:1A:2165:G:H2'	1:1A:2166:G:C4	2.51	0.46
1:1A:2630:G:H2'	1:1A:2631:G:H8	1.80	0.46
14:1S:41:ASP:O	14:1S:45:GLY:N	2.47	0.46
20:1Y:7:VAL:HG23	20:1Y:74:PRO:HD3	1.98	0.46
22:10:47:PRO:HB3	22:10:59:LEU:HD22	1.98	0.46
35:1d:158:ILE:H	35:1d:158:ILE:HG13	1.33	0.46
38:1g:43:PHE:O	38:1g:47:CYS:HB2	2.16	0.46
47:1p:17:TYR:HB2	47:1p:39:TYR:HB3	1.98	0.46
1:2A:103:A:H5'	24:22:3:LEU:HD21	1.97	0.46
1:2A:2131:G:H22	1:2A:2158:A:N6	2.14	0.46
1:2A:2360:A:OP2	62:2A:3951:HOH:O	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2749:A:O3'	7:2H:62:LYS:NZ	2.42	0.46
5:2F:36:VAL:HB	5:2F:183:VAL:HG21	1.98	0.46
5:2F:93:LYS:HD3	5:2F:93:LYS:HA	1.74	0.46
32:2a:137:C:H2'	32:2a:138:G:H8	1.81	0.46
32:2a:519:C:H2'	32:2a:520:A:O4'	2.15	0.46
32:2a:762:C:H2'	32:2a:763:G:H8	1.81	0.46
32:2a:1103:C:P	33:2b:96:ARG:HH22	2.39	0.46
32:2a:1236:A:O2'	32:2a:1304:G:H4'	2.15	0.46
32:2a:1530:G:OP1	32:2a:1530:G:H4'	2.16	0.46
33:2b:74:LYS:NZ	33:2b:206:ASP:OD1	2.43	0.46
34:2c:40:ARG:HA	34:2c:43:LEU:HB2	1.97	0.46
35:2d:112:VAL:HG22	35:2d:116:GLN:NE2	2.30	0.46
35:2d:175:SER:HB3	35:2d:186:LEU:HD21	1.97	0.46
36:2e:7:GLU:CD	36:2e:37:ARG:HH21	2.23	0.46
41:2j:5:ARG:O	41:2j:98:ILE:HA	2.16	0.46
48:2q:78:GLU:OE1	48:2q:81:ARG:NH1	2.46	0.46
1:1A:191:A:H2'	1:1A:192:C:C6	2.51	0.46
1:1A:630:G:OP1	30:18:47:LYS:NZ	2.46	0.46
1:1A:1045:A:OP1	1:1A:1045:A:H4'	2.17	0.46
1:1A:1065:U:O2'	1:1A:1073:A:N6	2.46	0.46
1:1A:1300:U:H4'	1:1A:1301:A:H5"	1.97	0.46
1:1A:1453:U:OP1	13:1R:77:ARG:HD3	2.16	0.46
1:1A:1630:G:H2'	1:1A:1631:C:C6	2.51	0.46
1:1A:1853:A:H2'	1:1A:1854:A:C8	2.51	0.46
9:1N:111:PRO:O	9:1N:115:ARG:HG3	2.16	0.46
10:1O:68:GLU:HB3	10:1O:78:ARG:HH11	1.79	0.46
51:1t:63:ILE:HD12	51:1t:81:LYS:HG2	1.97	0.46
57:1y:19:G:C6	57:1y:56:C:N4	2.84	0.46
1:2A:699:A:H2'	1:2A:700:G:O4'	2.16	0.46
1:2A:1952:A:OP1	10:2O:44:LYS:NZ	2.40	0.46
1:2A:2447:G:N2	1:2A:2450:A:OP2	2.48	0.46
6:2G:68:PRO:HB3	6:2G:92:VAL:HB	1.96	0.46
32:2a:920:U:H2'	32:2a:921:U:H6	1.81	0.46
33:2b:27:LYS:O	33:2b:194:PRO:HG2	2.16	0.46
1:1A:270:A:OP2	1:1A:271(X):G:N1	2.38	0.45
1:1A:2121:G:N2	1:1A:2177:C:N3	2.53	0.45
13:1R:79:LEU:HA	13:1R:83:ILE:HG13	1.97	0.45
15:1T:127:ALA:O	15:1T:129:ARG:N	2.45	0.45
32:1a:174:C:OP2	32:1a:174:C:H6	1.98	0.45
32:1a:341:C:H2'	32:1a:342:C:C6	2.51	0.45
32:1a:1239:A:H62	32:1a:1299:A:H62	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1347:G:N2	32:1a:1373:G:H2'	2.31	0.45
34:1c:22:TRP:CZ2	45:1n:54:PRO:HG2	2.51	0.45
51:1t:47:GLY:N	51:1t:48:LYS:HB2	2.31	0.45
1:2A:2115:G:O2'	1:2A:2117:A:N7	2.40	0.45
8:2I:43:ASN:ND2	23:21:75:GLU:OE2	2.49	0.45
15:2T:18:ASP:OD1	15:2T:18:ASP:N	2.40	0.45
15:2T:74:ARG:HG2	15:2T:76:PHE:CZ	2.51	0.45
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.16	0.45
24:22:1:MET:HB3	24:22:5:GLU:OE1	2.16	0.45
32:2a:547:A:OP2	35:2d:2:GLY:N	2.49	0.45
32:2a:857:C:H2'	32:2a:858:G:O4'	2.16	0.45
35:2d:11:LEU:HD23	35:2d:66:ARG:HD3	1.98	0.45
46:2o:24:SER:HB3	46:2o:27:VAL:HG13	1.98	0.45
51:2t:24:LEU:HD23	51:2t:24:LEU:HA	1.81	0.45
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.50	0.45
32:1a:1316:G:N1	32:1a:1319:A:OP2	2.43	0.45
32:1a:1402:4OC:O5'	32:1a:1402:4OC:H6	2.14	0.45
35:1d:154:ASN:HA	35:1d:159:ARG:HE	1.81	0.45
37:1f:17:SER:O	37:1f:21:LEU:HG	2.17	0.45
39:1h:64:LYS:HD2	39:1h:79:VAL:HG11	1.98	0.45
1:2A:31:C:H5"	1:2A:1239:G:OP1	2.16	0.45
1:2A:1016:G:O6	62:2A:3947:HOH:O	2.19	0.45
11:2P:135:LEU:HD23	11:2P:135:LEU:HA	1.84	0.45
19:2X:1:MET:HE1	24:22:22:GLU:HB3	1.98	0.45
32:2a:404:U:OP2	35:2d:118:ARG:NH2	2.49	0.45
32:2a:1132:C:H2'	32:2a:1133:G:C8	2.50	0.45
33:2b:213:LEU:HB3	33:2b:214:ILE:HD12	1.98	0.45
49:2r:25:THR:OG1	49:2r:42:ARG:NH2	2.49	0.45
57:2y:18:G:N1	57:2y:55:PSU:C4	2.85	0.45
1:1A:489:G:N7	18:1W:49:LYS:NZ	2.64	0.45
1:1A:839:U:H2'	1:1A:840:C:C6	2.51	0.45
1:1A:2305:A:H5"	6:1G:134:GLY:HA3	1.97	0.45
10:1O:86:ILE:HG22	10:1O:94:ARG:HD3	1.98	0.45
32:1a:404:U:H2'	32:1a:405:U:C6	2.51	0.45
32:1a:1028:C:H2'	32:1a:1029:C:O4'	2.17	0.45
35:1d:33:MET:HB2	61:1d:302:SF4:S2	2.56	0.45
36:1e:145:LYS:HA	36:1e:148:VAL:HG22	1.97	0.45
57:1y:71:G:O2'	57:1y:72:C:H5'	2.15	0.45
1:2A:251:A:C5	1:2A:252:G:H1'	2.52	0.45
1:2A:903:C:H2'	1:2A:904:C:C6	2.51	0.45
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2086:U:H2'	1:2A:2087:G:H8	1.80	0.45
1:2A:2156:G:H2'	1:2A:2157:G:C6	2.51	0.45
1:2A:2815:C:H2'	1:2A:2816:C:H6	1.81	0.45
6:2G:114:ILE:HD12	6:2G:117:PHE:CE1	2.51	0.45
12:2Q:57:HIS:CD2	12:2Q:117:ALA:HB2	2.51	0.45
32:2a:472:A:OP1	47:2p:75:ARG:NH2	2.36	0.45
32:2a:738:C:H2'	32:2a:739:C:H6	1.81	0.45
32:2a:1133:G:H2'	32:2a:1134:G:O4'	2.16	0.45
32:2a:1216:G:OP1	45:2n:2:ALA:HA	2.15	0.45
32:2a:1368:G:OP2	40:2i:112:LYS:NZ	2.48	0.45
32:2a:1457:G:OP1	51:2t:39:LYS:NZ	2.38	0.45
36:2e:24:ARG:NH1	53:2v:24:A:OP2	2.50	0.45
37:2f:10:LEU:HD21	37:2f:26:ILE:HD11	1.99	0.45
49:2r:53:ARG:HH21	49:2r:59:SER:HA	1.81	0.45
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.80	0.45
1:1A:1341:U:OP2	1:1A:1394:U:O2'	2.25	0.45
1:1A:2820:A:C8	4:1E:109:LYS:HE2	2.52	0.45
32:1a:265:G:H2'	32:1a:267:C:C5	2.52	0.45
32:1a:1040:U:H2'	32:1a:1041:A:C8	2.50	0.45
32:1a:1251:A:H2'	32:1a:1252:A:O4'	2.16	0.45
33:1b:55:PHE:CD1	33:1b:221:LEU:HD22	2.51	0.45
33:1b:201:ILE:HG21	33:1b:214:ILE:HG21	1.97	0.45
35:1d:138:TYR:C	35:1d:138:TYR:CD2	2.95	0.45
37:1f:69:GLU:H	37:1f:69:GLU:CD	2.24	0.45
38:1g:64:GLN:HE21	38:1g:68:ASN:ND2	2.10	0.45
38:1g:79:ARG:O	38:1g:82:GLY:N	2.48	0.45
48:1q:11:VAL:HA	48:1q:85:VAL:HG13	1.98	0.45
6:2G:114:ILE:HG12	6:2G:140:ILE:HG12	1.97	0.45
9:2N:15:LEU:HB2	9:2N:135:PRO:HB2	1.99	0.45
10:2O:119:PRO:HB2	15:2T:68:TYR:CZ	2.52	0.45
19:2X:32:PRO:O	19:2X:77:LYS:HE3	2.15	0.45
32:2a:412:A:O4'	35:2d:35:ARG:NH2	2.50	0.45
32:2a:423:G:H3'	32:2a:423:G:N3	2.31	0.45
32:2a:596:C:OP2	62:2a:1917:HOH:O	2.20	0.45
32:2a:1259:C:C4	32:2a:1260:C:H1'	2.52	0.45
33:2b:54:THR:HG23	33:2b:199:TYR:HB3	1.97	0.45
38:2g:18:TYR:CG	38:2g:59:LEU:HD13	2.51	0.45
57:2y:33:U:H1'	57:2y:36:A:N6	2.31	0.45
1:1A:288:C:H2'	1:1A:289:A:H8	1.81	0.45
1:1A:1712:C:H2'	1:1A:1713:U:O4'	2.16	0.45
1:1A:2067:G:N7	62:1A:4342:HOH:O	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.32	0.45
5:1F:101:LEU:O	5:1F:106:ARG:NH1	2.46	0.45
21:1Z:1:MET:HA	21:1Z:2:GLU:HA	1.62	0.45
32:1a:922:G:C6	32:1a:923:A:C6	3.05	0.45
50:1s:12:ASP:OD2	50:1s:37:ARG:NE	2.49	0.45
54:1w:66:U:O4	54:1w:67:C:N4	2.50	0.45
57:1y:36:A:H2'	57:1y:37:MIA:O4'	2.17	0.45
1:2A:388:G:O2'	1:2A:389:G:N7	2.49	0.45
1:2A:856:C:HO2'	1:2A:857:C:P	2.39	0.45
1:2A:2319:G:N2	14:2S:3:ARG:HD2	2.31	0.45
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.99	0.45
17:2V:62:LEU:HD21	17:2V:95:LEU:HB2	1.98	0.45
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.51	0.45
32:2a:757:U:O2'	32:2a:879:C:O2	2.33	0.45
33:2b:43:ASP:OD2	33:2b:46:LYS:N	2.32	0.45
41:2j:8:LEU:HD11	41:2j:20:ALA:HB2	1.97	0.45
41:2j:21:GLN:NE2	41:2j:25:GLU:HG2	2.30	0.45
57:2y:24:G:C6	57:2y:25:C:C4	3.04	0.45
1:1A:1057:A:N6	1:1A:1081:U:H3	2.14	0.45
1:1A:1816:G:O6	3:1D:35:LYS:NZ	2.31	0.45
1:1A:2817:G:OP1	13:1R:99:LYS:NZ	2.50	0.45
9:1N:15:LEU:HB2	9:1N:135:PRO:HB2	1.98	0.45
25:13:3:ARG:NE	25:13:60:GLU:OE1	2.40	0.45
26:14:69:LYS:HD2	26:14:69:LYS:HA	1.56	0.45
32:1a:708:C:H2'	32:1a:709:G:H8	1.81	0.45
32:1a:1278:U:H5'	32:1a:1279:A:O4'	2.16	0.45
34:1c:6:HIS:CD2	34:1c:8:ILE:H	2.28	0.45
34:1c:36:ASP:OD1	34:1c:59:ARG:NH2	2.46	0.45
6:2G:129:GLY:O	6:2G:161:THR:HB	2.17	0.45
13:2R:44:LEU:HA	13:2R:44:LEU:HD23	1.84	0.45
32:2a:36:C:H2'	32:2a:37:U:O4'	2.17	0.45
32:2a:447:G:O6	32:2a:485:G:O2'	2.25	0.45
32:2a:1263:C:H1'	32:2a:1273:G:N2	2.31	0.45
32:2a:1271:G:C2	32:2a:1272:G:C8	3.05	0.45
32:2a:1401:G:C2	32:2a:1402:4OC:H1'	2.51	0.45
38:2g:22:LEU:HG	38:2g:62:PHE:HE2	1.80	0.45
42:2k:50:TYR:CD1	42:2k:54:ARG:HB3	2.51	0.45
46:2o:7:GLU:H	46:2o:7:GLU:HG3	1.54	0.45
1:1A:1359:A:H2	1:1A:1372:U:O4	1.99	0.45
3:1D:19:ALA:HB3	3:1D:21:PHE:CE1	2.52	0.45
11:1P:121:LYS:O	11:1P:123:LEU:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1004:A:H5"	32:1a:1025:U:H5	1.82	0.45
39:1h:40:ALA:HA	39:1h:45:ILE:HG13	1.98	0.45
46:1o:8:LYS:HE3	46:1o:31:LEU:HD22	1.99	0.45
1:2A:27:G:HO2'	1:2A:28:A:P	2.37	0.45
1:2A:100:G:O2'	24:22:7:ARG:NH2	2.49	0.45
1:2A:287:C:H42	1:2A:354:G:H1	1.64	0.45
1:2A:597:U:H2'	1:2A:598:G:H8	1.82	0.45
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	1.99	0.45
5:2F:64:ILE:HG23	5:2F:76:GLY:O	2.17	0.45
24:22:44:LEU:HD12	24:22:44:LEU:HA	1.77	0.45
32:2a:1292:U:H2'	32:2a:1293:G:H8	1.81	0.45
34:2c:12:LEU:HA	34:2c:16:ARG:HB3	1.99	0.45
34:2c:53:ALA:HB2	34:2c:115:LEU:CD1	2.46	0.45
41:2j:65:LEU:HD13	45:2n:56:VAL:HG22	1.98	0.45
1:1A:2356:C:H2'	1:1A:2357:U:O4'	2.16	0.45
1:1A:2574:G:OP1	62:1A:4263:HOH:O	2.21	0.45
3:1D:37:LEU:HD13	3:1D:87:ASN:ND2	2.32	0.45
32:1a:343:U:O2'	32:1a:344:A:H2'	2.17	0.45
32:1a:567:G:H2'	32:1a:568:G:O4'	2.17	0.45
32:1a:1025:U:O2	32:1a:1036:G:C6	2.70	0.45
1:2A:274:G:C2	1:2A:363:G:C6	3.05	0.45
1:2A:386:G:O2'	62:2A:3948:HOH:O	2.20	0.45
1:2A:2291:U:OP1	1:2A:2380:C:O2'	2.31	0.45
1:2A:2318:G:H21	14:2S:3:ARG:NE	2.15	0.45
5:2F:113:ALA:HB1	5:2F:186:ILE:HG21	1.97	0.45
8:2I:77:LEU:O	8:2I:143:SER:OG	2.18	0.45
8:2I:87:LYS:HE3	8:2I:87:LYS:HB2	1.56	0.45
19:2X:94:GLY:H	19:2X:95:LEU:HB2	1.82	0.45
25:23:4:LEU:O	25:23:36:VAL:HA	2.17	0.45
32:2a:37:U:O2'	32:2a:500:G:H4'	2.17	0.45
32:2a:1490:C:H2'	32:2a:1491:G:O4'	2.17	0.45
37:2f:37:VAL:HG13	37:2f:65:VAL:HG12	1.97	0.45
37:2f:91:VAL:HG11	49:2r:72:ARG:NH1	2.32	0.45
40:2i:9:ARG:HG2	40:2i:14:VAL:HA	1.98	0.45
46:2o:11:VAL:HG21	46:2o:34:LEU:HD22	1.99	0.45
48:2q:26:GLN:HG2	48:2q:37:LYS:HG2	1.99	0.45
1:1A:387:U:O4	62:1A:4262:HOH:O	2.21	0.45
14:1S:83:LYS:HB3	14:1S:111:GLU:HG3	1.99	0.45
18:1W:27:LYS:HD2	18:1W:31:GLU:HG2	1.98	0.45
29:17:21:ARG:HD3	62:17:202:HOH:O	2.17	0.45
32:1a:60:A:N1	32:1a:107:G:O2'	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:219:C:H2'	32:1a:220:G:O4'	2.17	0.45
32:1a:299:G:C6	32:1a:300:A:C6	3.05	0.45
41:1j:57:LYS:O	41:1j:60:ARG:NE	2.39	0.45
1:2A:774:A:H2'	1:2A:774:A:N3	2.32	0.45
1:2A:1539:G:H2'	1:2A:1540:U:O4'	2.16	0.45
1:2A:2010:G:H5"	18:2W:42:ARG:HB2	1.98	0.45
1:2A:2106:G:H2'	1:2A:2107:C:O4'	2.16	0.45
1:2A:2130:U:H2'	1:2A:2158:A:H61	1.81	0.45
2:2B:77:U:H4'	21:2Z:84:GLU:OE1	2.17	0.45
9:2N:55:VAL:HB	9:2N:125:GLY:O	2.16	0.45
26:24:14:ILE:O	26:24:22:ILE:HD12	2.17	0.45
32:2a:1016:A:H2'	32:2a:1017:G:O4'	2.17	0.45
32:2a:1313:U:OP2	50:2s:5:LEU:HD13	2.17	0.45
35:2d:112:VAL:H	35:2d:116:GLN:NE2	2.15	0.45
41:2j:33:GLN:HG2	41:2j:34:VAL:N	2.30	0.45
45:2n:7:ILE:HG12	45:2n:23:ARG:HD3	1.99	0.45
57:2y:62:C:H2'	57:2y:63:G:C8	2.51	0.45
1:1A:363(A):A:H2'	1:1A:363(B):G:C8	2.51	0.45
1:1A:686:G:H21	1:1A:788:A:H61	1.65	0.45
6:1G:56:ALA:O	6:1G:59:GLU:HG2	2.17	0.45
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.65	0.45
11:1P:86:LYS:HG2	11:1P:87:ASP:N	2.30	0.45
14:1S:25:ARG:O	14:1S:39:ILE:HA	2.17	0.45
21:1Z:23:LYS:HD2	21:1Z:40:ASP:HA	1.98	0.45
32:1a:128:G:O2'	48:1q:3:LYS:NZ	2.50	0.45
32:1a:1194:U:H4'	36:1e:22:GLY:HA2	1.98	0.45
32:1a:1241:G:OP1	38:1g:35:LYS:NZ	2.49	0.45
33:1b:93:VAL:HG11	33:1b:97:TRP:HD1	1.83	0.45
35:1d:18:LYS:HG2	61:1d:302:SF4:S1	2.57	0.45
44:1m:9:ILE:HB	44:1m:18:ALA:HB1	1.99	0.45
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.52	0.45
1:2A:271(D):G:H1	1:2A:271(T):C:H42	1.65	0.45
1:2A:2507:C:H2'	1:2A:2508:G:O4'	2.17	0.45
6:2G:41:GLN:HG2	6:2G:154:GLY:O	2.17	0.45
7:2H:68:THR:O	7:2H:72:ILE:HG12	2.17	0.45
11:2P:94:GLU:HG3	11:2P:124:LYS:HE2	1.98	0.45
14:2S:23:ARG:HD3	14:2S:84:GLN:O	2.16	0.45
14:2S:84:GLN:HA	14:2S:111:GLU:HB2	1.97	0.45
16:2U:58:ARG:HA	16:2U:61:TRP:CE3	2.51	0.45
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.57	0.45
32:2a:165:C:H2'	32:2a:166:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:646:U:H2'	32:2a:647:C:C6	2.52	0.45
32:2a:807:A:H2'	32:2a:808:C:C6	2.52	0.45
32:2a:1105:A:H2'	32:2a:1106:G:C8	2.48	0.45
1:1A:859:G:O2'	1:1A:916:G:O6	2.30	0.44
1:1A:2112:G:C6	57:1y:19:G:C2	3.06	0.44
1:1A:2138:C:N3	1:1A:2153:G:O6	2.51	0.44
8:1I:48:GLU:HB3	8:1I:52:ARG:NH1	2.32	0.44
26:14:57:GLU:HA	26:14:58:ARG:HA	1.72	0.44
26:14:62:ARG:C	26:14:63:TYR:CG	2.95	0.44
32:1a:626:U:H2'	32:1a:627:G:H8	1.81	0.44
32:1a:735:C:H2'	32:1a:736:C:C6	2.52	0.44
32:1a:942:G:H21	40:1i:124:GLN:NE2	2.13	0.44
34:1c:152:ILE:HB	34:1c:199:LYS:HB2	1.99	0.44
36:1e:118:ILE:HG12	36:1e:119:LEU:N	2.32	0.44
49:1r:52:PRO:O	49:1r:56:THR:OG1	2.30	0.44
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.32	0.44
1:2A:1824:G:N3	3:2D:254:THR:OG1	2.49	0.44
7:2H:101:ARG:HH12	7:2H:122:THR:HA	1.82	0.44
22:20:36:ILE:HD12	22:20:58:THR:HG21	1.97	0.44
32:2a:688:G:C6	32:2a:700:G:C2	3.05	0.44
32:2a:1107:C:H5"	34:2c:173:VAL:O	2.17	0.44
32:2a:1359:C:H1'	32:2a:1362:C:H41	1.82	0.44
33:2b:100:GLY:N	33:2b:176:GLU:OE2	2.46	0.44
35:2d:100:ARG:NH2	35:2d:136:PRO:O	2.50	0.44
54:2w:12:U:H2'	54:2w:13:C:O4'	2.16	0.44
55:2x:66:C:H2'	55:2x:67:C:C6	2.53	0.44
1:1A:2102:U:H3	1:1A:2187:G:H1	1.63	0.44
5:1F:117:ARG:NH2	5:1F:189:THR:O	2.48	0.44
6:1G:76:SER:C	6:1G:77:ILE:HG13	2.41	0.44
8:1I:109:ILE:HG23	8:1I:130:TYR:CZ	2.51	0.44
32:1a:157:G:H1	32:1a:164:U:H3	1.63	0.44
32:1a:952:U:H2'	32:1a:953:G:C8	2.51	0.44
34:1c:119:ARG:HE	34:1c:140:ARG:CZ	2.29	0.44
36:1e:118:ILE:HG12	36:1e:119:LEU:H	1.82	0.44
43:1l:54:LYS:HD2	43:1l:54:LYS:N	2.32	0.44
1:2A:1908:C:O2	55:2x:12:G:H4'	2.17	0.44
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.52	0.44
7:2H:84:SER:HA	7:2H:133:VAL:O	2.17	0.44
11:2P:45:LEU:HD12	11:2P:45:LEU:HA	1.79	0.44
23:21:64:ALA:HA	23:21:67:ILE:HG13	1.99	0.44
32:2a:1002:G:N1	32:2a:1003:G:H8	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1053:G:H4'	32:2a:1054:C:H3'	2.00	0.44
35:2d:18:LYS:NZ	35:2d:31:CYS:SG	2.91	0.44
36:2e:60:TYR:CE1	36:2e:64:ARG:HD3	2.52	0.44
1:1A:2176:A:H2'	1:1A:2177:C:C6	2.53	0.44
1:1A:2836:U:C4	1:1A:2883:A:N6	2.86	0.44
2:1B:66:A:H61	2:1B:109:C:C5'	2.31	0.44
32:1a:137:C:H2'	32:1a:138:G:C8	2.53	0.44
32:1a:163:C:H2'	32:1a:164:U:C6	2.53	0.44
32:1a:626:U:H2'	32:1a:627:G:C8	2.53	0.44
32:1a:958:A:C2	50:1s:55:LYS:HB2	2.53	0.44
32:1a:1243:C:H2'	32:1a:1244:C:C6	2.52	0.44
33:1b:132:LYS:O	33:1b:136:VAL:HG22	2.18	0.44
39:1h:121:ASP:O	39:1h:125:ARG:HG3	2.17	0.44
41:1j:27:ALA:HA	41:1j:81:THR:HG21	1.99	0.44
42:1k:34:ASP:HB2	42:1k:35:PRO:HD2	1.99	0.44
43:1l:88:GLY:O	43:1l:99:HIS:HD2	2.00	0.44
1:2A:700:G:H2'	1:2A:701:G:O4'	2.18	0.44
1:2A:1022:G:N7	9:2N:66:LYS:HE2	2.32	0.44
1:2A:2336:A:H61	22:20:43:THR:CG2	2.30	0.44
3:2D:116:GLN:HE21	3:2D:116:GLN:HB3	1.53	0.44
5:2F:46:ARG:HB3	5:2F:48:THR:HG23	1.99	0.44
5:2F:166:ALA:C	5:2F:168:ARG:H	2.25	0.44
6:2G:65:GLY:HA2	26:24:7:PRO:HG2	2.00	0.44
16:2U:8:VAL:HG23	16:2U:11:ARG:HH21	1.82	0.44
27:25:49:CYS:SG	27:25:51:TYR:HB2	2.57	0.44
32:2a:60:A:N6	32:2a:110:C:N3	2.64	0.44
32:2a:126:G:O2'	32:2a:634:C:O2'	2.31	0.44
32:2a:742:G:OP2	46:2o:35:ARG:NH2	2.44	0.44
33:2b:80:ILE:HG21	33:2b:211:ILE:HG21	1.98	0.44
33:2b:124:SER:HB3	33:2b:125:PRO:HD3	1.98	0.44
34:2c:114:PRO:HA	34:2c:185:GLY:HA3	1.99	0.44
39:2h:39:LEU:HD12	39:2h:39:LEU:HA	1.80	0.44
1:1A:534:U:H2'	1:1A:535:C:C6	2.52	0.44
1:1A:839:U:H1'	1:1A:1191:G:H1'	1.99	0.44
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.32	0.44
4:1E:52:LEU:HB2	4:1E:76:ARG:HB2	1.98	0.44
4:1E:84:PHE:CZ	4:1E:86:PRO:HB3	2.52	0.44
5:1F:144:LYS:HB3	5:1F:144:LYS:HE3	1.63	0.44
32:1a:110:C:H2'	32:1a:111:G:O4'	2.18	0.44
32:1a:606:G:H21	32:1a:632:A:H62	1.65	0.44
32:1a:1030(B):C:H2'	32:1a:1030(B):C:O2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1118:C:H2'	32:1a:1119:C:C6	2.51	0.44
35:1d:107:ARG:HH22	35:1d:194:LEU:HD11	1.82	0.44
38:1g:50:ILE:HG13	38:1g:61:VAL:HG11	1.99	0.44
44:1m:19:LEU:HD21	44:1m:56:LEU:HD21	2.00	0.44
55:1x:50:U:H2'	55:1x:51:C:C6	2.53	0.44
1:2A:265:A:C8	1:2A:266:G:H1'	2.53	0.44
1:2A:446:G:OP1	16:2U:3:ARG:NH1	2.50	0.44
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.53	0.44
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.50	0.44
1:2A:2130:U:C2'	1:2A:2158:A:H61	2.29	0.44
1:2A:2420:C:H5'	28:26:54:ILE:HD11	2.00	0.44
1:2A:2769:C:H2'	1:2A:2770:G:O4'	2.18	0.44
4:2E:50:GLY:HA3	4:2E:75:VAL:HG21	2.00	0.44
8:2I:78:THR:O	8:2I:80:PRO:HD3	2.17	0.44
12:2Q:7:MET:HE1	12:2Q:73:PRO:HG3	2.00	0.44
32:2a:60:A:H4'	32:2a:61:G:O5'	2.18	0.44
32:2a:630:G:H2'	32:2a:631:G:C8	2.52	0.44
32:2a:1297:C:OP2	44:2m:44:ARG:NH2	2.48	0.44
33:2b:21:ARG:HA	33:2b:39:ILE:HA	2.00	0.44
36:2e:5:ASP:N	36:2e:5:ASP:OD1	2.50	0.44
1:1A:2805:G:H2'	1:1A:2807:G:C8	2.51	0.44
32:1a:512:U:H2'	32:1a:513:C:C6	2.53	0.44
32:1a:1227:A:P	44:1m:111:LYS:HZ2	2.41	0.44
36:1e:137:GLU:O	36:1e:141:GLN:HG3	2.16	0.44
40:1i:128:ARG:NH1	55:1x:35:A:OP2	2.50	0.44
50:1s:11:VAL:C	50:1s:13:ASP:H	2.26	0.44
55:1x:19:G:H3'	55:1x:20:U:H5	1.80	0.44
55:1x:25:C:H2'	55:1x:26:G:O4'	2.17	0.44
1:2A:90:U:H1'	1:2A:92:A:C8	2.52	0.44
1:2A:93:G:H2'	1:2A:94:C:C6	2.53	0.44
1:2A:403:U:H4'	1:2A:404:C:H5'	1.99	0.44
1:2A:1019:U:H2'	1:2A:1020:A:H8	1.83	0.44
1:2A:1114:G:H2'	1:2A:1115:G:C8	2.53	0.44
1:2A:1427:A:H4'	1:2A:1428:C:O5'	2.17	0.44
1:2A:2298:A:N6	1:2A:2318:G:H8	2.15	0.44
1:2A:2378:A:O5'	1:2A:2378:A:H8	2.00	0.44
1:2A:2747:G:OP1	7:2H:138:LYS:NZ	2.34	0.44
5:2F:51:THR:O	5:2F:93:LYS:HE2	2.18	0.44
5:2F:157:VAL:HG21	5:2F:181:LEU:HD13	2.00	0.44
14:2S:30:ARG:HB2	14:2S:35:ILE:HD12	2.00	0.44
26:24:50:VAL:HG11	44:2m:64:TRP:C	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:26:38:LYS:HB3	28:26:38:LYS:HE3	1.67	0.44
32:2a:1265:G:C2	32:2a:1271:G:C2	3.06	0.44
41:2j:8:LEU:HA	41:2j:96:ILE:HA	1.98	0.44
57:2y:68:C:H2'	57:2y:69:G:H5"	1.99	0.44
1:1A:196:A:H2'	1:1A:196:A:N3	2.32	0.44
1:1A:363(C):G:H2'	1:1A:363(D):G:C8	2.52	0.44
1:1A:1056:G:H1'	1:1A:1103:A:H61	1.82	0.44
1:1A:1429:G:H2'	1:1A:1430:C:H6	1.81	0.44
1:1A:1709:U:H2'	1:1A:1710:C:C6	2.52	0.44
1:1A:2576:G:H1'	62:1A:5318:HOH:O	2.17	0.44
1:1A:2745:C:H2'	1:1A:2746:U:O4'	2.17	0.44
1:1A:2790:A:H5'	1:1A:2893:G:H21	1.83	0.44
1:1A:2810:A:N6	1:1A:2891:G:O2'	2.47	0.44
8:1I:127:VAL:HA	8:1I:140:LEU:O	2.18	0.44
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.18	0.44
32:1a:620:C:H2'	32:1a:621:A:O4'	2.17	0.44
32:1a:1284:C:H3'	32:1a:1285:A:H8	1.82	0.44
32:1a:1360:A:H2'	32:1a:1361:G:O4'	2.18	0.44
32:1a:1469:G:H2'	32:1a:1470:G:H8	1.82	0.44
33:1b:12:GLU:O	33:1b:15:VAL:HG22	2.17	0.44
33:1b:60:ASP:CG	33:1b:64:ARG:HH21	2.25	0.44
35:1d:117:ALA:O	35:1d:121:VAL:HG23	2.18	0.44
36:1e:90:VAL:O	36:1e:120:THR:HA	2.18	0.44
37:1f:99:ALA:HB3	49:1r:29:PHE:CE1	2.53	0.44
38:1g:72:ARG:H	38:1g:72:ARG:HD3	1.82	0.44
48:1q:62:SER:OG	48:1q:72:ARG:NE	2.44	0.44
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.53	0.44
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.18	0.44
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.52	0.44
1:2A:2177:C:H2'	1:2A:2178:C:O4'	2.17	0.44
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.98	0.44
6:2G:114:ILE:HD12	6:2G:117:PHE:HE1	1.82	0.44
6:2G:127:GLY:N	6:2G:166:ASP:OD1	2.50	0.44
12:2Q:116:GLU:HG3	12:2Q:120:ILE:HD11	2.00	0.44
32:2a:9:G:H2'	32:2a:10:A:H8	1.83	0.44
32:2a:417:C:H2'	32:2a:418:C:C6	2.53	0.44
32:2a:1264:C:C4	32:2a:1272:G:O6	2.71	0.44
35:2d:173:TRP:CG	35:2d:189:PRO:HB3	2.52	0.44
35:2d:180:GLY:O	35:2d:182:LYS:HG3	2.18	0.44
37:2f:83:ASP:N	37:2f:83:ASP:OD1	2.51	0.44
50:2s:28:LYS:CB	50:2s:29:ARG:HA	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:2x:23:C:H2'	55:2x:24:U:C6	2.52	0.44
25:13:31:LEU:HD23	25:13:31:LEU:HA	1.84	0.44
32:1a:490:G:H2'	32:1a:491:G:H8	1.83	0.44
32:1a:867:G:O2'	32:1a:873:A:N1	2.47	0.44
33:1b:107:THR:O	33:1b:110:GLN:HB3	2.17	0.44
33:1b:140:HIS:O	33:1b:144:ARG:HG3	2.18	0.44
34:1c:30:ARG:NH1	45:1n:35:ARG:O	2.50	0.44
35:1d:81:GLU:CD	35:1d:139:ARG:HH12	2.26	0.44
40:1i:4:TYR:CG	40:1i:88:TYR:HB2	2.52	0.44
51:1t:92:LEU:HD23	51:1t:92:LEU:HA	1.82	0.44
1:2A:252:G:P	11:2P:50:ARG:HH12	2.41	0.44
1:2A:323:G:H2'	5:2F:169:ASN:OD1	2.17	0.44
1:2A:483:A:H3'	1:2A:484:C:C6	2.53	0.44
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.17	0.44
1:2A:2816:C:O3'	13:2R:99:LYS:NZ	2.51	0.44
1:2A:2821:A:H2'	1:2A:2822:G:H8	1.82	0.44
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	2.00	0.44
21:2Z:70:LEU:HD13	21:2Z:70:LEU:HA	1.85	0.44
32:2a:194:C:H2'	32:2a:195:A:H5"	2.00	0.44
32:2a:299:G:C6	32:2a:300:A:C6	3.05	0.44
32:2a:1080:A:H5"	32:2a:1081:G:OP2	2.17	0.44
48:2q:67:LYS:HA	48:2q:70:ARG:HH12	1.82	0.44
51:2t:57:ARG:HH12	51:2t:100:ILE:HD12	1.83	0.44
1:1A:723:G:H2'	1:1A:724:U:O4'	2.18	0.44
1:1A:1465:G:O2'	1:1A:1545:A:N1	2.43	0.44
1:1A:2522:U:O2'	1:1A:2647:U:OP1	2.32	0.44
1:1A:2629:A:HO2'	1:1A:2630:G:P	2.39	0.44
3:1D:246:PRO:O	3:1D:254:THR:HG22	2.17	0.44
20:1Y:68:HIS:ND1	20:1Y:70:SER:HB3	2.32	0.44
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.07	0.44
32:1a:690:G:C6	32:1a:691:G:C6	3.06	0.44
32:1a:743:U:H2'	32:1a:744:C:C6	2.53	0.44
32:1a:757:U:H2'	32:1a:758:G:O4'	2.17	0.44
32:1a:976:G:OP1	45:1n:32:SER:N	2.49	0.44
32:1a:1346:A:N1	32:1a:1374:A:H5"	2.32	0.44
35:1d:76:ARG:HG3	35:1d:207:TYR:CE1	2.53	0.44
37:1f:9:VAL:HA	37:1f:59:TYR:O	2.18	0.44
41:1j:65:LEU:HD13	45:1n:56:VAL:HG13	2.00	0.44
46:1o:24:SER:OG	46:1o:25:THR:N	2.51	0.44
1:2A:913:U:H4'	1:2A:914:C:OP1	2.18	0.44
1:2A:1198:U:H2'	1:2A:1199:U:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2113:U:H3	1:2A:2169:A:H62	1.65	0.44
1:2A:2334:G:H4'	1:2A:2335:A:OP2	2.17	0.44
1:2A:2540:C:H2'	1:2A:2541:A:O4'	2.18	0.44
8:2I:51:ILE:HD12	8:2I:51:ILE:HA	1.86	0.44
8:2I:110:ASP:H	8:2I:130:TYR:HE1	1.66	0.44
14:2S:30:ARG:HE	14:2S:98:VAL:HG23	1.83	0.44
34:2c:45:LYS:HG3	34:2c:46:GLU:N	2.32	0.44
34:2c:101:LEU:HD13	34:2c:102:ASN:H	1.83	0.44
36:2e:63:ARG:C	36:2e:66:MET:HE1	2.43	0.44
36:2e:89:ILE:HD12	36:2e:89:ILE:HA	1.87	0.44
37:2f:12:PRO:HG3	37:2f:57:GLN:O	2.17	0.44
45:2n:29:ARG:HG2	45:2n:31:ARG:H	1.82	0.44
45:2n:53:LEU:HD23	45:2n:53:LEU:HA	1.86	0.44
1:1A:583:G:OP2	16:1U:10:ARG:NH1	2.45	0.44
1:1A:882:G:H4'	54:1w:19:G:C6	2.53	0.44
1:1A:1082:U:C4	1:1A:1086:A:N1	2.76	0.44
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.53	0.44
1:1A:1697:G:OP2	1:1A:1698:A:O2'	2.33	0.44
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.25	0.44
6:1G:25:TYR:CZ	6:1G:32:PRO:HD3	2.53	0.44
32:1a:975:A:H5'	32:1a:975:A:H8	1.83	0.44
32:1a:1004:A:H61	32:1a:1037:C:H42	1.66	0.44
34:1c:116:VAL:HG21	34:1c:202:ILE:HD11	2.00	0.44
35:1d:196:LEU:O	35:1d:198:VAL:N	2.45	0.44
37:1f:76:ALA:O	37:1f:80:ARG:HG3	2.18	0.44
40:1i:41:VAL:C	40:1i:43:ALA:H	2.25	0.44
47:1p:6:LEU:HB3	47:1p:17:TYR:CD1	2.53	0.44
3:2D:97:TYR:C	3:2D:99:ASP:N	2.76	0.44
3:2D:112:GLN:O	3:2D:115:GLN:HG2	2.18	0.44
8:2I:5:LEU:HD11	8:2I:19:VAL:HG22	1.99	0.44
32:2a:376:G:O2'	47:2p:5:ARG:NH2	2.51	0.44
32:2a:692:U:O2'	32:2a:694:A:N7	2.46	0.44
32:2a:719:C:N4	49:2r:71:LYS:HE2	2.32	0.44
32:2a:748:C:H4'	32:2a:749:C:O5'	2.18	0.44
32:2a:1294:G:H2'	32:2a:1295:G:C8	2.53	0.44
34:2c:134:ILE:HG22	34:2c:168:ALA:HB3	1.99	0.44
40:2i:55:ALA:HA	40:2i:58:HIS:CD2	2.47	0.44
54:2w:67:C:H2'	54:2w:68:C:C6	2.52	0.44
55:2x:40:C:H5"	57:2y:36:A:OP1	2.17	0.44
1:1A:2840:C:O5'	1:1A:2840:C:H6	2.01	0.43
6:1G:22:ARG:NH1	6:1G:175:LEU:HD21	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1S:25:ARG:HG3	14:1S:88:ASP:HB2	2.00	0.43
32:1a:21:G:H2'	32:1a:22:G:C8	2.53	0.43
32:1a:145:G:H1	32:1a:177:C:H42	1.65	0.43
32:1a:250:A:H4'	32:1a:251:G:O5'	2.17	0.43
32:1a:477:A:H2'	32:1a:479:C:C6	2.53	0.43
32:1a:607:A:H2'	32:1a:608:A:C8	2.53	0.43
32:1a:668:G:O2'	46:1o:46:HIS:HB3	2.18	0.43
35:1d:120:LEU:HD23	35:1d:120:LEU:HA	1.82	0.43
41:1j:38:ILE:HG13	41:1j:38:ILE:O	2.17	0.43
1:2A:208:C:H2'	1:2A:209:C:C6	2.53	0.43
1:2A:1717:G:H2'	1:2A:1718:G:C8	2.52	0.43
1:2A:2818:G:OP2	13:2R:42:LYS:NZ	2.26	0.43
6:2G:43:LEU:C	6:2G:45:GLU:H	2.26	0.43
32:2a:162:A:H8	32:2a:162:A:O5'	2.01	0.43
32:2a:354:G:O2'	32:2a:389:A:OP1	2.31	0.43
32:2a:381:C:H2'	32:2a:382:A:O4'	2.18	0.43
32:2a:409:G:H2'	32:2a:410:G:O4'	2.18	0.43
32:2a:663:A:O3'	49:2r:64:ARG:NH2	2.44	0.43
32:2a:685:G:C2	32:2a:686:U:C4	3.06	0.43
32:2a:1265:G:C4	32:2a:1271:G:N2	2.86	0.43
37:2f:46:ARG:HH22	49:2r:37:VAL:HG11	1.84	0.43
44:2m:29:ARG:HD3	44:2m:64:TRP:CE2	2.53	0.43
1:1A:143:G:H2'	1:1A:143(A):C:C6	2.53	0.43
1:1A:403:U:H3'	62:1A:5220:HOH:O	2.18	0.43
1:1A:677:A:OP1	62:1A:4265:HOH:O	2.21	0.43
1:1A:1287:A:H8	13:1R:104:ARG:HD3	1.83	0.43
1:1A:1512:U:O2'	1:1A:1513:C:H5'	2.18	0.43
1:1A:2167:U:O2	1:1A:2167:U:H2'	2.18	0.43
1:1A:2492:U:H2'	1:1A:2493:U:C6	2.53	0.43
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	2.00	0.43
10:1O:63:VAL:HG12	10:1O:106:LEU:HD21	2.00	0.43
27:15:11:THR:HG23	27:15:15:ARG:HB3	2.00	0.43
32:1a:673:G:H2'	32:1a:674:G:C8	2.52	0.43
32:1a:1464:G:H2'	32:1a:1465:C:H6	1.83	0.43
37:1f:19:LEU:HD11	37:1f:59:TYR:CE1	2.53	0.43
37:1f:100:ASN:C	49:1r:28:GLU:HG3	2.43	0.43
40:1i:52:ALA:HB2	40:1i:101:PHE:HE2	1.82	0.43
1:2A:871:U:OP1	12:2Q:5:ARG:HG3	2.19	0.43
1:2A:1344:G:O2'	1:2A:1385:G:H2'	2.17	0.43
1:2A:1717:G:H2'	1:2A:1718:G:H8	1.83	0.43
1:2A:1951:U:O2	1:2A:1953:A:H8	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2063:C:H5”	62:2A:4197:HOH:O	2.16	0.43
1:2A:2402:C:H1’	1:2A:2403:C:H5	1.83	0.43
1:2A:2466:C:OP1	31:29:4:ARG:HB2	2.18	0.43
1:2A:2747:G:O6	1:2A:2755:C:H5”	2.17	0.43
8:2I:122:GLU:O	8:2I:126:TYR:OH	2.36	0.43
26:24:13:ARG:HD3	26:24:23:GLU:OE2	2.18	0.43
32:2a:533:A:OP1	62:2a:1919:HOH:O	2.21	0.43
32:2a:1133:G:H1	32:2a:1141:C:H42	1.66	0.43
36:2e:77:PRO:HD2	36:2e:142:LEU:HD13	2.00	0.43
41:2j:6:ILE:N	41:2j:72:VAL:O	2.44	0.43
43:2l:60:LEU:C	43:2l:62:SER:H	2.24	0.43
57:2y:33:U:H1’	57:2y:36:A:H61	1.83	0.43
57:2y:57:G:N3	57:2y:57:G:H2’	2.33	0.43
32:1a:78:G:H1	32:1a:91:C:N4	2.15	0.43
32:1a:707:C:H4’	42:1k:20:TYR:CG	2.54	0.43
32:1a:1000:U:H2’	32:1a:1001:A:C8	2.53	0.43
32:1a:1005:A:H5”	32:1a:1006:C:C5	2.53	0.43
32:1a:1066:C:O2’	32:1a:1067:A:H5’	2.18	0.43
32:1a:1229:A:OP2	44:1m:114:ARG:HD3	2.17	0.43
57:1y:22:G:N7	57:1y:46:G7M:N2	2.66	0.43
1:2A:141:A:C8	1:2A:1408:C:O2’	2.71	0.43
1:2A:1561:G:H2’	1:2A:1562:A:C8	2.52	0.43
1:2A:1630:G:H2’	1:2A:1631:C:C6	2.52	0.43
6:2G:148:MET:HE3	6:2G:148:MET:HB3	1.83	0.43
12:2Q:130:LYS:HE2	12:2Q:130:LYS:HB3	1.76	0.43
13:2R:72:ASP:O	13:2R:76:VAL:HG23	2.17	0.43
15:2T:1:MET:HE2	15:2T:1:MET:HB3	1.82	0.43
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.17	0.43
32:2a:18:C:H1’	32:2a:1079:G:N2	2.33	0.43
32:2a:299:G:H8	32:2a:299:G:O5’	2.00	0.43
32:2a:539:A:H2’	32:2a:540:G:C8	2.52	0.43
32:2a:627:G:H2’	32:2a:628:G:C8	2.54	0.43
32:2a:1122:U:C4	32:2a:1123:A:N7	2.86	0.43
32:2a:1513:A:H2’	32:2a:1514:C:C6	2.53	0.43
37:2f:22:GLU:OE2	37:2f:82:ARG:NE	2.52	0.43
44:2m:73:GLU:O	44:2m:77:ASN:HB2	2.19	0.43
46:2o:55:GLY:HA2	46:2o:58:MET:HE2	1.99	0.43
50:2s:28:LYS:HB3	50:2s:29:ARG:CA	2.42	0.43
1:1A:437:G:H2’	1:1A:438:G:C8	2.53	0.43
1:1A:1421:G:N2	1:1A:1495:A:N1	2.63	0.43
1:1A:1960:A:O2’	32:1a:1484:C:O2’	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2150:U:H2'	1:1A:2151:G:C8	2.53	0.43
1:1A:2162:G:H1'	1:1A:2173:A:H1'	2.00	0.43
1:1A:2183:C:H2'	1:1A:2184:G:C8	2.52	0.43
1:1A:2322:A:N6	62:1A:4481:HOH:O	2.51	0.43
16:1U:97:ASP:OD1	16:1U:101:ARG:HD2	2.18	0.43
34:1c:19:GLU:O	34:1c:40:ARG:NH2	2.50	0.43
34:1c:71:ALA:HA	34:1c:106:VAL:HG21	2.00	0.43
34:1c:77:ILE:H	34:1c:77:ILE:HG12	1.52	0.43
1:2A:83:G:N1	1:2A:102:G:O2'	2.40	0.43
1:2A:297:C:H2'	1:2A:298:G:O4'	2.17	0.43
1:2A:882:G:N1	1:2A:893:C:H5	2.16	0.43
1:2A:1783:A:H5'	1:2A:2608:G:H4'	2.00	0.43
1:2A:2532:G:C6	1:2A:2533:A:C6	3.06	0.43
5:2F:177:ALA:HB1	5:2F:178:PRO:HD2	1.99	0.43
30:28:26:LYS:HB2	30:28:44:LYS:O	2.18	0.43
32:2a:643:C:H2'	32:2a:644:G:H8	1.83	0.43
32:2a:772:U:H2'	32:2a:773:G:O4'	2.18	0.43
32:2a:918:A:H2'	32:2a:919:A:C8	2.53	0.43
32:2a:986:A:H2'	32:2a:987:G:H8	1.82	0.43
32:2a:1237:C:O2'	32:2a:1300:G:N2	2.43	0.43
32:2a:1242:C:H2'	32:2a:1243:C:C6	2.53	0.43
32:2a:1518:MA6:H93	32:2a:1519:MA6:C9	2.48	0.43
37:2f:100:ASN:HD21	49:2r:23:LYS:HG2	1.83	0.43
42:2k:18:ARG:NH2	42:2k:35:PRO:O	2.51	0.43
47:2p:15:PRO:HD2	47:2p:42:ARG:CD	2.49	0.43
50:2s:36:ARG:NH1	50:2s:75:ALA:O	2.49	0.43
55:2x:69:C:H2'	55:2x:70:G:O4'	2.18	0.43
1:1A:1506:C:H2'	1:1A:1507:A:C8	2.53	0.43
1:1A:1837:C:OP1	32:1a:784:C:H4'	2.19	0.43
3:1D:19:ALA:HB2	3:1D:204:ILE:HD11	2.01	0.43
8:1I:77:LEU:HG	8:1I:101:LEU:HD22	2.00	0.43
15:1T:29:ARG:HG3	15:1T:46:GLU:HB2	2.01	0.43
32:1a:718:G:OP2	32:1a:720:C:N4	2.51	0.43
32:1a:945:G:OP1	62:1a:1916:HOH:O	2.21	0.43
40:1i:4:TYR:O	40:1i:19:LEU:HB2	2.17	0.43
45:1n:5:ALA:O	45:1n:9:LYS:HB2	2.18	0.43
50:1s:22:LEU:HD13	50:1s:29:ARG:H	1.83	0.43
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.52	0.43
1:2A:655:A:H8	1:2A:656:G:O4'	2.01	0.43
1:2A:1021:A:H3'	1:2A:1021:A:C8	2.54	0.43
1:2A:1927:A:C6	1:2A:1928:A:C6	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:77:ALA:HA	3:2D:97:TYR:HA	2.00	0.43
14:2S:94:TYR:CZ	14:2S:99:LYS:HG3	2.53	0.43
32:2a:416:G:C5	32:2a:417:C:C4	3.07	0.43
32:2a:1149:C:O2'	32:2a:1280:A:N1	2.51	0.43
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.51	0.43
34:2c:108:ASN:HB3	34:2c:111:LEU:HB2	1.99	0.43
37:2f:53:ALA:HB3	37:2f:86:ARG:NH1	2.34	0.43
43:2l:6:THR:HG23	43:2l:9:GLN:OE1	2.19	0.43
1:1A:336:C:HO2'	20:1Y:35:TYR:HH	1.61	0.43
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.53	0.43
1:1A:2818:G:O2'	1:1A:2819:G:H5'	2.19	0.43
62:1A:4417:HOH:O	13:1R:15:SER:HB3	2.16	0.43
10:1O:7:TYR:HE2	10:1O:20:MET:HE2	1.84	0.43
11:1P:90:ARG:HG2	11:1P:90:ARG:HH11	1.83	0.43
26:14:16:CYS:HB3	26:14:20:ASN:HB3	2.00	0.43
32:1a:262:A:C6	32:1a:263:A:C6	3.07	0.43
40:1i:25:LYS:N	40:1i:60:ASP:OD1	2.52	0.43
54:1w:60:U:H5"	54:1w:61:C:C5	2.51	0.43
1:2A:852:G:H2'	1:2A:853:G:C8	2.53	0.43
1:2A:1171:G:H8	1:2A:1171:G:O5'	2.02	0.43
1:2A:1886:C:H2'	1:2A:1887:C:C6	2.53	0.43
1:2A:2037:G:H2'	1:2A:2038:G:C8	2.54	0.43
5:2F:116:ASP:O	5:2F:120:GLU:HG2	2.19	0.43
10:2O:48:PRO:CB	32:2a:1422:G:H5"	2.37	0.43
11:2P:86:LYS:HE2	11:2P:87:ASP:OD1	2.18	0.43
20:2Y:37:VAL:HG21	20:2Y:72:VAL:HG21	1.99	0.43
20:2Y:38:ILE:HD13	20:2Y:66:PRO:HA	2.00	0.43
32:2a:73:G:H1	32:2a:96:U:H3	1.65	0.43
32:2a:448:A:OP2	32:2a:485:G:N2	2.32	0.43
32:2a:1105:A:H8	32:2a:1105:A:OP2	2.02	0.43
32:2a:1189:C:OP1	34:2c:5:ILE:HD12	2.18	0.43
32:2a:1256:A:O3'	32:2a:1257:U:H4'	2.18	0.43
36:2e:28:PHE:O	36:2e:47:LYS:HA	2.19	0.43
38:2g:113:GLU:OE2	38:2g:119:ARG:HA	2.19	0.43
39:2h:119:LEU:HB3	39:2h:123:GLU:HB3	2.00	0.43
41:2j:8:LEU:HD23	41:2j:8:LEU:H	1.82	0.43
51:2t:9:ASN:OD1	51:2t:9:ASN:N	2.51	0.43
1:1A:303:U:H2'	1:1A:304:G:C8	2.53	0.43
1:1A:376:C:H2'	1:1A:377:C:C6	2.53	0.43
1:1A:493:G:H2'	1:1A:494:G:O4'	2.19	0.43
1:1A:748:G:P	18:1W:88:ARG:HH21	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1851:U:H2'	1:1A:1852:C:O4'	2.18	0.43
3:1D:274:ARG:H	3:1D:274:ARG:HG2	1.64	0.43
13:1R:96:ARG:HD2	13:1R:115:GLU:OE2	2.19	0.43
21:1Z:138:GLU:H	21:1Z:156:LYS:CE	2.27	0.43
32:1a:376:G:H1	32:1a:387:U:H3	1.67	0.43
32:1a:654:G:H2'	32:1a:655:A:O4'	2.18	0.43
32:1a:909:A:H2'	32:1a:910:C:O4'	2.18	0.43
32:1a:952:U:H2'	32:1a:953:G:H8	1.82	0.43
35:1d:67:ILE:HD13	35:1d:196:LEU:HD22	1.99	0.43
36:1e:102:ALA:HA	36:1e:120:THR:OG1	2.19	0.43
1:2A:118:A:H5'	1:2A:119:A:C8	2.52	0.43
1:2A:304:G:H2'	1:2A:305:U:H6	1.84	0.43
1:2A:857:C:H1'	22:20:26:TYR:CE1	2.53	0.43
1:2A:2869:G:H2'	1:2A:2870:C:O4'	2.18	0.43
1:2A:2872:G:O2'	1:2A:2873:A:H5'	2.18	0.43
1:2A:2888:C:H2'	1:2A:2889:C:C6	2.53	0.43
6:2G:63:ILE:HD12	6:2G:141:PHE:HB3	2.00	0.43
21:2Z:31:ARG:HD2	21:2Z:94:GLU:OE2	2.19	0.43
32:2a:1128:C:H2'	32:2a:1129:C:C6	2.54	0.43
32:2a:1178:G:N2	32:2a:1180:A:H3'	2.33	0.43
51:2t:39:LYS:O	51:2t:43:LEU:HG	2.19	0.43
1:1A:548:A:H3'	1:1A:548:A:OP2	2.18	0.43
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.84	0.43
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.34	0.43
1:1A:2773:C:H2'	1:1A:2774:C:H6	1.84	0.43
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	2.01	0.43
5:1F:192:LEU:HD23	5:1F:192:LEU:HA	1.87	0.43
26:14:40:HIS:O	26:14:44:THR:HG23	2.19	0.43
27:15:33:CYS:HB2	27:15:40:LYS:HD3	2.00	0.43
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.53	0.43
32:1a:1162:C:H2'	32:1a:1163:C:C6	2.53	0.43
32:1a:1191:A:OP1	34:1c:4:LYS:NZ	2.42	0.43
32:1a:1456:G:O3'	51:1t:39:LYS:HE3	2.19	0.43
37:1f:22:GLU:O	37:1f:26:ILE:HG13	2.19	0.43
45:1n:53:LEU:O	45:1n:56:VAL:HG23	2.19	0.43
47:1p:55:ARG:HH21	47:1p:59:TRP:NE1	2.17	0.43
1:2A:265:A:H1'	1:2A:266:G:O4'	2.18	0.43
1:2A:506:G:O3'	1:2A:507:A:H8	2.02	0.43
1:2A:854:G:H2'	1:2A:855:G:H8	1.84	0.43
1:2A:878:A:H61	1:2A:899:A:H1'	1.83	0.43
1:2A:1240:U:O2'	1:2A:1241:A:O5'	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1526:G:C6	1:2A:1527:G:C2	3.07	0.43
1:2A:2483:C:N3	12:2Q:124:LYS:NZ	2.47	0.43
6:2G:63:ILE:HD13	6:2G:143:GLU:HB2	2.00	0.43
8:2I:96:ASP:OD1	8:2I:96:ASP:N	2.52	0.43
14:2S:84:GLN:H	14:2S:111:GLU:HB2	1.82	0.43
18:2W:37:ARG:HD2	18:2W:38:TYR:CE2	2.53	0.43
21:2Z:52:SER:O	21:2Z:54:HIS:N	2.51	0.43
21:2Z:91:LEU:O	21:2Z:92:SER:OG	2.30	0.43
32:2a:109:A:H5'	32:2a:110:C:H5	1.83	0.43
32:2a:143:A:O2'	32:2a:144:G:OP2	2.35	0.43
32:2a:794:A:OP2	62:2a:1920:HOH:O	2.21	0.43
32:2a:955:U:O2'	50:2s:83:HIS:HD2	2.02	0.43
32:2a:1013:G:N2	32:2a:1016:A:OP2	2.48	0.43
32:2a:1298:C:N4	38:2g:114:ARG:HB3	2.34	0.43
32:2a:1352:C:H2'	32:2a:1353:G:C8	2.53	0.43
32:2a:1402:4OC:CM2	32:2a:1403:C:H5'	2.48	0.43
34:2c:51:GLY:O	34:2c:70:VAL:HG12	2.18	0.43
39:2h:110:ALA:HB3	39:2h:121:ASP:HB3	2.01	0.43
41:2j:47:PHE:N	41:2j:63:PHE:O	2.36	0.43
1:1A:64:A:C5	19:1X:66:LEU:HD13	2.53	0.43
1:1A:1093:G:H3'	1:1A:1094:U:H5"	2.00	0.43
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.83	0.43
1:1A:2722:G:H2'	1:1A:2723:C:C6	2.54	0.43
12:1Q:89:ASN:HB2	55:1x:1:C:C4	2.54	0.43
15:1T:56:GLY:O	15:1T:59:THR:HG22	2.18	0.43
17:1V:60:GLU:HB2	17:1V:97:LYS:HE2	2.01	0.43
21:1Z:157:LEU:HD22	21:1Z:161:VAL:HG23	2.01	0.43
32:1a:194:C:H2'	32:1a:195:A:H5"	2.00	0.43
32:1a:741:G:H2'	32:1a:742:G:O4'	2.19	0.43
42:1k:24:SER:O	42:1k:88:GLY:HA3	2.19	0.43
42:1k:59:TYR:CE2	42:1k:63:LEU:HD11	2.54	0.43
44:1m:123:ALA:HA	44:1m:124:PRO:HD3	1.91	0.43
49:1r:52:PRO:HB2	49:1r:54:ARG:HG3	2.01	0.43
51:1t:100:ILE:HG12	51:1t:100:ILE:H	1.58	0.43
52:1u:3:LYS:HD3	52:1u:14:TRP:CD1	2.54	0.43
1:2A:395:U:O2'	62:2A:3952:HOH:O	2.21	0.43
1:2A:900:A:H2'	1:2A:901:A:C8	2.52	0.43
1:2A:1686:C:H2'	1:2A:1687:G:O4'	2.19	0.43
1:2A:1785:A:OP1	62:2A:3953:HOH:O	2.22	0.43
1:2A:2360:A:H2'	1:2A:2361:A:O4'	2.19	0.43
1:2A:2630:G:H2'	1:2A:2631:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:55:LYS:O	6:2G:59:GLU:N	2.48	0.43
16:2U:76:TYR:CE2	16:2U:80:ILE:HG13	2.54	0.43
17:2V:69:LYS:HA	17:2V:88:ARG:HG2	1.99	0.43
32:2a:109:A:C6	32:2a:326:G:C6	3.07	0.43
32:2a:827:U:H5"	32:2a:828:A:OP2	2.19	0.43
33:2b:115:LEU:HD22	33:2b:153:ARG:NH2	2.34	0.43
41:2j:6:ILE:HG23	41:2j:98:ILE:HD11	2.00	0.43
41:2j:23:ILE:HD12	41:2j:23:ILE:HA	1.86	0.43
1:1A:69:C:O2'	1:1A:70:G:H5'	2.18	0.43
1:1A:271(O):C:H2'	1:1A:271(P):C:C6	2.54	0.43
1:1A:437:G:H2'	1:1A:438:G:H8	1.84	0.43
1:1A:603:A:H4'	1:1A:604:G:H5'	2.01	0.43
1:1A:819:A:C4	1:1A:1189:A:C2	3.06	0.43
1:1A:1012:U:C5	9:1N:28:THR:HG21	2.54	0.43
1:1A:1891:G:H2'	1:1A:1892:C:O4'	2.19	0.43
1:1A:1916:A:H2'	1:1A:1917:PSU:O4'	2.19	0.43
1:1A:2006:C:OP2	62:1A:4266:HOH:O	2.21	0.43
32:1a:749:C:H2'	32:1a:750:G:H8	1.84	0.43
32:1a:1101:A:N6	33:1b:176:GLU:OE2	2.52	0.43
33:1b:119:GLU:O	33:1b:123:ALA:HB2	2.18	0.43
57:1y:68:C:C2	57:1y:69:G:C8	3.07	0.43
1:2A:493:G:H2'	1:2A:494:G:O4'	2.19	0.43
1:2A:570:G:H2'	1:2A:2030:A:C5	2.54	0.43
1:2A:884:C:H3'	1:2A:885:C:H6	1.82	0.43
1:2A:1515:G:C6	1:2A:1516:C:C4	3.07	0.43
1:2A:1882:C:H2'	1:2A:1883:G:O4'	2.19	0.43
1:2A:2150:U:H2'	1:2A:2151:G:H8	1.83	0.43
1:2A:2290:G:C6	1:2A:2291:U:C4	3.07	0.43
1:2A:2641:G:H5"	9:2N:76:SER:HB3	1.99	0.43
5:2F:103:LYS:HA	5:2F:106:ARG:HD3	1.99	0.43
6:2G:49:ASP:O	6:2G:50:ALA:C	2.61	0.43
7:2H:8:PRO:O	7:2H:10:PRO:HD3	2.18	0.43
8:2I:1:MET:HE3	8:2I:1:MET:HB2	1.83	0.43
14:2S:87:PHE:CZ	14:2S:102:ALA:HB2	2.54	0.43
32:2a:523:A:N1	43:2l:92:0TD:H6	2.33	0.43
32:2a:1288:A:N1	32:2a:1371:G:H1'	2.34	0.43
33:2b:19:HIS:CE1	33:2b:206:ASP:HB2	2.54	0.43
38:2g:22:LEU:HG	38:2g:62:PHE:CE2	2.54	0.43
46:2o:5:LYS:H	46:2o:5:LYS:HG3	1.59	0.43
1:1A:53:A:H2'	1:1A:54:G:O4'	2.19	0.42
1:1A:1859:A:N6	1:1A:1883:G:O2'	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2406:U:H6	1:1A:2406:U:H2'	1.61	0.42
13:1R:104:ARG:HB2	13:1R:111:LEU:HD21	2.00	0.42
27:15:35:GLU:HG3	27:15:51:TYR:CD1	2.54	0.42
32:1a:438:G:H4'	35:1d:123:HIS:CE1	2.54	0.42
32:1a:1000:U:H2'	32:1a:1001:A:H8	1.84	0.42
33:1b:74:LYS:NZ	33:1b:166:ASP:OD2	2.45	0.42
34:1c:114:PRO:HA	34:1c:185:GLY:HA3	1.99	0.42
34:1c:122:GLU:O	34:1c:126:ARG:HD2	2.18	0.42
36:1e:85:GLY:C	36:1e:87:SER:H	2.26	0.42
42:1k:51:LYS:HD3	42:1k:51:LYS:HA	1.89	0.42
1:2A:567:A:H4'	1:2A:808:G:OP1	2.19	0.42
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.53	0.42
1:2A:1529:G:O6	1:2A:1530:C:N4	2.52	0.42
1:2A:2100:G:H2'	1:2A:2101:G:C8	2.54	0.42
32:2a:900:A:H2'	32:2a:901:A:C8	2.54	0.42
35:2d:104:VAL:HG21	35:2d:140:VAL:HG21	2.01	0.42
1:1A:749:C:H4'	1:1A:1271:G:N3	2.34	0.42
1:1A:836:G:C5	1:1A:837:C:C4	3.08	0.42
1:1A:987:G:N7	62:1A:4344:HOH:O	2.36	0.42
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.54	0.42
1:1A:1773:A:N1	62:1A:4340:HOH:O	2.36	0.42
1:1A:2752:C:O5'	1:1A:2752:C:H6	2.03	0.42
2:1B:77:U:H4'	21:1Z:84:GLU:OE1	2.19	0.42
8:1I:12:LEU:HA	8:1I:12:LEU:HD23	1.74	0.42
10:1O:68:GLU:H	10:1O:68:GLU:CD	2.27	0.42
12:1Q:103:MET:HE1	12:1Q:125:LEU:HD13	2.01	0.42
18:1W:24:ILE:HA	18:1W:27:LYS:HG3	2.01	0.42
22:10:18:ALA:HB3	22:10:20:ARG:HH11	1.84	0.42
32:1a:502:G:H2'	32:1a:503:C:O4'	2.19	0.42
32:1a:679:C:H2'	32:1a:680:C:C6	2.54	0.42
33:1b:219:VAL:O	33:1b:223:ILE:HG13	2.19	0.42
34:1c:52:LEU:CD1	34:1c:68:VAL:HG13	2.48	0.42
34:1c:68:VAL:HG12	34:1c:70:VAL:HB	2.01	0.42
35:1d:119:GLN:HG2	35:1d:123:HIS:CD2	2.54	0.42
35:1d:175:SER:HB3	35:1d:184:LYS:HB2	2.01	0.42
1:2A:140:G:N2	1:2A:1596:A:H4'	2.34	0.42
1:2A:775:G:N3	62:2A:4034:HOH:O	2.37	0.42
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.54	0.42
1:2A:1257:C:H2'	1:2A:1258:C:C6	2.54	0.42
1:2A:2059:A:H2'	1:2A:2503:2MA:HM23	2.00	0.42
1:2A:2078:C:C4	1:2A:2079:U:C4	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2637:U:H5”	4:2E:82:ARG:NH1	2.33	0.42
2:2B:31:C:H4’	6:2G:29:TRP:CH2	2.53	0.42
2:2B:56:G:H5’	6:2G:27:ASN:ND2	2.34	0.42
6:2G:79:ASN:N	6:2G:79:ASN:OD1	2.52	0.42
17:2V:71:LEU:HD23	17:2V:71:LEU:HA	1.85	0.42
26:24:64:GLY:C	26:24:66:SER:N	2.77	0.42
32:2a:157:G:H2’	32:2a:158:G:H8	1.84	0.42
32:2a:441:A:H3’	32:2a:442:C:C6	2.54	0.42
32:2a:642:A:N3	39:2h:113:SER:OG	2.49	0.42
32:2a:1084:G:OP1	32:2a:1086:U:C2	2.72	0.42
32:2a:1187:G:C6	32:2a:1188:A:C6	3.07	0.42
33:2b:8:LYS:HE2	33:2b:51:LEU:HB3	2.02	0.42
33:2b:144:ARG:HA	33:2b:144:ARG:HD2	1.84	0.42
34:2c:37:GLN:O	34:2c:40:ARG:N	2.52	0.42
38:2g:88:PRO:HG3	38:2g:149:ARG:HA	2.01	0.42
42:2k:65:ALA:O	42:2k:69:ALA:N	2.46	0.42
1:1A:303:U:H2’	1:1A:304:G:H8	1.85	0.42
1:1A:649:G:H2’	1:1A:650:C:C6	2.54	0.42
5:1F:182:ASN:HD21	5:1F:185:ASP:CG	2.27	0.42
10:1O:24:VAL:HG13	10:1O:33:ALA:HB2	2.01	0.42
18:1W:4:LYS:HE2	18:1W:6:ILE:HD11	2.00	0.42
18:1W:68:ARG:HH12	18:1W:112:GLY:H	1.67	0.42
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.55	0.42
26:14:46:GLN:O	26:14:47:GLN:C	2.62	0.42
32:1a:236:G:H5”	48:1q:42:TYR:OH	2.18	0.42
32:1a:332:G:H2’	32:1a:333:G:H8	1.83	0.42
32:1a:1182:G:H4’	32:1a:1183:A:H5”	1.99	0.42
32:1a:1460:A:H2’	32:1a:1461:G:O4’	2.18	0.42
32:1a:1464:G:H2’	32:1a:1465:C:C6	2.54	0.42
37:1f:2:ARG:HD2	37:1f:69:GLU:HB3	2.01	0.42
43:1l:8:ASN:O	43:1l:12:ARG:HG3	2.19	0.42
45:1n:21:TYR:HE1	45:1n:23:ARG:HE	1.67	0.42
1:2A:184:C:H2’	1:2A:185:U:C6	2.54	0.42
1:2A:690:G:H2’	1:2A:691:C:C6	2.54	0.42
1:2A:1169:G:C2	1:2A:1170:G:N7	2.88	0.42
1:2A:1423:G:H2’	1:2A:1424:G:C8	2.54	0.42
1:2A:1847:A:H3’	1:2A:1848:A:H5’	2.02	0.42
1:2A:1991:U:H2’	1:2A:1992:G:H5”	2.01	0.42
1:2A:2116:G:H8	1:2A:2166:G:N2	2.17	0.42
1:2A:2309:A:H2’	1:2A:2310:A:O4’	2.18	0.42
1:2A:2400:G:H2’	1:2A:2401:U:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:130:ALA:HB3	5:2F:142:TRP:HD1	1.84	0.42
7:2H:20:ALA:HB1	7:2H:21:PRO:HD2	2.01	0.42
7:2H:127:GLU:C	7:2H:129:THR:H	2.27	0.42
11:2P:98:GLU:O	11:2P:101:VAL:HG12	2.19	0.42
15:2T:77:PRO:HB2	15:2T:80:SER:HB2	2.01	0.42
19:2X:94:GLY:HA3	19:2X:95:LEU:HB2	1.99	0.42
32:2a:126:G:H4'	32:2a:634:C:O2	2.19	0.42
35:2d:92:VAL:HG22	35:2d:96:LEU:HD22	2.02	0.42
44:2m:66:LEU:HA	44:2m:70:LEU:HD12	1.99	0.42
57:2y:14:A:HO2'	57:2y:15:G:P	2.36	0.42
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.55	0.42
1:1A:1399:C:OP1	19:1X:25:LYS:NZ	2.52	0.42
1:1A:1800:C:OP1	3:1D:260:ARG:NH2	2.53	0.42
1:1A:2051:A:H5'	1:1A:2578:G:O4'	2.19	0.42
1:1A:2345:G:N3	1:1A:2381:C:H2'	2.34	0.42
26:14:63:TYR:HA	26:14:64:GLY:HA2	1.68	0.42
32:1a:204:U:H4'	32:1a:216:G:H5"	2.01	0.42
32:1a:1112:C:C2	34:1c:178:LEU:HB2	2.54	0.42
32:1a:1264:C:N4	32:1a:1271:G:H1	2.18	0.42
32:1a:1438:G:H2'	32:1a:1439:C:H6	1.84	0.42
33:1b:21:ARG:H	33:1b:21:ARG:HG2	1.57	0.42
35:1d:135:LEU:HD12	35:1d:135:LEU:HA	1.85	0.42
36:1e:53:LEU:O	36:1e:57:LYS:N	2.52	0.42
39:1h:95:VAL:HB	39:1h:99:GLU:HB2	2.00	0.42
41:1j:30:SER:HB3	41:1j:81:THR:HG23	2.00	0.42
54:1w:63:G:H2'	54:1w:64:A:H8	1.82	0.42
1:2A:1019:U:H3	1:2A:1142(A):A:N6	2.14	0.42
1:2A:1489:U:H2'	62:2A:4011:HOH:O	2.20	0.42
1:2A:1580:A:H3'	1:2A:1581:G:H8	1.84	0.42
1:2A:2031:A:N3	1:2A:2455:G:O2'	2.44	0.42
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.19	0.42
9:2N:103:VAL:O	9:2N:107:LEU:HG	2.18	0.42
15:2T:83:ILE:HD13	15:2T:86:ILE:HD11	2.02	0.42
32:2a:287:U:H2'	32:2a:288:A:C8	2.55	0.42
32:2a:994:A:N7	32:2a:1216:G:H4'	2.33	0.42
32:2a:1007:C:N3	32:2a:1022:G:O6	2.53	0.42
34:2c:131:ARG:HE	34:2c:135:LYS:HZ1	1.66	0.42
37:2f:41:GLU:CD	49:2r:35:ARG:HH22	2.27	0.42
38:2g:20:ASP:HB3	38:2g:23:VAL:HB	2.02	0.42
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.45	0.42
57:2y:9:A:H5'	57:2y:46:G7M:N3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:924:C:H2'	1:1A:925:C:C6	2.54	0.42
1:1A:1062:G:P	1:1A:1070:A:H1'	2.59	0.42
1:1A:1354:A:H4'	3:1D:38:LYS:HE3	2.01	0.42
1:1A:1799:G:N7	3:1D:179:SER:OG	2.52	0.42
1:1A:1825:A:OP1	3:1D:249:PRO:HD3	2.19	0.42
1:1A:1899:G:O2'	1:1A:1900:A:OP2	2.36	0.42
1:1A:2633:G:H2'	1:1A:2634:G:O4'	2.20	0.42
5:1F:161:GLU:HG2	5:1F:164:ARG:NH2	2.34	0.42
15:1T:39:ARG:NH2	32:1a:345:C:H5"	2.34	0.42
16:1U:82:GLY:HA3	16:1U:113:ALA:HB1	2.01	0.42
25:13:8:LEU:HA	25:13:54:VAL:HG23	2.01	0.42
32:1a:1430:C:H2'	32:1a:1431:C:C6	2.55	0.42
33:1b:19:HIS:HA	33:1b:39:ILE:CG2	2.49	0.42
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.20	0.42
1:2A:652(B):A:N6	1:2A:655:A:H1'	2.34	0.42
1:2A:870:A:OP1	12:2Q:6:ARG:NH2	2.53	0.42
1:2A:1400:G:H2'	1:2A:1401:G:C8	2.55	0.42
1:2A:1862:G:H2'	1:2A:1863:G:H8	1.84	0.42
2:2B:16:G:C2'	2:2B:17:C:H5'	2.49	0.42
2:2B:72:G:O2'	2:2B:105:A:N6	2.52	0.42
3:2D:206:LEU:HD22	3:2D:211:ARG:HG2	2.02	0.42
4:2E:78:LEU:HD12	4:2E:78:LEU:HA	1.80	0.42
7:2H:73:ALA:O	7:2H:76:VAL:HG12	2.19	0.42
7:2H:137:ASP:OD1	7:2H:140:LYS:N	2.40	0.42
21:2Z:151:HIS:HB3	21:2Z:152:ALA:H	1.73	0.42
23:21:98:LEU:HD23	23:21:98:LEU:HA	1.81	0.42
35:2d:119:GLN:HG2	35:2d:123:HIS:CD2	2.53	0.42
44:2m:65:LYS:HB2	44:2m:65:LYS:HE3	1.66	0.42
49:2r:84:LYS:N	49:2r:84:LYS:HD2	2.34	0.42
51:2t:79:ARG:HD2	51:2t:83:ARG:NH2	2.29	0.42
1:1A:141:A:C6	1:1A:142:A:N1	2.87	0.42
1:1A:271(L):U:O2'	1:1A:271(M):G:OP2	2.30	0.42
1:1A:531:C:H4'	1:1A:532:A:H5"	2.01	0.42
1:1A:862:G:H2'	1:1A:863:A:O4'	2.20	0.42
1:1A:1064:C:N3	1:1A:1074:G:C6	2.87	0.42
1:1A:1075:C:O2	1:1A:1076:C:H2'	2.19	0.42
1:1A:1364:G:N7	23:11:3:LYS:HE2	2.34	0.42
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.20	0.42
6:1G:110:ALA:HB1	6:1G:140:ILE:HG23	2.02	0.42
23:11:65:SER:HB2	23:11:66:HIS:ND1	2.34	0.42
32:1a:115:G:H4'	32:1a:116:A:O5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:987:G:N2	32:1a:1219:U:O2	2.53	0.42
38:1g:144:MET:HE2	38:1g:144:MET:HB3	1.82	0.42
41:1j:13:HIS:O	41:1j:17:ASP:N	2.39	0.42
57:1y:8:4SU:O2'	57:1y:21:A:N1	2.53	0.42
1:2A:74:A:H4'	1:2A:75:G:O5'	2.20	0.42
1:2A:271(J):C:OP2	1:2A:271(J):C:H6	2.02	0.42
1:2A:1114:G:H2'	1:2A:1115:G:H8	1.85	0.42
1:2A:1219:G:N2	1:2A:1221:C:N3	2.67	0.42
32:2a:397:A:H5'	32:2a:398:C:OP1	2.19	0.42
32:2a:933:G:O6	38:2g:3:ARG:NH2	2.53	0.42
32:2a:966:M2G:H2'	32:2a:967:5MC:C6	2.54	0.42
32:2a:1005:A:H5"	32:2a:1006:C:H5	1.84	0.42
32:2a:1081:G:N7	36:2e:47:LYS:HE3	2.34	0.42
32:2a:1134:G:N1	32:2a:1135:U:H1'	2.34	0.42
32:2a:1256:A:H5'	32:2a:1258:G:O4'	2.20	0.42
39:2h:56:LYS:HB2	39:2h:58:TYR:HE2	1.83	0.42
45:2n:3:ARG:HG3	45:2n:4:LYS:N	2.33	0.42
50:2s:22:LEU:HD11	50:2s:28:LYS:O	2.20	0.42
55:2x:8:4SU:O5'	55:2x:8:4SU:H6	2.19	0.42
57:2y:12:U:C2	57:2y:24:G:N2	2.87	0.42
1:1A:1421:G:C2	1:1A:1422:G:C8	3.08	0.42
1:1A:1740:G:H2'	1:1A:1741:A:C8	2.54	0.42
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.49	0.42
1:1A:2663:G:C6	1:1A:2664:G:C4	3.07	0.42
1:1A:2685:G:H5'	10:1O:68:GLU:OE2	2.19	0.42
5:1F:123:LEU:HD11	5:1F:194:MET:HE2	2.00	0.42
6:1G:148:MET:HE2	6:1G:148:MET:HB2	1.72	0.42
18:1W:71:VAL:HA	18:1W:107:LEU:HD23	2.02	0.42
32:1a:1284:C:OP2	32:1a:1285:A:O2'	2.35	0.42
33:1b:32:ILE:HD13	33:1b:40:HIS:CD2	2.55	0.42
38:1g:58:PRO:O	38:1g:61:VAL:HG12	2.19	0.42
1:2A:840:C:H2'	1:2A:841:A:C8	2.54	0.42
1:2A:1027:A:C6	1:2A:1126:A:C4	3.07	0.42
1:2A:1359:A:H2	1:2A:1372:U:O4	2.03	0.42
1:2A:1468:C:C2	1:2A:1525:G:N2	2.88	0.42
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.43	0.42
1:2A:2758:A:C4	7:2H:67:LEU:HD21	2.54	0.42
6:2G:5:VAL:HG21	6:2G:100:TRP:HB3	2.02	0.42
32:2a:137:C:H2'	32:2a:138:G:C8	2.55	0.42
32:2a:707:C:H2'	32:2a:708:C:C6	2.55	0.42
32:2a:792:A:H4'	32:2a:793:U:C5'	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:840:C:H4'	32:2a:841:U:OP1	2.20	0.42
34:2c:52:LEU:HD12	34:2c:53:ALA:H	1.84	0.42
39:2h:7:ALA:O	39:2h:11:THR:OG1	2.29	0.42
51:2t:54:LYS:HB3	51:2t:54:LYS:HE2	1.78	0.42
1:1A:150:C:C2'	1:1A:151:C:H5'	2.50	0.42
1:1A:445:C:O2'	1:1A:446:G:H5'	2.20	0.42
1:1A:884:C:N4	1:1A:892:G:H1	2.14	0.42
1:1A:1174:A:H1'	1:1A:1175:U:O5'	2.19	0.42
1:1A:2115:G:H2'	1:1A:2116:G:H5"	2.01	0.42
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.35	0.42
6:1G:122:PRO:HB3	6:1G:170:ARG:HH12	1.84	0.42
8:1I:17:GLN:HG2	8:1I:18:VAL:N	2.35	0.42
16:1U:47:TYR:HA	16:1U:50:ARG:NH2	2.34	0.42
32:1a:582:U:H2'	32:1a:583:A:C8	2.55	0.42
32:1a:1152:A:H2'	32:1a:1153:C:H6	1.84	0.42
1:2A:39:C:H2'	1:2A:40:C:C6	2.55	0.42
1:2A:315:G:H2'	1:2A:316:C:C6	2.55	0.42
1:2A:956:G:H2'	1:2A:957:A:H2'	2.02	0.42
1:2A:1009:A:OP2	9:2N:37:LYS:NZ	2.53	0.42
1:2A:1837:C:OP1	32:2a:784:C:H4'	2.19	0.42
1:2A:2262:U:H4'	1:2A:2328:A:C2	2.55	0.42
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.50	0.42
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	2.02	0.42
3:2D:20:ASP:HB2	3:2D:22:SER:OG	2.20	0.42
11:2P:88:LEU:HA	11:2P:91:PHE:CD2	2.54	0.42
14:2S:110:LEU:HD12	14:2S:110:LEU:HA	1.83	0.42
18:2W:5:ALA:C	18:2W:6:ILE:HG13	2.45	0.42
20:2Y:30:VAL:O	20:2Y:32:PRO:HD3	2.19	0.42
32:2a:23:C:H5	32:2a:561:U:O4	2.02	0.42
32:2a:458:C:H2'	32:2a:460:G:O4'	2.19	0.42
32:2a:580:U:H5"	46:2o:58:MET:HG2	2.01	0.42
32:2a:715:A:H2'	32:2a:716:A:C8	2.55	0.42
32:2a:841:U:C5	32:2a:848:C:H1'	2.55	0.42
32:2a:1041:A:H2'	32:2a:1042:G:C8	2.55	0.42
34:2c:58:GLU:HB3	41:2j:92:THR:CG2	2.41	0.42
35:2d:114:ARG:O	35:2d:118:ARG:N	2.49	0.42
40:2i:88:TYR:C	40:2i:88:TYR:CD2	2.98	0.42
54:2w:21:A:N6	54:2w:46:G7M:C4	2.82	0.42
54:2w:70:G:H8	54:2w:70:G:OP2	2.02	0.42
1:1A:478:A:C6	1:1A:480:A:C6	3.08	0.42
1:1A:1006:C:C2	1:1A:1138:G:N2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1253:A:OP1	62:1A:4264:HOH:O	2.21	0.42
1:1A:1301:A:O2'	1:1A:1302:A:H3'	2.20	0.42
1:1A:2512:C:H2'	1:1A:2513:G:O4'	2.20	0.42
1:1A:2857:G:N2	1:1A:2860:A:OP2	2.44	0.42
4:1E:37:ARG:HA	4:1E:42:ASP:OD2	2.20	0.42
5:1F:64:ILE:HD12	5:1F:65:TRP:CZ3	2.55	0.42
7:1H:154:PRO:HB3	7:1H:163:TYR:CE1	2.55	0.42
7:1H:170:ARG:O	7:1H:171:LEU:HD23	2.20	0.42
8:1I:5:LEU:HD21	8:1I:12:LEU:HB3	2.02	0.42
15:1T:33:LYS:O	15:1T:82:LEU:HD23	2.19	0.42
35:1d:128:VAL:HB	35:1d:133:VAL:HG21	2.01	0.42
44:1m:11:ARG:C	44:1m:13:LYS:H	2.27	0.42
44:1m:53:VAL:O	44:1m:57:ARG:HB3	2.20	0.42
1:2A:272(D):G:C2	1:2A:272(E):G:C8	3.08	0.42
1:2A:323:G:H1'	1:2A:1205:U:O2	2.19	0.42
1:2A:763:G:H1'	1:2A:765:G:O4'	2.20	0.42
1:2A:773:U:O2'	3:2D:48:ARG:HD3	2.20	0.42
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.44	0.42
1:2A:2286:A:H4'	1:2A:2287:A:O4'	2.20	0.42
1:2A:2320:A:H2'	1:2A:2320:A:N3	2.35	0.42
1:2A:2335:A:O2'	1:2A:2336:A:OP2	2.38	0.42
1:2A:2572:A:C8	4:2E:144:ARG:HD3	2.54	0.42
4:2E:127:ASP:OD2	62:2E:401:HOH:O	2.21	0.42
6:2G:45:GLU:H	6:2G:45:GLU:HG2	1.48	0.42
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.55	0.42
8:2I:58:LEU:HD22	8:2I:62:LYS:HG3	2.01	0.42
9:2N:32:THR:HG23	9:2N:37:LYS:HB2	2.02	0.42
10:2O:48:PRO:HB2	10:2O:49:ARG:CZ	2.50	0.42
14:2S:26:LEU:HD13	14:2S:85:VAL:HG11	2.01	0.42
16:2U:97:ASP:OD1	16:2U:101:ARG:HD2	2.20	0.42
18:2W:57:ASN:HA	18:2W:61:ASN:ND2	2.34	0.42
19:2X:46:ALA:HB1	24:22:33:MET:HE1	2.02	0.42
32:2a:110:C:O2'	47:2p:25:ARG:O	2.35	0.42
32:2a:913:A:OP1	43:2l:46:LYS:NZ	2.53	0.42
32:2a:1442:G:O2'	32:2a:1442(A):G:H5'	2.20	0.42
34:2c:101:LEU:HD22	34:2c:101:LEU:HA	1.91	0.42
34:2c:114:PRO:CA	34:2c:185:GLY:HA3	2.49	0.42
40:2i:85:LEU:HB3	40:2i:92:TYR:CD2	2.55	0.42
49:2r:32:ARG:HA	49:2r:69:THR:HG21	2.02	0.42
1:1A:41:C:H2'	1:1A:42:G:O4'	2.20	0.42
1:1A:861:A:C2	1:1A:917:A:C4	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2483:C:N3	12:1Q:124:LYS:NZ	2.62	0.42
4:1E:119:ARG:HG2	4:1E:120:TRP:CE2	2.54	0.42
4:1E:119:ARG:HD2	4:1E:160:TYR:HB2	2.02	0.42
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.20	0.42
11:1P:106:LEU:HD22	11:1P:112:LEU:HB2	2.02	0.42
12:1Q:8:LYS:HG2	12:1Q:9:TYR:CE2	2.55	0.42
13:1R:61:HIS:O	13:1R:65:LEU:HG	2.19	0.42
19:1X:94:GLY:H	19:1X:95:LEU:C	2.27	0.42
32:1a:31:G:N2	32:1a:47:C:O5'	2.53	0.42
32:1a:381:C:H2'	32:1a:382:A:O4'	2.20	0.42
32:1a:790:A:OP1	55:1x:38:A:O2'	2.34	0.42
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.55	0.42
32:1a:1169:A:H2'	32:1a:1170:A:C8	2.55	0.42
32:1a:1328:C:H2'	32:1a:1329:A:O4'	2.20	0.42
32:1a:1511:G:H2'	32:1a:1512:U:O4'	2.19	0.42
33:1b:158:LEU:HD23	33:1b:158:LEU:HA	1.91	0.42
40:1i:11:LYS:C	40:1i:13:ALA:H	2.27	0.42
40:1i:53:VAL:HG11	40:1i:92:TYR:CD1	2.55	0.42
1:2A:524:U:H2'	1:2A:525:U:C6	2.55	0.42
1:2A:1149:G:H2'	1:2A:1150:C:H6	1.84	0.42
1:2A:1591:G:H2'	1:2A:1592:C:C6	2.55	0.42
1:2A:1791:A:H3'	1:2A:1792:G:H8	1.85	0.42
1:2A:1851:U:C4	1:2A:1852:C:C4	3.08	0.42
1:2A:1920:OMC:HM22	1:2A:1921:G:H5'	2.02	0.42
1:2A:2493:U:H2'	1:2A:2494:G:O4'	2.20	0.42
4:2E:108:SER:HB3	4:2E:165:VAL:HG21	2.02	0.42
9:2N:4:TYR:HB2	16:2U:101:ARG:NH1	2.35	0.42
14:2S:80:LEU:HD23	14:2S:80:LEU:HA	1.84	0.42
16:2U:107:ALA:O	16:2U:111:GLU:HG2	2.20	0.42
32:2a:532:A:C2	32:2a:1055:A:H1'	2.55	0.42
32:2a:945:G:N1	32:2a:1337:G:C2	2.88	0.42
32:2a:1004:A:N6	32:2a:1037:C:O2	2.47	0.42
32:2a:1273:G:H3'	32:2a:1274:G:H8	1.85	0.42
33:2b:169:LYS:O	33:2b:169:LYS:HD3	2.20	0.42
40:2i:104:ARG:HG2	40:2i:105:ASP:N	2.34	0.42
44:2m:50:GLU:O	44:2m:54:VAL:HG22	2.20	0.42
1:1A:628:G:H2'	1:1A:629:G:C8	2.55	0.41
1:1A:774:A:N3	1:1A:774:A:H2'	2.35	0.41
2:1B:66:A:N6	2:1B:109:C:H5'	2.33	0.41
4:1E:77:ILE:HD12	4:1E:195:LEU:HD13	2.01	0.41
7:1H:77:LYS:HD3	7:1H:83:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:6:LEU:HD11	8:1I:37:VAL:HG23	2.02	0.41
18:1W:84:ARG:HG3	18:1W:98:LYS:HD2	2.02	0.41
26:14:18:CYS:SG	26:14:20:ASN:HB2	2.59	0.41
32:1a:333:G:H4'	51:1t:16:HIS:CE1	2.55	0.41
32:1a:1158:C:H2'	32:1a:1159:U:H4'	2.02	0.41
33:1b:87:ARG:CZ	33:1b:233:SER:HB3	2.50	0.41
39:1h:58:TYR:O	39:1h:59:LEU:HD23	2.20	0.41
44:1m:49:THR:HB	44:1m:52:GLU:H	1.85	0.41
44:1m:67:GLU:HG3	44:1m:71:ARG:HH21	1.84	0.41
57:1y:26:A:N6	57:1y:44:G:H1	2.16	0.41
1:2A:996:A:H4'	16:2U:91:ASP:OD2	2.19	0.41
1:2A:2024:G:H2'	1:2A:2025:C:C6	2.55	0.41
1:2A:2690:C:N4	1:2A:2713:A:H1'	2.35	0.41
10:2O:63:VAL:HG22	10:2O:84:ALA:HA	2.02	0.41
12:2Q:1:MET:HE2	12:2Q:1:MET:HB2	1.96	0.41
14:2S:105:ALA:HB1	14:2S:110:LEU:HD23	2.01	0.41
30:28:14:VAL:HG13	30:28:22:VAL:HG13	2.01	0.41
32:2a:109:A:H5'	32:2a:110:C:C5	2.55	0.41
32:2a:130:A:H1'	32:2a:263:A:O2'	2.20	0.41
32:2a:445:G:H2'	32:2a:446:G:H8	1.85	0.41
32:2a:583:A:N6	32:2a:758:G:O2'	2.52	0.41
32:2a:1041:A:H2'	32:2a:1042:G:H8	1.84	0.41
32:2a:1446:U:H3	32:2a:1452:C:C1'	2.33	0.41
33:2b:58:ILE:O	33:2b:62:ALA:N	2.45	0.41
43:2l:117:ARG:HB3	43:2l:122:THR:O	2.20	0.41
44:2m:44:ARG:O	44:2m:48:LEU:HG	2.20	0.41
1:1A:593:G:H4'	30:18:4:MET:HE2	2.02	0.41
1:1A:971:C:O2'	1:1A:983:A:N3	2.48	0.41
1:1A:2143:C:H2'	1:1A:2144:U:O4'	2.20	0.41
1:1A:2168:G:N2	1:1A:2171:A:N7	2.67	0.41
2:1B:78:A:C2	2:1B:100:A:C4	3.08	0.41
3:1D:130:ALA:C	3:1D:131:LEU:HD12	2.44	0.41
23:11:50:ARG:HG2	23:11:59:THR:CG2	2.50	0.41
32:1a:444:C:H2'	32:1a:445:G:H8	1.86	0.41
34:1c:82:GLU:O	34:1c:85:ARG:HG3	2.20	0.41
36:1e:83:GLU:HA	36:1e:87:SER:O	2.20	0.41
55:1x:20:U:H6	55:1x:20:U:O5'	2.03	0.41
1:2A:272(E):G:C2	1:2A:364:C:C2	3.08	0.41
1:2A:693:C:H2'	1:2A:694:U:C6	2.55	0.41
1:2A:940:G:H2'	1:2A:941:A:O4'	2.20	0.41
1:2A:1283:G:O2'	1:2A:1285:G:N7	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1945:G:H2'	1:2A:1946:U:C6	2.56	0.41
1:2A:2080:G:H2'	1:2A:2081:C:H6	1.85	0.41
1:2A:2127:G:C2	1:2A:2161:C:C4	3.08	0.41
9:2N:62:VAL:CG1	9:2N:66:LYS:HB2	2.51	0.41
15:2T:61:PHE:CE2	15:2T:76:PHE:HB2	2.54	0.41
35:2d:18:LYS:HE3	35:2d:20:TYR:CE1	2.56	0.41
36:2e:72:GLN:O	36:2e:75:THR:HG22	2.20	0.41
39:2h:23:SER:OG	39:2h:24:THR:N	2.53	0.41
41:2j:49:VAL:HG21	45:2n:41:ARG:O	2.20	0.41
49:2r:26:LEU:HD11	49:2r:42:ARG:HD3	2.02	0.41
51:2t:77:ALA:O	51:2t:81:LYS:HG3	2.20	0.41
1:1A:484:C:H2'	1:1A:485:C:H6	1.85	0.41
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.54	0.41
1:1A:1274:A:N3	1:1A:1297:C:H1'	2.35	0.41
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.19	0.41
23:11:73:LEU:HD22	23:11:97:LEU:HB2	2.01	0.41
23:11:82:LEU:O	23:11:85:LEU:HD12	2.21	0.41
32:1a:193:C:H2'	32:1a:194:C:C6	2.54	0.41
32:1a:341:C:H2'	32:1a:342:C:H6	1.85	0.41
32:1a:401:C:H2'	32:1a:402:G:C8	2.55	0.41
32:1a:1219:U:OP1	45:1n:19:ARG:NH1	2.48	0.41
38:1g:26:PHE:CE2	38:1g:30:ILE:HD11	2.55	0.41
44:1m:2:ALA:N	44:1m:8:GLU:HB2	2.35	0.41
51:1t:59:ALA:O	51:1t:63:ILE:HG13	2.21	0.41
57:1y:58:A:N3	57:1y:60:U:C5	2.88	0.41
1:2A:196:A:N3	1:2A:196:A:H2'	2.36	0.41
1:2A:645:C:H5"	1:2A:646:A:OP2	2.21	0.41
1:2A:807:U:P	11:2P:36:LYS:HD3	2.60	0.41
1:2A:1561:G:H2'	1:2A:1562:A:H8	1.84	0.41
1:2A:2114:A:H2'	1:2A:2114:A:N3	2.34	0.41
6:2G:67:LYS:H	26:24:6:HIS:CE1	2.38	0.41
6:2G:124:SER:O	6:2G:124:SER:OG	2.35	0.41
11:2P:67:MET:HE3	11:2P:67:MET:HB2	1.93	0.41
21:2Z:150:LEU:O	21:2Z:171:ILE:HG13	2.20	0.41
21:2Z:157:LEU:HD23	21:2Z:161:VAL:O	2.20	0.41
26:24:50:VAL:HG11	44:2m:64:TRP:O	2.19	0.41
32:2a:48:C:OP2	62:2a:1918:HOH:O	2.22	0.41
32:2a:790:A:C6	32:2a:791:G:C6	3.08	0.41
32:2a:1411:C:H2'	32:2a:1412:C:C6	2.54	0.41
54:2w:9:A:O2'	54:2w:10:G:N7	2.50	0.41
1:1A:285:C:H2'	1:1A:286:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:963:U:H5'	1:1A:2497:A:OP1	2.20	0.41
1:1A:2304:G:H22	1:1A:2312:U:H3	1.68	0.41
1:1A:2889:C:H2'	1:1A:2891:G:O4'	2.20	0.41
5:1F:34:TRP:NE1	11:1P:8:PRO:HD3	2.35	0.41
10:1O:78:ARG:NH2	15:1T:73:GLU:OE1	2.50	0.41
13:1R:87:TYR:OH	13:1R:117:VAL:O	2.36	0.41
21:1Z:48:PHE:HA	21:1Z:51:ALA:HB3	2.02	0.41
32:1a:194:C:C2'	32:1a:195:A:H5"	2.50	0.41
32:1a:270:A:H2'	32:1a:271:C:O4'	2.20	0.41
32:1a:317:G:C6	32:1a:318:G:C5	3.08	0.41
32:1a:396:G:O2'	32:1a:398:C:OP1	2.17	0.41
32:1a:487:A:H2'	32:1a:488:C:O4'	2.21	0.41
32:1a:1284:C:H3'	32:1a:1285:A:C8	2.55	0.41
40:1i:96:LEU:HD13	40:1i:101:PHE:CD2	2.49	0.41
55:1x:19:G:H4'	55:1x:20:U:OP2	2.20	0.41
1:2A:271(P):C:O2'	8:2I:42:SER:OG	2.32	0.41
1:2A:896:A:H4'	1:2A:897:C:OP1	2.20	0.41
1:2A:1021:A:H3'	1:2A:1021:A:H8	1.85	0.41
1:2A:1508:A:H4'	1:2A:1509(A):A:C5	2.55	0.41
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.56	0.41
1:2A:2102:U:H2'	1:2A:2103:C:C6	2.55	0.41
1:2A:2271:G:OP1	22:20:18:ALA:HB1	2.21	0.41
1:2A:2296:U:H4'	1:2A:2297:C:OP1	2.20	0.41
1:2A:2626:C:H2'	1:2A:2627:G:O4'	2.20	0.41
3:2D:8:PRO:HB3	3:2D:14:ARG:HG3	2.02	0.41
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	2.02	0.41
5:2F:28:ILE:HD11	5:2F:115:ALA:HB3	2.03	0.41
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.36	0.41
8:2I:64:GLU:O	8:2I:68:LEU:HD12	2.21	0.41
8:2I:133:HIS:HD2	8:2I:134:PRO:HD2	1.85	0.41
13:2R:26:LYS:HE2	13:2R:70:LEU:O	2.21	0.41
16:2U:27:LEU:HB3	16:2U:31:SER:HB3	2.03	0.41
18:2W:18:ARG:HG2	18:2W:76:VAL:HB	2.02	0.41
24:22:25:VAL:HG11	24:22:61:LEU:HD21	2.01	0.41
32:2a:224:C:H2'	32:2a:225:C:C6	2.55	0.41
32:2a:1258:G:H2'	32:2a:1259:C:C6	2.55	0.41
36:2e:36:ASP:O	36:2e:38:GLN:N	2.44	0.41
36:2e:140:ARG:O	36:2e:143:ARG:NH1	2.40	0.41
37:2f:91:VAL:HG12	37:2f:92:LYS:O	2.20	0.41
50:2s:28:LYS:HA	50:2s:28:LYS:HD3	1.93	0.41
57:2y:14:A:N6	57:2y:21:A:H2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1100:C:H5'	1:1A:1101:U:OP2	2.20	0.41
1:1A:1253:A:OP1	62:1A:4269:HOH:O	2.22	0.41
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.55	0.41
1:1A:2203:U:O4'	3:1D:151:LYS:HE2	2.20	0.41
1:1A:2271:G:H5"	22:10:20:ARG:NH1	2.34	0.41
8:1I:38:LEU:H	8:1I:38:LEU:CD2	2.32	0.41
32:1a:309:G:O2'	32:1a:607:A:N1	2.54	0.41
32:1a:453:A:C5	32:1a:454:C:C4	3.08	0.41
32:1a:503:C:OP1	43:1l:119:LYS:NZ	2.42	0.41
32:1a:1098:C:C2	32:1a:1099:G:C8	3.09	0.41
33:1b:139:LYS:O	33:1b:143:GLU:HG3	2.20	0.41
35:1d:131:ARG:O	35:1d:133:VAL:HG23	2.21	0.41
42:1k:82:VAL:HB	42:1k:108:ILE:HG12	2.02	0.41
57:1y:57:G:C2'	57:1y:58:A:H5'	2.49	0.41
1:2A:463:G:OP2	62:2A:3954:HOH:O	2.22	0.41
1:2A:2129:C:H5'	1:2A:2130:U:OP2	2.20	0.41
1:2A:2387:U:H4'	22:20:41:ARG:NH2	2.34	0.41
1:2A:2785:C:H1'	4:2E:66:HIS:CE1	2.56	0.41
2:2B:88:C:H2'	2:2B:89:G:O4'	2.20	0.41
6:2G:7:LEU:HD22	6:2G:104:GLU:N	2.34	0.41
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.55	0.41
8:2I:71:ILE:O	8:2I:75:LEU:HG	2.21	0.41
11:2P:6:LEU:HA	11:2P:6:LEU:HD23	1.67	0.41
11:2P:50:ARG:HH21	30:28:7:HIS:HD2	1.68	0.41
15:2T:102:ILE:HB	15:2T:110:ILE:HG12	2.02	0.41
21:2Z:40:ASP:OD2	21:2Z:43:GLU:N	2.38	0.41
32:2a:99:U:H2'	32:2a:100:C:C6	2.55	0.41
32:2a:232:G:H1'	32:2a:262:A:N1	2.35	0.41
32:2a:664:G:P	49:2r:64:ARG:HH21	2.43	0.41
32:2a:1360:A:H8	32:2a:1360:A:OP1	2.04	0.41
35:2d:94:LEU:O	35:2d:98:GLU:N	2.54	0.41
35:2d:107:ARG:HH12	35:2d:194:LEU:HD23	1.85	0.41
39:2h:2:LEU:HD11	39:2h:8:ASP:HB2	2.02	0.41
41:2j:55:LYS:HE3	41:2j:56:HIS:NE2	2.36	0.41
43:2l:53:ARG:HB3	43:2l:69:TYR:HE1	1.84	0.41
43:2l:89:ARG:NH2	43:2l:91:LYS:HA	2.34	0.41
46:2o:82:ILE:HD12	46:2o:88:ARG:HB2	2.02	0.41
1:1A:2252:G:OP2	62:1A:4267:HOH:O	2.22	0.41
7:1H:121:ILE:HG13	7:1H:144:VAL:HG21	2.03	0.41
13:1R:65:LEU:HD23	13:1R:65:LEU:HA	1.81	0.41
15:1T:108:ARG:HG3	15:1T:109:GLU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1X:50:LYS:NZ	62:1X:201:HOH:O	2.49	0.41
32:1a:397:A:H3'	32:1a:397:A:N3	2.35	0.41
32:1a:511:C:H4'	35:1d:43:HIS:CD2	2.56	0.41
32:1a:1304:G:C6	32:1a:1305:G:N1	2.89	0.41
35:1d:164:ALA:O	35:1d:168:ARG:HG3	2.20	0.41
41:1j:31:GLY:HA3	41:1j:32:ALA:HA	1.77	0.41
44:1m:34:LEU:HD13	44:1m:41:PRO:HA	2.01	0.41
51:1t:10:LEU:HD13	51:1t:10:LEU:HA	1.81	0.41
1:2A:995:C:O2	9:2N:3:THR:OG1	2.34	0.41
1:2A:1312:U:OP2	19:2X:63:LYS:HD2	2.20	0.41
1:2A:2125:G:H1'	1:2A:2173:A:N6	2.36	0.41
1:2A:2555:U:C4	1:2A:2556:C:C2	3.08	0.41
1:2A:2774:C:H2'	1:2A:2775:A:O4'	2.20	0.41
1:2A:2848:G:H1'	1:2A:2867:G:N2	2.35	0.41
2:2B:17:C:H2'	2:2B:18:G:O4'	2.20	0.41
3:2D:71:ASP:HB2	3:2D:103:ARG:HH12	1.85	0.41
5:2F:53:THR:HG22	5:2F:56:GLU:CD	2.46	0.41
7:2H:20:ALA:HB3	7:2H:23:ARG:HB2	2.03	0.41
14:2S:29:PHE:O	14:2S:35:ILE:HA	2.20	0.41
17:2V:76:LYS:HB2	17:2V:81:TYR:HD2	1.85	0.41
32:2a:8:A:N6	35:2d:209:ARG:HB2	2.35	0.41
32:2a:664:G:N2	32:2a:741:G:H1	2.19	0.41
32:2a:914:A:H2'	32:2a:915:A:H8	1.85	0.41
32:2a:946:A:H2'	32:2a:947:G:C8	2.55	0.41
32:2a:963:G:H5'	62:2a:1990:HOH:O	2.19	0.41
32:2a:986:A:H1'	50:2s:54:GLY:O	2.20	0.41
32:2a:1157:A:C5	32:2a:1181:G:C6	3.09	0.41
32:2a:1375:A:H2'	32:2a:1376:U:O4'	2.21	0.41
33:2b:83:MET:HG3	33:2b:234:PRO:HG3	2.01	0.41
33:2b:150:SER:OG	33:2b:151:GLY:N	2.54	0.41
35:2d:57:ARG:H	35:2d:57:ARG:HG2	1.64	0.41
35:2d:155:LEU:O	35:2d:159:ARG:HG3	2.21	0.41
36:2e:62:ALA:C	36:2e:64:ARG:H	2.29	0.41
37:2f:67:MET:HE1	37:2f:75:LEU:HD22	2.03	0.41
41:2j:74:ILE:HG22	62:2j:302:HOH:O	2.21	0.41
48:2q:4:LYS:HE3	48:2q:6:LEU:HD21	2.03	0.41
49:2r:68:LYS:HE2	49:2r:68:LYS:HB2	1.91	0.41
50:2s:6:LYS:H	50:2s:6:LYS:HG2	1.59	0.41
1:1A:75:G:H4'	24:12:55:ARG:NH2	2.35	0.41
1:1A:1486:A:H2'	1:1A:1487:G:C8	2.56	0.41
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:155:SER:HB3	7:1H:158:HIS:O	2.21	0.41
32:1a:383:A:H5"	32:1a:384:G:OP2	2.20	0.41
32:1a:1166:G:N2	32:1a:1170:A:OP2	2.53	0.41
55:1x:21:A:H3'	55:1x:46:G:O6	2.20	0.41
1:2A:667:U:O2	30:28:2:PRO:HD2	2.21	0.41
1:2A:811:U:H2'	11:2P:21:ARG:HA	2.01	0.41
1:2A:2313:C:H4'	6:2G:91:ARG:HG3	2.01	0.41
1:2A:2412:A:H2'	1:2A:2413:G:O4'	2.20	0.41
14:2S:25:ARG:NH1	14:2S:42:ASP:OD2	2.54	0.41
23:21:3:LYS:O	23:21:12:PRO:HD3	2.20	0.41
31:29:18:ARG:NH1	31:29:21:GLY:HA2	2.36	0.41
32:2a:251:G:N1	32:2a:266:G:O6	2.54	0.41
32:2a:445:G:H2'	32:2a:446:G:C8	2.55	0.41
32:2a:540:G:C6	32:2a:541:G:C5	3.09	0.41
32:2a:762:C:H2'	32:2a:763:G:C8	2.55	0.41
32:2a:964:A:N3	32:2a:969:A:O2'	2.45	0.41
32:2a:1118:C:H1'	32:2a:1179:A:C5	2.55	0.41
32:2a:1270:C:H2'	32:2a:1271:G:C8	2.55	0.41
34:2c:87:LEU:O	34:2c:91:LEU:HD12	2.20	0.41
48:2q:81:ARG:HH21	48:2q:84:LEU:HD21	1.86	0.41
57:2y:23:A:C5	57:2y:24:G:C8	3.08	0.41
1:1A:30:G:C5	1:1A:31:C:C4	3.09	0.41
1:1A:1063:G:H2'	1:1A:1064:C:H5	1.86	0.41
1:1A:1256:G:H1'	5:1F:82:ILE:HD11	2.02	0.41
1:1A:1796:U:H2'	1:1A:1797:C:H6	1.82	0.41
1:1A:2093:G:C6	1:1A:2225:A:C8	3.09	0.41
1:1A:2175:C:H2'	1:1A:2176:A:O4'	2.21	0.41
1:1A:2712:U:OP1	1:1A:2714:G:H4'	2.21	0.41
3:1D:218:ARG:HB3	3:1D:219:PRO:HD2	2.02	0.41
7:1H:35:VAL:HG11	7:1H:71:LEU:HB3	2.02	0.41
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.69	0.41
26:14:40:HIS:ND1	26:14:42:PHE:HB3	2.35	0.41
27:15:11:THR:CG2	27:15:15:ARG:HB3	2.50	0.41
32:1a:1324:A:H2'	32:1a:1325:C:O4'	2.20	0.41
33:1b:204:ASN:OD1	33:1b:206:ASP:N	2.30	0.41
35:1d:94:LEU:HD23	35:1d:94:LEU:HA	1.94	0.41
45:1n:33:VAL:HA	45:1n:40:CYS:HA	2.02	0.41
50:1s:40:ILE:HA	50:1s:44:MET:SD	2.60	0.41
1:2A:36:G:OP1	62:2A:3955:HOH:O	2.22	0.41
1:2A:272(A):U:H5'	1:2A:272(B):G:OP2	2.21	0.41
1:2A:1024:G:C6	1:2A:1025:G:C6	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1199:U:H2'	1:2A:1200:C:C6	2.56	0.41
1:2A:1359:A:C2	1:2A:1360:A:C8	3.09	0.41
1:2A:1359:A:C2	1:2A:1372:U:O4	2.74	0.41
1:2A:1490:A:O2'	3:2D:99:ASP:OD1	2.31	0.41
1:2A:1668:A:O2'	1:2A:1674:G:N7	2.37	0.41
1:2A:2128:C:H2'	1:2A:2129:C:O4'	2.21	0.41
1:2A:2156:G:H2'	1:2A:2157:G:C2	2.55	0.41
1:2A:2400:G:H2'	1:2A:2401:U:C6	2.56	0.41
1:2A:2734:A:H62	1:2A:2770:G:H21	1.69	0.41
4:2E:7:VAL:HG23	4:2E:51:PHE:HE2	1.85	0.41
9:2N:73:THR:OG1	9:2N:82:LEU:HD11	2.21	0.41
21:2Z:44:PHE:CE1	21:2Z:86:VAL:HG21	2.55	0.41
21:2Z:54:HIS:HB2	21:2Z:55:HIS:CD2	2.56	0.41
21:2Z:100:VAL:HA	21:2Z:101:PRO:HD3	1.94	0.41
21:2Z:144:LEU:HD21	21:2Z:173:ALA:HB1	2.01	0.41
32:2a:20:U:H2'	32:2a:21:G:O4'	2.20	0.41
32:2a:44:G:H2'	32:2a:45:U:O4'	2.20	0.41
32:2a:141:A:O2'	32:2a:182:U:H1'	2.19	0.41
32:2a:340:U:C2	32:2a:350:G:N2	2.89	0.41
32:2a:657:G:H4'	46:2o:28:GLN:HG2	2.02	0.41
32:2a:1085:U:H3'	32:2a:1086:U:C6	2.56	0.41
32:2a:1123:A:H4'	41:2j:36:GLY:HA3	2.03	0.41
32:2a:1369:C:H2'	32:2a:1370:G:O4'	2.21	0.41
33:2b:182:ILE:HA	33:2b:183:PRO:HD3	1.97	0.41
35:2d:20:TYR:HD1	35:2d:26:CYS:HB3	1.85	0.41
35:2d:200:GLU:OE1	35:2d:200:GLU:N	2.52	0.41
40:2i:9:ARG:HG2	40:2i:14:VAL:HG12	2.02	0.41
42:2k:82:VAL:O	42:2k:109:VAL:HG12	2.21	0.41
43:2l:28:LYS:HE2	43:2l:28:LYS:HB3	1.91	0.41
44:2m:50:GLU:O	44:2m:53:VAL:HG22	2.21	0.41
55:2x:58:A:H4'	55:2x:59:A:OP1	2.20	0.41
1:1A:271(E):U:H2'	1:1A:271(F):C:C6	2.56	0.41
1:1A:292:C:H2'	1:1A:293:U:C6	2.56	0.41
1:1A:563:G:H22	1:1A:578:A:H2	1.69	0.41
1:1A:956:G:H2'	1:1A:957:A:H2'	2.02	0.41
1:1A:1268:A:C2	1:1A:2013:A:C4	3.09	0.41
1:1A:1359:A:C2	1:1A:1372:U:O4	2.73	0.41
1:1A:1669:A:H5"	1:1A:2550:G:OP1	2.20	0.41
1:1A:1882:C:H2'	1:1A:1883:G:O4'	2.21	0.41
1:1A:2439:A:H5'	1:1A:2439:A:C8	2.56	0.41
2:1B:119:G:C6	2:1B:120:A:C6	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:116:GLN:HE21	3:1D:116:GLN:HB3	1.70	0.41
4:1E:28:ALA:HB3	4:1E:93:VAL:CG1	2.51	0.41
11:1P:98:GLU:O	11:1P:101:VAL:HG12	2.21	0.41
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.85	0.41
21:1Z:62:PRO:C	21:1Z:64:GLY:H	2.29	0.41
25:13:4:LEU:O	25:13:36:VAL:HA	2.21	0.41
32:1a:911:U:H2'	32:1a:912:C:C6	2.56	0.41
32:1a:1112:C:N3	34:1c:178:LEU:HB2	2.36	0.41
32:1a:1309:G:OP2	44:1m:99:ARG:NH2	2.53	0.41
33:1b:102:LEU:HB3	33:1b:180:LEU:CD1	2.51	0.41
35:1d:65:ARG:HH11	35:1d:72:GLU:HB2	1.84	0.41
35:1d:112:VAL:H	35:1d:116:GLN:NE2	2.19	0.41
37:1f:42:GLU:OE2	37:1f:59:TYR:OH	2.36	0.41
38:1g:52:GLU:HB2	38:1g:53:LYS:H	1.71	0.41
44:1m:16:ASP:OD1	44:1m:16:ASP:N	2.53	0.41
44:1m:87:TYR:HA	44:1m:90:LEU:HD12	2.02	0.41
57:1y:8:4SU:S4	57:1y:14:A:N7	2.93	0.41
57:1y:15:G:N2	57:1y:48:C:H42	2.19	0.41
57:1y:71:G:H2'	57:1y:72:C:H6	1.86	0.41
1:2A:522:G:H2'	1:2A:523:C:C6	2.56	0.41
1:2A:652(U):G:H2'	1:2A:652(V):C:O4'	2.20	0.41
1:2A:747:U:O2	1:2A:2014:A:H1'	2.20	0.41
1:2A:1005:C:H2'	1:2A:1006:C:H6	1.85	0.41
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.55	0.41
1:2A:1374:G:H2'	1:2A:1375:C:C6	2.55	0.41
1:2A:1423:G:OP1	1:2A:1492:G:O2'	2.38	0.41
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.21	0.41
1:2A:1651:G:H2'	1:2A:1652:A:O4'	2.21	0.41
1:2A:1682:G:H1'	1:2A:1762:A:C6	2.56	0.41
1:2A:1754:C:H2'	1:2A:1755:A:O4'	2.21	0.41
1:2A:2390:U:O2'	1:2A:2391:G:H5'	2.21	0.41
4:2E:119:ARG:HG2	4:2E:120:TRP:CE2	2.55	0.41
6:2G:116:ASP:CG	44:2m:68:GLY:HA3	2.46	0.41
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.56	0.41
11:2P:63:PRO:HG2	30:28:25:MET:HB2	2.03	0.41
11:2P:101:VAL:HG21	11:2P:108:LYS:HG2	2.01	0.41
12:2Q:1:MET:HB3	12:2Q:44:ALA:HB1	2.03	0.41
12:2Q:43:THR:HA	12:2Q:94:VAL:HG12	2.03	0.41
18:2W:4:LYS:HG2	18:2W:5:ALA:N	2.34	0.41
21:2Z:47:VAL:O	21:2Z:50:GLN:NE2	2.54	0.41
21:2Z:70:LEU:HD12	21:2Z:71:VAL:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:5:U:H5'	32:2a:6:G:C5	2.55	0.41
32:2a:107:G:H2'	32:2a:108:G:O4'	2.21	0.41
32:2a:193:C:H2'	32:2a:194:C:C6	2.56	0.41
32:2a:424:G:H2'	32:2a:425:G:C8	2.56	0.41
32:2a:607:A:H2'	32:2a:608:A:O4'	2.21	0.41
32:2a:923:A:OP1	36:2e:21:ALA:HB2	2.21	0.41
32:2a:1003:G:H2'	32:2a:1004:A:O4'	2.21	0.41
32:2a:1128:C:H1'	32:2a:1147:C:N4	2.35	0.41
32:2a:1250:A:H4'	40:2i:68:GLY:N	2.36	0.41
32:2a:1478:C:H2'	32:2a:1479:C:H6	1.86	0.41
35:2d:58:LEU:HD23	35:2d:58:LEU:HA	1.89	0.41
37:2f:94:GLN:HE22	49:2r:72:ARG:HH12	1.69	0.41
37:2f:99:ALA:HB1	49:2r:23:LYS:NZ	2.35	0.41
44:2m:113:PRO:O	44:2m:115:LYS:NZ	2.54	0.41
45:2n:32:SER:O	45:2n:40:CYS:HA	2.20	0.41
47:2p:22:THR:HA	47:2p:33:ILE:HG13	2.03	0.41
49:2r:33:ASP:CG	49:2r:36:ASN:HB2	2.46	0.41
51:2t:38:LYS:HE2	51:2t:38:LYS:HB3	1.95	0.41
55:2x:15:G:H2'	55:2x:59:A:N1	2.36	0.41
57:2y:35:A:C6	57:2y:36:A:C2	3.08	0.41
57:2y:75:C:HO2'	57:2y:76:A:H8	1.64	0.41
1:1A:271(P):C:H2'	1:1A:271(Q):G:O4'	2.21	0.41
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.21	0.41
1:1A:504:U:H5"	1:1A:505:A:OP1	2.21	0.41
1:1A:882:G:H4'	54:1w:19:G:O6	2.21	0.41
1:1A:1092:C:C2'	1:1A:1093:G:H5'	2.51	0.41
1:1A:2028:U:H2'	1:1A:2029:G:O4'	2.20	0.41
1:1A:2064:C:H2'	1:1A:2065:C:C6	2.56	0.41
1:1A:2153:G:H2'	1:1A:2154:G:C8	2.56	0.41
62:1A:5687:HOH:O	9:1N:28:THR:HG23	2.20	0.41
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	2.02	0.41
5:1F:8:GLN:NE2	5:1F:21:ALA:HB2	2.36	0.41
9:1N:61:ARG:HD3	9:1N:61:ARG:HA	1.86	0.41
14:1S:77:ALA:HB3	14:1S:110:LEU:HD11	2.02	0.41
21:1Z:132:ASN:N	21:1Z:132:ASN:OD1	2.52	0.41
22:10:46:LYS:NZ	22:10:75:LEU:O	2.45	0.41
26:14:62:ARG:HB2	26:14:63:TYR:CD1	2.56	0.41
32:1a:636:U:H2'	32:1a:637:G:C8	2.49	0.41
32:1a:955:U:O2'	50:1s:83:HIS:HD2	2.03	0.41
32:1a:1106:G:O3'	34:1c:172:ARG:HB2	2.21	0.41
32:1a:1239:A:C4	32:1a:1298:C:N4	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:11:LEU:HD23	35:1d:66:ARG:HB3	2.03	0.41
36:1e:12:LEU:HB3	36:1e:31:LEU:HB3	2.02	0.41
40:1i:128:ARG:HD2	55:1x:35:A:OP1	2.22	0.41
46:1o:11:VAL:HG21	46:1o:34:LEU:HD22	2.03	0.41
49:1r:25:THR:O	49:1r:26:LEU:HG	2.21	0.41
57:1y:53:G:H1	57:1y:61:C:H42	1.68	0.41
1:2A:2061:G:OP1	5:2F:68:LYS:NZ	2.53	0.41
6:2G:116:ASP:OD1	44:2m:68:GLY:HA3	2.21	0.41
17:2V:2:PHE:CZ	17:2V:41:GLY:HA3	2.56	0.41
32:2a:129(A):G:C6	32:2a:189(E):U:H4'	2.56	0.41
32:2a:1045:C:H2'	32:2a:1046:A:O4'	2.21	0.41
35:2d:61:LYS:HE2	35:2d:61:LYS:HB3	1.85	0.41
51:2t:18:GLN:O	51:2t:22:ARG:HG3	2.21	0.41
57:2y:62:C:H2'	57:2y:63:G:H8	1.85	0.41
1:1A:620:G:N3	1:1A:620:G:H2'	2.35	0.40
1:1A:2540:C:H2'	1:1A:2541:A:O4'	2.21	0.40
1:1A:2740:A:H2'	1:1A:2741:A:C8	2.55	0.40
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.20	0.40
19:1X:11:PRO:HB2	19:1X:92:LEU:HD21	2.02	0.40
20:1Y:86:ARG:HB2	20:1Y:98:VAL:HG23	2.02	0.40
26:14:40:HIS:HB3	26:14:43:TYR:HD2	1.86	0.40
32:1a:411:A:OP2	35:1d:30:LYS:HD2	2.21	0.40
33:1b:85:ALA:HB1	33:1b:90:MET:O	2.21	0.40
44:1m:82:MET:O	44:1m:93:ARG:NH2	2.54	0.40
1:2A:584:C:OP2	16:2U:6:THR:OG1	2.37	0.40
1:2A:612:C:C2	1:2A:616:G:N2	2.89	0.40
1:2A:652(T):C:H5'	1:2A:652(U):G:OP2	2.21	0.40
1:2A:861:A:H2'	1:2A:862:G:O4'	2.20	0.40
1:2A:1155:A:H5"	16:2U:55:ARG:NE	2.36	0.40
1:2A:1287:A:C8	13:2R:104:ARG:HD3	2.54	0.40
5:2F:129:PHE:O	5:2F:130:ALA:C	2.64	0.40
12:2Q:16:ARG:HG3	12:2Q:17:LEU:H	1.85	0.40
23:21:82:LEU:HA	23:21:85:LEU:HD12	2.02	0.40
26:24:12:ALA:HB3	26:24:26:SER:HB3	2.02	0.40
32:2a:103:C:O2'	32:2a:172:A:N1	2.48	0.40
32:2a:684:A:C6	32:2a:685:G:C6	3.09	0.40
32:2a:942:G:C2	32:2a:1342:C:C2	3.08	0.40
33:2b:47:THR:HA	33:2b:202:PRO:HG2	2.03	0.40
50:2s:80:TYR:CZ	50:2s:82:GLY:HA2	2.56	0.40
52:2u:12:LYS:HB2	52:2u:22:ARG:HD3	2.03	0.40
54:2w:21:A:O2'	54:2w:22:G:P	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:2x:50:U:H2'	55:2x:51:C:C6	2.56	0.40
1:1A:11:G:C2'	1:1A:12:U:H5'	2.50	0.40
1:1A:330:A:H2'	1:1A:330:A:N3	2.36	0.40
1:1A:568:U:H5'	1:1A:945:A:N6	2.36	0.40
1:1A:1095:A:H2'	1:1A:1096:A:H8	1.87	0.40
1:1A:1491:G:O2'	3:1D:101:GLU:HB2	2.21	0.40
1:1A:1526:G:C6	1:1A:1527:G:C2	3.09	0.40
1:1A:2128:C:N4	1:1A:2160:G:C6	2.90	0.40
3:1D:26:LYS:NZ	3:1D:83:GLU:OE2	2.52	0.40
24:12:30:ARG:O	24:12:34:GLU:HG3	2.21	0.40
32:1a:595:G:H22	32:1a:643:C:H41	1.67	0.40
32:1a:674:G:H2'	32:1a:675:A:H8	1.86	0.40
32:1a:869:G:OP2	62:1a:1918:HOH:O	2.22	0.40
32:1a:1003:G:H2'	32:1a:1004:A:N3	2.36	0.40
32:1a:1005:A:C2	32:1a:1025:U:H1'	2.55	0.40
32:1a:1017:G:H2'	32:1a:1018:C:C6	2.56	0.40
32:1a:1060:C:C5	34:1c:2:GLY:HA3	2.56	0.40
34:1c:11:ARG:HB3	34:1c:15:THR:HB	2.03	0.40
39:1h:33:GLU:HG2	39:1h:48:TYR:OH	2.21	0.40
40:1i:75:ASP:HA	40:1i:78:LYS:HB3	2.03	0.40
57:1y:52:G:C6	57:1y:63:G:C6	3.10	0.40
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.21	0.40
1:2A:1220:A:OP2	16:2U:19:LYS:NZ	2.49	0.40
1:2A:2103:C:H2'	1:2A:2104:G:O4'	2.21	0.40
1:2A:2516:G:C6	1:2A:2517:C:C4	3.09	0.40
1:2A:2801(A):A:O2'	1:2A:2895:U:O4'	2.39	0.40
2:2B:119:G:C6	2:2B:120:A:C6	3.10	0.40
3:2D:29:PRO:HA	3:2D:83:GLU:OE1	2.22	0.40
4:2E:5:LEU:HD11	4:2E:79:ARG:HB2	2.03	0.40
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	2.02	0.40
9:2N:40:PRO:HA	16:2U:67:ALA:HB3	2.02	0.40
10:2O:26:LYS:O	10:2O:30:ALA:HB2	2.20	0.40
15:2T:20:PRO:HG2	15:2T:88:ILE:HD11	2.04	0.40
32:2a:958:A:H2'	32:2a:959:A:C8	2.56	0.40
32:2a:978:A:O2'	32:2a:1322:C:N3	2.49	0.40
32:2a:1015:A:O2'	32:2a:1219:U:H5'	2.21	0.40
32:2a:1273:G:C6	32:2a:1274:G:C4	3.09	0.40
33:2b:118:LEU:HD23	33:2b:142:LEU:HB2	2.03	0.40
33:2b:149:LEU:HD22	33:2b:152:PHE:CD2	2.56	0.40
42:2k:45:GLY:O	42:2k:50:TYR:HB2	2.21	0.40
1:1A:970:C:H2'	1:1A:971:C:H6	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2206:G:H5”	1:1A:2207:G:N7	2.36	0.40
3:1D:245:PRO:HA	3:1D:246:PRO:HD3	1.94	0.40
5:1F:64:ILE:HD12	5:1F:65:TRP:CE3	2.57	0.40
12:1Q:34:LEU:HD21	12:1Q:129:THR:HG21	2.02	0.40
15:1T:18:ASP:OD1	15:1T:18:ASP:N	2.50	0.40
22:10:43:THR:HG23	22:10:43:THR:O	2.21	0.40
32:1a:585:G:N3	32:1a:879:C:H4’	2.36	0.40
32:1a:1368:G:OP1	40:1i:114:TYR:N	2.54	0.40
32:1a:1504:G:OP1	32:1a:1507:A:H4’	2.21	0.40
35:1d:138:TYR:C	35:1d:138:TYR:HD2	2.29	0.40
38:1g:50:ILE:HD11	38:1g:125:MET:HG2	2.03	0.40
54:1w:8:4SU:O5’	54:1w:8:4SU:H6	2.21	0.40
1:2A:142:A:N1	1:2A:1595:G:O2’	2.46	0.40
1:2A:1446:C:H42	1:2A:1465:G:H1	1.68	0.40
1:2A:1607:C:H5”	1:2A:1608:A:H5’	2.03	0.40
1:2A:1668:A:C8	1:2A:1674:G:C6	3.09	0.40
1:2A:1779:U:H2’	62:2A:4449:HOH:O	2.21	0.40
1:2A:1848:A:C6	32:2a:702:A:C6	3.10	0.40
1:2A:2615:U:C6	27:25:7:PRO:HA	2.57	0.40
2:2B:75:G:N2	21:2Z:87:ASP:OD1	2.54	0.40
7:2H:3:ARG:HH22	7:2H:65:HIS:HB3	1.85	0.40
10:2O:49:ARG:NH1	32:2a:1422:G:O3’	2.33	0.40
23:21:4:VAL:HG21	23:21:11:ARG:HH21	1.86	0.40
32:2a:376:G:H4’	47:2p:5:ARG:HH21	1.85	0.40
32:2a:719:C:H42	49:2r:71:LYS:HE2	1.87	0.40
32:2a:919:A:O2’	32:2a:1080:A:N1	2.43	0.40
32:2a:1288:A:H2	32:2a:1352:C:O2	2.04	0.40
33:2b:19:HIS:ND1	33:2b:20:GLU:HG2	2.37	0.40
33:2b:50:GLU:HB3	33:2b:200:ILE:O	2.22	0.40
38:2g:53:LYS:HE2	38:2g:53:LYS:HB3	1.82	0.40
43:2l:8:ASN:OD1	48:2q:34:LYS:NZ	2.29	0.40
48:2q:27:PHE:CE1	48:2q:36:ILE:HD11	2.56	0.40
57:2y:66:U:C4	57:2y:67:C:C4	3.10	0.40
1:1A:1550:C:H4’	1:1A:1743:C:O2	2.22	0.40
1:1A:2462:U:H2’	1:1A:2463:C:O4’	2.21	0.40
1:1A:2492:U:H2’	1:1A:2493:U:H6	1.87	0.40
5:1F:150:GLY:HA2	5:1F:172:TRP:CE3	2.57	0.40
18:1W:4:LYS:HB2	18:1W:106:ILE:HG12	2.03	0.40
32:1a:7:G:H21	36:1e:121:LYS:HG2	1.87	0.40
32:1a:56:U:H2’	32:1a:57:G:H8	1.85	0.40
32:1a:1027:C:N1	32:1a:1034:G:N2	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1117:G:H5”	40:1i:104:ARG:NH1	2.36	0.40
33:1b:169:LYS:O	33:1b:169:LYS:HD3	2.20	0.40
1:2A:277:C:H4’	1:2A:278:A:OP2	2.22	0.40
1:2A:858:U:O2	1:2A:2268:A:H2’	2.21	0.40
1:2A:1185:C:H5”	1:2A:1186:G:OP1	2.21	0.40
1:2A:1268:A:C2	1:2A:2013:A:C4	3.10	0.40
1:2A:1891:G:C6	1:2A:1892:C:C4	3.10	0.40
1:2A:2351:G:O6	30:28:39:LYS:HD2	2.22	0.40
1:2A:2838:G:N7	62:2A:4041:HOH:O	2.37	0.40
5:2F:184:TYR:O	5:2F:188:ARG:HG3	2.21	0.40
8:2I:89:TYR:CD2	8:2I:89:TYR:N	2.89	0.40
10:2O:101:PRO:HG3	15:2T:67:SER:HB3	2.02	0.40
12:2Q:2:LEU:H	12:2Q:2:LEU:HG	1.74	0.40
12:2Q:43:THR:HG22	12:2Q:94:VAL:HG12	2.04	0.40
15:2T:64:ARG:NH1	15:2T:103:ARG:HA	2.35	0.40
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.56	0.40
24:22:25:VAL:CG2	24:22:60:LEU:HB3	2.52	0.40
26:24:46:GLN:C	26:24:48:ARG:N	2.74	0.40
32:2a:958:A:N6	50:2s:77:THR:O	2.54	0.40
32:2a:1030(A):G:O2’	32:2a:1030(C):G:N7	2.38	0.40
32:2a:1304:G:C6	32:2a:1305:G:N1	2.89	0.40
32:2a:1314:C:H2’	32:2a:1315:U:H6	1.85	0.40
32:2a:1338:G:H21	55:2x:41:C:H1’	1.85	0.40
32:2a:1350:A:C2	32:2a:1351:U:C2	3.09	0.40
35:2d:22:LYS:HB2	35:2d:26:CYS:SG	2.62	0.40
36:2e:20:GLN:OE1	36:2e:25:ARG:NH1	2.54	0.40
1:1A:705:A:C2	1:1A:727:A:H1’	2.56	0.40
1:1A:918:A:H5”	2:1B:98:G:O2’	2.21	0.40
1:1A:1028:A:N3	1:1A:2486:G:O2’	2.46	0.40
1:1A:1394:U:H6	1:1A:1394:U:H3’	1.87	0.40
1:1A:1466:G:H2’	1:1A:1547:C:N4	2.36	0.40
1:1A:1924:C:H4’	55:1x:13:C:O2’	2.21	0.40
1:1A:2820:A:C5	13:1R:4:LEU:HD11	2.57	0.40
5:1F:89:VAL:HG12	5:1F:90:PHE:CD2	2.56	0.40
9:1N:75:TYR:OH	62:1N:301:HOH:O	2.22	0.40
10:1O:16:ALA:HB2	10:1O:52:VAL:HG21	2.04	0.40
11:1P:84:ASN:CG	11:1P:117:GLU:HB3	2.46	0.40
26:14:44:THR:OG1	26:14:47:GLN:HB2	2.22	0.40
30:18:8:LYS:HD3	30:18:8:LYS:HA	1.67	0.40
32:1a:182:U:C4	32:1a:183:G:H1’	2.56	0.40
32:1a:729:A:H2’	32:1a:730:G:C8	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1201:A:H4'	32:1a:1202:G:O5'	2.21	0.40
32:1a:1202:G:H1'	45:1n:29:ARG:HD2	2.03	0.40
32:1a:1532:U:H6	32:1a:1532:U:O5'	2.04	0.40
36:1e:33:VAL:HG13	36:1e:112:LEU:HD12	2.03	0.40
40:1i:85:LEU:HD23	40:1i:85:LEU:HA	1.91	0.40
41:1j:7:LYS:HG2	41:1j:70:ARG:O	2.22	0.40
41:1j:38:ILE:HD11	41:1j:71:LEU:HB3	2.04	0.40
54:1w:2:C:H2'	54:1w:3:C:C6	2.56	0.40
57:1y:20:U:O3'	57:1y:21:A:H4'	2.21	0.40
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.56	0.40
1:2A:304:G:H2'	1:2A:305:U:C6	2.57	0.40
1:2A:658:C:H2'	1:2A:659:C:H6	1.84	0.40
1:2A:1027:A:N6	1:2A:1126:A:N3	2.70	0.40
1:2A:2116:G:O6	1:2A:2162:G:H5"	2.21	0.40
1:2A:2164:C:C4	1:2A:2165:G:H1'	2.56	0.40
1:2A:2193:G:H2'	1:2A:2194:G:C8	2.56	0.40
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.21	0.40
2:2B:19:G:H2'	2:2B:20:C:O4'	2.21	0.40
15:2T:118:ARG:HA	15:2T:121:ILE:HD12	2.04	0.40
21:2Z:40:ASP:OD2	21:2Z:42:VAL:HG13	2.21	0.40
23:21:94:LEU:HD23	23:21:94:LEU:HA	1.96	0.40
32:2a:22:G:H5'	32:2a:885:G:OP2	2.22	0.40
32:2a:232:G:H2'	32:2a:233:C:C6	2.56	0.40
32:2a:593:G:C6	32:2a:594:G:C5	3.10	0.40
32:2a:811:C:O2'	32:2a:901:A:N1	2.53	0.40
32:2a:1008:C:C2	32:2a:1022:G:C2	3.10	0.40
32:2a:1290:G:H2'	32:2a:1291:G:H8	1.86	0.40
37:2f:62:TRP:CH2	37:2f:64:GLN:HB2	2.56	0.40
39:2h:83:ILE:HB	39:2h:137:VAL:HG13	2.03	0.40
46:2o:39:LEU:HD23	46:2o:39:LEU:HA	1.92	0.40
46:2o:46:HIS:C	46:2o:48:LYS:H	2.30	0.40
51:2t:75:ASN:HD22	51:2t:75:ASN:N	2.19	0.40
57:2y:18:G:N2	57:2y:55:PSU:C4	2.89	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%)	255 (93%)	18 (7%)	0	100 100
3	2D	273/276 (99%)	255 (93%)	18 (7%)	0	100 100
4	1E	202/206 (98%)	190 (94%)	10 (5%)	2 (1%)	12 20
4	2E	202/206 (98%)	188 (93%)	13 (6%)	1 (0%)	24 37
5	1F	200/210 (95%)	194 (97%)	5 (2%)	1 (0%)	24 37
5	2F	200/210 (95%)	178 (89%)	18 (9%)	4 (2%)	6 7
6	1G	179/182 (98%)	162 (90%)	16 (9%)	1 (1%)	21 32
6	2G	179/182 (98%)	155 (87%)	19 (11%)	5 (3%)	4 3
7	1H	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	21 32
7	2H	172/180 (96%)	155 (90%)	15 (9%)	2 (1%)	10 16
8	1I	144/148 (97%)	126 (88%)	17 (12%)	1 (1%)	18 28
8	2I	144/148 (97%)	121 (84%)	22 (15%)	1 (1%)	18 28
9	1N	138/140 (99%)	135 (98%)	2 (1%)	1 (1%)	18 28
9	2N	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	18 28
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100 100
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100 100
11	1P	147/150 (98%)	129 (88%)	15 (10%)	3 (2%)	6 7
11	2P	147/150 (98%)	129 (88%)	12 (8%)	6 (4%)	2 2
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100 100
12	2Q	139/141 (99%)	125 (90%)	14 (10%)	0	100 100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100 100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100 100
14	1S	108/112 (96%)	106 (98%)	2 (2%)	0	100 100
14	2S	108/112 (96%)	97 (90%)	10 (9%)	1 (1%)	14 22
15	1T	129/146 (88%)	121 (94%)	6 (5%)	2 (2%)	7 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100 100
16	1U	114/118 (97%)	114 (100%)	0	0	100 100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
17	1V	99/101 (98%)	93 (94%)	4 (4%)	2 (2%)	6 7
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	12 20
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
19	1X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	11 18
19	2X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11 18
20	1Y	105/110 (96%)	97 (92%)	8 (8%)	0	100 100
20	2Y	105/110 (96%)	95 (90%)	10 (10%)	0	100 100
21	1Z	148/206 (72%)	135 (91%)	11 (7%)	2 (1%)	9 13
21	2Z	156/206 (76%)	127 (81%)	29 (19%)	0	100 100
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100 100
22	20	81/85 (95%)	78 (96%)	3 (4%)	0	100 100
23	11	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11 18
23	21	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11 18
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
24	22	68/72 (94%)	68 (100%)	0	0	100 100
25	13	57/60 (95%)	57 (100%)	0	0	100 100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
26	14	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1 0
26	24	67/71 (94%)	50 (75%)	14 (21%)	3 (4%)	2 1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100 100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100 100
29	17	46/49 (94%)	46 (100%)	0	0	100 100
29	27	46/49 (94%)	46 (100%)	0	0	100 100
30	18	62/65 (95%)	62 (100%)	0	0	100 100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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%)	195 (85%)	28 (12%)	6 (3%)	4 4
33	2b	229/256 (90%)	195 (85%)	30 (13%)	4 (2%)	7 10
34	1c	204/239 (85%)	188 (92%)	16 (8%)	0	100 100
34	2c	204/239 (85%)	176 (86%)	27 (13%)	1 (0%)	24 37
35	1d	206/209 (99%)	189 (92%)	16 (8%)	1 (0%)	24 37
35	2d	206/209 (99%)	190 (92%)	16 (8%)	0	100 100
36	1e	146/162 (90%)	132 (90%)	11 (8%)	3 (2%)	5 7
36	2e	146/162 (90%)	132 (90%)	13 (9%)	1 (1%)	18 28
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100 100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100 100
38	1g	153/156 (98%)	136 (89%)	15 (10%)	2 (1%)	9 14
38	2g	153/156 (98%)	132 (86%)	16 (10%)	5 (3%)	3 2
39	1h	135/138 (98%)	129 (96%)	6 (4%)	0	100 100
39	2h	135/138 (98%)	128 (95%)	6 (4%)	1 (1%)	18 28
40	1i	125/128 (98%)	110 (88%)	13 (10%)	2 (2%)	7 11
40	2i	125/128 (98%)	106 (85%)	19 (15%)	0	100 100
41	1j	95/105 (90%)	84 (88%)	7 (7%)	4 (4%)	2 2
41	2j	94/105 (90%)	79 (84%)	13 (14%)	2 (2%)	5 7
42	1k	112/129 (87%)	99 (88%)	11 (10%)	2 (2%)	6 9
42	2k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	14 22
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100 100
43	2l	119/132 (90%)	108 (91%)	9 (8%)	2 (2%)	7 10
44	1m	121/126 (96%)	104 (86%)	15 (12%)	2 (2%)	7 10
44	2m	120/126 (95%)	103 (86%)	15 (12%)	2 (2%)	7 10
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100 100
45	2n	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7 10
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100 100
46	2o	86/89 (97%)	79 (92%)	7 (8%)	0	100 100
47	1p	80/88 (91%)	77 (96%)	3 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
47	2p	80/88 (91%)	71 (89%)	8 (10%)	1 (1%)	9 14
48	1q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	12 20
48	2q	97/105 (92%)	87 (90%)	8 (8%)	2 (2%)	5 7
49	1r	66/88 (75%)	61 (92%)	5 (8%)	0	100 100
49	2r	66/88 (75%)	66 (100%)	0	0	100 100
50	1s	81/93 (87%)	68 (84%)	13 (16%)	0	100 100
50	2s	81/93 (87%)	65 (80%)	15 (18%)	1 (1%)	10 16
51	1t	94/106 (89%)	81 (86%)	10 (11%)	3 (3%)	3 3
51	2t	94/106 (89%)	83 (88%)	9 (10%)	2 (2%)	5 7
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100 100
56	1z	2/5 (40%)	1 (50%)	1 (50%)	0	100 100
56	2z	1/5 (20%)	1 (100%)	0	0	100 100
All	All	11371/12138 (94%)	10427 (92%)	842 (7%)	102 (1%)	14 22

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	1P	29	LYS
21	1Z	53	ILE
23	11	3	LYS
33	1b	17	PHE
40	1i	54	ASP
44	1m	67	GLU
44	1m	107	ALA
11	2P	29	LYS
11	2P	36	LYS
33	2b	17	PHE
33	2b	123	ALA
38	2g	80	VAL
44	2m	67	GLU
48	2q	68	ARG
50	2s	81	ARG
26	14	47	GLN
26	14	49	PHE
26	14	53	GLU
26	14	62	ARG

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Mol	Chain	Res	Type
33	1b	8	LYS
33	1b	126	GLU
38	1g	52	GLU
41	1j	79	ARG
42	1k	49	GLY
5	2F	130	ALA
6	2G	42	GLY
6	2G	43	LEU
6	2G	181	ARG
11	2P	38	GLN
17	2V	79	VAL
26	24	3	GLU
26	24	45	GLY
33	2b	20	GLU
34	2c	54	ARG
38	2g	55	GLY
41	2j	79	ARG
43	2l	91	LYS
44	2m	106	ASN
48	2q	67	LYS
4	1E	28	ALA
4	1E	52	LEU
5	1F	130	ALA
11	1P	38	GLN
15	1T	55	ASN
33	1b	231	GLU
42	1k	74	ALA
48	1q	68	ARG
4	2E	52	LEU
5	2F	21	ALA
5	2F	195	ASP
9	2N	2	LYS
14	2S	84	GLN
19	2X	93	GLU
43	2l	105	TYR
47	2p	52	ASP
51	2t	47	GLY
7	1H	126	PRO
8	1I	10	GLU
9	1N	2	LYS
17	1V	53	GLU
33	1b	124	SER

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Mol	Chain	Res	Type
38	1g	79	ARG
41	1j	78	ASN
51	1t	47	GLY
6	2G	50	ALA
11	2P	45	LEU
26	24	47	GLN
39	2h	133	LEU
41	2j	78	ASN
42	2k	49	GLY
6	1G	43	LEU
11	1P	45	LEU
17	1V	79	VAL
51	1t	96	GLY
7	2H	55	PRO
7	2H	126	PRO
8	2I	40	THR
23	21	3	LYS
38	2g	52	GLU
19	1X	2	LYS
36	1e	86	ALA
40	1i	40	LEU
5	2F	166	ALA
6	2G	24	GLY
36	2e	69	VAL
38	2g	39	ALA
51	2t	102	GLY
15	1T	37	GLY
21	1Z	120	ILE
35	1d	88	VAL
11	2P	44	GLY
41	1j	77	PRO
51	1t	98	PRO
26	14	56	VAL
36	1e	85	GLY
33	2b	125	PRO
38	2g	130	GLY
41	1j	91	PRO
11	2P	122	PRO
36	1e	69	VAL
45	2n	14	PRO
33	1b	125	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1D	215/218 (99%)	207 (96%)	8 (4%)	30 51
3	2D	215/218 (99%)	201 (94%)	14 (6%)	15 27
4	1E	164/166 (99%)	153 (93%)	11 (7%)	15 26
4	2E	164/166 (99%)	154 (94%)	10 (6%)	17 30
5	1F	160/166 (96%)	142 (89%)	18 (11%)	5 8
5	2F	159/166 (96%)	147 (92%)	12 (8%)	12 21
6	1G	143/156 (92%)	129 (90%)	14 (10%)	7 12
6	2G	143/156 (92%)	125 (87%)	18 (13%)	4 6
7	1H	144/148 (97%)	130 (90%)	14 (10%)	8 12
7	2H	144/148 (97%)	127 (88%)	17 (12%)	5 7
8	1I	113/124 (91%)	92 (81%)	21 (19%)	1 2
8	2I	105/124 (85%)	81 (77%)	24 (23%)	1 1
9	1N	118/119 (99%)	111 (94%)	7 (6%)	18 31
9	2N	118/119 (99%)	110 (93%)	8 (7%)	14 25
10	1O	100/100 (100%)	97 (97%)	3 (3%)	36 58
10	2O	100/100 (100%)	97 (97%)	3 (3%)	36 58
11	1P	115/116 (99%)	104 (90%)	11 (10%)	8 12
11	2P	115/116 (99%)	105 (91%)	10 (9%)	9 16
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	11 18
12	2Q	111/111 (100%)	103 (93%)	8 (7%)	13 23
13	1R	101/101 (100%)	93 (92%)	8 (8%)	11 19
13	2R	101/101 (100%)	97 (96%)	4 (4%)	28 47
14	1S	86/88 (98%)	80 (93%)	6 (7%)	14 24
14	2S	85/88 (97%)	74 (87%)	11 (13%)	4 6
15	1T	115/127 (91%)	108 (94%)	7 (6%)	17 30
15	2T	113/127 (89%)	100 (88%)	13 (12%)	5 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	1U	93/94 (99%)	84 (90%)	9 (10%)	8 12
16	2U	93/94 (99%)	88 (95%)	5 (5%)	20 35
17	1V	80/82 (98%)	73 (91%)	7 (9%)	9 15
17	2V	80/82 (98%)	75 (94%)	5 (6%)	16 29
18	1W	90/92 (98%)	82 (91%)	8 (9%)	9 15
18	2W	90/92 (98%)	85 (94%)	5 (6%)	19 33
19	1X	77/78 (99%)	76 (99%)	1 (1%)	61 80
19	2X	77/78 (99%)	73 (95%)	4 (5%)	21 36
20	1Y	85/91 (93%)	78 (92%)	7 (8%)	10 18
20	2Y	85/91 (93%)	73 (86%)	12 (14%)	3 4
21	1Z	135/179 (75%)	120 (89%)	15 (11%)	6 9
21	2Z	137/179 (76%)	117 (85%)	20 (15%)	3 4
22	10	65/67 (97%)	65 (100%)	0	100 100
22	20	65/67 (97%)	63 (97%)	2 (3%)	35 57
23	11	80/83 (96%)	74 (92%)	6 (8%)	12 21
23	21	80/83 (96%)	73 (91%)	7 (9%)	9 15
24	12	65/67 (97%)	61 (94%)	4 (6%)	16 29
24	22	65/67 (97%)	59 (91%)	6 (9%)	8 14
25	13	51/52 (98%)	45 (88%)	6 (12%)	5 7
25	23	50/52 (96%)	46 (92%)	4 (8%)	11 19
26	14	59/63 (94%)	49 (83%)	10 (17%)	2 3
26	24	53/63 (84%)	39 (74%)	14 (26%)	0 0
27	15	50/52 (96%)	44 (88%)	6 (12%)	5 7
27	25	50/52 (96%)	47 (94%)	3 (6%)	17 31
28	16	51/52 (98%)	46 (90%)	5 (10%)	7 12
28	26	50/52 (96%)	42 (84%)	8 (16%)	2 3
29	17	41/42 (98%)	37 (90%)	4 (10%)	7 12
29	27	41/42 (98%)	39 (95%)	2 (5%)	22 39
30	18	54/55 (98%)	50 (93%)	4 (7%)	13 22
30	28	54/55 (98%)	51 (94%)	3 (6%)	19 33
31	19	34/34 (100%)	32 (94%)	2 (6%)	18 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
31	29	34/34 (100%)	34 (100%)	0	100 100
33	1b	192/220 (87%)	168 (88%)	24 (12%)	4 6
33	2b	187/220 (85%)	160 (86%)	27 (14%)	3 4
34	1c	142/188 (76%)	129 (91%)	13 (9%)	8 14
34	2c	140/188 (74%)	121 (86%)	19 (14%)	3 5
35	1d	169/181 (93%)	146 (86%)	23 (14%)	3 5
35	2d	173/181 (96%)	159 (92%)	14 (8%)	11 18
36	1e	113/123 (92%)	108 (96%)	5 (4%)	25 43
36	2e	114/123 (93%)	106 (93%)	8 (7%)	14 24
37	1f	84/90 (93%)	75 (89%)	9 (11%)	6 10
37	2f	85/90 (94%)	79 (93%)	6 (7%)	13 23
38	1g	119/127 (94%)	107 (90%)	12 (10%)	7 11
38	2g	120/127 (94%)	107 (89%)	13 (11%)	6 9
39	1h	114/119 (96%)	105 (92%)	9 (8%)	11 19
39	2h	114/119 (96%)	103 (90%)	11 (10%)	8 12
40	1i	90/99 (91%)	81 (90%)	9 (10%)	7 11
40	2i	89/99 (90%)	78 (88%)	11 (12%)	4 6
41	1j	66/92 (72%)	59 (89%)	7 (11%)	6 10
41	2j	69/92 (75%)	58 (84%)	11 (16%)	2 3
42	1k	82/99 (83%)	72 (88%)	10 (12%)	5 7
42	2k	83/99 (84%)	74 (89%)	9 (11%)	6 9
43	1l	96/108 (89%)	90 (94%)	6 (6%)	16 29
43	2l	96/108 (89%)	87 (91%)	9 (9%)	8 13
44	1m	93/101 (92%)	82 (88%)	11 (12%)	5 7
44	2m	92/101 (91%)	79 (86%)	13 (14%)	3 4
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5 7
45	2n	49/50 (98%)	47 (96%)	2 (4%)	27 46
46	1o	78/80 (98%)	71 (91%)	7 (9%)	9 15
46	2o	78/80 (98%)	73 (94%)	5 (6%)	16 28
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7 11
47	2p	68/74 (92%)	62 (91%)	6 (9%)	9 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
48	1q	94/97 (97%)	87 (93%)	7 (7%)	13 22
48	2q	94/97 (97%)	88 (94%)	6 (6%)	16 28
49	1r	59/77 (77%)	56 (95%)	3 (5%)	21 37
49	2r	59/77 (77%)	52 (88%)	7 (12%)	5 7
50	1s	69/80 (86%)	61 (88%)	8 (12%)	5 8
50	2s	67/80 (84%)	57 (85%)	10 (15%)	3 3
51	1t	70/82 (85%)	61 (87%)	9 (13%)	4 6
51	2t	70/82 (85%)	66 (94%)	4 (6%)	18 33
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6 9
52	2u	18/22 (82%)	18 (100%)	0	100 100
56	1z	3/3 (100%)	3 (100%)	0	100 100
56	2z	2/3 (67%)	2 (100%)	0	100 100
All	All	9308/10070 (92%)	8447 (91%)	861 (9%)	8 14

All (861) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	22	SER
3	1D	32	SER
3	1D	99	ASP
3	1D	142	VAL
3	1D	154	LYS
3	1D	221	VAL
3	1D	242	ARG
4	1E	12	THR
4	1E	33	VAL
4	1E	47	VAL
4	1E	61	ARG
4	1E	78	LEU
4	1E	89	ASP
4	1E	90	THR
4	1E	116	VAL
4	1E	134	ILE
4	1E	184	VAL
4	1E	195	LEU
5	1F	33	LEU
5	1F	53	THR

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Mol	Chain	Res	Type
5	1F	57	VAL
5	1F	70	THR
5	1F	72	ARG
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	127	GLU
5	1F	132	VAL
5	1F	140	LEU
5	1F	158	THR
5	1F	162	LEU
5	1F	168	ARG
5	1F	175	THR
5	1F	183	VAL
5	1F	192	LEU
5	1F	197	ASP
6	1G	3	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	8	LYS
6	1G	21	ARG
6	1G	31	VAL
6	1G	35	GLU
6	1G	36	LYS
6	1G	43	LEU
6	1G	99	MET
6	1G	132	ASN
6	1G	140	ILE
6	1G	148	MET
6	1G	159	VAL
7	1H	16	SER
7	1H	45	VAL
7	1H	57	ASP
7	1H	76	VAL
7	1H	84	SER
7	1H	88	LEU
7	1H	92	ILE
7	1H	99	VAL
7	1H	103	LEU
7	1H	116	GLU
7	1H	122	THR
7	1H	127	GLU

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Mol	Chain	Res	Type
7	1H	129	THR
7	1H	149	ARG
8	1I	10	GLU
8	1I	15	VAL
8	1I	20	ASP
8	1I	27	ARG
8	1I	38	LEU
8	1I	45	LYS
8	1I	47	LEU
8	1I	61	ARG
8	1I	76	THR
8	1I	77	LEU
8	1I	78	THR
8	1I	85	GLU
8	1I	87	LYS
8	1I	92	VAL
8	1I	101	LEU
8	1I	116	LEU
8	1I	123	LEU
8	1I	127	VAL
8	1I	129	THR
8	1I	140	LEU
8	1I	142	VAL
9	1N	2	LYS
9	1N	9	VAL
9	1N	28	THR
9	1N	46	VAL
9	1N	48	MET
9	1N	71	ILE
9	1N	140	VAL
10	1O	28	SER
10	1O	106	LEU
10	1O	112	MET
11	1P	3	LEU
11	1P	86	LYS
11	1P	92	GLU
11	1P	95	VAL
11	1P	96	THR
11	1P	98	GLU
11	1P	101	VAL
11	1P	114	ILE
11	1P	125	VAL

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Mol	Chain	Res	Type
11	1P	133	SER
11	1P	147	LEU
12	1Q	1	MET
12	1Q	7	MET
12	1Q	8	LYS
12	1Q	12	GLN
12	1Q	75	THR
12	1Q	98	LYS
12	1Q	115	MET
12	1Q	127	ILE
12	1Q	133	ARG
13	1R	15	SER
13	1R	36	THR
13	1R	44	LEU
13	1R	73	VAL
13	1R	83	ILE
13	1R	100	LEU
13	1R	111	LEU
13	1R	114	VAL
14	1S	14	VAL
14	1S	36	TYR
14	1S	49	VAL
14	1S	52	SER
14	1S	69	VAL
14	1S	73	LEU
15	1T	28	VAL
15	1T	30	VAL
15	1T	36	GLU
15	1T	65	LYS
15	1T	96	ARG
15	1T	125	ARG
15	1T	128	GLU
16	1U	9	VAL
16	1U	17	ILE
16	1U	27	LEU
16	1U	31	SER
16	1U	55	ARG
16	1U	59	ARG
16	1U	74	LEU
16	1U	95	LEU
16	1U	108	GLU
17	1V	10	LYS

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Mol	Chain	Res	Type
17	1V	32	THR
17	1V	46	VAL
17	1V	53	GLU
17	1V	61	VAL
17	1V	79	VAL
17	1V	85	LYS
18	1W	4	LYS
18	1W	11	ARG
18	1W	18	ARG
18	1W	24	ILE
18	1W	35	ILE
18	1W	50	VAL
18	1W	67	ASP
18	1W	96	ILE
19	1X	92	LEU
20	1Y	7	VAL
20	1Y	31	LEU
20	1Y	38	ILE
20	1Y	44	ILE
20	1Y	72	VAL
20	1Y	85	VAL
20	1Y	99	CYS
21	1Z	18	LEU
21	1Z	28	MET
21	1Z	42	VAL
21	1Z	46	LYS
21	1Z	53	ILE
21	1Z	56	VAL
21	1Z	61	LEU
21	1Z	86	VAL
21	1Z	124	ILE
21	1Z	129	SER
21	1Z	132	ASN
21	1Z	139	VAL
21	1Z	154	ASP
21	1Z	170	THR
21	1Z	171	ILE
23	11	3	LYS
23	11	11	ARG
23	11	46	LEU
23	11	59	THR
23	11	65	SER

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Mol	Chain	Res	Type
23	11	78	LYS
24	12	24	LEU
24	12	41	ILE
24	12	53	LEU
24	12	55	ARG
25	13	6	VAL
25	13	23	LEU
25	13	37	LEU
25	13	54	VAL
25	13	56	VAL
25	13	60	GLU
26	14	14	ILE
26	14	15	ILE
26	14	44	THR
26	14	49	PHE
26	14	50	VAL
26	14	52	THR
26	14	53	GLU
26	14	59	PHE
26	14	63	TYR
26	14	69	LYS
27	15	6	VAL
27	15	26	THR
27	15	35	GLU
27	15	40	LYS
27	15	57	VAL
27	15	59	GLU
28	16	5	VAL
28	16	6	ARG
28	16	14	THR
28	16	45	LYS
28	16	47	THR
29	17	24	THR
29	17	29	LYS
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	23	VAL
30	18	34	TRP
30	18	50	LEU
31	19	4	ARG
31	19	10	ILE

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Mol	Chain	Res	Type
33	1b	8	LYS
33	1b	12	GLU
33	1b	20	GLU
33	1b	21	ARG
33	1b	35	GLU
33	1b	39	ILE
33	1b	43	ASP
33	1b	44	LEU
33	1b	54	THR
33	1b	64	ARG
33	1b	67	THR
33	1b	78	GLN
33	1b	80	ILE
33	1b	101	MET
33	1b	112	VAL
33	1b	127	ILE
33	1b	187	LEU
33	1b	189	ASP
33	1b	192	SER
33	1b	200	ILE
33	1b	208	ILE
33	1b	212	GLN
33	1b	215	LEU
33	1b	236	TYR
34	1c	3	ASN
34	1c	28	GLN
34	1c	36	ASP
34	1c	77	ILE
34	1c	85	ARG
34	1c	87	LEU
34	1c	89	GLU
34	1c	98	ASN
34	1c	105	GLU
34	1c	175	LEU
34	1c	178	LEU
34	1c	195	VAL
34	1c	196	LEU
35	1d	3	ARG
35	1d	5	ILE
35	1d	19	LEU
35	1d	22	LYS
35	1d	70	ILE

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Mol	Chain	Res	Type
35	1d	76	ARG
35	1d	77	ASN
35	1d	83	SER
35	1d	85	LYS
35	1d	86	LYS
35	1d	127	THR
35	1d	135	LEU
35	1d	138	TYR
35	1d	140	VAL
35	1d	144	ASP
35	1d	158	ILE
35	1d	170	VAL
35	1d	175	SER
35	1d	177	ASP
35	1d	178	VAL
35	1d	184	LYS
35	1d	188	LEU
35	1d	194	LEU
36	1e	12	LEU
36	1e	41	VAL
36	1e	56	GLN
36	1e	68	GLU
36	1e	79	GLU
37	1f	36	ARG
37	1f	43	LEU
37	1f	70	ASP
37	1f	72	VAL
37	1f	75	LEU
37	1f	78	GLU
37	1f	81	ILE
37	1f	91	VAL
37	1f	93	SER
38	1g	21	VAL
38	1g	24	THR
38	1g	27	ILE
38	1g	32	ARG
38	1g	41	ARG
38	1g	50	ILE
38	1g	59	LEU
38	1g	61	VAL
38	1g	85	TYR
38	1g	104	LEU

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Mol	Chain	Res	Type
38	1g	114	ARG
38	1g	115	ARG
39	1h	13	ILE
39	1h	33	GLU
39	1h	39	LEU
39	1h	51	VAL
39	1h	77	GLU
39	1h	86	ILE
39	1h	109	ILE
39	1h	112	LEU
39	1h	133	LEU
40	1i	25	LYS
40	1i	50	LEU
40	1i	53	VAL
40	1i	64	THR
40	1i	88	TYR
40	1i	89	ASN
40	1i	96	LEU
40	1i	103	THR
40	1i	128	ARG
41	1j	23	ILE
41	1j	35	SER
41	1j	49	VAL
41	1j	81	THR
41	1j	92	THR
41	1j	94	VAL
41	1j	100	THR
42	1k	14	VAL
42	1k	31	THR
42	1k	48	ILE
42	1k	80	VAL
42	1k	87	THR
42	1k	104	GLN
42	1k	107	SER
42	1k	109	VAL
42	1k	114	VAL
42	1k	117	ASN
43	1l	18	VAL
43	1l	36	VAL
43	1l	46	LYS
43	1l	57	LYS
43	1l	58	VAL

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Mol	Chain	Res	Type
43	1l	83	VAL
44	1m	3	ARG
44	1m	4	ILE
44	1m	17	VAL
44	1m	43	THR
44	1m	57	ARG
44	1m	64	TRP
44	1m	67	GLU
44	1m	70	LEU
44	1m	106	ASN
44	1m	109	THR
44	1m	121	LYS
45	1n	3	ARG
45	1n	9	LYS
45	1n	13	THR
45	1n	33	VAL
45	1n	56	VAL
45	1n	60	SER
46	1o	24	SER
46	1o	27	VAL
46	1o	39	LEU
46	1o	47	LYS
46	1o	76	GLU
46	1o	84	LYS
46	1o	87	ILE
47	1p	11	SER
47	1p	20	VAL
47	1p	21	VAL
47	1p	27	LYS
47	1p	45	THR
47	1p	62	VAL
47	1p	67	THR
48	1q	9	VAL
48	1q	19	VAL
48	1q	26	GLN
48	1q	39	SER
48	1q	60	ILE
48	1q	85	VAL
48	1q	100	LYS
49	1r	36	ASN
49	1r	54	ARG
49	1r	76	LEU

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Mol	Chain	Res	Type
50	1s	6	LYS
50	1s	12	ASP
50	1s	16	LEU
50	1s	19	VAL
50	1s	28	LYS
50	1s	37	ARG
50	1s	38	SER
50	1s	41	VAL
51	1t	10	LEU
51	1t	13	LEU
51	1t	24	LEU
51	1t	37	SER
51	1t	53	LEU
51	1t	71	THR
51	1t	84	LEU
51	1t	86	ARG
51	1t	100	ILE
52	1u	6	ARG
52	1u	15	ARG
3	2D	3	VAL
3	2D	20	ASP
3	2D	22	SER
3	2D	37	LEU
3	2D	61	LEU
3	2D	73	VAL
3	2D	116	GLN
3	2D	141	VAL
3	2D	142	VAL
3	2D	173	VAL
3	2D	204	ILE
3	2D	242	ARG
3	2D	253	GLN
3	2D	270	ILE
4	2E	11	MET
4	2E	12	THR
4	2E	33	VAL
4	2E	38	THR
4	2E	41	LYS
4	2E	78	LEU
4	2E	90	THR
4	2E	116	VAL
4	2E	145	LYS

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Mol	Chain	Res	Type
4	2E	175	VAL
5	2F	20	LEU
5	2F	28	ILE
5	2F	33	LEU
5	2F	57	VAL
5	2F	74	ARG
5	2F	107	LYS
5	2F	145	GLU
5	2F	161	GLU
5	2F	162	LEU
5	2F	175	THR
5	2F	183	VAL
5	2F	195	ASP
6	2G	4	ASP
6	2G	19	LEU
6	2G	20	ILE
6	2G	26	GLN
6	2G	28	VAL
6	2G	43	LEU
6	2G	45	GLU
6	2G	53	LEU
6	2G	59	GLU
6	2G	60	LEU
6	2G	79	ASN
6	2G	91	ARG
6	2G	105	LYS
6	2G	109	VAL
6	2G	140	ILE
6	2G	145	THR
6	2G	148	MET
6	2G	165	THR
7	2H	7	LEU
7	2H	15	VAL
7	2H	24	VAL
7	2H	45	VAL
7	2H	57	ASP
7	2H	76	VAL
7	2H	88	LEU
7	2H	92	ILE
7	2H	99	VAL
7	2H	122	THR
7	2H	124	GLU

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Mol	Chain	Res	Type
7	2H	127	GLU
7	2H	129	THR
7	2H	130	ARG
7	2H	134	SER
7	2H	141	VAL
7	2H	160	LYS
8	2I	2	LYS
8	2I	12	LEU
8	2I	14	ASP
8	2I	38	LEU
8	2I	45	LYS
8	2I	58	LEU
8	2I	61	ARG
8	2I	69	LYS
8	2I	74	ASN
8	2I	75	LEU
8	2I	78	THR
8	2I	82	ARG
8	2I	85	GLU
8	2I	87	LYS
8	2I	89	TYR
8	2I	108	THR
8	2I	117	GLU
8	2I	123	LEU
8	2I	127	VAL
8	2I	129	THR
8	2I	142	VAL
8	2I	143	SER
8	2I	144	VAL
8	2I	145	VAL
9	2N	9	VAL
9	2N	16	ILE
9	2N	28	THR
9	2N	48	MET
9	2N	60	ILE
9	2N	62	VAL
9	2N	73	THR
9	2N	83	LYS
10	2O	32	TYR
10	2O	96	THR
10	2O	116	SER
11	2P	3	LEU

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Mol	Chain	Res	Type
11	2P	7	ARG
11	2P	45	LEU
11	2P	86	LYS
11	2P	95	VAL
11	2P	98	GLU
11	2P	101	VAL
11	2P	131	SER
11	2P	133	SER
11	2P	135	LEU
12	2Q	1	MET
12	2Q	6	ARG
12	2Q	10	ARG
12	2Q	21	THR
12	2Q	75	THR
12	2Q	106	VAL
12	2Q	110	THR
12	2Q	115	MET
13	2R	36	THR
13	2R	44	LEU
13	2R	100	LEU
13	2R	114	VAL
14	2S	12	PHE
14	2S	25	ARG
14	2S	26	LEU
14	2S	27	SER
14	2S	43	GLU
14	2S	58	LEU
14	2S	63	THR
14	2S	65	VAL
14	2S	84	GLN
14	2S	103	GLU
14	2S	110	LEU
15	2T	9	LEU
15	2T	17	THR
15	2T	18	ASP
15	2T	39	ARG
15	2T	64	ARG
15	2T	66	VAL
15	2T	67	SER
15	2T	72	VAL
15	2T	87	ASP
15	2T	89	VAL

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Mol	Chain	Res	Type
15	2T	96	ARG
15	2T	102	ILE
15	2T	113	LYS
16	2U	5	LYS
16	2U	17	ILE
16	2U	74	LEU
16	2U	77	SER
16	2U	95	LEU
17	2V	46	VAL
17	2V	52	VAL
17	2V	61	VAL
17	2V	79	VAL
17	2V	98	GLU
18	2W	4	LYS
18	2W	11	ARG
18	2W	17	VAL
18	2W	67	ASP
18	2W	96	ILE
19	2X	35	THR
19	2X	45	THR
19	2X	81	VAL
19	2X	92	LEU
20	2Y	1	MET
20	2Y	3	VAL
20	2Y	5	MET
20	2Y	14	LEU
20	2Y	26	LYS
20	2Y	30	VAL
20	2Y	39	VAL
20	2Y	72	VAL
20	2Y	96	ILE
20	2Y	97	ARG
20	2Y	98	VAL
20	2Y	99	CYS
21	2Z	27	VAL
21	2Z	42	VAL
21	2Z	61	LEU
21	2Z	67	LEU
21	2Z	70	LEU
21	2Z	71	VAL
21	2Z	81	ARG
21	2Z	90	VAL

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Mol	Chain	Res	Type
21	2Z	91	LEU
21	2Z	96	VAL
21	2Z	100	VAL
21	2Z	121	HIS
21	2Z	128	VAL
21	2Z	136	PHE
21	2Z	154	ASP
21	2Z	161	VAL
21	2Z	163	LEU
21	2Z	170	THR
21	2Z	171	ILE
21	2Z	174	VAL
22	20	14	ARG
22	20	40	GLN
23	21	11	ARG
23	21	59	THR
23	21	65	SER
23	21	78	LYS
23	21	80	LEU
23	21	89	GLU
23	21	92	LYS
24	22	19	VAL
24	22	24	LEU
24	22	32	LEU
24	22	50	ILE
24	22	53	LEU
24	22	70	GLN
25	23	31	LEU
25	23	37	LEU
25	23	54	VAL
25	23	59	VAL
26	24	3	GLU
26	24	22	ILE
26	24	24	THR
26	24	26	SER
26	24	27	THR
26	24	33	VAL
26	24	34	GLU
26	24	37	SER
26	24	48	ARG
26	24	50	VAL
26	24	59	PHE

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Mol	Chain	Res	Type
26	24	63	TYR
26	24	67	TYR
26	24	68	ARG
27	25	6	VAL
27	25	35	GLU
27	25	55	ARG
28	26	7	ILE
28	26	9	LEU
28	26	14	THR
28	26	19	ARG
28	26	20	ASN
28	26	32	ASN
28	26	34	LEU
28	26	48	VAL
29	27	43	THR
29	27	46	VAL
30	28	14	VAL
30	28	23	VAL
30	28	50	LEU
33	2b	7	VAL
33	2b	8	LYS
33	2b	9	GLU
33	2b	16	HIS
33	2b	35	GLU
33	2b	52	GLU
33	2b	68	ILE
33	2b	76	GLN
33	2b	83	MET
33	2b	107	THR
33	2b	110	GLN
33	2b	112	VAL
33	2b	115	LEU
33	2b	117	GLU
33	2b	118	LEU
33	2b	127	ILE
33	2b	142	LEU
33	2b	157	ARG
33	2b	164	VAL
33	2b	168	THR
33	2b	172	ILE
33	2b	185	ILE
33	2b	187	LEU

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Mol	Chain	Res	Type
33	2b	189	ASP
33	2b	215	LEU
33	2b	224	GLN
33	2b	236	TYR
34	2c	16	ARG
34	2c	26	LYS
34	2c	30	ARG
34	2c	32	LEU
34	2c	39	ILE
34	2c	45	LYS
34	2c	57	ILE
34	2c	91	LEU
34	2c	101	LEU
34	2c	103	VAL
34	2c	115	LEU
34	2c	116	VAL
34	2c	132	ARG
34	2c	153	VAL
34	2c	161	GLU
34	2c	190	ARG
34	2c	192	THR
34	2c	195	VAL
34	2c	196	LEU
35	2d	5	ILE
35	2d	52	SER
35	2d	58	LEU
35	2d	67	ILE
35	2d	76	ARG
35	2d	78	LEU
35	2d	86	LYS
35	2d	96	LEU
35	2d	118	ARG
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	158	ILE
35	2d	193	ASP
36	2e	13	ILE
36	2e	41	VAL
36	2e	51	VAL
36	2e	55	VAL
36	2e	83	GLU

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Mol	Chain	Res	Type
36	2e	87	SER
36	2e	118	ILE
36	2e	150	ARG
37	2f	30	LEU
37	2f	63	TYR
37	2f	69	GLU
37	2f	81	ILE
37	2f	92	LYS
37	2f	95	GLU
38	2g	6	ARG
38	2g	9	VAL
38	2g	21	VAL
38	2g	27	ILE
38	2g	30	ILE
38	2g	53	LYS
38	2g	78	ARG
38	2g	79	ARG
38	2g	85	TYR
38	2g	98	SER
38	2g	114	ARG
38	2g	139	GLU
38	2g	144	MET
39	2h	29	SER
39	2h	45	ILE
39	2h	50	ARG
39	2h	51	VAL
39	2h	52	ASP
39	2h	99	GLU
39	2h	109	ILE
39	2h	112	LEU
39	2h	119	LEU
39	2h	133	LEU
39	2h	137	VAL
40	2i	27	THR
40	2i	40	LEU
40	2i	41	VAL
40	2i	56	LEU
40	2i	64	THR
40	2i	65	VAL
40	2i	66	ARG
40	2i	88	TYR
40	2i	89	ASN

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Mol	Chain	Res	Type
40	2i	103	THR
40	2i	113	LYS
41	2j	23	ILE
41	2j	38	ILE
41	2j	55	LYS
41	2j	61	GLU
41	2j	66	ARG
41	2j	67	THR
41	2j	81	THR
41	2j	94	VAL
41	2j	97	GLU
41	2j	98	ILE
41	2j	100	THR
42	2k	21	ILE
42	2k	29	ILE
42	2k	41	THR
42	2k	43	SER
42	2k	48	ILE
42	2k	62	GLN
42	2k	87	THR
42	2k	105	VAL
42	2k	107	SER
43	2l	34	ARG
43	2l	36	VAL
43	2l	39	VAL
43	2l	40	VAL
43	2l	46	LYS
43	2l	62	SER
43	2l	83	VAL
43	2l	97	ARG
43	2l	117	ARG
44	2m	32	GLU
44	2m	49	THR
44	2m	53	VAL
44	2m	57	ARG
44	2m	70	LEU
44	2m	90	LEU
44	2m	94	ARG
44	2m	102	ARG
44	2m	103	THR
44	2m	106	ASN
44	2m	117	VAL

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Mol	Chain	Res	Type
44	2m	121	LYS
44	2m	122	LYS
45	2n	3	ARG
45	2n	33	VAL
46	2o	3	ILE
46	2o	7	GLU
46	2o	13	GLN
46	2o	27	VAL
46	2o	60	VAL
47	2p	2	VAL
47	2p	20	VAL
47	2p	21	VAL
47	2p	42	ARG
47	2p	53	VAL
47	2p	67	THR
48	2q	5	VAL
48	2q	36	ILE
48	2q	52	LYS
48	2q	60	ILE
48	2q	84	LEU
48	2q	96	GLU
49	2r	37	VAL
49	2r	47	THR
49	2r	56	THR
49	2r	69	THR
49	2r	75	ILE
49	2r	82	THR
49	2r	86	VAL
50	2s	5	LEU
50	2s	16	LEU
50	2s	27	GLU
50	2s	37	ARG
50	2s	39	THR
50	2s	45	VAL
50	2s	48	THR
50	2s	49	ILE
50	2s	51	VAL
50	2s	57	HIS
51	2t	45	GLN
51	2t	51	GLU
51	2t	71	THR
51	2t	75	ASN

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

Mol	Chain	Res	Type
3	1D	116	GLN
3	1D	126	GLN
3	1D	166	GLN
4	1E	48	GLN
4	1E	143	ASN
5	1F	8	GLN
5	1F	203	GLN
6	1G	26	GLN
6	1G	132	ASN
8	1I	133	HIS
9	1N	94	HIS
9	1N	133	GLN
10	1O	3	GLN
11	1P	81	GLN
12	1Q	12	GLN
12	1Q	123	HIS
13	1R	13	HIS
15	1T	58	ASN
15	1T	90	GLN
16	1U	72	HIS
16	1U	94	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	32	HIS
21	1Z	73	GLN
21	1Z	151	HIS
22	10	35	ASN
24	12	43	GLN
25	13	32	GLN
33	1b	40	HIS
33	1b	78	GLN
34	1c	6	HIS
34	1c	37	GLN
34	1c	162	GLN
34	1c	170	GLN
34	1c	181	ASN
35	1d	77	ASN
35	1d	116	GLN
35	1d	123	HIS
35	1d	125	HIS

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Mol	Chain	Res	Type
36	1e	78	HIS
36	1e	141	GLN
37	1f	7	ASN
37	1f	13	ASN
37	1f	18	GLN
37	1f	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	68	ASN
38	1g	86	GLN
39	1h	15	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	58	HIS
40	1i	124	GLN
41	1j	56	HIS
41	1j	69	ASN
42	1k	104	GLN
43	1l	99	HIS
44	1m	77	ASN
44	1m	92	HIS
46	1o	9	GLN
46	1o	46	HIS
47	1p	13	HIS
47	1p	14	ASN
50	1s	47	HIS
50	1s	83	HIS
51	1t	16	HIS
51	1t	75	ASN
3	2D	116	GLN
3	2D	143	HIS
5	2F	69	HIS
6	2G	27	ASN
7	2H	74	ASN
7	2H	111	HIS
8	2I	133	HIS
10	2O	3	GLN
10	2O	5	GLN
12	2Q	12	GLN
13	2R	50	HIS

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Mol	Chain	Res	Type
13	2R	61	HIS
14	2S	38	GLN
15	2T	84	GLN
16	2U	94	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	32	HIS
21	2Z	50	GLN
21	2Z	55	HIS
21	2Z	151	HIS
23	21	56	GLN
25	23	32	GLN
28	26	20	ASN
30	28	35	GLN
33	2b	76	GLN
33	2b	95	GLN
33	2b	110	GLN
33	2b	135	GLN
34	2c	6	HIS
34	2c	31	HIS
34	2c	98	ASN
34	2c	162	GLN
35	2d	45	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
36	2e	141	GLN
37	2f	73	ASN
37	2f	94	GLN
37	2f	100	ASN
38	2g	11	GLN
38	2g	28	ASN
38	2g	37	ASN
38	2g	86	GLN
38	2g	148	ASN
40	2i	3	GLN
40	2i	31	GLN
40	2i	58	HIS
41	2j	21	GLN
41	2j	33	GLN

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Mol	Chain	Res	Type
41	2j	68	HIS
42	2k	104	GLN
42	2k	116	HIS
42	2k	117	ASN
43	2l	99	HIS
44	2m	77	ASN
46	2o	9	GLN
47	2p	14	ASN
49	2r	63	GLN
50	2s	69	HIS
50	2s	83	HIS
51	2t	75	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	442 (15%)	27 (0%)
1	2A	2791/2915 (95%)	449 (16%)	25 (0%)
2	1B	119/121 (98%)	13 (10%)	0
2	2B	118/121 (97%)	23 (19%)	0
32	1a	1497/1521 (98%)	240 (16%)	0
32	2a	1501/1521 (98%)	275 (18%)	0
53	1v	12/24 (50%)	0	0
53	2v	12/24 (50%)	0	0
54	1w	71/76 (93%)	21 (29%)	0
54	2w	68/76 (89%)	23 (33%)	0
55	1x	75/77 (97%)	8 (10%)	0
55	2x	75/77 (97%)	10 (13%)	0
57	1y	72/76 (94%)	25 (34%)	0
57	2y	70/76 (92%)	19 (27%)	0
All	All	9345/9620 (97%)	1548 (16%)	52 (0%)

All (1548) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	11	G
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	36	G

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Mol	Chain	Res	Type
1	1A	45	C
1	1A	61	G
1	1A	63	U
1	1A	71	A
1	1A	72	U
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	151	C
1	1A	154	G
1	1A	154(A)	C
1	1A	181	A
1	1A	182	A
1	1A	196	A
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	225	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	271(B)	C
1	1A	271(C)	C
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	271(X)	G
1	1A	272(B)	G
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G

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Mol	Chain	Res	Type
1	1A	353	G
1	1A	354	G
1	1A	357	A
1	1A	363	G
1	1A	363(B)	G
1	1A	386	G
1	1A	389	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	455	C
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	586	A
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	616	G
1	1A	627	A
1	1A	637	A
1	1A	645	C

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Mol	Chain	Res	Type
1	1A	646	A
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	668	G
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	746	A
1	1A	747	U
1	1A	764	A
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	783	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
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	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	892	G

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Mol	Chain	Res	Type
1	1A	893	C
1	1A	894	C
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	985	C
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1033	U
1	1A	1040	C
1	1A	1044	G
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G
1	1A	1065	U
1	1A	1068	G
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C

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Mol	Chain	Res	Type
1	1A	1081	U
1	1A	1083	U
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1093	G
1	1A	1094	U
1	1A	1098	A
1	1A	1099	G
1	1A	1101	U
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1128	A
1	1A	1135	C
1	1A	1136	G
1	1A	1142	U
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	1205	U
1	1A	1220	A
1	1A	1229	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	1281	G
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A

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Mol	Chain	Res	Type
1	1A	1365	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
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	1497	U
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1513	C
1	1A	1540	U
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1610	A
1	1A	1616	A
1	1A	1648	C
1	1A	1674	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1756	G

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Mol	Chain	Res	Type
1	1A	1763	G
1	1A	1764	G
1	1A	1769	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1786	A
1	1A	1791	A
1	1A	1800	C
1	1A	1812	A
1	1A	1816	G
1	1A	1829	A
1	1A	1839	G
1	1A	1847	A
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1927	A
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1960	A
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

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Mol	Chain	Res	Type
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2108	C
1	1A	2110	G
1	1A	2113	U
1	1A	2116	G
1	1A	2118	U
1	1A	2119	A
1	1A	2120	G
1	1A	2121	G
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2137	C
1	1A	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2150	U
1	1A	2151	G
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2161	C
1	1A	2166	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2181	G

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Mol	Chain	Res	Type
1	1A	2182	G
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	2208	A
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2283	C
1	1A	2286	A
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G
1	1A	2309	A
1	1A	2312	U
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2361	A
1	1A	2379	G
1	1A	2383	G
1	1A	2385	C
1	1A	2396	G
1	1A	2400	G
1	1A	2406	U
1	1A	2422	A
1	1A	2423	U
1	1A	2424	C
1	1A	2425	A
1	1A	2428	G
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U

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Mol	Chain	Res	Type
1	1A	2435	A
1	1A	2439	A
1	1A	2440	C
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	2554	U
1	1A	2562	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2578	G
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2660	A
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2721	A
1	1A	2726	U
1	1A	2733	A
1	1A	2757	A
1	1A	2765	A

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Mol	Chain	Res	Type
1	1A	2778	A
1	1A	2783	G
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2802	G
1	1A	2803	C
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2836	U
1	1A	2872	G
1	1A	2876	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
2	1B	2	C
2	1B	13	A
2	1B	25	A
2	1B	35	U
2	1B	45	A
2	1B	50	G
2	1B	56	G
2	1B	57	A
2	1B	67	G
2	1B	73	A
2	1B	85	G
2	1B	92	C
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	31	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	52	G
32	1a	61	G
32	1a	73	G
32	1a	77	G
32	1a	79	G

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Mol	Chain	Res	Type
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	142	G
32	1a	144	G
32	1a	145	G
32	1a	147	G
32	1a	163	C
32	1a	164	U
32	1a	174	C
32	1a	180	U
32	1a	182	U
32	1a	189(C)	C
32	1a	189(F)	U
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	347	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G

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Mol	Chain	Res	Type
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	441	A
32	1a	442	C
32	1a	451	A
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	483	C
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	531	U
32	1a	532	A
32	1a	533	A
32	1a	547	A
32	1a	559	A
32	1a	560	U
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	596	C
32	1a	607	A
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	666	G
32	1a	671	G
32	1a	672	U

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Mol	Chain	Res	Type
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	738	C
32	1a	749	C
32	1a	755	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	806	C
32	1a	815	A
32	1a	816	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	860	A
32	1a	870	U
32	1a	874	G
32	1a	902	G
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	932	C
32	1a	934	C
32	1a	936	C
32	1a	942	G
32	1a	950	U
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A

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Mol	Chain	Res	Type
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1011	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1035	A
32	1a	1037	C
32	1a	1039	C
32	1a	1044	A
32	1a	1045	C
32	1a	1068	G
32	1a	1081	G
32	1a	1086	U
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1127	G
32	1a	1132	C
32	1a	1134	G

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Mol	Chain	Res	Type
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G
32	1a	1157	A
32	1a	1159	U
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1213	A
32	1a	1219	U
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1312	G
32	1a	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1370	G

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Mol	Chain	Res	Type
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	1456	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1519	MA6
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
54	1w	2	C
54	1w	6	G
54	1w	7	A
54	1w	8	4SU
54	1w	9	A
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	36	A
54	1w	45	U
54	1w	46	G7M
54	1w	47	U
54	1w	48	C
54	1w	62	C
54	1w	67	C
54	1w	68	C
54	1w	73	A
54	1w	74	C
55	1x	5	G
55	1x	7	G
55	1x	9	G
55	1x	21	A

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Mol	Chain	Res	Type
55	1x	47	U
55	1x	61	C
55	1x	63	G
55	1x	64	G
57	1y	5	G
57	1y	6	G
57	1y	9	A
57	1y	13	C
57	1y	14	A
57	1y	19	G
57	1y	20	U
57	1y	21	A
57	1y	29	G
57	1y	35	A
57	1y	39	PSU
57	1y	44	G
57	1y	45	U
57	1y	46	G7M
57	1y	47	U
57	1y	48	C
57	1y	52	G
57	1y	56	C
57	1y	57	G
57	1y	58	A
57	1y	59	U
57	1y	61	C
57	1y	66	U
57	1y	70	G
57	1y	72	C
1	2A	8	A
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	36	G
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U

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Mol	Chain	Res	Type
1	2A	94	C
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	154	G
1	2A	154(A)	C
1	2A	157	U
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	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	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	346	A
1	2A	352	G
1	2A	354	G
1	2A	363	G
1	2A	363(B)	G
1	2A	370	G

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Mol	Chain	Res	Type
1	2A	386	G
1	2A	389	G
1	2A	399	G
1	2A	403	U
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	435	C
1	2A	442	G
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	479	A
1	2A	481	G
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	573	G
1	2A	574	C
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C
1	2A	637	A

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Mol	Chain	Res	Type
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	656	G
1	2A	669	G
1	2A	686	G
1	2A	701	G
1	2A	730	C
1	2A	740	U
1	2A	752	A
1	2A	753	C
1	2A	774	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	793	A
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	857	C
1	2A	859	G
1	2A	869	G
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	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	900	A

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Mol	Chain	Res	Type
1	2A	901	A
1	2A	904	C
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	933	A
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	950	G
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	990	A
1	2A	996	A
1	2A	999	U
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1021	A
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1114	G
1	2A	1116	C
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1143	A
1	2A	1167	U
1	2A	1171	G
1	2A	1206	G

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Mol	Chain	Res	Type
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1241	A
1	2A	1248	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1345	C
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	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
1	2A	1460	A
1	2A	1461	G
1	2A	1463	C
1	2A	1467	C
1	2A	1471	A

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Mol	Chain	Res	Type
1	2A	1482	G
1	2A	1486	A
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U
1	2A	1506	C
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1547	C
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1648	C
1	2A	1654	A
1	2A	1667	G
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G

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Mol	Chain	Res	Type
1	2A	1816	G
1	2A	1828	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1861	G
1	2A	1866	C
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1931	U
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	1984	G
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
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	2093	G
1	2A	2099	U
1	2A	2110	G
1	2A	2111	C

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Mol	Chain	Res	Type
1	2A	2112	G
1	2A	2116	G
1	2A	2117	A
1	2A	2120	G
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C
1	2A	2140	C
1	2A	2142	C
1	2A	2145	C
1	2A	2149	G
1	2A	2150	U
1	2A	2151	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2176	A
1	2A	2178	C
1	2A	2183	C
1	2A	2185	C
1	2A	2189	U
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G

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Mol	Chain	Res	Type
1	2A	2208	A
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	2297	C
1	2A	2298	A
1	2A	2305	A
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2366	A
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2391	G
1	2A	2403	C
1	2A	2406	U
1	2A	2410	G
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2459	A
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A
1	2A	2478	A

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Mol	Chain	Res	Type
1	2A	2491	U
1	2A	2494	G
1	2A	2497	A
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2549	G
1	2A	2554	U
1	2A	2555	U
1	2A	2562	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2574	G
1	2A	2578	G
1	2A	2582	G
1	2A	2585	U
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2634	G
1	2A	2645	G
1	2A	2654	A
1	2A	2660	A
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2748	A
1	2A	2751	G
1	2A	2757	A
1	2A	2758	A
1	2A	2765	A

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Mol	Chain	Res	Type
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
1	2A	2802	G
1	2A	2803	C
1	2A	2807	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2836	U
1	2A	2872	G
1	2A	2873	A
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	3	C
2	2B	8	U
2	2B	12	C
2	2B	13	A
2	2B	17	C
2	2B	19	G
2	2B	20	C
2	2B	33	G
2	2B	41	U
2	2B	45	A
2	2B	53	A
2	2B	54	G
2	2B	67	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	89	G
2	2B	106	G
2	2B	109	C
2	2B	110	G
2	2B	116	G
2	2B	120	A
32	2a	9	G
32	2a	22	G
32	2a	31	G

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Mol	Chain	Res	Type
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	66	G
32	2a	70	G
32	2a	73	G
32	2a	79	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	93	G
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	133	U
32	2a	144	G
32	2a	162	A
32	2a	163	C
32	2a	175	C
32	2a	182	U
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	231	G
32	2a	244	U
32	2a	247	G
32	2a	249	U
32	2a	250	A
32	2a	251	G
32	2a	258	G
32	2a	262	A
32	2a	266	G
32	2a	267	C

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Mol	Chain	Res	Type
32	2a	289	G
32	2a	301	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	345	C
32	2a	350	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	355	C
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	381	C
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	442	C
32	2a	452	A
32	2a	458	C
32	2a	470	C
32	2a	485	G
32	2a	492	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	527	G7M
32	2a	531	U
32	2a	532	A
32	2a	533	A

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Mol	Chain	Res	Type
32	2a	547	A
32	2a	559	A
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	630	G
32	2a	639	G
32	2a	641	U
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
32	2a	731	G
32	2a	749	C
32	2a	755	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	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	855	G
32	2a	859	A
32	2a	874	G

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Mol	Chain	Res	Type
32	2a	902	G
32	2a	914	A
32	2a	924	C
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	938	A
32	2a	942	G
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
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	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

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Mol	Chain	Res	Type
32	2a	1032	G
32	2a	1033	G
32	2a	1035	A
32	2a	1036	G
32	2a	1037	C
32	2a	1039	C
32	2a	1040	U
32	2a	1043	C
32	2a	1045	C
32	2a	1051	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1079	G
32	2a	1081	G
32	2a	1085	U
32	2a	1086	U
32	2a	1092	A
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1105	A
32	2a	1125	U
32	2a	1127	G
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1143	G
32	2a	1144	G
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1160	G

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Mol	Chain	Res	Type
32	2a	1182	G
32	2a	1184	G
32	2a	1186	G
32	2a	1191	A
32	2a	1192	C
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1201	A
32	2a	1202	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1215	G
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1255	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1264	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1281	U
32	2a	1287	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1316	G
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G
32	2a	1352	C
32	2a	1359	C
32	2a	1363	C

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Mol	Chain	Res	Type
32	2a	1368	G
32	2a	1370	G
32	2a	1380	U
32	2a	1397	C
32	2a	1404	5MC
32	2a	1405	G
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1487	G
32	2a	1492	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
54	2w	4	C
54	2w	6	G
54	2w	8	4SU
54	2w	9	A
54	2w	12	U
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	46	G7M
54	2w	47	U
54	2w	48	C
54	2w	50	U
54	2w	51	U
54	2w	58	A
54	2w	62	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

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Mol	Chain	Res	Type
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	19	G
55	2x	20	U
55	2x	21	A
55	2x	47	U
55	2x	56	C
55	2x	61	C
55	2x	69	C
57	2y	15	G
57	2y	19	G
57	2y	23	A
57	2y	27	G
57	2y	38	A
57	2y	40	C
57	2y	48	C
57	2y	49	C
57	2y	52	G
57	2y	53	G
57	2y	54	5MU
57	2y	56	C
57	2y	58	A
57	2y	59	U
57	2y	65	G
57	2y	68	C
57	2y	69	G
57	2y	70	G
57	2y	73	A

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	271(J)	C
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	685	A
1	1A	746	A

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Mol	Chain	Res	Type
1	1A	764	A
1	1A	974	G
1	1A	1067	A
1	1A	1174	A
1	1A	1176	G
1	1A	1379	A
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2430	A
1	1A	2439	A
1	1A	2629	A
1	1A	2689	U
1	1A	2756	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1240	U
1	2A	1420	U
1	2A	1442	G
1	2A	1460	A
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2335	A
1	2A	2439	A

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Mol	Chain	Res	Type
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	5MU	2x	54	55	19,22,23	1.39	5 (26%)	27,32,35	2.34	6 (22%)
57	5MU	2y	54	57	19,22,23	1.52	5 (26%)	27,32,35	1.67	8 (29%)
57	PSU	1y	55	57	18,21,22	1.39	2 (11%)	21,30,33	2.03	4 (19%)
32	5MC	2a	1407	32	19,22,23	1.62	3 (15%)	26,32,35	1.17	3 (11%)
54	MIA	1w	37	54	28,31,32	2.26	6 (21%)	38,44,47	2.98	14 (36%)
55	4SU	2x	8	55	18,21,22	2.08	6 (33%)	25,30,33	1.51	4 (16%)
43	0TD	2l	92	43	8,9,10	4.59	1 (12%)	6,11,13	3.45	3 (50%)
57	PSU	2y	32	57	18,21,22	1.37	2 (11%)	21,30,33	2.00	4 (19%)
54	5MU	2w	54	54	19,22,23	1.37	4 (21%)	27,32,35	1.80	5 (18%)
32	5MC	2a	1404	32	19,22,23	1.72	3 (15%)	26,32,35	1.17	2 (7%)
57	MIA	1y	37	57	21,24,32	1.58	4 (19%)	30,35,47	2.03	7 (23%)
54	PSU	2w	32	54	18,21,22	1.41	2 (11%)	21,30,33	1.87	4 (19%)
57	PSU	1y	32	57	18,21,22	1.38	2 (11%)	21,30,33	1.93	4 (19%)
57	5MU	1y	54	57	19,22,23	1.43	4 (21%)	27,32,35	1.91	6 (22%)
1	PSU	1A	1911	1	18,21,22	1.35	2 (11%)	21,30,33	2.12	5 (23%)
1	PSU	1A	2605	1	18,21,22	1.41	3 (16%)	21,30,33	2.14	5 (23%)
32	5MC	1a	1407	32	19,22,23	1.59	2 (10%)	26,32,35	1.15	3 (11%)
1	2MA	2A	2503	58,1	22,25,26	1.54	4 (18%)	32,37,40	2.42	8 (25%)
1	2MA	1A	2503	58,1	22,25,26	1.59	5 (22%)	32,37,40	2.19	9 (28%)
54	G7M	2w	46	54	23,26,27	1.47	3 (13%)	34,39,42	1.72	5 (14%)
1	5MC	1A	1942	1	19,22,23	1.60	3 (15%)	26,32,35	1.23	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMC	2A	1920	1	19,22,23	0.80	0	25,31,34	0.96	0
32	5MC	2a	1400	32	19,22,23	1.74	3 (15%)	26,32,35	1.18	2 (7%)
54	5MU	1w	54	54	19,22,23	1.30	3 (15%)	27,32,35	2.17	6 (22%)
54	PSU	2w	39	54	18,21,22	1.41	2 (11%)	21,30,33	1.85	4 (19%)
1	OMG	1A	2251	55,58,1	23,26,27	1.22	3 (13%)	32,38,41	2.03	6 (18%)
32	2MG	2a	1207	32	23,26,27	1.26	3 (13%)	33,38,41	2.16	9 (27%)
57	4SU	1y	8	57	18,21,22	1.75	4 (22%)	25,30,33	2.14	5 (20%)
57	PSU	1y	39	57	18,21,22	1.36	2 (11%)	21,30,33	1.98	4 (19%)
1	OMU	2A	2552	58,1	19,22,23	1.25	2 (10%)	25,31,34	1.80	5 (20%)
55	4SU	1x	8	55	18,21,22	2.17	5 (27%)	25,30,33	1.86	6 (24%)
55	5MC	2x	32	55	19,22,23	1.77	3 (15%)	26,32,35	1.34	5 (19%)
54	PSU	2w	55	54	18,21,22	1.38	2 (11%)	21,30,33	1.94	3 (14%)
55	PSU	2x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.02	4 (19%)
57	G7M	1y	46	57	23,26,27	1.55	4 (17%)	34,39,42	1.76	4 (11%)
32	5MC	1a	967	32	19,22,23	1.67	3 (15%)	26,32,35	1.17	3 (11%)
55	8AN	2x	76	55,58,56,59	21,24,25	1.41	3 (14%)	26,35,38	2.31	11 (42%)
32	5MC	2a	967	32	19,22,23	1.69	3 (15%)	26,32,35	1.14	3 (11%)
32	UR3	1a	1498	32	19,22,23	1.06	1 (5%)	26,32,35	1.75	4 (15%)
1	PSU	2A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	2.11	4 (19%)
54	PSU	1w	32	54,58	18,21,22	1.36	2 (11%)	21,30,33	1.95	3 (14%)
54	F3N	2w	76	54,1	33,36,37	1.46	4 (12%)	41,51,54	1.72	9 (21%)
55	5MU	1x	54	55	19,22,23	1.41	5 (26%)	27,32,35	1.94	6 (22%)
54	PSU	1w	55	54	18,21,22	1.39	2 (11%)	21,30,33	1.97	3 (14%)
1	5MC	2A	1962	58,1	19,22,23	1.70	3 (15%)	26,32,35	1.16	3 (11%)
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.13	8 (24%)
32	4OC	1a	1402	32	20,23,24	0.76	0	25,32,35	0.92	1 (4%)
32	M2G	2a	966	32	24,27,28	1.30	4 (16%)	33,40,43	1.89	5 (15%)
54	F3N	1w	76	54,1	33,36,37	1.43	4 (12%)	41,51,54	1.75	9 (21%)
43	0TD	1l	92	43	8,9,10	4.59	2 (25%)	6,11,13	9.08	2 (33%)
32	5MC	1a	1400	32	19,22,23	1.63	3 (15%)	26,32,35	1.18	3 (11%)
55	5MC	1x	32	55	19,22,23	1.57	3 (15%)	26,32,35	1.24	2 (7%)
1	5MC	2A	1942	1	19,22,23	1.67	2 (10%)	26,32,35	1.13	2 (7%)
55	PSU	1x	55	55	18,21,22	1.42	2 (11%)	21,30,33	1.90	3 (14%)
32	G7M	2a	527	58,32	23,26,27	1.45	3 (13%)	34,39,42	1.66	5 (14%)
32	5MC	1a	1404	32	19,22,23	1.66	3 (15%)	26,32,35	1.13	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMC	1A	1920	1	19,22,23	0.84	0	25,31,34	0.87	0
32	MA6	2a	1518	32	23,26,27	0.43	0	33,38,41	2.10	9 (27%)
1	PSU	2A	2605	1	18,21,22	1.33	4 (22%)	21,30,33	2.19	4 (19%)
32	UR3	2a	1498	32	19,22,23	1.02	0	26,32,35	1.73	3 (11%)
1	5MU	2A	1939	1	19,22,23	1.41	6 (31%)	27,32,35	2.12	6 (22%)
57	4SU	2y	8	57	18,21,22	1.78	4 (22%)	25,30,33	2.09	5 (20%)
55	8AN	1x	76	55,58,56	21,24,25	1.50	3 (14%)	26,35,38	2.58	11 (42%)
57	PSU	2y	55	57	18,21,22	1.40	3 (16%)	21,30,33	1.97	4 (19%)
54	4SU	2w	8	54	18,21,22	1.78	3 (16%)	25,30,33	2.52	5 (20%)
57	G7M	2y	46	57	23,26,27	1.56	3 (13%)	34,39,42	1.86	4 (11%)
54	4SU	1w	8	54	18,21,22	1.97	5 (27%)	25,30,33	1.65	6 (24%)
32	PSU	1a	516	58,32	18,21,22	1.40	2 (11%)	21,30,33	1.92	5 (23%)
1	PSU	2A	1917	1	18,21,22	1.36	2 (11%)	21,30,33	2.07	3 (14%)
54	PSU	1w	39	54	18,21,22	1.30	2 (11%)	21,30,33	2.02	4 (19%)
54	G7M	1w	46	54	23,26,27	1.50	4 (17%)	34,39,42	1.70	4 (11%)
1	OMU	1A	2552	58,1	19,22,23	1.23	3 (15%)	25,31,34	1.75	5 (20%)
1	5MC	1A	1962	1	19,22,23	1.66	3 (15%)	26,32,35	1.13	2 (7%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.07	3 (14%)
1	OMG	2A	2251	55,58,1	23,26,27	1.18	3 (13%)	32,38,41	2.04	8 (25%)
32	G7M	1a	527	32	23,26,27	1.50	4 (17%)	34,39,42	1.71	5 (14%)
57	PSU	2y	39	57	18,21,22	1.38	2 (11%)	21,30,33	1.86	4 (19%)
32	2MG	1a	1207	32	23,26,27	1.26	3 (13%)	33,38,41	2.20	7 (21%)
32	4OC	2a	1402	32	20,23,24	0.75	0	25,32,35	1.24	3 (12%)
1	5MU	1A	1939	58,1	19,22,23	1.51	6 (31%)	27,32,35	2.20	6 (22%)
32	MA6	1a	1518	32	23,26,27	0.43	0	33,38,41	2.04	9 (27%)
32	M2G	1a	966	32	24,27,28	1.30	3 (12%)	33,40,43	1.93	5 (15%)
1	5MU	2A	1915	1	19,22,23	1.48	5 (26%)	27,32,35	2.09	7 (25%)
32	PSU	2a	516	32	18,21,22	1.34	2 (11%)	21,30,33	2.00	4 (19%)
32	MA6	2a	1519	32	23,26,27	0.42	0	33,38,41	2.17	10 (30%)
57	MIA	2y	37	57	21,24,32	1.62	4 (19%)	30,35,47	2.07	7 (23%)
1	5MU	1A	1915	1	19,22,23	1.31	5 (26%)	27,32,35	2.15	7 (25%)
54	MIA	2w	37	54	24,27,32	2.18	5 (20%)	32,39,47	2.69	11 (34%)

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	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
57	5MU	2y	54	57	-	2/7/25/26	0/2/2/2
57	PSU	1y	55	57	-	2/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	3/15/33/34	0/3/3/3
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
57	PSU	2y	32	57	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	1/7/25/26	0/2/2/2
57	MIA	1y	37	57	-	0/7/25/34	0/3/3/3
54	PSU	2w	32	54	-	2/7/25/26	0/2/2/2
57	PSU	1y	32	57	-	0/7/25/26	0/2/2/2
57	5MU	1y	54	57	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	58,1	-	2/7/25/26	0/3/3/3
1	2MA	1A	2503	58,1	-	1/7/25/26	0/3/3/3
54	G7M	2w	46	54	-	3/7/25/26	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	1/7/25/26	0/2/2/2
1	OMG	1A	2251	55,58,1	-	0/9/27/28	0/3/3/3
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
57	4SU	1y	8	57	-	2/7/25/26	0/2/2/2
57	PSU	1y	39	57	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	58,1	-	0/9/27/28	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
57	G7M	1y	46	57	-	2/7/25/26	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
55	8AN	2x	76	55,58,56,59	-	3/7/25/26	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	1w	32	54,58	-	0/7/25/26	0/2/2/2
54	F3N	2w	76	54,1	-	2/19/37/38	0/4/4/4
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	58,1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
54	F3N	1w	76	54,1	-	0/19/37/38	0/4/4/4
43	0TD	1l	92	43	-	2/7/12/14	-
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	58,32	-	3/7/25/26	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
57	4SU	2y	8	57	-	1/7/25/26	0/2/2/2
55	8AN	1x	76	55,58,56	-	3/7/25/26	0/3/3/3
57	PSU	2y	55	57	-	1/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	2/7/25/26	0/2/2/2
57	G7M	2y	46	57	-	2/7/25/26	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	58,32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
1	OMU	1A	2552	58,1	-	0/9/27/28	0/2/2/2
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,58,1	-	0/9/27/28	0/3/3/3
32	G7M	1a	527	32	-	3/7/25/26	0/3/3/3
57	PSU	2y	39	57	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
32	4OC	2a	1402	32	-	3/9/29/30	0/2/2/2
1	5MU	1A	1939	58,1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
57	MIA	2y	37	57	-	2/7/25/34	0/3/3/3
1	5MU	1A	1915	1	-	1/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/11/29/34	0/3/3/3

All (254) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.53	1.69	1.82
43	1l	92	0TD	CB-SB	-12.41	1.69	1.82
54	2w	37	MIA	C2-S10	-7.51	1.69	1.75
55	2x	32	5MC	C5-C4	6.63	1.49	1.44
54	1w	37	MIA	C13-C14	6.60	1.52	1.32
54	1w	37	MIA	C2-S10	-6.35	1.70	1.75
32	2a	1404	5MC	C5-C4	6.34	1.48	1.44
32	2a	1400	5MC	C5-C4	6.29	1.48	1.44
32	2a	967	5MC	C5-C4	6.25	1.48	1.44
32	1a	967	5MC	C5-C4	6.19	1.48	1.44
1	2A	1942	5MC	C5-C4	6.09	1.48	1.44
1	2A	1962	5MC	C5-C4	6.08	1.48	1.44
1	1A	1962	5MC	C5-C4	6.03	1.48	1.44
32	2a	1407	5MC	C5-C4	5.97	1.48	1.44
32	1a	1404	5MC	C5-C4	5.88	1.48	1.44
1	1A	1942	5MC	C5-C4	5.83	1.48	1.44
32	1a	1407	5MC	C5-C4	5.81	1.48	1.44
32	1a	1400	5MC	C5-C4	5.76	1.48	1.44
55	1x	32	5MC	C5-C4	5.53	1.48	1.44
57	2y	37	MIA	C5-C4	5.15	1.48	1.39
54	2w	8	4SU	C4-S4	-5.10	1.59	1.68
54	1w	37	MIA	C5-C4	5.07	1.48	1.39
54	2w	37	MIA	C5-C4	5.03	1.48	1.39
57	1y	37	MIA	C5-C4	5.03	1.48	1.39
54	2w	76	F3N	CB-CG	-4.86	1.39	1.51
54	1w	8	4SU	C4-S4	-4.86	1.60	1.68
55	1x	8	4SU	C4-N3	-4.82	1.32	1.37
1	1A	2503	2MA	C5-C4	4.76	1.47	1.39
57	2y	8	4SU	C4-S4	-4.73	1.60	1.68
55	2x	8	4SU	C4-S4	-4.67	1.60	1.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	527	G7M	C5-N7	-4.66	1.33	1.39
1	2A	2503	2MA	C5-C4	4.64	1.47	1.39
55	2x	8	4SU	C4-N3	-4.64	1.32	1.37
54	1w	46	G7M	C5-N7	-4.64	1.33	1.39
54	1w	76	F3N	CB-CG	-4.62	1.40	1.51
57	1y	8	4SU	C4-S4	-4.53	1.60	1.68
54	2w	46	G7M	C5-N7	-4.41	1.34	1.39
57	2y	46	G7M	C5-N7	-4.37	1.34	1.39
55	1x	8	4SU	C4-S4	-4.36	1.61	1.68
57	1y	46	G7M	C5-N7	-4.25	1.34	1.39
54	2w	39	PSU	C6-C5	4.21	1.40	1.35
32	2a	527	G7M	C5-N7	-4.20	1.34	1.39
57	2y	39	PSU	C6-C5	4.19	1.39	1.35
54	1w	8	4SU	C4-N3	-4.18	1.33	1.37
54	1w	55	PSU	C6-C5	4.13	1.39	1.35
57	1y	32	PSU	C6-C5	4.02	1.39	1.35
57	1y	39	PSU	C6-C5	4.00	1.39	1.35
54	2w	55	PSU	C6-C5	3.98	1.39	1.35
57	1y	55	PSU	C6-C5	3.94	1.39	1.35
54	2w	76	F3N	C5-N7	-3.90	1.32	1.39
32	2a	516	PSU	C6-C5	3.90	1.39	1.35
57	2y	32	PSU	C6-C5	3.86	1.39	1.35
55	2x	76	8AN	C5-N7	-3.84	1.32	1.39
54	2w	32	PSU	C6-C5	3.84	1.39	1.35
55	1x	76	8AN	C5-N7	-3.82	1.32	1.39
55	1x	8	4SU	C2-N3	-3.78	1.31	1.38
54	1w	76	F3N	C5-N7	-3.77	1.32	1.39
55	1x	55	PSU	C6-C5	3.71	1.39	1.35
57	2y	46	G7M	C5-C4	3.66	1.47	1.38
57	1y	46	G7M	C5-C4	3.65	1.47	1.38
1	2A	1917	PSU	C6-C5	3.54	1.39	1.35
1	1A	1917	PSU	C6-C5	3.51	1.39	1.35
32	1a	516	PSU	C6-C5	3.50	1.39	1.35
55	2x	55	PSU	C6-C5	3.49	1.39	1.35
54	1w	32	PSU	C6-C5	3.48	1.39	1.35
55	1x	8	4SU	C5-C4	-3.46	1.38	1.42
57	2y	55	PSU	C6-C5	3.42	1.39	1.35
1	2A	1911	PSU	C6-C5	3.39	1.39	1.35
32	1a	527	G7M	C5-C4	3.38	1.46	1.38
54	1w	39	PSU	C6-C5	3.35	1.39	1.35
54	2w	46	G7M	C5-C4	3.33	1.46	1.38
32	2a	1207	2MG	C5-C4	3.31	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	46	G7M	C5-C4	3.27	1.46	1.38
1	1A	2251	OMG	C5-C4	3.23	1.47	1.38
1	1A	1911	PSU	C6-C5	3.23	1.38	1.35
55	2x	8	4SU	C5-C4	-3.22	1.38	1.42
1	2A	2605	PSU	C6-C5	3.20	1.38	1.35
1	1A	2605	PSU	C4-N3	-3.17	1.32	1.38
32	2a	966	M2G	C5-C4	3.16	1.47	1.38
57	2y	54	5MU	C2-N1	3.16	1.43	1.38
57	2y	54	5MU	C6-C5	3.15	1.39	1.34
32	1a	966	M2G	C5-C4	3.14	1.47	1.38
55	1x	76	8AN	C5-C4	-3.14	1.33	1.39
54	1w	76	F3N	C5-C4	-3.13	1.33	1.39
55	2x	76	8AN	C5-C4	-3.12	1.33	1.39
32	2a	527	G7M	C5-C4	3.12	1.46	1.38
32	1a	1207	2MG	C5-C4	3.10	1.47	1.38
1	1A	2605	PSU	C6-C5	3.09	1.38	1.35
57	2y	8	4SU	C4-N3	-3.08	1.34	1.37
54	2w	76	F3N	C5-C4	-3.07	1.33	1.39
1	2A	2251	OMG	C5-C4	3.06	1.47	1.38
1	2A	1939	5MU	C6-C5	3.00	1.39	1.34
32	1a	966	M2G	C2-N2	2.99	1.40	1.35
54	2w	37	MIA	C5-C6	2.98	1.49	1.41
1	2A	1942	5MC	C6-C5	2.96	1.39	1.34
1	2A	1962	5MC	C6-C5	2.95	1.39	1.34
54	2w	54	5MU	C6-C5	2.95	1.39	1.34
54	2w	8	4SU	C4-N3	-2.95	1.34	1.37
32	1a	1400	5MC	C6-C5	2.90	1.39	1.34
57	2y	37	MIA	C5-C6	2.90	1.49	1.41
1	2A	1915	5MU	C6-C5	2.88	1.39	1.34
55	1x	54	5MU	C4-N3	-2.88	1.33	1.38
32	2a	1400	5MC	C6-C5	2.85	1.39	1.34
57	1y	54	5MU	C6-C5	2.85	1.39	1.34
57	1y	8	4SU	C4-N3	-2.84	1.34	1.37
32	1a	1407	5MC	C6-C5	2.84	1.39	1.34
32	2a	966	M2G	C2-N2	2.83	1.40	1.35
1	2A	1915	5MU	C4-C5	2.83	1.49	1.44
55	2x	8	4SU	C2-N3	-2.82	1.33	1.38
54	1w	37	MIA	C5-C6	2.82	1.48	1.41
32	2a	1404	5MC	C6-C5	2.80	1.39	1.34
1	1A	1962	5MC	C6-C5	2.80	1.39	1.34
54	1w	8	4SU	C5-C4	-2.79	1.39	1.42
55	1x	54	5MU	C6-C5	2.79	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1y	8	4SU	C2-N1	2.79	1.42	1.38
57	1y	37	MIA	C5-C6	2.78	1.48	1.41
1	2A	1915	5MU	C2-N1	2.78	1.42	1.38
1	1A	1939	5MU	C4-C5	2.75	1.49	1.44
1	1A	2552	OMU	C4-N3	-2.73	1.33	1.38
54	1w	32	PSU	C4-N3	-2.73	1.33	1.38
1	1A	1942	5MC	C6-C5	2.72	1.39	1.34
57	2y	8	4SU	C2-N1	2.69	1.42	1.38
1	1A	2503	2MA	C5-C6	2.69	1.48	1.41
55	2x	76	8AN	C5-C6	-2.67	1.33	1.41
55	2x	54	5MU	C6-C5	2.67	1.39	1.34
1	2A	2552	OMU	C4-N3	-2.66	1.34	1.38
57	2y	54	5MU	C4-N3	-2.66	1.33	1.38
57	1y	54	5MU	C4-C5	2.65	1.49	1.44
54	1w	54	5MU	C6-C5	2.63	1.38	1.34
32	1a	1404	5MC	C6-C5	2.63	1.38	1.34
1	1A	1911	PSU	C4-N3	-2.60	1.34	1.38
1	1A	1939	5MU	C4-N3	-2.59	1.34	1.38
1	1A	1939	5MU	C6-N1	-2.59	1.33	1.38
1	2A	1911	PSU	C4-N3	-2.59	1.34	1.38
32	1a	516	PSU	C4-N3	-2.59	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.58	1.33	1.38
32	1a	1207	2MG	C6-N1	-2.57	1.34	1.38
1	1A	1939	5MU	C6-C5	2.57	1.38	1.34
55	2x	54	5MU	C4-N3	-2.57	1.34	1.38
54	2w	8	4SU	C5-C4	-2.56	1.39	1.42
32	1a	1498	UR3	C2-N1	2.56	1.42	1.38
1	2A	2503	2MA	C5-N7	-2.56	1.34	1.39
32	2a	967	5MC	C6-C5	2.56	1.38	1.34
55	1x	8	4SU	O2-C2	2.54	1.27	1.23
55	1x	32	5MC	C6-C5	2.54	1.38	1.34
1	2A	1917	PSU	C4-N3	-2.54	1.34	1.38
54	1w	8	4SU	C2-N3	-2.54	1.33	1.38
55	1x	76	8AN	C5-C6	-2.53	1.33	1.41
57	1y	8	4SU	C5-C4	-2.53	1.39	1.42
57	2y	55	PSU	C4-N3	-2.52	1.34	1.38
54	2w	76	F3N	C5-C6	-2.52	1.34	1.41
1	1A	2503	2MA	C8-N7	2.52	1.36	1.31
1	2A	2503	2MA	C5-C6	2.52	1.48	1.41
1	2A	2251	OMG	C6-N1	-2.51	1.34	1.38
54	1w	54	5MU	C2-N1	2.50	1.42	1.38
32	1a	966	M2G	C6-N1	-2.49	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	967	5MC	C6-C5	2.49	1.38	1.34
55	2x	55	PSU	C4-N3	-2.48	1.34	1.38
1	2A	1939	5MU	C4-N3	-2.47	1.34	1.38
55	2x	54	5MU	C4-C5	2.47	1.48	1.44
1	2A	2552	OMU	C5-C4	2.46	1.49	1.43
54	1w	76	F3N	C5-C6	-2.46	1.34	1.41
55	2x	32	5MC	C6-C5	2.46	1.38	1.34
55	2x	54	5MU	C2-N1	2.45	1.42	1.38
1	1A	1917	PSU	C4-N3	-2.45	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.44	1.34	1.38
55	1x	55	PSU	C4-N3	-2.44	1.34	1.38
1	2A	1939	5MU	C2-N1	2.43	1.42	1.38
57	1y	37	MIA	C8-N7	2.43	1.36	1.31
54	2w	32	PSU	C4-N3	-2.43	1.34	1.38
32	2a	527	G7M	C6-N1	-2.40	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.39	1.33	1.38
54	1w	39	PSU	C4-N3	-2.39	1.34	1.38
55	1x	32	5MC	C6-N1	-2.39	1.33	1.38
32	2a	1400	5MC	C6-N1	-2.39	1.33	1.38
54	1w	37	MIA	C5-N7	-2.38	1.34	1.39
57	2y	37	MIA	C8-N7	2.38	1.36	1.31
57	1y	54	5MU	C4-N3	-2.38	1.34	1.38
32	2a	1407	5MC	C6-C5	2.38	1.38	1.34
57	1y	39	PSU	C4-N3	-2.37	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.37	1.34	1.38
55	2x	32	5MC	C6-N1	-2.36	1.34	1.38
55	2x	8	4SU	O2-C2	2.36	1.27	1.23
32	2a	966	M2G	C6-N1	-2.35	1.34	1.38
57	2y	8	4SU	C5-C4	-2.35	1.39	1.42
54	2w	54	5MU	C4-N3	-2.35	1.34	1.38
1	1A	1915	5MU	C6-C5	2.34	1.38	1.34
57	1y	54	5MU	C2-N1	2.34	1.42	1.38
1	2A	1915	5MU	C4-N3	-2.33	1.34	1.38
1	1A	1915	5MU	C4-C5	2.33	1.48	1.44
54	1w	37	MIA	C8-N7	2.33	1.36	1.31
32	1a	967	5MC	C6-N1	-2.33	1.34	1.38
1	1A	1915	5MU	C2-N1	2.32	1.42	1.38
54	2w	54	5MU	C2-N1	2.31	1.42	1.38
1	1A	1915	5MU	C4-N3	-2.31	1.34	1.38
57	2y	54	5MU	C2-N3	-2.30	1.34	1.38
57	2y	46	G7M	C6-N1	-2.30	1.34	1.38
1	2A	1939	5MU	C4-C5	2.29	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2503	2MA	C8-N7	2.29	1.36	1.31
32	1a	1404	5MC	C6-N1	-2.29	1.34	1.38
57	2y	32	PSU	C4-N3	-2.28	1.34	1.38
57	1y	32	PSU	C4-N3	-2.28	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.27	1.34	1.38
54	2w	37	MIA	C5-N7	-2.27	1.34	1.39
1	1A	1939	5MU	C2-N1	2.27	1.42	1.38
1	1A	2251	OMG	C5-N7	-2.27	1.34	1.39
32	2a	1404	5MC	C6-N1	-2.26	1.34	1.38
54	2w	55	PSU	C4-N3	-2.26	1.34	1.38
1	1A	2503	2MA	C5-N7	-2.25	1.35	1.39
55	1x	54	5MU	C2-N3	-2.23	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.23	1.34	1.38
54	1w	55	PSU	C4-N3	-2.23	1.34	1.38
57	1y	55	PSU	C4-N3	-2.22	1.34	1.38
1	1A	2503	2MA	C4-N9	-2.22	1.33	1.37
32	1a	527	G7M	C4-N9	-2.22	1.32	1.38
57	2y	39	PSU	C4-N3	-2.21	1.34	1.38
32	1a	527	G7M	C6-N1	-2.21	1.34	1.38
54	1w	8	4SU	C2-N1	2.20	1.41	1.38
57	1y	46	G7M	C6-N1	-2.20	1.34	1.38
57	2y	54	5MU	O2-C2	2.19	1.26	1.23
1	1A	2251	OMG	C6-N1	-2.19	1.34	1.38
54	2w	54	5MU	C4-C5	2.18	1.48	1.44
1	1A	2552	OMU	C5-C4	2.15	1.48	1.43
54	2w	37	MIA	C8-N7	2.15	1.35	1.31
54	1w	46	G7M	C6-N1	-2.14	1.34	1.38
57	2y	37	MIA	C5-N7	-2.14	1.35	1.39
57	1y	46	G7M	C5-C6	2.14	1.49	1.43
54	2w	39	PSU	C4-N3	-2.14	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.13	1.34	1.38
1	1A	1915	5MU	C6-N1	-2.12	1.34	1.38
32	2a	967	5MC	C6-N1	-2.12	1.34	1.38
32	2a	516	PSU	C4-N3	-2.12	1.34	1.38
54	1w	54	5MU	C4-N3	-2.12	1.34	1.38
1	1A	2605	PSU	C2-N3	-2.12	1.34	1.37
55	2x	8	4SU	C2-N1	2.11	1.41	1.38
1	2A	1939	5MU	C2-N3	-2.11	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.10	1.34	1.38
32	2a	1207	2MG	C5-N7	-2.10	1.34	1.39
55	2x	54	5MU	C6-N1	-2.10	1.34	1.38
55	1x	54	5MU	C6-N1	-2.10	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1y	37	MIA	C5-N7	-2.09	1.35	1.39
55	1x	54	5MU	C2-N1	2.08	1.41	1.38
1	2A	2605	PSU	C2-N1	-2.08	1.34	1.36
1	2A	2605	PSU	C4-N3	-2.07	1.35	1.38
43	1l	92	0TD	CB-CG	2.07	1.55	1.52
54	2w	46	G7M	C5-C6	2.05	1.48	1.43
32	1a	1207	2MG	C2-N3	2.03	1.35	1.32
1	2A	1939	5MU	C6-N1	-2.03	1.34	1.38
54	1w	46	G7M	C4-N9	-2.02	1.32	1.38
1	2A	2605	PSU	C2-N3	-2.02	1.34	1.37
1	2A	2251	OMG	C5-N7	-2.02	1.35	1.39
32	2a	966	M2G	C5-N7	-2.02	1.35	1.39
57	2y	55	PSU	C2-N1	-2.02	1.34	1.36
1	1A	2552	OMU	C2-N3	-2.01	1.34	1.38

All (442) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	-21.82	63.14	102.36
54	1w	37	MIA	C12-C13-C14	-10.41	108.32	127.01
54	2w	37	MIA	C5-C4-N3	-9.12	117.58	127.18
1	2A	2503	2MA	C5-C4-N3	-8.69	118.02	127.18
54	1w	37	MIA	C5-C4-N3	-8.20	118.55	127.18
54	2w	8	4SU	C4-N3-C2	-7.69	119.94	127.31
54	2w	37	MIA	N3-C4-N9	7.40	136.39	126.99
43	2l	92	0TD	CSB-SB-CB	-7.23	89.37	102.36
32	2a	1498	UR3	C4-N3-C2	-7.08	118.89	124.58
1	2A	2503	2MA	N3-C4-N9	7.05	135.94	126.99
32	1a	1207	2MG	C2-N3-C4	7.01	120.77	112.00
1	1A	2503	2MA	C5-C4-N3	-6.93	119.88	127.18
1	1A	2605	PSU	N1-C2-N3	6.70	122.24	115.17
32	1a	1498	UR3	C4-N3-C2	-6.67	119.21	124.58
54	2w	8	4SU	C5-C4-N3	6.50	120.79	114.75
32	2a	1207	2MG	C2-N3-C4	6.49	120.12	112.00
1	2A	1917	PSU	N1-C2-N3	6.49	122.02	115.17
1	1A	1911	PSU	N1-C2-N3	6.45	121.97	115.17
54	1w	37	MIA	N3-C4-N9	6.35	135.05	126.99
55	2x	55	PSU	N1-C2-N3	6.32	121.84	115.17
1	2A	2251	OMG	C5-C4-N3	-6.30	118.36	128.39
1	1A	2251	OMG	C5-C4-N3	-6.30	118.37	128.39
57	1y	55	PSU	N1-C2-N3	6.29	121.81	115.17
1	2A	1911	PSU	N1-C2-N3	6.27	121.79	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2605	PSU	N1-C2-N3	6.25	121.76	115.17
57	2y	37	MIA	C5-C4-N3	-6.21	118.16	126.72
57	2y	46	G7M	N9-C4-N3	6.20	138.36	125.95
57	2y	32	PSU	N1-C2-N3	6.20	121.71	115.17
32	2a	966	M2G	C5-C4-N3	-6.20	118.53	128.39
32	1a	966	M2G	C5-C4-N3	-6.18	118.56	128.39
54	1w	32	PSU	N1-C2-N3	6.14	121.65	115.17
1	1A	1917	PSU	N1-C2-N3	6.12	121.62	115.17
57	1y	37	MIA	C5-C4-N3	-6.08	118.35	126.72
54	1w	39	PSU	N1-C2-N3	6.07	121.57	115.17
55	1x	76	8AN	O4'-C1'-N9	6.06	119.74	108.09
32	1a	516	PSU	N1-C2-N3	6.03	121.53	115.17
32	2a	1207	2MG	C5-C4-N3	-6.03	118.79	128.39
57	2y	8	4SU	C4-N3-C2	-6.03	121.54	127.31
57	1y	39	PSU	N1-C2-N3	6.02	121.51	115.17
32	2a	516	PSU	N1-C2-N3	5.98	121.48	115.17
32	1a	1207	2MG	C5-C4-N3	-5.95	118.92	128.39
54	2w	55	PSU	N1-C2-N3	5.94	121.43	115.17
54	1w	55	PSU	N1-C2-N3	5.92	121.42	115.17
55	1x	55	PSU	N1-C2-N3	5.89	121.38	115.17
55	2x	54	5MU	C4-N3-C2	-5.88	119.62	127.34
55	1x	76	8AN	N1-C2-N3	-5.76	119.87	128.58
57	1y	46	G7M	N9-C4-N3	5.73	137.42	125.95
57	2y	55	PSU	N1-C2-N3	5.73	121.21	115.17
54	1w	76	F3N	N1-C2-N3	-5.71	119.93	128.58
57	1y	32	PSU	N1-C2-N3	5.71	121.19	115.17
54	2w	32	PSU	N1-C2-N3	5.71	121.19	115.17
54	2w	76	F3N	N1-C2-N3	-5.66	120.01	128.58
55	2x	76	8AN	N1-C2-N3	-5.66	120.02	128.58
1	1A	2503	2MA	N3-C4-N9	5.65	134.16	126.99
57	1y	8	4SU	C4-N3-C2	-5.63	121.92	127.31
57	2y	39	PSU	N1-C2-N3	5.61	121.08	115.17
57	2y	46	G7M	C5-C4-N3	-5.60	117.57	128.15
55	2x	54	5MU	N3-C2-N1	5.60	122.18	114.89
1	1A	1939	5MU	C5-C4-N3	5.45	120.06	115.32
57	1y	46	G7M	C5-C4-N3	-5.45	117.86	128.15
57	2y	8	4SU	C5-C4-N3	5.44	119.81	114.75
32	2a	527	G7M	N9-C4-N3	5.40	136.76	125.95
54	2w	39	PSU	N1-C2-N3	5.40	120.87	115.17
1	1A	2552	OMU	N3-C2-N1	5.36	121.87	114.89
54	1w	46	G7M	N9-C4-N3	5.34	136.63	125.95
32	2a	1519	MA6	N1-C2-N3	-5.33	120.52	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1939	5MU	C4-N3-C2	-5.32	120.37	127.34
54	1w	54	5MU	O4-C4-C5	-5.23	118.93	124.92
32	1a	527	G7M	N9-C4-N3	5.23	136.41	125.95
1	1A	2251	OMG	C2-N3-C4	5.23	121.30	112.30
32	2a	527	G7M	C5-C4-N3	-5.19	118.34	128.15
54	1w	54	5MU	C4-N3-C2	-5.18	120.54	127.34
32	1a	1518	MA6	N1-C2-N3	-5.17	120.76	128.58
32	2a	1518	MA6	N1-C2-N3	-5.17	120.76	128.58
54	2w	46	G7M	C5-C4-N3	-5.08	118.54	128.15
55	2x	76	8AN	C5-C4-N3	-5.07	119.73	126.72
1	1A	1915	5MU	C4-N3-C2	-5.06	120.70	127.34
55	1x	76	8AN	C5-C4-N3	-5.06	119.75	126.72
1	2A	2251	OMG	N9-C4-N3	5.03	136.02	125.95
1	2A	2251	OMG	C2-N3-C4	5.02	120.95	112.30
54	1w	8	4SU	C5-C4-N3	5.01	119.41	114.75
1	2A	1939	5MU	C4-N3-C2	-5.00	120.79	127.34
54	2w	46	G7M	N9-C4-N3	4.99	135.93	125.95
54	1w	76	F3N	C5-C4-N3	-4.99	119.85	126.72
32	1a	1519	MA6	N1-C2-N3	-4.98	121.04	128.58
1	2A	1915	5MU	C4-N3-C2	-4.98	120.81	127.34
57	2y	46	G7M	C2-N3-C4	4.97	120.86	112.30
57	1y	8	4SU	C5-C4-N3	4.96	119.37	114.75
55	2x	54	5MU	C5-C4-N3	4.96	119.64	115.32
1	2A	2552	OMU	N3-C2-N1	4.96	121.34	114.89
54	1w	54	5MU	N3-C2-N1	4.94	121.33	114.89
57	1y	46	G7M	C2-N3-C4	4.94	120.81	112.30
57	2y	37	MIA	N3-C4-N9	4.91	135.52	127.17
54	2w	76	F3N	C5-C4-N3	-4.90	119.97	126.72
1	2A	1915	5MU	N3-C2-N1	4.89	121.26	114.89
54	1w	46	G7M	C5-C4-N3	-4.88	118.93	128.15
1	2A	1939	5MU	N3-C2-N1	4.86	121.22	114.89
57	1y	37	MIA	N3-C4-N9	4.85	135.41	127.17
32	1a	527	G7M	C5-C4-N3	-4.81	119.07	128.15
32	1a	966	M2G	C2-N3-C4	4.81	121.40	112.51
55	1x	8	4SU	O2-C2-N1	4.77	129.01	122.80
1	1A	1915	5MU	N3-C2-N1	4.72	121.03	114.89
54	2w	8	4SU	C5-C4-S4	-4.69	118.94	124.31
1	1A	2605	PSU	C4-N3-C2	-4.69	119.91	126.37
54	1w	54	5MU	C5-C4-N3	4.67	119.38	115.32
1	1A	1915	5MU	O4-C4-C5	-4.67	119.58	124.92
1	2A	1939	5MU	C5-C4-N3	4.64	119.36	115.32
32	2a	527	G7M	C2-N3-C4	4.63	120.28	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2605	PSU	C4-N3-C2	-4.63	119.99	126.37
32	1a	1519	MA6	C5-C4-N3	-4.60	120.39	126.72
54	2w	46	G7M	C2-N3-C4	4.59	120.21	112.30
1	1A	2251	OMG	N9-C4-N3	4.58	135.12	125.95
1	1A	1915	5MU	C5-C4-N3	4.56	119.29	115.32
55	1x	54	5MU	C4-N3-C2	-4.55	121.38	127.34
55	1x	54	5MU	N3-C2-N1	4.53	120.79	114.89
32	2a	966	M2G	C2-N3-C4	4.52	120.88	112.51
57	1y	54	5MU	N3-C2-N1	4.50	120.75	114.89
1	2A	1911	PSU	C4-N3-C2	-4.47	120.22	126.37
32	2a	1518	MA6	C5-C4-N3	-4.47	120.57	126.72
1	2A	2552	OMU	C4-N3-C2	-4.46	121.08	126.61
57	1y	54	5MU	C4-N3-C2	-4.46	121.50	127.34
1	2A	2605	PSU	O2-C2-N1	-4.41	118.24	122.79
54	1w	39	PSU	C4-N3-C2	-4.40	120.31	126.37
1	2A	1939	5MU	O4-C4-C5	-4.37	119.92	124.92
32	2a	966	M2G	N9-C4-N3	4.35	134.66	125.95
32	1a	527	G7M	C2-N3-C4	4.33	119.77	112.30
1	1A	1917	PSU	O2-C2-N1	-4.32	118.33	122.79
54	1w	37	MIA	C15-C14-C13	-4.32	109.69	122.66
1	2A	1915	5MU	C5-C4-N3	4.32	119.08	115.32
1	1A	1911	PSU	C4-N3-C2	-4.31	120.43	126.37
54	2w	8	4SU	N3-C2-N1	4.30	120.49	114.89
1	1A	1939	5MU	N3-C2-N1	4.30	120.49	114.89
54	2w	54	5MU	N3-C2-N1	4.28	120.46	114.89
55	1x	54	5MU	C5-C4-N3	4.24	119.01	115.32
54	1w	46	G7M	C2-N3-C4	4.21	119.56	112.30
55	2x	54	5MU	O4-C4-C5	-4.21	120.10	124.92
32	1a	1518	MA6	C2-N1-C6	4.21	122.11	111.83
1	1A	1911	PSU	O2-C2-N1	-4.19	118.47	122.79
54	2w	54	5MU	O4-C4-C5	-4.18	120.14	124.92
32	1a	966	M2G	N9-C4-N3	4.17	134.29	125.95
1	1A	1939	5MU	C5-C6-N1	-4.17	118.78	123.31
1	2A	1917	PSU	C4-N3-C2	-4.16	120.64	126.37
32	2a	1518	MA6	C2-N1-C6	4.14	121.94	111.83
54	1w	55	PSU	O2-C2-N1	-4.14	118.52	122.79
55	2x	55	PSU	C4-N3-C2	-4.14	120.67	126.37
57	1y	39	PSU	C4-N3-C2	-4.13	120.68	126.37
57	1y	55	PSU	O2-C2-N1	-4.12	118.54	122.79
32	2a	1519	MA6	C5-N7-C8	4.10	109.89	103.45
32	1a	1518	MA6	C5-C4-N3	-4.09	121.08	126.72
57	1y	54	5MU	C5-C4-N3	4.09	118.88	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1917	PSU	C4-N3-C2	-4.08	120.75	126.37
32	1a	1519	MA6	C4-C5-N7	-4.07	105.93	110.58
32	2a	1519	MA6	C5-C4-N3	-4.06	121.13	126.72
32	2a	1519	MA6	C2-N1-C6	4.06	121.74	111.83
32	1a	1519	MA6	C5-N7-C8	4.04	109.80	103.45
55	1x	8	4SU	C6-C5-C4	-4.04	116.46	119.95
32	2a	1519	MA6	C4-C5-N7	-4.03	105.97	110.58
32	2a	1207	2MG	N9-C4-N3	4.03	134.00	125.95
1	2A	1917	PSU	O2-C2-N1	-4.00	118.66	122.79
32	2a	516	PSU	C4-N3-C2	-4.00	120.86	126.37
55	1x	54	5MU	O4-C4-C5	-4.00	120.35	124.92
32	1a	1207	2MG	N9-C4-N3	3.99	133.92	125.95
54	2w	54	5MU	C4-N3-C2	-3.98	122.13	127.34
57	2y	32	PSU	C4-N3-C2	-3.97	120.90	126.37
57	1y	8	4SU	C1'-N1-C2	3.95	124.69	117.59
57	1y	8	4SU	C5-C4-S4	-3.91	119.84	124.31
57	1y	32	PSU	O2-C2-N1	-3.91	118.76	122.79
32	2a	1518	MA6	C5-N7-C8	3.90	109.59	103.45
1	2A	1911	PSU	O2-C2-N1	-3.89	118.78	122.79
54	2w	37	MIA	C12-N6-C6	-3.87	119.26	122.85
57	2y	54	5MU	O4-C4-C5	-3.87	120.49	124.92
54	1w	32	PSU	C4-N3-C2	-3.86	121.06	126.37
32	1a	1207	2MG	C6-C5-N7	3.84	137.28	130.29
57	1y	37	MIA	C2-N3-C4	3.84	121.20	111.83
32	1a	516	PSU	C4-N3-C2	-3.83	121.09	126.37
55	2x	8	4SU	C5-C4-N3	3.82	118.30	114.75
32	1a	1518	MA6	C5-N7-C8	3.81	109.44	103.45
32	2a	1404	5MC	C5-C6-N1	-3.81	119.18	123.31
32	1a	1519	MA6	C2-N1-C6	3.79	121.09	111.83
32	1a	966	M2G	C6-C5-N7	3.76	137.13	130.29
55	2x	32	5MC	C5-C6-N1	-3.76	119.23	123.31
54	2w	54	5MU	C5-C4-N3	3.75	118.59	115.32
57	2y	8	4SU	N3-C2-N1	3.74	119.77	114.89
57	2y	55	PSU	C4-N3-C2	-3.74	121.22	126.37
32	2a	1518	MA6	C4-C5-N7	-3.74	106.31	110.58
1	1A	2552	OMU	O2-C2-N1	-3.71	117.96	122.80
57	1y	8	4SU	N3-C2-N1	3.70	119.71	114.89
32	2a	1519	MA6	N9-C8-N7	-3.70	108.69	113.94
57	2y	37	MIA	C2-N3-C4	3.70	120.87	111.83
1	1A	2552	OMU	C4-N3-C2	-3.70	122.02	126.61
1	1A	2503	2MA	C2-N1-C6	3.68	123.76	118.10
57	2y	54	5MU	C5-C4-N3	3.68	118.52	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	37	MIA	C6-C5-N7	3.67	136.43	132.43
55	1x	55	PSU	C4-N3-C2	-3.66	121.32	126.37
54	1w	37	MIA	C16-C14-C13	-3.66	111.67	122.66
57	2y	37	MIA	C4-C5-N7	-3.66	106.40	110.58
1	2A	2552	OMU	O2-C2-N1	-3.66	118.03	122.80
54	2w	55	PSU	O2-C2-N1	-3.66	119.02	122.79
32	1a	1519	MA6	C2-N3-C4	3.65	120.74	111.83
54	2w	55	PSU	C4-N3-C2	-3.62	121.39	126.37
32	2a	1400	5MC	C5-C6-N1	-3.60	119.40	123.31
32	2a	516	PSU	O2-C2-N1	-3.60	119.08	122.79
54	2w	32	PSU	C4-N3-C2	-3.60	121.41	126.37
55	1x	54	5MU	C5-C6-N1	-3.60	119.41	123.31
57	1y	54	5MU	O4-C4-C5	-3.59	120.81	124.92
32	2a	1407	5MC	C5-C6-N1	-3.58	119.42	123.31
54	1w	8	4SU	C4-N3-C2	-3.58	123.88	127.31
55	1x	8	4SU	C1'-N1-C2	3.58	124.02	117.59
32	1a	1518	MA6	C4-C5-N7	-3.58	106.49	110.58
57	1y	32	PSU	C4-N3-C2	-3.57	121.45	126.37
32	2a	1519	MA6	C2-N3-C4	3.57	120.55	111.83
32	2a	1518	MA6	N9-C8-N7	-3.56	108.88	113.94
54	2w	37	MIA	C4-C5-N7	-3.55	106.53	110.58
32	1a	1518	MA6	N9-C8-N7	-3.54	108.92	113.94
32	2a	1518	MA6	C2-N3-C4	3.53	120.46	111.83
57	1y	55	PSU	C4-N3-C2	-3.53	121.51	126.37
1	1A	1942	5MC	C5-C6-N1	-3.53	119.48	123.31
57	1y	37	MIA	N3-C2-N1	-3.53	123.25	128.58
55	2x	54	5MU	C5-C6-N1	-3.52	119.49	123.31
1	2A	1915	5MU	O4-C4-C5	-3.52	120.89	124.92
1	2A	1962	5MC	C5-C6-N1	-3.51	119.50	123.31
32	1a	1519	MA6	N9-C8-N7	-3.50	108.97	113.94
1	2A	2503	2MA	C4-C5-N7	-3.48	106.60	110.58
55	2x	55	PSU	O2-C2-N1	-3.46	119.22	122.79
57	2y	39	PSU	C4-N3-C2	-3.45	121.61	126.37
1	1A	1939	5MU	O4-C4-C5	-3.45	120.97	124.92
54	2w	39	PSU	C4-N3-C2	-3.44	121.63	126.37
54	2w	76	F3N	N9-C8-N7	-3.43	109.06	113.94
54	2w	37	MIA	C11-S10-C2	-3.43	99.67	102.25
55	2x	76	8AN	N9-C8-N7	-3.43	109.06	113.94
54	1w	76	F3N	N9-C8-N7	-3.43	109.07	113.94
54	1w	37	MIA	C4-C5-N7	-3.43	106.66	110.58
55	1x	76	8AN	N9-C8-N7	-3.42	109.08	113.94
32	1a	1518	MA6	C2-N3-C4	3.42	120.18	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	2y	32	PSU	O2-C2-N1	-3.41	119.27	122.79
55	1x	76	8AN	C2-N3-C4	3.40	120.14	111.83
57	2y	8	4SU	C5-C4-S4	-3.40	120.42	124.31
1	2A	1939	5MU	C5-C6-N1	-3.39	119.63	123.31
54	1w	76	F3N	C2-N3-C4	3.39	120.11	111.83
54	1w	37	MIA	C2-N3-C4	3.38	121.15	112.29
57	2y	55	PSU	O2-C2-N1	-3.37	119.31	122.79
54	1w	55	PSU	C4-N3-C2	-3.36	121.74	126.37
1	2A	1942	5MC	C5-C6-N1	-3.35	119.68	123.31
55	2x	76	8AN	C2-N3-C4	3.35	120.00	111.83
32	1a	967	5MC	C5-C6-N1	-3.34	119.69	123.31
55	1x	32	5MC	C5-C6-N1	-3.34	119.69	123.31
32	2a	966	M2G	C6-C5-N7	3.33	136.35	130.29
55	2x	8	4SU	C1'-N1-C2	3.33	123.57	117.59
32	1a	1400	5MC	C5-C6-N1	-3.33	119.70	123.31
54	2w	76	F3N	C2-N3-C4	3.32	119.94	111.83
1	1A	2503	2MA	C4-N9-C8	3.30	109.20	105.74
43	2l	92	0TD	OD2-CG-CB	3.29	120.25	113.15
43	1l	92	0TD	OD2-CG-CB	3.28	120.23	113.15
32	1a	1498	UR3	C5-C4-N3	3.26	119.34	115.04
57	1y	37	MIA	C4-C5-N7	-3.26	106.85	110.58
32	2a	1207	2MG	C6-C5-N7	3.24	136.19	130.29
55	2x	8	4SU	C6-C5-C4	-3.24	117.14	119.95
54	2w	37	MIA	C2-N3-C4	3.24	120.77	112.29
55	1x	55	PSU	O2-C2-N1	-3.23	119.46	122.79
54	1w	39	PSU	O2-C2-N1	-3.23	119.46	122.79
57	2y	37	MIA	N3-C2-N1	-3.22	123.71	128.58
1	2A	1915	5MU	C5-C6-N1	-3.21	119.83	123.31
55	1x	8	4SU	C5-C4-N3	3.19	117.72	114.75
57	2y	55	PSU	C6-C5-C4	-3.18	116.03	118.17
32	1a	1404	5MC	C5-C4-N3	-3.18	118.49	121.75
1	1A	2503	2MA	C4-C5-N7	-3.18	106.95	110.58
32	1a	1207	2MG	C4-C5-N7	-3.16	105.66	110.67
1	1A	2503	2MA	N6-C6-N1	3.15	121.28	117.03
55	2x	76	8AN	C5-N7-C8	3.14	108.39	103.45
54	2w	39	PSU	O2-C2-N1	-3.13	119.56	122.79
1	1A	2251	OMG	C6-C5-N7	3.13	135.98	130.29
57	2y	54	5MU	N3-C2-N1	3.11	118.94	114.89
32	2a	967	5MC	C5-C6-N1	-3.08	119.97	123.31
54	2w	76	F3N	C5-N7-C8	3.07	108.28	103.45
32	1a	1407	5MC	C5-C6-N1	-3.07	119.98	123.31
54	1w	76	F3N	C5-N7-C8	3.06	108.27	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	76	8AN	C4'-O4'-C1'	-3.06	102.70	109.47
1	1A	1962	5MC	C5-C6-N1	-3.06	119.99	123.31
55	2x	54	5MU	O2-C2-N1	-3.05	118.82	122.80
55	1x	32	5MC	C5-C4-N3	-3.05	118.63	121.75
1	2A	2503	2MA	N6-C6-N1	3.03	121.12	117.03
32	1a	966	M2G	C4-C5-N7	-3.02	105.88	110.67
32	2a	1498	UR3	C5-C4-N3	3.02	119.02	115.04
55	1x	76	8AN	C5-N7-C8	3.00	108.16	103.45
32	1a	1404	5MC	C5-C6-N1	-2.99	120.07	123.31
57	2y	39	PSU	O2-C2-N1	-2.97	119.72	122.79
55	2x	76	8AN	C4'-O4'-C1'	-2.95	102.95	109.47
54	2w	32	PSU	O2-C2-N1	-2.95	119.75	122.79
55	2x	76	8AN	C5-C4-N9	2.94	109.02	105.81
32	2a	1207	2MG	N2-C2-N3	-2.93	116.78	120.51
54	1w	37	MIA	C2-N1-C6	2.91	123.06	117.54
32	2a	1207	2MG	C4-C5-N7	-2.91	106.06	110.67
32	1a	527	G7M	O6-C6-C5	-2.90	121.54	128.01
1	2A	2251	OMG	C6-C5-N7	2.88	135.54	130.29
32	2a	1402	4OC	CM4-N4-C4	-2.87	116.84	122.45
32	2a	1518	MA6	N3-C4-N9	2.86	132.04	127.17
1	1A	1939	5MU	C5M-C5-C4	2.86	121.84	118.78
54	2w	39	PSU	C6-C5-C4	-2.86	116.25	118.17
1	2A	1942	5MC	C5-C4-N3	-2.84	118.84	121.75
32	2a	966	M2G	C4-C5-N7	-2.84	106.18	110.67
57	1y	54	5MU	C5-C6-N1	-2.83	120.24	123.31
54	2w	8	4SU	O2-C2-N1	-2.80	119.15	122.80
32	2a	1407	5MC	C5-C4-N3	-2.80	118.89	121.75
1	2A	1962	5MC	C5-C4-N3	-2.77	118.91	121.75
32	1a	1400	5MC	C5-C4-N3	-2.77	118.92	121.75
57	1y	39	PSU	O2-C2-N1	-2.76	119.94	122.79
32	1a	516	PSU	O2-C2-N1	-2.75	119.95	122.79
55	2x	32	5MC	C5-C4-N3	-2.75	118.93	121.75
32	2a	1400	5MC	C5-C4-N3	-2.75	118.93	121.75
54	2w	37	MIA	C5-N7-C8	2.74	107.76	103.45
32	2a	1402	4OC	O2-C2-N3	-2.74	118.01	122.33
1	1A	1962	5MC	C5-C4-N3	-2.74	118.94	121.75
54	1w	32	PSU	O2-C2-N1	-2.74	119.96	122.79
54	1w	54	5MU	C5-C6-N1	-2.74	120.34	123.31
57	2y	54	5MU	C1'-N1-C2	2.74	122.50	117.59
55	1x	8	4SU	O2-C2-N3	-2.73	116.46	121.49
1	1A	1915	5MU	C5-C6-N1	-2.72	120.36	123.31
54	1w	37	MIA	C11-S10-C2	-2.72	100.21	102.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	46	G7M	O6-C6-C5	-2.72	121.94	128.01
57	2y	37	MIA	C5-N7-C8	2.71	107.71	103.45
1	2A	2503	2MA	C4-N9-C8	2.70	108.58	105.74
1	2A	2503	2MA	C5-N7-C8	2.70	107.69	103.45
54	2w	46	G7M	O6-C6-C5	-2.69	122.00	128.01
32	2a	1404	5MC	C5-C4-N3	-2.69	119.00	121.75
55	1x	76	8AN	C5-C4-N9	2.69	108.74	105.81
57	2y	54	5MU	C4-N3-C2	-2.69	123.82	127.34
1	2A	1915	5MU	C5M-C5-C4	2.68	121.65	118.78
1	1A	1915	5MU	C5M-C5-C4	2.68	121.65	118.78
1	2A	2552	OMU	C5-C4-N3	2.68	118.55	114.80
1	1A	1915	5MU	O2-C2-N1	-2.68	119.31	122.80
1	1A	2605	PSU	C5-C6-N1	-2.67	118.44	122.14
32	1a	1519	MA6	N3-C4-N9	2.66	131.69	127.17
1	1A	1942	5MC	C5-C4-N3	-2.64	119.05	121.75
54	1w	76	F3N	C5-C4-N9	2.64	108.69	105.81
32	1a	1518	MA6	N3-C4-N9	2.63	131.65	127.17
54	1w	37	MIA	N3-C2-N1	-2.61	122.23	127.00
43	2l	92	0TD	OD1-CG-CB	-2.60	116.99	122.44
32	1a	1407	5MC	C5-C4-N3	-2.60	119.09	121.75
54	2w	76	F3N	C5-C4-N9	2.59	108.64	105.81
1	1A	2605	PSU	O2-C2-N3	-2.58	117.27	121.86
1	2A	2251	OMG	O6-C6-C5	-2.58	119.72	126.53
57	2y	8	4SU	C1'-N1-C2	2.57	122.22	117.59
1	2A	2503	2MA	C2-N1-C6	2.56	122.03	118.10
32	1a	1498	UR3	C1'-N1-C2	2.56	121.23	117.04
1	1A	2251	OMG	C4-C5-N7	-2.55	106.62	110.67
55	1x	76	8AN	N3-C4-N9	2.55	131.51	127.17
54	1w	76	F3N	N3-C4-N9	2.52	131.46	127.17
1	1A	2251	OMG	O6-C6-C5	-2.52	119.89	126.53
1	2A	2552	OMU	O4-C4-C5	-2.51	120.83	125.16
54	2w	32	PSU	C6-C5-C4	-2.51	116.48	118.17
54	2w	37	MIA	C6-C5-N7	2.49	135.15	132.43
54	1w	54	5MU	O2-C2-N1	-2.49	119.55	122.80
54	2w	76	F3N	N3-C4-N9	2.48	131.39	127.17
57	2y	54	5MU	O2-C2-N3	-2.47	116.93	121.49
54	1w	8	4SU	N3-C2-N1	2.47	118.11	114.89
55	2x	32	5MC	O2-C2-N3	-2.45	118.47	122.33
55	2x	32	5MC	CM5-C5-C6	-2.44	119.54	122.85
54	2w	54	5MU	C5-C6-N1	-2.44	120.67	123.31
55	2x	76	8AN	C4-C5-N7	-2.44	107.80	110.58
57	1y	37	MIA	C5-N7-C8	2.42	107.26	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	37	MIA	C5-N7-C8	2.42	107.25	103.45
32	2a	1207	2MG	N1-C2-N2	2.41	119.02	116.56
1	2A	1911	PSU	C5-C6-N1	-2.41	118.80	122.14
1	1A	2503	2MA	C5-N7-C8	2.40	107.23	103.45
55	2x	76	8AN	N3-C4-N9	2.40	131.25	127.17
32	2a	967	5MC	C5-C4-N3	-2.38	119.31	121.75
32	1a	1402	4OC	C6-C5-C4	2.37	119.85	117.00
57	2y	54	5MU	C1'-N1-C6	-2.36	117.26	121.15
32	1a	1407	5MC	O2-C2-N3	-2.36	118.61	122.33
32	2a	1519	MA6	N3-C4-N9	2.35	131.16	127.17
57	1y	32	PSU	C6-C5-C4	-2.35	116.59	118.17
54	2w	37	MIA	C4-N9-C8	2.35	108.20	105.74
54	1w	8	4SU	C1'-N1-C2	2.34	121.79	117.59
1	2A	2251	OMG	C5-C6-N1	2.33	119.19	113.25
32	1a	1400	5MC	O2-C2-N3	-2.33	118.66	122.33
55	1x	76	8AN	C6-C5-C4	2.33	120.35	117.18
32	1a	1207	2MG	N1-C2-N2	2.33	118.94	116.56
1	1A	2503	2MA	N9-C8-N7	-2.30	110.67	113.94
32	1a	967	5MC	CM5-C5-C6	-2.29	119.76	122.85
32	2a	1518	MA6	C4-C5-C6	2.28	118.27	115.91
32	1a	1498	UR3	C3U-N3-C2	2.28	121.31	117.33
57	2y	37	MIA	C4-N9-C8	2.27	108.13	105.74
1	1A	2552	OMU	O4-C4-C5	-2.27	121.25	125.16
55	2x	32	5MC	C1'-N1-C6	-2.26	117.42	121.15
55	1x	8	4SU	S4-C4-N3	-2.25	117.85	120.20
57	1y	54	5MU	C5M-C5-C4	2.24	121.17	118.78
1	1A	2605	PSU	O2-C2-N1	-2.23	120.49	122.79
1	1A	2503	2MA	C6-C5-N7	2.22	136.38	132.09
32	1a	516	PSU	O4'-C1'-C2'	2.21	108.21	105.15
32	2a	1207	2MG	CM2-N2-C2	-2.21	118.90	123.65
55	2x	76	8AN	C6-C5-C4	2.21	120.19	117.18
32	2a	1402	4OC	C6-C5-C4	2.21	119.66	117.00
55	2x	8	4SU	O2-C2-N1	2.21	125.67	122.80
32	1a	967	5MC	C5-C4-N3	-2.20	119.50	121.75
55	2x	76	8AN	O2'-C2'-C3'	2.19	117.39	111.61
32	2a	967	5MC	CM5-C5-C6	-2.18	119.90	122.85
57	1y	37	MIA	C4-N9-C8	2.18	108.02	105.74
1	2A	2251	OMG	C4-C5-N7	-2.18	107.22	110.67
1	2A	2251	OMG	C2-N1-C6	-2.17	121.17	125.11
32	1a	1207	2MG	C8-N7-C5	2.17	108.13	104.26
57	2y	54	5MU	C5-C6-N1	-2.17	120.96	123.31
1	2A	2605	PSU	C5-C6-N1	-2.17	119.13	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	76	F3N	C4-C5-N7	-2.16	108.12	110.58
55	1x	76	8AN	C4-C5-N7	-2.16	108.12	110.58
57	1y	46	G7M	O6-C6-C5	-2.15	123.22	128.01
54	2w	76	F3N	C4-C5-N7	-2.14	108.13	110.58
57	2y	46	G7M	O6-C6-C5	-2.14	123.23	128.01
1	2A	1915	5MU	C5M-C5-C6	-2.14	119.96	122.85
32	1a	527	G7M	C5-C6-N1	2.13	116.25	111.84
54	1w	39	PSU	C5-C6-N1	-2.13	119.18	122.14
54	2w	46	G7M	C5-C6-N1	2.13	116.24	111.84
54	1w	76	F3N	C6-C5-C4	2.12	120.08	117.18
54	1w	37	MIA	C5-C6-N6	2.12	126.12	122.03
57	1y	55	PSU	O4'-C1'-C2'	2.12	108.08	105.15
57	2y	39	PSU	C6-C5-C4	-2.11	116.75	118.17
32	2a	516	PSU	C6-C5-C4	-2.11	116.75	118.17
54	2w	37	MIA	C1'-N9-C8	-2.11	122.42	127.09
57	2y	32	PSU	O4'-C1'-C2'	2.11	108.07	105.15
32	2a	527	G7M	C5-C6-N1	2.10	116.19	111.84
32	2a	1207	2MG	C2-N1-C6	-2.09	122.02	124.55
57	1y	39	PSU	C6-C5-C4	-2.09	116.76	118.17
54	2w	37	MIA	C2-N1-C6	2.09	121.52	117.54
1	2A	1939	5MU	O2-C2-N1	-2.09	120.08	122.80
54	1w	8	4SU	C5-C4-S4	-2.08	121.93	124.31
32	2a	1519	MA6	C6-C5-N7	2.07	136.74	133.43
1	1A	1911	PSU	O4'-C1'-C2'	2.07	108.01	105.15
55	1x	54	5MU	O2-C2-N1	-2.06	120.11	122.80
54	2w	76	F3N	C6-C5-C4	2.06	119.99	117.18
1	2A	1962	5MC	O2-C2-N3	-2.04	119.11	122.33
32	2a	527	G7M	O6-C6-C5	-2.04	123.46	128.01
32	1a	516	PSU	C5-C6-N1	-2.04	119.31	122.14
32	1a	1518	MA6	C4-N9-C8	2.04	107.88	105.74
54	1w	37	MIA	C4-N9-C8	2.03	107.87	105.74
32	2a	1498	UR3	C3U-N3-C4	2.03	120.68	117.87
54	1w	8	4SU	C6-C5-C4	-2.03	118.20	119.95
55	2x	55	PSU	C5-C6-N1	-2.02	119.33	122.14
1	1A	2552	OMU	C5-C4-N3	2.02	117.63	114.80
1	1A	1942	5MC	O2-C2-N3	-2.02	119.15	122.33
1	1A	1911	PSU	C5-C6-N1	-2.01	119.34	122.14
32	2a	1519	MA6	C4-N9-C1'	-2.01	121.92	126.63
1	2A	2503	2MA	N9-C8-N7	-2.01	111.08	113.94
32	2a	1407	5MC	CM5-C5-C6	-2.01	120.13	122.85

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
57	1y	46	G7M	C4'-C5'-O5'-P
43	2l	92	0TD	CG-CB-SB-CSB
55	2x	76	8AN	O4'-C4'-C5'-O5'
55	2x	76	8AN	C3'-C4'-C5'-O5'
57	2y	54	5MU	C3'-C4'-C5'-O5'
57	2y	54	5MU	O4'-C4'-C5'-O5'
54	2w	32	PSU	C2'-C1'-C5-C4
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16
55	1x	76	8AN	C3'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
57	2y	37	MIA	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
54	2w	46	G7M	C4'-C5'-O5'-P
57	2y	46	G7M	O4'-C1'-N9-C4
32	1a	527	G7M	C3'-C4'-C5'-O5'
55	1x	76	8AN	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
57	2y	37	MIA	O4'-C4'-C5'-O5'
54	2w	76	F3N	N-CA-CB-CG
32	1a	1400	5MC	C3'-C4'-C5'-O5'
54	1w	46	G7M	C4'-C5'-O5'-P
57	2y	46	G7M	O4'-C1'-N9-C8
32	2a	527	G7M	C4'-C5'-O5'-P
55	2x	76	8AN	C4'-C5'-O5'-P
32	2a	1402	4OC	C3'-C4'-C5'-O5'
54	2w	8	4SU	C3'-C4'-C5'-O5'
32	1a	527	G7M	O4'-C4'-C5'-O5'
57	1y	55	PSU	O4'-C1'-C5-C4
54	2w	39	PSU	O4'-C1'-C5-C4
32	2a	1404	5MC	C3'-C4'-C5'-O5'
54	2w	8	4SU	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
54	1w	37	MIA	N6-C12-C13-C14
1	2A	2503	2MA	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
54	2w	46	G7M	C3'-C4'-C5'-O5'
55	1x	76	8AN	C4'-C5'-O5'-P
54	2w	32	PSU	O4'-C4'-C5'-O5'
1	1A	2503	2MA	C4'-C5'-O5'-P
1	1A	1915	5MU	O4'-C4'-C5'-O5'
54	2w	46	G7M	O4'-C4'-C5'-O5'
43	2l	92	0TD	CA-CB-SB-CSB
54	2w	76	F3N	C-CA-CB-CG
57	1y	8	4SU	C2'-C1'-N1-C6
57	1y	55	PSU	O4'-C1'-C5-C6
57	2y	55	PSU	O4'-C1'-C5-C6
32	1a	1519	MA6	C4'-C5'-O5'-P
57	1y	46	G7M	C3'-C4'-C5'-O5'
57	1y	8	4SU	C2'-C1'-N1-C2
32	1a	527	G7M	C4'-C5'-O5'-P
1	1A	1920	OMC	C2'-C1'-N1-C2
32	2a	1402	4OC	C2'-C1'-N1-C2
57	2y	8	4SU	C2'-C1'-N1-C2
1	2A	2503	2MA	C3'-C4'-C5'-O5'

There are no ring outliers.

35 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	1y	55	PSU	1	0
55	2x	8	4SU	1	0
43	2l	92	0TD	2	0
54	2w	54	5MU	1	0
57	1y	37	MIA	1	0
54	2w	32	PSU	1	0
1	2A	2503	2MA	2	0
54	2w	46	G7M	2	0
1	2A	1920	OMC	1	0
54	2w	39	PSU	2	0
32	2a	1207	2MG	2	0
57	1y	8	4SU	3	0
57	1y	39	PSU	1	0
55	1x	8	4SU	1	0
54	2w	55	PSU	1	0
57	1y	46	G7M	2	0
32	2a	967	5MC	1	0
32	1a	1498	UR3	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2w	76	F3N	2	0
32	1a	1519	MA6	2	0
32	1a	1402	4OC	2	0
32	2a	966	M2G	1	0
32	1a	1404	5MC	1	0
32	2a	1518	MA6	1	0
57	2y	8	4SU	1	0
55	1x	76	8AN	1	0
57	2y	55	PSU	7	0
57	2y	46	G7M	2	0
54	1w	8	4SU	1	0
1	1A	2552	OMU	1	0
1	1A	1917	PSU	1	0
32	2a	1402	4OC	3	0
1	1A	1939	5MU	1	0
32	1a	1518	MA6	1	0
32	2a	1519	MA6	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2778 ligands modelled in this entry, 2776 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
61	SF4	2d	303	35	0,12,12	-	-	-		
61	SF4	1d	302	35	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	SF4	2d	303	35	-	-	0/6/5/5
61	SF4	1d	302	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	1d	302	SF4	2	0

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%)	-0.37	161 (5%) 30 26	14, 31, 78, 88	0
1	2A	2789/2915 (95%)	0.19	149 (5%) 32 28	28, 49, 76, 86	0
2	1B	120/121 (99%)	-0.26	0 100 100	25, 43, 53, 73	0
2	2B	120/121 (99%)	0.67	2 (1%) 69 65	49, 61, 68, 79	0
3	1D	275/276 (99%)	0.10	3 (1%) 78 74	18, 34, 46, 62	0
3	2D	275/276 (99%)	0.48	2 (0%) 84 81	27, 44, 56, 71	0
4	1E	204/206 (99%)	0.03	2 (0%) 79 76	14, 33, 53, 60	0
4	2E	204/206 (99%)	0.66	6 (2%) 53 50	28, 51, 60, 68	0
5	1F	202/210 (96%)	0.07	4 (1%) 65 60	15, 36, 58, 69	0
5	2F	202/210 (96%)	0.82	8 (3%) 42 38	28, 56, 66, 69	0
6	1G	181/182 (99%)	0.63	9 (4%) 34 30	33, 49, 60, 71	0
6	2G	181/182 (99%)	1.18	18 (9%) 13 9	52, 62, 70, 73	0
7	1H	174/180 (96%)	0.44	3 (1%) 69 65	32, 46, 57, 69	0
7	2H	174/180 (96%)	1.59	54 (31%) 1 1	56, 67, 74, 78	0
8	1I	146/148 (98%)	0.99	7 (4%) 35 32	39, 60, 67, 72	0
8	2I	146/148 (98%)	1.65	47 (32%) 1 1	46, 64, 73, 77	0
9	1N	140/140 (100%)	0.07	0 100 100	20, 33, 50, 57	0
9	2N	140/140 (100%)	0.98	12 (8%) 16 13	41, 54, 65, 71	0
10	1O	122/122 (100%)	0.08	1 (0%) 82 80	22, 35, 51, 57	0
10	2O	122/122 (100%)	0.66	0 100 100	41, 51, 60, 65	0
11	1P	149/150 (99%)	0.24	2 (1%) 75 71	16, 40, 57, 63	0
11	2P	149/150 (99%)	0.92	11 (7%) 20 17	30, 55, 68, 73	0
12	1Q	141/141 (100%)	0.07	0 100 100	22, 34, 47, 60	0
12	2Q	141/141 (100%)	0.99	11 (7%) 19 15	38, 54, 62, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.12	0 100 100	18, 29, 40, 50	0
13	2R	118/118 (100%)	0.52	2 (1%) 69 65	35, 45, 54, 62	0
14	1S	110/112 (98%)	0.28	0 100 100	31, 42, 52, 58	0
14	2S	110/112 (98%)	1.08	10 (9%) 15 12	51, 59, 65, 68	0
15	1T	131/146 (89%)	0.25	3 (2%) 61 57	25, 38, 59, 67	0
15	2T	131/146 (89%)	0.85	5 (3%) 44 40	41, 52, 61, 66	0
16	1U	116/118 (98%)	-0.30	0 100 100	15, 25, 40, 47	0
16	2U	116/118 (98%)	0.74	3 (2%) 57 53	35, 49, 61, 67	0
17	1V	101/101 (100%)	-0.18	1 (0%) 79 76	17, 33, 48, 57	0
17	2V	101/101 (100%)	1.01	5 (4%) 34 30	35, 57, 63, 76	0
18	1W	112/113 (99%)	-0.25	0 100 100	16, 26, 42, 65	0
18	2W	112/113 (99%)	0.42	4 (3%) 46 42	34, 43, 53, 71	0
19	1X	95/96 (98%)	0.06	2 (2%) 63 59	23, 33, 49, 71	0
19	2X	95/96 (98%)	0.93	9 (9%) 14 11	39, 51, 64, 72	0
20	1Y	107/110 (97%)	0.39	1 (0%) 81 78	31, 42, 57, 66	0
20	2Y	107/110 (97%)	1.37	18 (16%) 4 3	51, 59, 68, 72	0
21	1Z	154/206 (74%)	0.89	13 (8%) 17 14	34, 53, 68, 73	0
21	2Z	160/206 (77%)	1.74	61 (38%) 1 0	51, 65, 73, 76	0
22	10	83/85 (97%)	-0.01	0 100 100	21, 32, 42, 54	0
22	20	83/85 (97%)	0.77	3 (3%) 46 42	33, 52, 60, 64	0
23	11	97/98 (98%)	0.34	1 (1%) 79 76	24, 41, 58, 61	0
23	21	97/98 (98%)	0.83	5 (5%) 33 29	33, 50, 62, 65	0
24	12	70/72 (97%)	0.22	2 (2%) 53 50	30, 41, 50, 54	0
24	22	70/72 (97%)	1.00	3 (4%) 40 36	49, 59, 67, 76	0
25	13	59/60 (98%)	-0.03	0 100 100	17, 30, 50, 56	0
25	23	59/60 (98%)	0.72	2 (3%) 48 44	46, 54, 62, 70	0
26	14	69/71 (97%)	1.19	11 (15%) 5 4	43, 61, 71, 79	0
26	24	69/71 (97%)	1.59	20 (28%) 1 1	61, 67, 75, 78	0
27	15	59/60 (98%)	-0.27	0 100 100	15, 25, 43, 52	0
27	25	59/60 (98%)	0.36	0 100 100	32, 43, 56, 66	0
28	16	53/54 (98%)	-0.01	0 100 100	29, 37, 48, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.67	1 (1%) 66 62	39, 50, 58, 61	0
29	17	48/49 (97%)	-0.25	1 (2%) 63 59	16, 22, 41, 52	0
29	27	48/49 (97%)	0.41	3 (6%) 26 22	28, 38, 58, 62	0
30	18	64/65 (98%)	-0.10	0 100 100	23, 29, 36, 48	0
30	28	64/65 (98%)	0.64	0 100 100	40, 47, 54, 57	0
31	19	37/37 (100%)	-0.12	0 100 100	25, 33, 43, 48	0
31	29	37/37 (100%)	1.08	3 (8%) 18 14	48, 54, 59, 60	0
32	1a	1488/1521 (97%)	0.41	49 (3%) 49 45	32, 55, 75, 86	0
32	2a	1491/1521 (98%)	0.73	83 (5%) 30 26	43, 63, 77, 86	0
33	1b	231/256 (90%)	1.34	41 (17%) 4 3	50, 64, 70, 76	0
33	2b	231/256 (90%)	1.59	57 (24%) 2 1	59, 67, 73, 80	0
34	1c	206/239 (86%)	1.05	15 (7%) 21 17	49, 58, 65, 73	0
34	2c	206/239 (86%)	1.70	71 (34%) 1 1	57, 67, 73, 79	0
35	1d	208/209 (99%)	1.13	21 (10%) 12 9	45, 57, 64, 70	0
35	2d	208/209 (99%)	1.13	17 (8%) 17 14	49, 59, 66, 73	0
36	1e	148/162 (91%)	0.82	6 (4%) 41 37	44, 54, 62, 67	0
36	2e	148/162 (91%)	1.19	16 (10%) 11 8	53, 62, 66, 71	0
37	1f	100/101 (99%)	0.93	5 (5%) 34 30	47, 56, 63, 65	0
37	2f	100/101 (99%)	0.89	3 (3%) 52 48	48, 56, 63, 63	0
38	1g	155/156 (99%)	1.00	11 (7%) 22 18	51, 59, 69, 72	0
38	2g	155/156 (99%)	1.35	26 (16%) 4 3	56, 65, 70, 75	0
39	1h	137/138 (99%)	0.86	7 (5%) 33 30	48, 56, 62, 65	0
39	2h	137/138 (99%)	1.23	17 (12%) 8 6	53, 62, 68, 70	0
40	1i	127/128 (99%)	1.43	25 (19%) 3 2	48, 62, 68, 71	0
40	2i	127/128 (99%)	2.04	58 (45%) 0 0	57, 68, 72, 74	0
41	1j	97/105 (92%)	1.51	21 (21%) 2 2	47, 62, 69, 77	0
41	2j	96/105 (91%)	1.88	39 (40%) 0 0	57, 68, 72, 75	0
42	1k	114/129 (88%)	0.96	10 (8%) 15 12	35, 57, 63, 68	0
42	2k	114/129 (88%)	1.28	12 (10%) 11 8	48, 60, 66, 71	0
43	1l	121/132 (91%)	0.54	5 (4%) 41 37	36, 45, 55, 60	0
43	2l	121/132 (91%)	1.01	12 (9%) 13 9	46, 54, 62, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	1.18	15 (12%) 8 6	46, 58, 66, 72	0
44	2m	122/126 (96%)	1.53	25 (20%) 2 2	57, 65, 69, 72	0
45	1n	60/61 (98%)	1.48	13 (21%) 2 2	49, 55, 61, 67	0
45	2n	60/61 (98%)	2.40	35 (58%) 0 0	60, 67, 71, 73	0
46	1o	88/89 (98%)	0.95	4 (4%) 38 34	39, 53, 62, 67	0
46	2o	88/89 (98%)	1.10	11 (12%) 8 6	51, 59, 66, 69	0
47	1p	82/88 (93%)	1.41	18 (21%) 2 2	48, 58, 63, 69	0
47	2p	82/88 (93%)	1.40	12 (14%) 6 4	51, 58, 65, 68	0
48	1q	99/105 (94%)	1.05	7 (7%) 22 18	44, 57, 62, 69	0
48	2q	99/105 (94%)	1.26	13 (13%) 7 5	51, 59, 65, 67	0
49	1r	68/88 (77%)	0.92	5 (7%) 20 17	49, 56, 64, 66	0
49	2r	68/88 (77%)	0.93	3 (4%) 39 34	50, 58, 65, 67	0
50	1s	83/93 (89%)	0.97	6 (7%) 21 18	50, 58, 65, 68	0
50	2s	83/93 (89%)	1.51	20 (24%) 2 1	60, 66, 71, 74	0
51	1t	96/106 (90%)	1.21	13 (13%) 7 5	48, 58, 66, 71	0
51	2t	96/106 (90%)	1.31	18 (18%) 3 3	49, 59, 67, 71	0
52	1u	23/27 (85%)	1.46	4 (17%) 4 3	52, 56, 60, 62	0
52	2u	23/27 (85%)	1.93	9 (39%) 1 0	61, 65, 68, 71	0
53	1v	13/24 (54%)	0.67	3 (23%) 2 1	38, 44, 73, 76	0
53	2v	13/24 (54%)	1.35	4 (30%) 1 1	56, 61, 79, 89	0
54	1w	66/76 (86%)	1.15	8 (12%) 8 6	22, 69, 78, 84	0
54	2w	64/76 (84%)	1.59	15 (23%) 2 1	41, 74, 80, 86	0
55	1x	72/77 (93%)	0.41	1 (1%) 73 69	21, 53, 68, 74	0
55	2x	72/77 (93%)	0.74	2 (2%) 55 51	36, 62, 71, 78	0
56	1z	4/5 (80%)	0.18	0 100 100	22, 26, 31, 35	0
56	2z	3/5 (60%)	0.11	0 100 100	34, 34, 37, 40	0
57	1y	67/76 (88%)	1.91	31 (46%) 0 0	53, 80, 84, 85	0
57	2y	66/76 (86%)	2.01	31 (46%) 0 0	60, 80, 85, 86	0
All	All	20878/21758 (95%)	0.56	1657 (7%) 18 15	14, 54, 72, 89	0

All (1657) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	7.1
44	1m	123	ALA	6.7
45	1n	2	ALA	6.6
45	2n	2	ALA	6.1
1	1A	2145	C	5.4
44	2m	123	ALA	5.3
1	2A	883	G	5.3
1	2A	2802	G	5.3
23	11	2	SER	5.3
1	2A	2135	A	5.3
32	2a	1030(B)	C	5.1
1	2A	2142	C	5.1
38	1g	80	VAL	5.0
1	1A	2159	G	5.0
1	2A	2115	G	5.0
21	2Z	172	ALA	4.9
1	1A	896	A	4.9
1	1A	2803	C	4.9
40	2i	14	VAL	4.9
1	2A	2160	G	4.8
1	2A	2169	A	4.8
1	2A	884	C	4.8
1	2A	2147	G	4.8
1	2A	2111	C	4.8
40	2i	9	ARG	4.8
1	1A	2113	U	4.7
1	2A	896	A	4.7
1	2A	2159	G	4.7
1	2A	2117	A	4.7
21	1Z	141	VAL	4.7
21	2Z	149	SER	4.6
1	1A	1078	U	4.6
1	1A	2115	G	4.6
8	2I	83	ALA	4.6
20	2Y	55	TYR	4.6
1	1A	2143	C	4.6
40	2i	102	LEU	4.6
33	2b	165	VAL	4.6
1	1A	2114	A	4.6
33	2b	237	ALA	4.6
1	2A	2112	G	4.6
1	1A	2146	C	4.5
8	2I	81	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
40	2i	10	ARG	4.4
32	2a	1033	G	4.4
8	2I	80	PRO	4.4
41	2j	34	VAL	4.4
1	2A	2113	U	4.4
1	1A	2112	G	4.4
1	2A	2129	C	4.4
1	2A	2146	C	4.4
32	2a	1031	G	4.4
35	1d	2	GLY	4.4
44	2m	6	GLY	4.4
42	1k	14	VAL	4.4
1	2A	2128	C	4.4
54	2w	71	G	4.4
1	2A	2170	A	4.4
8	2I	68	LEU	4.4
7	1H	2	SER	4.3
44	1m	122	LYS	4.3
51	2t	99	LEU	4.3
45	2n	38	GLY	4.3
1	2A	2143	C	4.3
1	2A	2119	A	4.3
1	2A	2134	A	4.3
40	2i	62	TYR	4.3
21	1Z	146	ILE	4.3
1	1A	2142	C	4.3
1	2A	885	C	4.3
1	2A	2127	G	4.3
45	2n	22	THR	4.3
1	2A	2149	G	4.2
6	2G	147	ASP	4.2
1	1A	2141	G	4.2
21	2Z	150	LEU	4.2
36	2e	21	ALA	4.2
1	1A	897	C	4.2
44	2m	122	LYS	4.2
41	2j	74	ILE	4.2
45	2n	25	VAL	4.2
44	1m	124	PRO	4.2
34	2c	2	GLY	4.2
32	2a	1030(A)	G	4.2
33	1b	187	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
33	1b	237	ALA	4.1
19	2X	94	GLY	4.1
38	1g	81	GLY	4.1
40	2i	36	TYR	4.1
54	2w	72	C	4.1
32	2a	1030	C	4.0
1	1A	1064	C	4.0
1	1A	2174	C	4.0
1	2A	2145	C	4.0
1	1A	2130	U	4.0
26	14	54	GLY	4.0
8	2I	72	LEU	4.0
1	1A	2182	G	4.0
54	2w	70	G	4.0
1	2A	2144	U	4.0
38	1g	79	ARG	4.0
1	2A	2155	G	4.0
6	1G	146	TYR	4.0
1	2A	2133	G	3.9
1	2A	2793	G	3.9
1	1A	2111	C	3.9
1	2A	898	C	3.9
8	2I	75	LEU	3.9
33	2b	129	GLU	3.9
38	2g	80	VAL	3.9
1	1A	2160	G	3.9
8	2I	89	TYR	3.9
33	2b	122	PHE	3.9
40	2i	66	ARG	3.9
45	2n	18	VAL	3.9
1	1A	2133	G	3.8
1	2A	2116	G	3.8
54	1w	70	G	3.8
38	2g	82	GLY	3.8
51	1t	47	GLY	3.8
8	2I	79	ILE	3.8
32	1a	1257	U	3.8
38	2g	154	TYR	3.8
1	2A	2138	C	3.8
3	2D	275	LYS	3.8
32	2a	1026	G	3.8
54	2w	73	A	3.8

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Mol	Chain	Res	Type	RSRZ
3	1D	276	LYS	3.8
1	1A	898	C	3.8
1	2A	2803	C	3.8
33	2b	185	ILE	3.8
54	1w	72	C	3.8
1	1A	2131	G	3.8
41	1j	33	GLN	3.8
19	1X	95	LEU	3.8
41	1j	4	ILE	3.8
52	2u	24	ARG	3.7
55	2x	47	U	3.7
20	1Y	92	ASN	3.7
21	2Z	171	ILE	3.7
45	2n	34	TYR	3.7
7	1H	15	VAL	3.7
1	1A	2109	U	3.7
6	2G	52	ILE	3.7
35	1d	70	ILE	3.7
1	2A	2804	C	3.7
1	2A	2896	C	3.7
40	2i	64	THR	3.7
21	2Z	146	ILE	3.7
1	1A	1094	U	3.7
1	2A	1026	U	3.7
45	2n	14	PRO	3.7
44	2m	102	ARG	3.7
40	2i	28	VAL	3.7
40	2i	103	THR	3.7
54	2w	2	C	3.7
51	1t	12	ALA	3.7
8	2I	123	LEU	3.7
21	2Z	155	LEU	3.7
54	1w	71	G	3.7
1	2A	2126	A	3.6
45	2n	20	ALA	3.6
1	2A	2110	G	3.6
1	2A	2125	G	3.6
26	24	51	ASP	3.6
1	2A	2158	A	3.6
33	1b	136	VAL	3.6
15	2T	131	ALA	3.6
1	1A	885	C	3.6

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Mol	Chain	Res	Type	RSRZ
24	22	70	GLN	3.6
1	2A	2109	U	3.6
1	1A	2162	G	3.6
33	2b	112	VAL	3.6
1	1A	2135	A	3.6
38	1g	82	GLY	3.6
1	2A	2137	C	3.6
1	1A	2132	U	3.6
1	1A	882	G	3.6
1	1A	2165	G	3.6
1	2A	879	G	3.6
1	2A	2123	G	3.6
1	1A	2108	C	3.5
1	1A	2140	C	3.5
1	1A	2144	U	3.5
1	2A	2130	U	3.5
26	14	56	VAL	3.5
26	24	63	TYR	3.5
15	1T	130	ALA	3.5
38	2g	16	LEU	3.5
38	2g	81	GLY	3.5
45	2n	55	GLY	3.5
32	2a	1030(D)	A	3.5
50	2s	45	VAL	3.5
19	1X	94	GLY	3.5
34	1c	2	GLY	3.5
1	1A	1059	G	3.5
1	1A	2158	A	3.5
1	1A	2166	G	3.5
38	1g	84	ASN	3.5
1	1A	888	C	3.5
1	2A	888	C	3.5
29	27	47	ARG	3.5
6	2G	146	TYR	3.5
43	1l	64	TYR	3.5
44	1m	2	ALA	3.5
41	1j	98	ILE	3.5
36	1e	85	GLY	3.5
51	2t	29	LYS	3.5
1	1A	1063	G	3.4
1	2A	11	G	3.4
1	2A	2162	G	3.4

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Mol	Chain	Res	Type	RSRZ
1	2A	2168	G	3.4
32	2a	1036	G	3.4
33	1b	125	PRO	3.4
1	1A	2185	C	3.4
1	2A	2139	C	3.4
36	2e	20	GLN	3.4
1	2A	2154	G	3.4
6	2G	145	THR	3.4
36	2e	114	GLY	3.4
41	2j	93	GLY	3.4
8	2I	65	ALA	3.4
1	1A	1065	U	3.4
34	2c	201	TYR	3.4
52	2u	14	TRP	3.4
41	2j	44	VAL	3.4
1	1A	2805	G	3.4
1	2A	2807	G	3.4
34	2c	149	ALA	3.4
1	1A	1066	U	3.4
1	1A	2189	U	3.4
1	1A	2117	A	3.4
21	2Z	96	VAL	3.4
34	2c	195	VAL	3.4
50	2s	11	VAL	3.4
50	2s	2	PRO	3.4
51	2t	98	PRO	3.4
40	2i	45	ALA	3.4
1	1A	2147	G	3.3
1	1A	2181	G	3.3
32	2a	1034	G	3.3
33	2b	21	ARG	3.3
44	2m	100	GLY	3.3
26	14	32	TYR	3.3
38	1g	85	TYR	3.3
1	2A	882	G	3.3
3	2D	276	LYS	3.3
1	2A	2174	C	3.3
32	2a	999	C	3.3
48	2q	21	VAL	3.3
21	2Z	147	GLY	3.3
34	2c	157	ILE	3.3
40	2i	13	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
26	14	59	PHE	3.3
26	14	63	TYR	3.3
1	2A	2148	G	3.3
32	1a	1001(A)	G	3.3
1	2A	652(T)	C	3.3
41	1j	77	PRO	3.3
41	2j	40	LEU	3.3
26	24	55	ARG	3.3
21	2Z	126	VAL	3.3
1	2A	2114	A	3.3
21	1Z	166	SER	3.3
21	2Z	157	LEU	3.3
9	2N	9	VAL	3.3
36	1e	69	VAL	3.3
1	1A	884	C	3.3
1	1A	2137	C	3.3
1	2A	894	C	3.3
21	1Z	1	MET	3.3
47	1p	59	TRP	3.3
15	1T	131	ALA	3.3
47	2p	82	GLN	3.2
32	1a	204	U	3.2
32	2a	1257	U	3.2
45	2n	53	LEU	3.2
35	1d	133	VAL	3.2
1	1A	2793	G	3.2
1	2A	2131	G	3.2
1	2A	2141	G	3.2
26	14	58	ARG	3.2
33	2b	121	LEU	3.2
26	24	56	VAL	3.2
33	1b	15	VAL	3.2
46	2o	89	GLY	3.2
4	2E	204	ALA	3.2
1	2A	2151	G	3.2
45	2n	29	ARG	3.2
1	1A	1057	A	3.2
32	1a	1035	A	3.2
41	2j	65	LEU	3.2
45	2n	6	LEU	3.2
44	1m	120	LYS	3.2
8	2I	144	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
21	2Z	173	ALA	3.2
8	2I	67	ARG	3.2
45	2n	26	ARG	3.2
1	1A	2802	G	3.2
1	2A	881	G	3.2
1	1A	1096	A	3.2
34	2c	205	GLY	3.2
41	1j	36	GLY	3.2
1	1A	2897	U	3.2
41	2j	75	ILE	3.2
8	2I	146	ALA	3.1
45	2n	5	ALA	3.1
32	2a	1029	C	3.1
33	1b	9	GLU	3.1
40	2i	99	LEU	3.1
1	2A	2166	G	3.1
32	1a	1003	G	3.1
32	2a	1356	G	3.1
32	2a	1447	A	3.1
53	2v	12	A	3.1
1	2A	2897	U	3.1
36	2e	138	ALA	3.1
42	1k	74	ALA	3.1
6	2G	76	SER	3.1
45	2n	16	PHE	3.1
41	2j	71	LEU	3.1
7	1H	174	GLY	3.1
1	1A	2120	G	3.1
1	1A	2792	G	3.1
32	1a	1033	G	3.1
57	2y	57	G	3.1
1	2A	2132	U	3.1
20	2Y	53	PRO	3.1
34	2c	43	LEU	3.1
47	2p	48	TRP	3.1
1	1A	1072	C	3.1
1	1A	2136	C	3.1
11	1P	44	GLY	3.1
51	1t	103	GLY	3.1
44	2m	4	ILE	3.1
1	1A	879	G	3.1
1	1A	1091	G	3.1

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Mol	Chain	Res	Type	RSRZ
34	2c	109	PRO	3.1
7	2H	98	LEU	3.1
19	2X	95	LEU	3.1
21	2Z	144	LEU	3.1
51	1t	100	ILE	3.1
1	2A	2124	G	3.0
54	2w	15	G	3.0
57	1y	34	G	3.0
45	2n	11	LYS	3.0
33	1b	7	VAL	3.0
1	1A	886	C	3.0
32	1a	1027	C	3.0
43	2l	56	ALA	3.0
50	2s	24	ALA	3.0
34	2c	184	TYR	3.0
41	2j	41	PRO	3.0
1	2A	2153	G	3.0
1	2A	2805	G	3.0
40	1i	126	SER	3.0
33	1b	133	LYS	3.0
1	1A	2129	C	3.0
1	1A	2138	C	3.0
1	1A	2164	C	3.0
1	2A	2108	C	3.0
54	2w	3	C	3.0
40	2i	96	LEU	3.0
1	2A	2801(A)	A	3.0
40	1i	18	PHE	3.0
1	2A	2893	G	3.0
32	1a	1034	G	3.0
19	2X	81	VAL	3.0
21	1Z	165	VAL	3.0
33	2b	7	VAL	3.0
40	2i	63	ILE	3.0
40	2i	65	VAL	3.0
44	2m	9	ILE	3.0
33	1b	134	GLU	3.0
34	2c	129	ALA	3.0
35	2d	115	ARG	3.0
1	1A	271(K)	U	3.0
32	1a	841	U	3.0
8	2I	84	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
7	2H	17	VAL	2.9
34	2c	99	VAL	2.9
35	1d	5	ILE	2.9
1	2A	2104	G	2.9
8	2I	85	GLU	2.9
20	2Y	5	MET	2.9
32	1a	1023	G	2.9
32	2a	1032	G	2.9
33	2b	120	ALA	2.9
41	2j	32	ALA	2.9
44	2m	33	ALA	2.9
21	2Z	91	LEU	2.9
51	1t	13	LEU	2.9
32	2a	1249	C	2.9
33	2b	17	PHE	2.9
38	2g	26	PHE	2.9
1	1A	895	U	2.9
51	1t	69	GLY	2.9
45	2n	7	ILE	2.9
48	1q	36	ILE	2.9
5	2F	183	VAL	2.9
20	2Y	7	VAL	2.9
33	1b	81	VAL	2.9
45	2n	13	THR	2.9
40	2i	61	ALA	2.9
1	2A	1533	G	2.9
21	2Z	159	PRO	2.9
32	2a	1030(C)	G	2.9
38	1g	156	TRP	2.9
47	1p	48	TRP	2.9
39	2h	2	LEU	2.9
1	1A	2161	C	2.9
1	2A	2161	C	2.9
1	2A	2183	C	2.9
43	1l	14	GLY	2.9
32	1a	1286	A	2.9
48	1q	78	GLU	2.9
33	2b	200	ILE	2.9
41	1j	34	VAL	2.9
6	2G	50	ALA	2.9
7	2H	36	PRO	2.9
8	2I	63	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
19	2X	42	ALA	2.9
50	2s	76	PRO	2.9
45	2n	61	TRP	2.9
1	1A	1058	G	2.9
1	2A	2157	G	2.9
57	1y	19	G	2.9
40	2i	5	TYR	2.9
25	23	60	GLU	2.9
33	2b	228	GLY	2.9
1	2A	2167	U	2.9
42	2k	117	ASN	2.9
32	1a	999	C	2.9
41	1j	75	ILE	2.9
1	1A	2790	A	2.9
36	2e	55	VAL	2.9
50	2s	32	LYS	2.9
51	2t	97	ALA	2.9
11	2P	91	PHE	2.9
16	2U	117	GLN	2.9
20	2Y	89	PHE	2.9
24	22	1	MET	2.9
32	1a	1002	G	2.9
33	1b	236	TYR	2.9
50	2s	80	TYR	2.9
34	2c	74	GLY	2.9
41	2j	38	ILE	2.8
1	1A	2167	U	2.8
32	2a	1159	U	2.8
26	14	50	VAL	2.8
46	2o	60	VAL	2.8
1	1A	2804	C	2.8
32	1a	1029	C	2.8
1	1A	2169	A	2.8
1	2A	901	A	2.8
19	2X	91	ALA	2.8
32	1a	1030(D)	A	2.8
34	2c	61	ALA	2.8
45	2n	10	ALA	2.8
8	2I	12	LEU	2.8
33	2b	51	LEU	2.8
35	1d	194	LEU	2.8
40	2i	19	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
33	1b	17	PHE	2.8
45	2n	37	PHE	2.8
33	2b	199	TYR	2.8
40	2i	4	TYR	2.8
45	2n	21	TYR	2.8
12	2Q	22	LYS	2.8
20	2Y	54	LYS	2.8
33	1b	227	GLY	2.8
38	1g	4	ARG	2.8
41	2j	10	GLY	2.8
42	2k	102	GLY	2.8
1	1A	2110	G	2.8
1	2A	2156	G	2.8
40	2i	126	SER	2.8
6	2G	160	VAL	2.8
21	2Z	161	VAL	2.8
33	2b	81	VAL	2.8
41	2j	77	PRO	2.8
1	1A	894	C	2.8
1	2A	1536	C	2.8
1	2A	2136	C	2.8
33	1b	120	ALA	2.8
41	1j	20	ALA	2.8
1	1A	890	A	2.8
1	2A	229	A	2.8
1	2A	2171	A	2.8
41	2j	86	MET	2.8
43	2l	16	GLU	2.8
40	2i	37	PHE	2.8
44	2m	121	LYS	2.8
35	1d	6	GLY	2.8
39	2h	58	TYR	2.8
51	2t	47	GLY	2.8
21	2Z	57	ILE	2.8
38	2g	84	ASN	2.8
45	2n	42	ILE	2.8
57	2y	71	G	2.8
1	1A	1081	U	2.8
1	2A	2895	U	2.8
7	2H	96	ALA	2.8
34	2c	87	LEU	2.8
34	2c	91	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	2A	2107	C	2.8
1	1A	2170	A	2.8
1	1A	2801(A)	A	2.8
32	2a	1157	A	2.8
7	2H	6	ARG	2.8
7	2H	123	PHE	2.8
21	2Z	104	PHE	2.8
41	2j	47	PHE	2.8
48	1q	27	PHE	2.8
33	1b	97	TRP	2.8
40	2i	39	GLY	2.8
16	2U	88	ILE	2.8
48	2q	99	SER	2.8
7	2H	49	VAL	2.8
8	2I	15	VAL	2.8
33	1b	71	VAL	2.8
40	2i	26	VAL	2.8
6	2G	3	LEU	2.8
32	1a	1000	U	2.8
39	1h	2	LEU	2.8
57	1y	20	U	2.8
1	2A	614(B)	G	2.8
1	2A	652(U)	G	2.8
32	1a	1036	G	2.8
1	1A	2188	C	2.8
7	2H	170	ARG	2.8
31	29	15	LYS	2.8
32	1a	848	C	2.8
47	2p	76	GLN	2.8
32	2a	1275	A	2.8
57	2y	75	C	2.8
33	1b	19	HIS	2.8
33	2b	16	HIS	2.8
26	24	59	PHE	2.8
33	2b	152	PHE	2.8
51	2t	103	GLY	2.7
34	2c	77	ILE	2.7
34	2c	182	ILE	2.7
35	2d	154	ASN	2.7
38	2g	85	TYR	2.7
49	1r	86	VAL	2.7
41	1j	90	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
41	2j	90	LEU	2.7
5	2F	21	ALA	2.7
15	2T	130	ALA	2.7
1	1A	2150	U	2.7
32	2a	202	U	2.7
32	2a	1150	U	2.7
1	2A	2181	G	2.7
32	1a	1032	G	2.7
54	1w	1	G	2.7
57	2y	5	G	2.7
1	1A	899	A	2.7
1	2A	2173	A	2.7
32	2a	1531	A	2.7
53	1v	13	A	2.7
53	2v	13	A	2.7
33	2b	66	GLY	2.7
33	2b	214	ILE	2.7
51	2t	100	ILE	2.7
6	2G	149	VAL	2.7
34	2c	29	TYR	2.7
35	1d	170	VAL	2.7
9	2N	23	LEU	2.7
21	2Z	125	LEU	2.7
35	1d	19	LEU	2.7
40	1i	19	LEU	2.7
51	2t	13	LEU	2.7
38	2g	83	ALA	2.7
43	2l	19	ARG	2.7
51	2t	8	ARG	2.7
8	1I	117	GLU	2.7
1	1A	2121	G	2.7
1	2A	2894	G	2.7
7	2H	120	GLY	2.7
32	2a	1202	G	2.7
57	2y	34	G	2.7
1	1A	1095	A	2.7
1	1A	2107	C	2.7
1	2A	897	C	2.7
1	2A	2140	C	2.7
1	2A	2175	C	2.7
32	1a	1001	A	2.7
32	2a	1004	A	2.7

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Mol	Chain	Res	Type	RSRZ
32	2a	1286	A	2.7
42	2k	32	ILE	2.7
33	2b	37	ASN	2.7
7	2H	113	VAL	2.7
21	2Z	56	VAL	2.7
33	2b	15	VAL	2.7
34	2c	141	VAL	2.7
40	1i	26	VAL	2.7
48	1q	77	VAL	2.7
48	2q	82	MET	2.7
51	2t	24	LEU	2.7
12	2Q	53	ALA	2.7
45	2n	35	ARG	2.7
47	1p	24	ALA	2.7
32	2a	1532	U	2.7
50	2s	13	ASP	2.7
46	2o	86	GLY	2.7
40	1i	59	PHE	2.7
7	2H	39	PRO	2.7
33	1b	131	PRO	2.7
52	2u	13	ILE	2.7
1	1A	887	A	2.7
1	1A	2101	G	2.7
1	1A	2156	G	2.7
1	1A	2190	G	2.7
32	1a	1447	A	2.7
32	2a	1276	G	2.7
9	2N	118	LYS	2.7
15	2T	49	VAL	2.7
18	2W	92	ARG	2.7
20	2Y	1	MET	2.7
21	2Z	105	VAL	2.7
21	2Z	129	SER	2.7
21	2Z	166	SER	2.7
33	2b	71	VAL	2.7
34	2c	190	ARG	2.7
43	2l	18	VAL	2.7
45	2n	31	ARG	2.7
50	2s	71	LEU	2.7
34	2c	60	ALA	2.7
32	2a	1358	U	2.7
17	2V	50	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
36	2e	106	PRO	2.6
12	2Q	10	ARG	2.6
19	2X	1	MET	2.6
51	2t	57	ARG	2.6
1	1A	2171	A	2.6
1	2A	652(B)	A	2.6
10	1O	91	LEU	2.6
23	21	98	LEU	2.6
34	2c	76	VAL	2.6
36	2e	41	VAL	2.6
38	2g	75	VAL	2.6
40	1i	14	VAL	2.6
46	2o	11	VAL	2.6
57	2y	73	A	2.6
1	1A	881	G	2.6
1	2A	2120	G	2.6
57	2y	25	C	2.6
7	2H	145	ALA	2.6
12	2Q	137	TYR	2.6
20	2Y	78	ALA	2.6
40	1i	4	TYR	2.6
42	1k	75	TYR	2.6
44	1m	105	THR	2.6
47	2p	32	TYR	2.6
6	2G	29	TRP	2.6
32	2a	1000	U	2.6
34	1c	62	ASP	2.6
38	2g	34	GLY	2.6
39	1h	54	ASP	2.6
40	2i	11	LYS	2.6
26	24	29	PRO	2.6
46	2o	87	ILE	2.6
20	2Y	31	LEU	2.6
44	1m	70	LEU	2.6
45	2n	39	LEU	2.6
51	2t	9	ASN	2.6
8	2I	107	VAL	2.6
26	24	50	VAL	2.6
40	2i	53	VAL	2.6
1	1A	1098	A	2.6
14	2S	31	SER	2.6
35	1d	152	SER	2.6

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Mol	Chain	Res	Type	RSRZ
57	2y	14	A	2.6
32	2a	1149	C	2.6
41	2j	67	THR	2.6
57	1y	75	C	2.6
57	2y	68	C	2.6
1	2A	2792	G	2.6
32	2a	1117	G	2.6
21	2Z	148	ASP	2.6
6	1G	83	ARG	2.6
33	1b	21	ARG	2.6
46	2o	88	ARG	2.6
6	2G	139	LEU	2.6
12	2Q	2	LEU	2.6
8	2I	142	VAL	2.6
48	2q	12	SER	2.6
21	2Z	51	ALA	2.6
33	1b	188	ALA	2.6
42	1k	64	ALA	2.6
1	1A	1076	C	2.6
1	1A	2794	C	2.6
1	2A	2185	C	2.6
32	1a	1038	C	2.6
32	2a	1027	C	2.6
57	2y	74	C	2.6
34	2c	93	LYS	2.6
1	1A	2116	G	2.6
32	1a	1030(A)	G	2.6
57	2y	19	G	2.6
57	2y	44	G	2.6
7	2H	51	ARG	2.6
8	2I	82	ARG	2.6
21	2Z	62	PRO	2.6
26	24	65	ASP	2.6
34	2c	41	GLY	2.6
39	1h	100	ILE	2.6
55	1x	47	U	2.6
7	2H	33	LEU	2.6
21	2Z	168	GLU	2.6
46	1o	57	LEU	2.6
50	2s	30	LEU	2.6
7	2H	114	VAL	2.6
7	2H	133	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
34	2c	3	ASN	2.6
47	1p	21	VAL	2.6
7	2H	56	SER	2.6
39	2h	110	ALA	2.6
19	2X	33	LYS	2.6
45	1n	11	LYS	2.6
1	2A	887	A	2.6
26	14	67	TYR	2.6
38	1g	154	TYR	2.6
50	1s	80	TYR	2.6
52	1u	18	TYR	2.6
32	2a	1018	C	2.5
57	1y	67	C	2.5
5	2F	61	GLY	2.5
7	2H	48	GLY	2.5
11	2P	109	GLY	2.5
46	2o	2	PRO	2.5
1	1A	880	G	2.5
1	1A	2148	G	2.5
1	1A	2149	G	2.5
1	1A	2157	G	2.5
1	1A	2807	G	2.5
1	2A	2165	G	2.5
1	2A	2318	G	2.5
40	2i	77	ILE	2.5
21	2Z	136	PHE	2.5
50	2s	10	PHE	2.5
1	2A	2189	U	2.5
13	2R	111	LEU	2.5
33	1b	10	LEU	2.5
33	2b	154	LEU	2.5
34	2c	12	LEU	2.5
48	2q	22	LEU	2.5
54	1w	20	U	2.5
8	2I	37	VAL	2.5
43	1l	18	VAL	2.5
43	2l	55	VAL	2.5
47	1p	62	VAL	2.5
33	1b	132	LYS	2.5
34	2c	189	ALA	2.5
51	1t	95	ALA	2.5
44	2m	11	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
45	2n	12	ARG	2.5
52	1u	24	ARG	2.5
1	1A	2119	A	2.5
32	1a	1531	A	2.5
33	2b	31	TYR	2.5
40	2i	114	TYR	2.5
57	2y	36	A	2.5
18	2W	112	GLY	2.5
32	2a	1129	C	2.5
42	1k	49	GLY	2.5
50	2s	84	GLY	2.5
33	2b	39	ILE	2.5
1	1A	1087	G	2.5
1	1A	1099	G	2.5
1	1A	2124	G	2.5
1	2A	2152	G	2.5
20	2Y	90	LEU	2.5
54	2w	19	G	2.5
57	2y	69	G	2.5
57	2y	70	G	2.5
4	2E	172	VAL	2.5
21	2Z	90	VAL	2.5
33	1b	165	VAL	2.5
34	2c	75	VAL	2.5
34	2c	198	VAL	2.5
44	2m	106	ASN	2.5
33	2b	123	ALA	2.5
7	2H	38	SER	2.5
33	1b	107	THR	2.5
52	1u	17	THR	2.5
45	2n	3	ARG	2.5
8	2I	1	MET	2.5
33	2b	236	TYR	2.5
40	1i	88	TYR	2.5
1	2A	878	A	2.5
1	2A	1847	A	2.5
26	24	54	GLY	2.5
34	2c	25	GLY	2.5
40	1i	6	GLY	2.5
52	2u	4	GLY	2.5
41	2j	58	ASP	2.5
53	2v	14	A	2.5

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Mol	Chain	Res	Type	RSRZ
8	1I	70	GLU	2.5
8	2I	138	ILE	2.5
33	1b	127	ILE	2.5
33	2b	223	ILE	2.5
1	2A	2164	C	2.5
38	2g	156	TRP	2.5
47	2p	59	TRP	2.5
34	2c	47	LEU	2.5
34	2c	186	PHE	2.5
37	1f	19	LEU	2.5
45	2n	44	LEU	2.5
49	1r	85	LEU	2.5
48	2q	100	LYS	2.5
1	1A	2102	U	2.5
21	2Z	121	HIS	2.5
21	2Z	165	VAL	2.5
21	2Z	174	VAL	2.5
28	26	20	ASN	2.5
39	2h	97	VAL	2.5
45	1n	56	VAL	2.5
57	2y	33	U	2.5
1	1A	1056	G	2.5
1	1A	2123	G	2.5
1	2A	2100	G	2.5
32	1a	79	G	2.5
32	2a	1002	G	2.5
14	2S	20	ARG	2.5
33	1b	137	ARG	2.5
40	1i	82	ALA	2.5
40	2i	42	ARG	2.5
26	24	66	SER	2.5
41	1j	86	MET	2.5
11	2P	93	GLY	2.5
26	24	45	GLY	2.5
35	1d	138	TYR	2.5
40	1i	2	GLU	2.5
8	1I	120	ILE	2.5
21	2Z	53	ILE	2.5
34	2c	8	ILE	2.5
41	1j	74	ILE	2.5
1	1A	1086	A	2.5
14	2S	58	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
35	1d	120	LEU	2.5
35	2d	155	LEU	2.5
45	2n	9	LYS	2.5
51	1t	38	LYS	2.5
33	2b	97	TRP	2.5
35	1d	173	TRP	2.5
41	1j	47	PHE	2.5
42	2k	125	PHE	2.5
1	1A	893	C	2.5
1	2A	886	C	2.5
1	2A	2794	C	2.5
41	2j	68	HIS	2.5
54	2w	68	C	2.5
8	1I	136	VAL	2.5
29	27	46	VAL	2.5
40	1i	41	VAL	2.5
38	2g	4	ARG	2.5
38	2g	5	ARG	2.5
41	1j	76	ASN	2.5
45	1n	3	ARG	2.5
5	2F	22	ALA	2.5
8	2I	53	ALA	2.5
40	2i	84	ALA	2.5
33	2b	48	MET	2.5
34	1c	177	THR	2.5
1	1A	1538	G	2.5
1	2A	171	G	2.5
1	2A	1170	G	2.5
1	2A	2106	G	2.5
1	2A	2182	G	2.5
1	2A	2319	G	2.5
32	1a	78	G	2.5
57	1y	53	G	2.5
57	2y	18	G	2.5
20	2Y	79	CYS	2.4
48	2q	2	PRO	2.4
7	2H	167	GLU	2.4
12	2Q	15	GLY	2.4
33	2b	126	GLU	2.4
35	2d	167	GLY	2.4
35	2d	179	GLU	2.4
44	2m	38	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
20	2Y	38	ILE	2.4
42	1k	25	TYR	2.4
35	2d	19	LEU	2.4
37	1f	45	LEU	2.4
21	2Z	85	HIS	2.4
53	1v	12	A	2.4
52	2u	22	ARG	2.4
1	1A	652(S)	C	2.4
1	1A	1092	C	2.4
1	1A	2128	C	2.4
7	2H	35	VAL	2.4
21	2Z	74	VAL	2.4
32	1a	1028	C	2.4
54	2w	56	C	2.4
54	2w	67	C	2.4
1	1A	2180	U	2.4
29	27	45	ALA	2.4
32	1a	1025	U	2.4
34	2c	53	ALA	2.4
34	2c	160	ALA	2.4
39	2h	9	MET	2.4
40	1i	45	ALA	2.4
21	2Z	170	THR	2.4
41	2j	92	THR	2.4
21	1Z	149	SER	2.4
33	1b	129	GLU	2.4
35	1d	179	GLU	2.4
1	1A	2125	G	2.4
1	1A	2127	G	2.4
1	1A	2154	G	2.4
1	1A	2186	G	2.4
1	2A	892	G	2.4
8	2I	69	LYS	2.4
32	1a	77	G	2.4
32	2a	630	G	2.4
32	2a	1011	G	2.4
32	2a	1182	G	2.4
32	2a	1253	G	2.4
32	2a	1283	G	2.4
33	1b	203	GLY	2.4
57	1y	27	G	2.4
9	2N	116	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
33	2b	10	LEU	2.4
39	1h	62	TYR	2.4
44	1m	56	LEU	2.4
45	1n	6	LEU	2.4
11	2P	102	ARG	2.4
38	2g	6	ARG	2.4
40	2i	18	PHE	2.4
1	1A	1073	A	2.4
1	2A	899	A	2.4
57	2y	23	A	2.4
7	2H	19	VAL	2.4
33	2b	197	VAL	2.4
35	1d	128	VAL	2.4
1	1A	1509	C	2.4
1	2A	1040	C	2.4
34	2c	24	ALA	2.4
45	1n	59	ALA	2.4
51	2t	28	ALA	2.4
1	2A	2180	U	2.4
41	2j	100	THR	2.4
34	2c	154	SER	2.4
38	2g	77	SER	2.4
52	1u	23	PRO	2.4
8	2I	106	GLY	2.4
34	1c	81	GLY	2.4
34	2c	145	GLY	2.4
36	1e	22	GLY	2.4
41	1j	93	GLY	2.4
7	2H	57	ASP	2.4
40	1i	81	ILE	2.4
47	1p	33	ILE	2.4
1	1A	1055	G	2.4
1	2A	2184	G	2.4
9	2N	82	LEU	2.4
21	2Z	102	LEU	2.4
22	20	84	LEU	2.4
32	1a	1024	G	2.4
32	1a	1031	G	2.4
33	2b	61	LEU	2.4
34	2c	33	LEU	2.4
35	2d	162	LEU	2.4
41	2j	16	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
41	2j	88	LEU	2.4
54	2w	5	G	2.4
34	2c	48	TYR	2.4
44	1m	59	TYR	2.4
6	1G	149	VAL	2.4
38	2g	21	VAL	2.4
1	2A	2176	A	2.4
32	2a	1035	A	2.4
32	2a	1248	A	2.4
44	1m	106	ASN	2.4
8	1I	146	ALA	2.4
33	1b	24	TRP	2.4
34	2c	100	ALA	2.4
40	2i	119	ALA	2.4
44	1m	75	ALA	2.4
33	2b	35	GLU	2.4
33	2b	168	THR	2.4
44	1m	121	LYS	2.4
47	1p	22	THR	2.4
1	2A	889	C	2.4
35	2d	29	PRO	2.4
40	2i	90	PRO	2.4
1	2A	895	U	2.4
21	2Z	153	SER	2.4
32	1a	90	U	2.4
32	2a	1025	U	2.4
8	2I	16	GLY	2.4
11	2P	28	GLY	2.4
35	1d	167	GLY	2.4
33	1b	41	ILE	2.4
34	2c	124	ILE	2.4
46	2o	3	ILE	2.4
6	1G	82	LEU	2.4
8	2I	101	LEU	2.4
33	1b	11	LEU	2.4
33	1b	40	HIS	2.4
34	1c	32	LEU	2.4
39	2h	112	LEU	2.4
40	1i	104	ARG	2.4
42	1k	126	ARG	2.4
43	1l	9	GLN	2.4
50	1s	13	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	2A	880	G	2.4
1	2A	2101	G	2.4
32	1a	216	G	2.4
32	1a	1030(C)	G	2.4
32	2a	1001(A)	G	2.4
36	2e	84	PHE	2.4
46	1o	69	TYR	2.4
7	2H	24	VAL	2.4
20	2Y	45	VAL	2.4
21	2Z	86	VAL	2.4
34	2c	86	VAL	2.4
37	1f	85	VAL	2.4
47	1p	20	VAL	2.4
51	2t	88	VAL	2.4
1	1A	1103	A	2.4
41	1j	32	ALA	2.4
26	14	57	GLU	2.4
26	24	27	THR	2.3
47	2p	45	THR	2.3
51	2t	70	SER	2.3
32	2a	1148	U	2.3
1	2A	1509	C	2.3
32	2a	1038	C	2.3
40	2i	30	GLY	2.3
40	2i	67	GLY	2.3
42	2k	86	GLY	2.3
57	2y	2	C	2.3
57	2y	56	C	2.3
7	2H	88	LEU	2.3
8	1I	9	LEU	2.3
22	20	62	LEU	2.3
26	24	9	LEU	2.3
41	2j	82	ILE	2.3
34	2c	36	ASP	2.3
34	2c	62	ASP	2.3
40	2i	105	ASP	2.3
44	1m	90	LEU	2.3
14	2S	7	TYR	2.3
26	24	49	PHE	2.3
40	2i	92	TYR	2.3
40	2i	125	TYR	2.3
5	2F	193	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
7	2H	44	VAL	2.3
34	2c	4	LYS	2.3
34	2c	138	VAL	2.3
43	2l	39	VAL	2.3
1	1A	2155	G	2.3
1	1A	2207	G	2.3
32	1a	1021	G	2.3
32	1a	1026	G	2.3
32	2a	1127	G	2.3
42	1k	117	ASN	2.3
57	1y	15	G	2.3
57	1y	18	G	2.3
6	2G	48	GLU	2.3
38	2g	40	ALA	2.3
41	1j	64	GLU	2.3
45	2n	46	GLU	2.3
39	2h	5	PRO	2.3
8	2I	78	THR	2.3
33	2b	47	THR	2.3
44	2m	37	THR	2.3
50	2s	77	THR	2.3
1	1A	229	A	2.3
1	1A	878	A	2.3
1	1A	1070	A	2.3
1	1A	1077	A	2.3
32	1a	1041	A	2.3
32	2a	1245	A	2.3
53	2v	24	A	2.3
57	1y	35	A	2.3
21	1Z	52	SER	2.3
41	2j	66	ARG	2.3
49	1r	87	ARG	2.3
1	1A	1097	U	2.3
1	1A	1175	U	2.3
1	1A	2118	U	2.3
1	2A	2118	U	2.3
32	1a	1532	U	2.3
57	1y	51	U	2.3
7	2H	121	ILE	2.3
14	2S	35	ILE	2.3
20	2Y	44	ILE	2.3
34	1c	14	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
39	1h	127	LEU	2.3
41	1j	6	ILE	2.3
51	1t	24	LEU	2.3
1	1A	889	C	2.3
21	2Z	58	VAL	2.3
33	1b	93	VAL	2.3
33	2b	136	VAL	2.3
34	1c	76	VAL	2.3
34	2c	151	VAL	2.3
40	2i	17	VAL	2.3
40	2i	109	VAL	2.3
4	1E	56	PRO	2.3
7	2H	21	PRO	2.3
8	2I	98	ALA	2.3
1	1A	1068	G	2.3
1	1A	2100	G	2.3
32	2a	1003	G	2.3
41	1j	100	THR	2.3
52	2u	9	ARG	2.3
17	2V	41	GLY	2.3
32	2a	1001	A	2.3
32	2a	1005	A	2.3
32	2a	1251	A	2.3
40	2i	57	GLY	2.3
6	1G	52	ILE	2.3
14	2S	80	LEU	2.3
31	29	17	ILE	2.3
38	1g	12	LEU	2.3
40	2i	56	LEU	2.3
50	1s	40	ILE	2.3
1	1A	1060	U	2.3
21	2Z	63	ASP	2.3
36	2e	10	MET	2.3
1	1A	1079	C	2.3
1	1A	2178	C	2.3
1	2A	2188	C	2.3
3	1D	38	LYS	2.3
32	2a	1007	C	2.3
43	2l	17	LYS	2.3
34	2c	203	PHE	2.3
6	2G	15	VAL	2.3
21	1Z	168	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
8	2I	29	TYR	2.3
26	24	10	VAL	2.3
26	24	32	TYR	2.3
34	2c	130	VAL	2.3
35	1d	20	TYR	2.3
35	2d	20	TYR	2.3
7	2H	12	PRO	2.3
8	1I	65	ALA	2.3
9	2N	45	ASN	2.3
29	17	45	ALA	2.3
36	1e	138	ALA	2.3
36	2e	30	ALA	2.3
41	2j	76	ASN	2.3
8	2I	76	THR	2.3
40	2i	27	THR	2.3
47	2p	69	THR	2.3
19	2X	86	GLY	2.3
40	2i	100	GLY	2.3
50	2s	68	GLY	2.3
1	1A	1176	G	2.3
1	1A	2168	G	2.3
8	2I	143	SER	2.3
1	2A	900	A	2.3
2	2B	59	A	2.3
7	2H	72	ILE	2.3
21	2Z	137	ILE	2.3
32	2a	1156	G	2.3
32	2a	1258	G	2.3
41	2j	59	SER	2.3
42	2k	40	ILE	2.3
49	2r	85	LEU	2.3
57	1y	24	G	2.3
57	2y	1	G	2.3
57	2y	65	G	2.3
54	1w	73	A	2.3
57	1y	23	A	2.3
45	2n	4	LYS	2.3
1	1A	9	U	2.3
1	1A	2172	U	2.3
32	1a	65	U	2.3
1	1A	2103	C	2.3
1	1A	2896	C	2.3

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Mol	Chain	Res	Type	RSRZ
1	2A	277	C	2.3
1	2A	893	C	2.3
4	1E	73	GLU	2.3
9	2N	10	GLU	2.3
15	2T	128	GLU	2.3
26	14	49	PHE	2.3
32	1a	163	C	2.3
32	2a	1028	C	2.3
33	2b	163	PHE	2.3
17	2V	51	VAL	2.3
34	2c	120	VAL	2.3
39	2h	19	VAL	2.3
9	2N	11	PRO	2.3
31	29	30	PRO	2.3
34	2c	73	PRO	2.3
6	1G	50	ALA	2.2
24	22	13	ALA	2.2
35	2d	164	ALA	2.2
4	2E	10	GLY	2.2
21	1Z	151	HIS	2.2
21	2Z	106	GLY	2.2
34	1c	13	GLY	2.2
34	2c	80	GLY	2.2
52	2u	16	GLY	2.2
7	2H	7	LEU	2.2
35	1d	126	ILE	2.2
36	2e	101	ILE	2.2
49	1r	31	LEU	2.2
51	1t	10	LEU	2.2
1	2A	528	A	2.2
1	2A	2892	A	2.2
6	2G	49	ASP	2.2
32	2a	1252	A	2.2
41	2j	17	ASP	2.2
57	1y	64	A	2.2
1	1A	2184	G	2.2
1	2A	652(C)	G	2.2
57	1y	22	G	2.2
1	1A	12	U	2.2
1	2A	9	U	2.2
1	2A	2150	U	2.2
57	1y	12	U	2.2

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Mol	Chain	Res	Type	RSRZ
21	2Z	169	GLU	2.2
26	24	57	GLU	2.2
43	1l	16	GLU	2.2
1	1A	1075	C	2.2
1	1A	1080	C	2.2
1	1A	2105	C	2.2
1	1A	2183	C	2.2
1	2A	2177	C	2.2
1	2A	2178	C	2.2
7	2H	26	VAL	2.2
9	2N	140	VAL	2.2
21	1Z	139	VAL	2.2
33	2b	226	ARG	2.2
40	1i	9	ARG	2.2
32	2a	1019	C	2.2
47	1p	51	VAL	2.2
57	1y	3	C	2.2
57	1y	68	C	2.2
57	1y	74	C	2.2
57	2y	43	C	2.2
12	2Q	28	ALA	2.2
35	2d	149	ALA	2.2
44	2m	87	TYR	2.2
50	1s	52	TYR	2.2
21	2Z	151	HIS	2.2
41	1j	42	THR	2.2
4	2E	115	GLY	2.2
26	24	69	LYS	2.2
33	2b	132	LYS	2.2
35	2d	183	GLY	2.2
51	2t	96	GLY	2.2
21	2Z	67	LEU	2.2
47	1p	49	LEU	2.2
48	1q	98	LEU	2.2
50	2s	16	LEU	2.2
33	2b	210	SER	2.2
37	2f	93	SER	2.2
45	1n	42	ILE	2.2
5	2F	172	TRP	2.2
1	1A	1054	A	2.2
32	2a	1179	A	2.2
1	1A	2122	U	2.2

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Mol	Chain	Res	Type	RSRZ
1	2A	272(A)	U	2.2
1	1A	1093	G	2.2
1	2A	1114	G	2.2
1	2A	1171	G	2.2
32	2a	1024	G	2.2
38	2g	78	ARG	2.2
45	1n	57	ARG	2.2
54	1w	44	G	2.2
54	2w	18	G	2.2
57	1y	69	G	2.2
24	12	37	PHE	2.2
34	2c	128	PHE	2.2
40	2i	101	PHE	2.2
47	2p	9	PHE	2.2
7	2H	15	VAL	2.2
7	2H	52	VAL	2.2
7	2H	99	VAL	2.2
12	2Q	106	VAL	2.2
20	2Y	42	VAL	2.2
34	2c	70	VAL	2.2
40	1i	21	PRO	2.2
41	2j	49	VAL	2.2
42	2k	39	PRO	2.2
8	2I	100	ALA	2.2
21	2Z	7	ALA	2.2
33	1b	123	ALA	2.2
33	2b	13	ALA	2.2
34	2c	92	ALA	2.2
35	1d	195	ALA	2.2
40	2i	122	ALA	2.2
41	1j	78	ASN	2.2
42	2k	26	ASN	2.2
50	2s	53	ASN	2.2
34	2c	199	LYS	2.2
39	2h	17	THR	2.2
39	2h	70	GLN	2.2
40	1i	5	TYR	2.2
41	2j	13	HIS	2.2
47	1p	16	HIS	2.2
5	1F	131	GLY	2.2
23	21	55	GLY	2.2
38	2g	22	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
38	2g	124	LEU	2.2
40	1i	69	GLY	2.2
42	1k	98	LEU	2.2
47	2p	10	GLY	2.2
49	2r	66	LEU	2.2
21	1Z	171	ILE	2.2
34	2c	39	ILE	2.2
34	2c	57	ILE	2.2
46	1o	12	ILE	2.2
33	1b	189	ASP	2.2
15	1T	115	ARG	2.2
34	2c	167	TRP	2.2
32	2a	1250	A	2.2
57	1y	33	U	2.2
57	2y	38	A	2.2
33	2b	131	PRO	2.2
7	2H	169	VAL	2.2
8	2I	145	VAL	2.2
12	2Q	109	VAL	2.2
21	2Z	139	VAL	2.2
34	2c	55	VAL	2.2
38	2g	66	VAL	2.2
32	2a	1160	G	2.2
32	2a	1175	G	2.2
33	2b	22	LYS	2.2
57	2y	6	G	2.2
6	2G	79	ASN	2.2
11	2P	84	ASN	2.2
41	2j	62	HIS	2.2
49	1r	20	ALA	2.2
1	1A	2791	C	2.2
7	2H	31	GLY	2.2
7	2H	103	LEU	2.2
13	2R	65	LEU	2.2
32	2a	1116	C	2.2
32	2a	1260	C	2.2
33	1b	14	GLY	2.2
33	1b	18	GLY	2.2
33	2b	118	LEU	2.2
34	2c	193	TYR	2.2
39	2h	24	THR	2.2
47	1p	45	THR	2.2

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Mol	Chain	Res	Type	RSRZ
40	1i	50	LEU	2.2
44	1m	24	GLY	2.2
57	2y	13	C	2.2
45	2n	40	CYS	2.2
5	2F	28	ILE	2.2
6	1G	144	ILE	2.2
7	2H	136	ILE	2.2
33	2b	162	ILE	2.2
34	1c	124	ILE	2.2
5	1F	13	SER	2.2
36	2e	125	SER	2.2
48	1q	97	SER	2.2
48	2q	97	SER	2.2
11	1P	98	GLU	2.2
40	2i	83	ARG	2.2
8	2I	137	PRO	2.2
36	1e	96	PRO	2.2
39	2h	101	PRO	2.2
45	1n	14	PRO	2.2
52	2u	23	PRO	2.2
21	2Z	44	PHE	2.2
1	1A	228	A	2.1
1	2A	2122	U	2.2
11	2P	101	VAL	2.1
32	1a	1446	U	2.2
32	2a	997	U	2.2
34	2c	207	VAL	2.1
57	1y	21	A	2.1
3	1D	2	ALA	2.1
7	2H	111	HIS	2.1
7	2H	156	ALA	2.1
7	2H	165	ALA	2.1
8	2I	94	ALA	2.1
11	2P	68	GLN	2.1
33	2b	77	ALA	2.1
34	2c	71	ALA	2.1
38	1g	83	ALA	2.1
39	2h	15	ASN	2.1
40	1i	46	ALA	2.1
41	1j	69	ASN	2.1
47	1p	82	GLN	2.1
51	1t	76	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	1A	892	G	2.1
19	2X	92	LEU	2.1
32	1a	630	G	2.1
32	2a	1021	G	2.1
41	2j	52	GLY	2.1
48	2q	43	LEU	2.1
50	2s	8	GLY	2.1
57	1y	5	G	2.1
57	1y	57	G	2.1
57	1y	70	G	2.1
7	2H	83	TYR	2.1
33	1b	39	ILE	2.1
47	1p	36	ILE	2.1
1	1A	2175	C	2.1
32	2a	1043	C	2.1
57	1y	48	C	2.1
57	2y	67	C	2.1
8	2I	103	ARG	2.1
11	2P	79	ARG	2.1
33	2b	111	ARG	2.1
36	2e	27	ARG	2.1
42	1k	92	GLU	2.1
45	2n	45	ARG	2.1
50	2s	35	SER	2.1
7	2H	29	PRO	2.1
41	2j	91	PRO	2.1
45	1n	50	LYS	2.1
48	2q	14	LYS	2.1
21	2Z	88	PHE	2.1
21	2Z	128	VAL	2.1
38	2g	103	TRP	2.1
33	2b	40	HIS	2.1
49	2r	86	VAL	2.1
1	1A	2173	A	2.1
26	24	60	GLN	2.1
8	2I	49	ALA	2.1
14	2S	51	ALA	2.1
32	2a	1176	A	2.1
40	2i	73	GLN	2.1
34	2c	137	ALA	2.1
40	2i	52	ALA	2.1
54	2w	31	A	2.1

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Mol	Chain	Res	Type	RSRZ
57	2y	26	A	2.1
34	2c	102	ASN	2.1
37	1f	13	ASN	2.1
4	2E	29	GLY	2.1
17	2V	101	GLY	2.1
21	2Z	26	GLY	2.1
34	2c	148	GLY	2.1
37	1f	79	LEU	2.1
40	2i	79	LEU	2.1
41	2j	8	LEU	2.1
44	2m	105	THR	2.1
50	1s	71	LEU	2.1
50	2s	63	THR	2.1
15	2T	110	ILE	2.1
39	2h	6	ILE	2.1
43	2l	7	ILE	2.1
24	12	69	ARG	2.1
35	2d	163	GLU	2.1
37	2f	63	TYR	2.1
1	1A	171	G	2.1
1	2A	2121	G	2.1
32	2a	976	G	2.1
32	2a	1190	G	2.1
46	2o	76	GLU	2.1
57	1y	1	G	2.1
1	2A	2105	C	2.1
8	2I	20	ASP	2.1
32	2a	1452	C	2.1
57	1y	49	C	2.1
6	2G	47	LYS	2.1
52	2u	3	LYS	2.1
33	2b	125	PRO	2.1
33	2b	19	HIS	2.1
47	1p	1	MET	2.1
12	2Q	113	GLN	2.1
44	2m	15	VAL	2.1
1	2A	2172	U	2.1
25	23	25	ALA	2.1
33	1b	225	ALA	2.1
33	2b	188	ALA	2.1
34	1c	18	TRP	2.1
32	2a	1040	U	2.1

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Mol	Chain	Res	Type	RSRZ
36	2e	17	ALA	2.1
51	2t	67	ALA	2.1
57	1y	66	U	2.1
57	2y	66	U	2.1
1	2A	2629	A	2.1
7	2H	142	GLY	2.1
12	2Q	17	LEU	2.1
32	1a	162	A	2.1
23	21	22	GLY	2.1
23	21	28	GLY	2.1
34	2c	188	LEU	2.1
33	1b	190	THR	2.1
36	1e	97	GLY	2.1
40	1i	8	GLY	2.1
47	2p	73	LEU	2.1
48	2q	76	LEU	2.1
5	1F	17	ARG	2.1
8	2I	27	ARG	2.1
9	2N	115	ARG	2.1
35	2d	47	ARG	2.1
45	2n	19	ARG	2.1
34	1c	5	ILE	2.1
34	1c	23	TYR	2.1
47	2p	38	TYR	2.1
21	2Z	66	SER	2.1
26	24	39	CYS	2.1
1	1A	1089	G	2.1
1	1A	2152	G	2.1
32	2a	1131	G	2.1
54	2w	69	G	2.1
55	2x	46	G	2.1
57	2y	52	G	2.1
21	1Z	167	PRO	2.1
21	2Z	95	PRO	2.1
32	2a	840	C	2.1
32	2a	1037	C	2.1
32	2a	1254	C	2.1
47	1p	41	PRO	2.1
57	1y	13	C	2.1
14	2S	34	HIS	2.1
9	2N	124	ALA	2.1
33	2b	88	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
35	2d	147	ALA	2.1
38	2g	7	ALA	2.1
42	2k	74	ALA	2.1
42	2k	89	ALA	2.1
44	2m	28	ALA	2.1
51	1t	59	ALA	2.1
18	2W	60	ASN	2.1
6	1G	51	ARG	2.1
6	2G	53	LEU	2.1
36	2e	142	LEU	2.1
39	2h	127	LEU	2.1
40	2i	29	ASN	2.1
21	2Z	131	ARG	2.1
21	2Z	143	GLY	2.1
26	14	64	GLY	2.1
34	2c	197	GLY	2.1
35	2d	130	GLY	2.1
6	2G	54	GLU	2.1
34	2c	206	GLU	2.1
40	1i	103	THR	2.1
1	1A	1460	A	2.1
18	2W	95	ILE	2.1
32	2a	1041	A	2.1
36	2e	109	ILE	2.1
40	2i	81	ILE	2.1
41	2j	23	ILE	2.1
41	2j	50	ILE	2.1
47	2p	33	ILE	2.1
57	1y	38	A	2.1
46	2o	10	LYS	2.1
51	2t	27	LYS	2.1
21	2Z	8	TYR	2.1
42	2k	75	TYR	2.1
43	2l	64	TYR	2.1
7	2H	10	PRO	2.1
35	1d	189	PRO	2.1
39	2h	72	PRO	2.1
1	1A	1062	G	2.0
32	1a	165	C	2.1
32	1a	1006	C	2.1
32	2a	470	C	2.1
32	2a	1263	C	2.1

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Mol	Chain	Res	Type	RSRZ
50	1s	14	HIS	2.1
32	2a	1272	G	2.0
57	2y	4	C	2.1
35	1d	201	GLN	2.0
7	2H	11	VAL	2.0
7	2H	107	VAL	2.0
8	2I	18	VAL	2.0
16	2U	106	PHE	2.0
17	2V	5	VAL	2.0
20	2Y	39	VAL	2.0
21	2Z	141	VAL	2.0
33	1b	230	VAL	2.0
39	1h	53	VAL	2.0
40	2i	33	PHE	2.0
47	1p	2	VAL	2.0
34	1c	65	ALA	2.0
40	2i	94	ALA	2.0
44	2m	5	ALA	2.0
51	1t	89	ARG	2.0
21	1Z	150	LEU	2.0
34	2c	94	LEU	2.0
37	2f	21	LEU	2.0
40	1i	102	LEU	2.0
42	2k	103	LEU	2.0
44	2m	90	LEU	2.0
6	1G	48	GLU	2.0
8	2I	70	GLU	2.0
11	2P	44	GLY	2.0
17	1V	54	GLY	2.0
21	2Z	11	GLU	2.0
33	2b	134	GLU	2.0
43	2l	29	GLY	2.0
14	2S	5	THR	2.0
32	1a	1040	U	2.0
34	1c	84	ILE	2.0
41	2j	55	LYS	2.0
44	1m	27	LYS	2.0
46	1o	3	ILE	2.0
1	2A	6	A	2.0
1	2A	1460	A	2.0
53	1v	14	A	2.0
39	1h	4	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
5	1F	14	PRO	2.0
5	2F	14	PRO	2.0
7	2H	118	PRO	2.0
7	2H	134	SER	2.0
11	2P	78	PRO	2.0
20	2Y	56	PRO	2.0
40	2i	21	PRO	2.0
43	2l	25	PRO	2.0
45	1n	21	TYR	2.0
1	2A	271(J)	C	2.0
7	2H	45	VAL	2.0
21	2Z	71	VAL	2.0
22	20	69	PHE	2.0
32	1a	1019	C	2.0
34	1c	207	VAL	2.0
39	2h	26	VAL	2.0
40	2i	16	ARG	2.0
40	2i	41	VAL	2.0
41	2j	11	PHE	2.0
41	2j	46	ARG	2.0
44	2m	53	VAL	2.0
45	1n	18	VAL	2.0
50	2s	58	VAL	2.0
1	2A	10	G	2.0
2	2B	106	G	2.0
4	2E	63	LEU	2.0
7	2H	20	ALA	2.0
21	2Z	164	ALA	2.0
32	1a	1010	G	2.0
8	2I	73	GLU	2.0
8	2I	77	LEU	2.0
8	2I	140	LEU	2.0
20	2Y	105	ALA	2.0
35	2d	196	LEU	2.0
38	2g	65	ALA	2.0
40	1i	106	ALA	2.0
40	2i	35	GLU	2.0
44	2m	48	LEU	2.0
44	2m	96	LEU	2.0
48	2q	98	LEU	2.0
14	2S	109	GLY	2.0
23	21	81	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
35	1d	171	GLY	2.0
43	2l	63	GLY	2.0
45	1n	17	LYS	2.0
7	2H	4	ILE	2.0
33	2b	107	THR	2.0
44	2m	22	ILE	2.0
47	1p	44	THR	2.0
48	2q	7	THR	2.0
32	2a	1126	U	2.0
9	2N	86	PRO	2.0
32	1a	344	A	2.0
54	1w	7	A	2.0
7	2H	2	SER	2.0
21	2Z	3	TYR	2.0
38	2g	151	TYR	2.0
44	2m	92	HIS	2.0
46	2o	69	TYR	2.0
48	1q	66	SER	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	G7M	2y	46	24/25	0.56	0.18	73,82,88,90	0
57	G7M	1y	46	24/25	0.58	0.17	75,80,85,93	0
57	4SU	2y	8	20/21	0.59	0.18	76,87,92,101	0
57	PSU	1y	55	20/21	0.63	0.18	76,81,89,94	0
57	MIA	2y	37	22/30	0.64	0.18	68,77,91,101	0
57	MIA	1y	37	22/30	0.65	0.18	72,78,86,95	0
57	PSU	2y	39	20/21	0.68	0.19	71,79,88,94	0
57	PSU	1y	39	20/21	0.69	0.16	71,77,86,86	0
57	5MU	1y	54	21/22	0.70	0.15	72,77,84,87	0
57	4SU	1y	8	20/21	0.70	0.14	76,80,87,101	0
57	5MU	2y	54	21/22	0.70	0.17	70,78,87,101	0
57	PSU	2y	55	20/21	0.71	0.16	75,80,90,90	0
54	G7M	2w	46	24/25	0.72	0.16	61,76,89,101	0
54	G7M	1w	46	24/25	0.75	0.15	59,69,79,99	0
57	PSU	1y	32	20/21	0.76	0.16	67,75,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	PSU	2y	32	20/21	0.78	0.14	70,77,83,86	0
54	4SU	1w	8	20/21	0.86	0.13	68,74,81,81	0
54	PSU	2w	55	20/21	0.86	0.12	58,70,73,73	0
32	2MG	2a	1207	24/25	0.87	0.15	56,67,72,76	0
54	4SU	2w	8	20/21	0.87	0.13	70,75,81,88	0
54	PSU	2w	32	20/21	0.87	0.17	57,63,75,78	0
54	MIA	2w	37	25/30	0.89	0.14	56,64,67,85	0
55	5MU	2x	54	21/22	0.90	0.15	58,66,73,77	0
55	PSU	2x	55	20/21	0.90	0.12	59,65,72,74	0
1	5MU	2A	1915	21/22	0.90	0.13	44,55,61,62	0
43	0TD	1l	92	10/11	0.90	0.12	39,44,45,60	0
54	PSU	2w	39	20/21	0.91	0.13	57,65,71,72	0
43	0TD	2l	92	10/11	0.91	0.13	49,51,56,67	0
55	5MC	2x	32	21/22	0.91	0.15	52,58,64,68	0
54	5MU	2w	54	21/22	0.91	0.13	50,64,66,69	0
55	5MU	1x	54	21/22	0.91	0.12	53,58,66,73	0
32	G7M	2a	527	24/25	0.92	0.12	43,56,61,65	0
54	MIA	1w	37	29/30	0.92	0.14	33,45,54,82	0
32	M2G	2a	966	25/26	0.92	0.14	53,56,64,73	0
55	4SU	2x	8	20/21	0.92	0.13	58,63,66,68	0
1	PSU	2A	1917	20/21	0.93	0.10	48,53,59,64	0
1	5MC	2A	1942	21/22	0.93	0.10	43,50,56,57	0
32	PSU	2a	516	20/21	0.93	0.10	54,62,66,67	0
55	4SU	1x	8	20/21	0.93	0.10	49,58,65,68	0
1	PSU	2A	1911	20/21	0.93	0.10	45,53,56,57	0
55	PSU	1x	55	20/21	0.93	0.11	48,54,60,65	0
32	5MC	2a	1400	21/22	0.93	0.14	52,60,64,68	0
54	PSU	1w	32	20/21	0.93	0.12	49,55,62,62	0
32	4OC	2a	1402	22/23	0.94	0.11	46,49,54,56	0
32	5MC	2a	1407	21/22	0.94	0.11	42,45,51,53	0
32	2MG	1a	1207	24/25	0.94	0.10	49,57,61,66	0
54	5MU	1w	54	21/22	0.94	0.11	40,54,60,62	0
1	OMC	2A	1920	21/22	0.94	0.10	45,53,55,56	0
54	PSU	1w	55	20/21	0.94	0.11	42,60,65,66	0
54	PSU	1w	39	20/21	0.94	0.11	37,55,60,68	0
54	F3N	2w	76	33/34	0.94	0.11	27,35,42,46	0
32	G7M	1a	527	24/25	0.95	0.10	33,42,46,52	0
1	5MC	2A	1962	21/22	0.95	0.10	32,40,49,62	0
32	5MC	2a	1404	21/22	0.95	0.11	40,46,50,63	0
1	OMU	2A	2552	21/22	0.95	0.10	36,42,46,51	0
32	MA6	2a	1519	24/25	0.95	0.12	44,53,59,62	0
32	M2G	1a	966	25/26	0.95	0.11	41,48,52,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MU	1A	1915	21/22	0.95	0.08	36,42,46,47	0
32	5MC	1a	1400	21/22	0.95	0.10	36,45,48,50	0
32	5MC	2a	967	21/22	0.95	0.11	51,57,60,65	0
32	5MC	1a	1407	21/22	0.95	0.09	31,36,40,42	0
55	8AN	2x	76	22/23	0.95	0.10	31,35,41,46	0
32	5MC	1a	967	21/22	0.96	0.10	43,48,53,56	0
32	MA6	1a	1519	24/25	0.96	0.09	34,40,43,51	0
1	PSU	1A	1917	20/21	0.96	0.09	31,40,44,45	0
32	PSU	1a	516	20/21	0.96	0.09	40,51,55,56	0
55	5MC	1x	32	21/22	0.96	0.11	34,45,50,62	0
32	UR3	2a	1498	21/22	0.96	0.10	43,49,55,60	0
32	MA6	2a	1518	24/25	0.96	0.09	42,50,55,58	0
32	5MC	1a	1404	21/22	0.96	0.10	31,40,45,46	0
1	5MU	2A	1939	21/22	0.96	0.09	30,37,41,45	0
1	OMG	2A	2251	24/25	0.97	0.08	30,35,39,41	0
1	2MA	2A	2503	23/24	0.97	0.08	28,35,39,42	0
32	UR3	1a	1498	21/22	0.97	0.08	33,38,41,43	0
1	PSU	2A	2605	20/21	0.97	0.07	25,32,37,38	0
55	8AN	1x	76	22/23	0.97	0.07	14,19,24,25	0
32	MA6	1a	1518	24/25	0.97	0.09	33,39,44,45	0
1	PSU	1A	1911	20/21	0.97	0.08	26,40,45,47	0
1	OMC	1A	1920	21/22	0.97	0.08	30,37,42,44	0
32	4OC	1a	1402	22/23	0.97	0.08	33,37,42,46	0
1	5MC	1A	1942	21/22	0.97	0.08	23,34,40,54	0
1	PSU	1A	2605	20/21	0.97	0.08	18,23,28,28	0
1	5MC	1A	1962	21/22	0.98	0.07	27,31,35,37	0
1	2MA	1A	2503	23/24	0.98	0.06	12,16,19,21	0
1	OMU	1A	2552	21/22	0.98	0.05	16,23,27,29	0
54	F3N	1w	76	33/34	0.98	0.08	13,17,21,24	0
1	5MU	1A	1939	21/22	0.98	0.07	21,24,30,31	0
1	OMG	1A	2251	24/25	0.99	0.05	17,22,24,25	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	4072	1/1	0.45	0.28	58,58,58,58	0
58	MG	10	105	1/1	0.54	0.26	58,58,58,58	0
58	MG	2A	3683	1/1	0.59	0.25	60,60,60,60	0
58	MG	2A	3844	1/1	0.59	0.28	74,74,74,74	0
58	MG	1A	3845	1/1	0.64	0.20	60,60,60,60	0
58	MG	1A	3621	1/1	0.66	0.17	24,24,24,24	0
58	MG	1A	3659	1/1	0.67	0.10	30,30,30,30	0
58	MG	2A	3752	1/1	0.68	0.15	42,42,42,42	0
58	MG	2A	3744	1/1	0.68	0.20	66,66,66,66	0
58	MG	20	102	1/1	0.69	0.20	56,56,56,56	0
58	MG	1a	1790	1/1	0.70	0.13	62,62,62,62	0
58	MG	1A	4006	1/1	0.70	0.16	40,40,40,40	0
58	MG	2A	3823	1/1	0.71	0.17	66,66,66,66	0
58	MG	1A	3865	1/1	0.71	0.14	68,68,68,68	0
58	MG	1a	1675	1/1	0.71	0.28	62,62,62,62	0
58	MG	1A	3802	1/1	0.72	0.20	73,73,73,73	0
58	MG	2A	3580	1/1	0.74	0.16	50,50,50,50	0
58	MG	1A	3851	1/1	0.75	0.17	52,52,52,52	0
58	MG	2A	3645	1/1	0.75	0.19	39,39,39,39	0
58	MG	1A	3773	1/1	0.75	0.10	19,19,19,19	0
58	MG	1E	311	1/1	0.75	0.18	60,60,60,60	0
58	MG	1A	4076	1/1	0.76	0.15	54,54,54,54	0
58	MG	1a	1807	1/1	0.76	0.17	67,67,67,67	0
58	MG	2A	3203	1/1	0.76	0.33	67,67,67,67	0
58	MG	2A	3253	1/1	0.76	0.23	62,62,62,62	0
58	MG	2a	1816	1/1	0.76	0.17	65,65,65,65	0
58	MG	1B	216	1/1	0.77	0.12	49,49,49,49	0
58	MG	2A	3803	1/1	0.77	0.14	57,57,57,57	0
58	MG	1a	1743	1/1	0.77	0.19	77,77,77,77	0
58	MG	2A	3659	1/1	0.77	0.16	67,67,67,67	0
58	MG	1B	225	1/1	0.77	0.17	57,57,57,57	0
58	MG	2a	1662	1/1	0.77	0.36	68,68,68,68	0
58	MG	2A	3342	1/1	0.77	0.16	69,69,69,69	0
58	MG	1A	3859	1/1	0.78	0.14	60,60,60,60	0
58	MG	2A	3717	1/1	0.78	0.21	56,56,56,56	0
58	MG	2A	3320	1/1	0.78	0.17	57,57,57,57	0
58	MG	1A	3814	1/1	0.78	0.13	40,40,40,40	0
58	MG	2A	3401	1/1	0.78	0.17	65,65,65,65	0
58	MG	2A	3528	1/1	0.78	0.18	62,62,62,62	0
58	MG	1A	3904	1/1	0.78	0.12	36,36,36,36	0
58	MG	2A	3619	1/1	0.78	0.17	50,50,50,50	0
58	MG	1A	3566	1/1	0.78	0.27	71,71,71,71	0
58	MG	1A	3717	1/1	0.78	0.14	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2j	201	1/1	0.78	0.15	65,65,65,65	0
58	MG	2A	3650	1/1	0.79	0.19	49,49,49,49	0
58	MG	1A	3693	1/1	0.79	0.16	56,56,56,56	0
58	MG	1A	4046	1/1	0.79	0.19	49,49,49,49	0
58	MG	2A	3684	1/1	0.79	0.16	73,73,73,73	0
58	MG	2a	1644	1/1	0.79	0.32	65,65,65,65	0
58	MG	2A	3296	1/1	0.79	0.18	62,62,62,62	0
58	MG	2a	1782	1/1	0.79	0.24	70,70,70,70	0
58	MG	1A	3991	1/1	0.79	0.19	60,60,60,60	0
58	MG	2a	1833	1/1	0.79	0.18	63,63,63,63	0
58	MG	1A	4002	1/1	0.79	0.12	41,41,41,41	0
58	MG	1B	230	1/1	0.80	0.12	54,54,54,54	0
58	MG	2A	3511	1/1	0.80	0.12	46,46,46,46	0
58	MG	2A	3521	1/1	0.80	0.22	60,60,60,60	0
58	MG	2A	3788	1/1	0.80	0.20	57,57,57,57	0
58	MG	1B	236	1/1	0.80	0.14	53,53,53,53	0
58	MG	1A	3899	1/1	0.80	0.16	37,37,37,37	0
58	MG	2A	3584	1/1	0.80	0.12	59,59,59,59	0
58	MG	2A	3611	1/1	0.80	0.14	57,57,57,57	0
58	MG	28	103	1/1	0.80	0.21	54,54,54,54	0
58	MG	2a	1627	1/1	0.80	0.21	65,65,65,65	0
58	MG	1A	3701	1/1	0.80	0.12	20,20,20,20	0
58	MG	1A	3896	1/1	0.80	0.18	31,31,31,31	0
58	MG	2a	1761	1/1	0.80	0.12	63,63,63,63	0
58	MG	2A	3316	1/1	0.80	0.13	65,65,65,65	0
58	MG	1A	4070	1/1	0.80	0.17	56,56,56,56	0
58	MG	1a	1744	1/1	0.80	0.18	64,64,64,64	0
58	MG	2A	3362	1/1	0.80	0.36	68,68,68,68	0
58	MG	1A	3837	1/1	0.81	0.15	36,36,36,36	0
58	MG	2A	3348	1/1	0.81	0.10	70,70,70,70	0
58	MG	1A	3881	1/1	0.81	0.18	38,38,38,38	0
58	MG	2A	3618	1/1	0.81	0.15	39,39,39,39	0
58	MG	1A	3937	1/1	0.81	0.11	30,30,30,30	0
58	MG	2a	1663	1/1	0.81	0.17	66,66,66,66	0
58	MG	2a	1748	1/1	0.81	0.12	78,78,78,78	0
58	MG	2a	1751	1/1	0.81	0.11	73,73,73,73	0
58	MG	2A	3765	1/1	0.81	0.17	56,56,56,56	0
58	MG	1A	3953	1/1	0.81	0.08	23,23,23,23	0
58	MG	1A	3722	1/1	0.81	0.14	47,47,47,47	0
58	MG	2A	3655	1/1	0.81	0.19	58,58,58,58	0
58	MG	1E	309	1/1	0.81	0.09	21,21,21,21	0
58	MG	2A	3809	1/1	0.82	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3777	1/1	0.82	0.11	25,25,25,25	0
58	MG	2A	3841	1/1	0.82	0.15	63,63,63,63	0
58	MG	1A	4104	1/1	0.82	0.11	44,44,44,44	0
58	MG	2A	3856	1/1	0.82	0.16	63,63,63,63	0
58	MG	1A	3783	1/1	0.82	0.08	46,46,46,46	0
58	MG	1a	1775	1/1	0.82	0.12	68,68,68,68	0
58	MG	1a	1784	1/1	0.82	0.11	40,40,40,40	0
58	MG	2a	1635	1/1	0.82	0.26	66,66,66,66	0
58	MG	1A	3645	1/1	0.82	0.15	50,50,50,50	0
58	MG	1A	3872	1/1	0.82	0.13	54,54,54,54	0
58	MG	2A	3709	1/1	0.82	0.19	71,71,71,71	0
58	MG	2a	1706	1/1	0.82	0.20	59,59,59,59	0
58	MG	2a	1722	1/1	0.82	0.14	71,71,71,71	0
58	MG	2A	3024	1/1	0.82	0.19	61,61,61,61	0
58	MG	2A	3718	1/1	0.82	0.20	59,59,59,59	0
58	MG	2a	1758	1/1	0.82	0.09	78,78,78,78	0
58	MG	2A	3559	1/1	0.82	0.17	52,52,52,52	0
58	MG	1A	3652	1/1	0.82	0.08	14,14,14,14	0
58	MG	1A	3830	1/1	0.82	0.12	50,50,50,50	0
58	MG	1A	3620	1/1	0.82	0.11	52,52,52,52	0
58	MG	1A	3356	1/1	0.82	0.13	47,47,47,47	0
58	MG	2l	204	1/1	0.82	0.11	49,49,49,49	0
58	MG	1A	3671	1/1	0.83	0.10	17,17,17,17	0
58	MG	1A	3677	1/1	0.83	0.10	37,37,37,37	0
58	MG	1A	3927	1/1	0.83	0.09	24,24,24,24	0
58	MG	2A	3282	1/1	0.83	0.13	53,53,53,53	0
58	MG	1A	3608	1/1	0.83	0.20	51,51,51,51	0
58	MG	1B	231	1/1	0.83	0.16	61,61,61,61	0
58	MG	2A	3769	1/1	0.83	0.15	38,38,38,38	0
58	MG	1B	235	1/1	0.83	0.16	50,50,50,50	0
58	MG	1A	3346	1/1	0.83	0.18	60,60,60,60	0
58	MG	1A	3102	1/1	0.83	0.12	56,56,56,56	0
58	MG	1A	3995	1/1	0.83	0.13	38,38,38,38	0
58	MG	2A	3839	1/1	0.83	0.11	57,57,57,57	0
58	MG	2A	3370	1/1	0.83	0.16	63,63,63,63	0
58	MG	2A	3843	1/1	0.83	0.14	41,41,41,41	0
58	MG	1Z	303	1/1	0.83	0.13	51,51,51,51	0
58	MG	2A	3433	1/1	0.83	0.24	53,53,53,53	0
58	MG	1A	3720	1/1	0.83	0.15	40,40,40,40	0
58	MG	18	104	1/1	0.83	0.14	43,43,43,43	0
58	MG	2a	1605	1/1	0.83	0.11	66,66,66,66	0
58	MG	2a	1613	1/1	0.83	0.16	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1a	1641	1/1	0.83	0.15	49,49,49,49	0
58	MG	2A	3532	1/1	0.83	0.16	59,59,59,59	0
58	MG	2A	3544	1/1	0.83	0.13	53,53,53,53	0
58	MG	1a	1672	1/1	0.83	0.18	60,60,60,60	0
58	MG	1A	3637	1/1	0.83	0.19	61,61,61,61	0
58	MG	1a	1697	1/1	0.83	0.16	56,56,56,56	0
58	MG	1a	1736	1/1	0.83	0.15	56,56,56,56	0
58	MG	1A	4030	1/1	0.83	0.12	52,52,52,52	0
58	MG	1A	3389	1/1	0.83	0.17	53,53,53,53	0
58	MG	1a	1763	1/1	0.83	0.15	58,58,58,58	0
58	MG	1a	1764	1/1	0.83	0.14	68,68,68,68	0
58	MG	1A	3465	1/1	0.83	0.14	56,56,56,56	0
58	MG	2a	1801	1/1	0.83	0.19	66,66,66,66	0
58	MG	2a	1802	1/1	0.83	0.20	66,66,66,66	0
58	MG	2a	1809	1/1	0.83	0.13	61,61,61,61	0
58	MG	1A	3781	1/1	0.83	0.09	25,25,25,25	0
58	MG	1A	3267	1/1	0.83	0.13	50,50,50,50	0
58	MG	1A	4096	1/1	0.83	0.18	71,71,71,71	0
58	MG	2A	3693	1/1	0.83	0.14	61,61,61,61	0
58	MG	2A	3829	1/1	0.84	0.14	37,37,37,37	0
58	MG	1a	1809	1/1	0.84	0.14	48,48,48,48	0
58	MG	1V	206	1/1	0.84	0.13	51,51,51,51	0
58	MG	2A	3587	1/1	0.84	0.12	56,56,56,56	0
58	MG	1A	4053	1/1	0.84	0.08	20,20,20,20	0
58	MG	1A	3663	1/1	0.84	0.13	34,34,34,34	0
58	MG	2B	206	1/1	0.84	0.17	60,60,60,60	0
58	MG	2B	215	1/1	0.84	0.17	59,59,59,59	0
58	MG	2R	202	1/1	0.84	0.16	55,55,55,55	0
58	MG	2A	3256	1/1	0.84	0.15	67,67,67,67	0
58	MG	2A	3265	1/1	0.84	0.14	65,65,65,65	0
58	MG	1A	3454	1/1	0.84	0.16	54,54,54,54	0
58	MG	2a	1612	1/1	0.84	0.25	66,66,66,66	0
58	MG	1A	3954	1/1	0.84	0.12	29,29,29,29	0
58	MG	2a	1624	1/1	0.84	0.13	55,55,55,55	0
58	MG	1A	3877	1/1	0.84	0.12	55,55,55,55	0
58	MG	2a	1632	1/1	0.84	0.14	55,55,55,55	0
58	MG	1A	3461	1/1	0.84	0.11	52,52,52,52	0
58	MG	1A	4001	1/1	0.84	0.11	50,50,50,50	0
58	MG	2a	1659	1/1	0.84	0.28	77,77,77,77	0
58	MG	1a	1699	1/1	0.84	0.16	57,57,57,57	0
58	MG	2A	3704	1/1	0.84	0.17	60,60,60,60	0
58	MG	1A	3226	1/1	0.84	0.20	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3654	1/1	0.84	0.18	52,52,52,52	0
58	MG	1A	4018	1/1	0.84	0.15	42,42,42,42	0
58	MG	2A	3735	1/1	0.84	0.15	65,65,65,65	0
58	MG	1A	3782	1/1	0.84	0.08	16,16,16,16	0
58	MG	1A	4038	1/1	0.84	0.10	42,42,42,42	0
58	MG	2A	3757	1/1	0.84	0.12	36,36,36,36	0
58	MG	2A	3515	1/1	0.84	0.14	33,33,33,33	0
58	MG	1A	4045	1/1	0.84	0.12	40,40,40,40	0
58	MG	1A	3527	1/1	0.84	0.18	66,66,66,66	0
58	MG	2A	3800	1/1	0.84	0.16	57,57,57,57	0
58	MG	1G	204	1/1	0.84	0.15	60,60,60,60	0
58	MG	1O	204	1/1	0.84	0.14	66,66,66,66	0
58	MG	1a	1808	1/1	0.84	0.27	58,58,58,58	0
58	MG	2v	103	1/1	0.84	0.13	70,70,70,70	0
58	MG	1a	1662	1/1	0.85	0.12	48,48,48,48	0
58	MG	1A	3999	1/1	0.85	0.08	20,20,20,20	0
58	MG	2B	219	1/1	0.85	0.20	71,71,71,71	0
58	MG	2E	305	1/1	0.85	0.12	37,37,37,37	0
58	MG	1A	3749	1/1	0.85	0.11	47,47,47,47	0
58	MG	1A	3882	1/1	0.85	0.15	37,37,37,37	0
58	MG	1A	3895	1/1	0.85	0.11	47,47,47,47	0
58	MG	2a	1604	1/1	0.85	0.17	65,65,65,65	0
58	MG	1A	3570	1/1	0.85	0.15	55,55,55,55	0
58	MG	2a	1607	1/1	0.85	0.21	64,64,64,64	0
58	MG	2a	1609	1/1	0.85	0.22	61,61,61,61	0
58	MG	2A	3689	1/1	0.85	0.14	44,44,44,44	0
58	MG	1A	3312	1/1	0.85	0.12	57,57,57,57	0
58	MG	2a	1619	1/1	0.85	0.22	56,56,56,56	0
58	MG	2a	1622	1/1	0.85	0.18	62,62,62,62	0
58	MG	1A	4037	1/1	0.85	0.16	50,50,50,50	0
58	MG	1A	3612	1/1	0.85	0.14	58,58,58,58	0
58	MG	2A	3374	1/1	0.85	0.11	58,58,58,58	0
58	MG	1A	3667	1/1	0.85	0.12	44,44,44,44	0
58	MG	1A	3858	1/1	0.85	0.14	44,44,44,44	0
58	MG	2a	1649	1/1	0.85	0.23	68,68,68,68	0
58	MG	1A	3494	1/1	0.85	0.14	56,56,56,56	0
58	MG	2A	3514	1/1	0.85	0.12	51,51,51,51	0
58	MG	1V	205	1/1	0.85	0.12	49,49,49,49	0
58	MG	2a	1687	1/1	0.85	0.20	57,57,57,57	0
58	MG	1A	4069	1/1	0.85	0.09	30,30,30,30	0
58	MG	2a	1710	1/1	0.85	0.21	55,55,55,55	0
58	MG	1A	3800	1/1	0.85	0.08	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3985	1/1	0.85	0.10	41,41,41,41	0
58	MG	2A	3799	1/1	0.85	0.12	63,63,63,63	0
58	MG	2A	3543	1/1	0.85	0.14	56,56,56,56	0
58	MG	1w	109	1/1	0.85	0.13	72,72,72,72	0
58	MG	2a	1766	1/1	0.85	0.14	55,55,55,55	0
58	MG	2A	3805	1/1	0.85	0.18	54,54,54,54	0
58	MG	2a	1796	1/1	0.85	0.13	54,54,54,54	0
58	MG	1A	3672	1/1	0.85	0.06	13,13,13,13	0
58	MG	2A	3109	1/1	0.85	0.11	72,72,72,72	0
58	MG	2a	1804	1/1	0.85	0.16	70,70,70,70	0
58	MG	2A	3115	1/1	0.85	0.29	60,60,60,60	0
58	MG	1a	1610	1/1	0.85	0.15	61,61,61,61	0
58	MG	2a	1824	1/1	0.85	0.14	59,59,59,59	0
58	MG	2A	3216	1/1	0.85	0.12	54,54,54,54	0
58	MG	1a	1623	1/1	0.85	0.17	54,54,54,54	0
58	MG	1A	3806	1/1	0.85	0.07	23,23,23,23	0
58	MG	2A	3621	1/1	0.85	0.15	47,47,47,47	0
58	MG	2w	104	1/1	0.85	0.20	67,67,67,67	0
58	MG	2A	3666	1/1	0.86	0.10	57,57,57,57	0
58	MG	2A	3675	1/1	0.86	0.12	51,51,51,51	0
58	MG	1A	3831	1/1	0.86	0.08	34,34,34,34	0
58	MG	1A	3705	1/1	0.86	0.10	25,25,25,25	0
58	MG	2A	3688	1/1	0.86	0.12	51,51,51,51	0
58	MG	1A	3898	1/1	0.86	0.12	38,38,38,38	0
58	MG	1A	3074	1/1	0.86	0.18	57,57,57,57	0
58	MG	2A	3386	1/1	0.86	0.24	54,54,54,54	0
58	MG	1w	102	1/1	0.86	0.27	67,67,67,67	0
58	MG	2A	3411	1/1	0.86	0.12	59,59,59,59	0
58	MG	1A	3850	1/1	0.86	0.15	48,48,48,48	0
58	MG	2A	3720	1/1	0.86	0.12	48,48,48,48	0
58	MG	2A	3480	1/1	0.86	0.17	70,70,70,70	0
58	MG	1A	3307	1/1	0.86	0.11	36,36,36,36	0
58	MG	2A	3050	1/1	0.86	0.12	67,67,67,67	0
58	MG	2A	3063	1/1	0.86	0.14	64,64,64,64	0
58	MG	2A	3758	1/1	0.86	0.15	47,47,47,47	0
58	MG	2A	3517	1/1	0.86	0.14	59,59,59,59	0
58	MG	2a	1682	1/1	0.86	0.23	58,58,58,58	0
58	MG	1A	3798	1/1	0.86	0.07	41,41,41,41	0
58	MG	2a	1690	1/1	0.86	0.14	51,51,51,51	0
58	MG	1A	3681	1/1	0.86	0.10	38,38,38,38	0
58	MG	2A	3146	1/1	0.86	0.16	55,55,55,55	0
58	MG	2A	3185	1/1	0.86	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
58	MG	1A	3747	1/1	0.86	0.11	54,54,54,54	0
58	MG	2A	3548	1/1	0.86	0.10	40,40,40,40	0
58	MG	2a	1757	1/1	0.86	0.11	66,66,66,66	0
58	MG	2A	3205	1/1	0.86	0.13	56,56,56,56	0
58	MG	2A	3563	1/1	0.86	0.18	38,38,38,38	0
58	MG	1A	3964	1/1	0.86	0.10	49,49,49,49	0
58	MG	2a	1775	1/1	0.86	0.12	53,53,53,53	0
58	MG	1A	4058	1/1	0.86	0.10	47,47,47,47	0
58	MG	1A	3440	1/1	0.86	0.13	44,44,44,44	0
58	MG	1A	3700	1/1	0.86	0.10	33,33,33,33	0
58	MG	1A	3820	1/1	0.86	0.13	57,57,57,57	0
58	MG	1a	1771	1/1	0.86	0.10	57,57,57,57	0
58	MG	2A	3868	1/1	0.86	0.18	63,63,63,63	0
58	MG	2a	1811	1/1	0.86	0.15	56,56,56,56	0
58	MG	2a	1812	1/1	0.86	0.11	58,58,58,58	0
58	MG	1A	3475	1/1	0.86	0.15	59,59,59,59	0
58	MG	2A	3623	1/1	0.86	0.09	43,43,43,43	0
58	MG	1a	1783	1/1	0.86	0.12	55,55,55,55	0
58	MG	2A	3333	1/1	0.86	0.14	48,48,48,48	0
58	MG	2l	202	1/1	0.86	0.24	62,62,62,62	0
58	MG	2A	3334	1/1	0.86	0.20	57,57,57,57	0
58	MG	1A	4085	1/1	0.86	0.11	31,31,31,31	0
58	MG	2w	103	1/1	0.86	0.23	63,63,63,63	0
58	MG	25	106	1/1	0.86	0.15	57,57,57,57	0
58	MG	2A	3576	1/1	0.87	0.14	53,53,53,53	0
58	MG	1A	3369	1/1	0.87	0.21	32,32,32,32	0
58	MG	1A	3811	1/1	0.87	0.08	36,36,36,36	0
58	MG	2B	216	1/1	0.87	0.16	46,46,46,46	0
58	MG	1a	1749	1/1	0.87	0.23	66,66,66,66	0
58	MG	2A	3603	1/1	0.87	0.19	62,62,62,62	0
58	MG	2F	303	1/1	0.87	0.19	51,51,51,51	0
58	MG	2A	3610	1/1	0.87	0.19	56,56,56,56	0
58	MG	1a	1753	1/1	0.87	0.10	45,45,45,45	0
58	MG	1A	3956	1/1	0.87	0.28	54,54,54,54	0
58	MG	2A	3288	1/1	0.87	0.26	67,67,67,67	0
58	MG	2a	1601	1/1	0.87	0.19	61,61,61,61	0
58	MG	1A	3767	1/1	0.87	0.14	57,57,57,57	0
58	MG	1a	1766	1/1	0.87	0.11	49,49,49,49	0
58	MG	2a	1606	1/1	0.87	0.27	62,62,62,62	0
58	MG	2A	3631	1/1	0.87	0.10	49,49,49,49	0
58	MG	2a	1608	1/1	0.87	0.24	67,67,67,67	0
58	MG	1a	1770	1/1	0.87	0.11	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3646	1/1	0.87	0.14	40,40,40,40	0
58	MG	2A	3328	1/1	0.87	0.15	64,64,64,64	0
58	MG	2a	1618	1/1	0.87	0.13	60,60,60,60	0
58	MG	2A	3330	1/1	0.87	0.22	68,68,68,68	0
58	MG	2A	3332	1/1	0.87	0.15	50,50,50,50	0
58	MG	2A	3664	1/1	0.87	0.24	62,62,62,62	0
58	MG	1A	3026	1/1	0.87	0.15	50,50,50,50	0
58	MG	1A	3329	1/1	0.87	0.30	60,60,60,60	0
58	MG	2A	3341	1/1	0.87	0.12	66,66,66,66	0
58	MG	1A	3992	1/1	0.87	0.15	60,60,60,60	0
58	MG	2a	1646	1/1	0.87	0.15	59,59,59,59	0
58	MG	2A	3685	1/1	0.87	0.14	49,49,49,49	0
58	MG	1A	3778	1/1	0.87	0.11	30,30,30,30	0
58	MG	1A	3998	1/1	0.87	0.09	29,29,29,29	0
58	MG	2A	3691	1/1	0.87	0.17	63,63,63,63	0
58	MG	1a	1806	1/1	0.87	0.15	68,68,68,68	0
58	MG	2A	3698	1/1	0.87	0.12	53,53,53,53	0
58	MG	1A	4081	1/1	0.87	0.20	40,40,40,40	0
58	MG	1A	3166	1/1	0.87	0.15	53,53,53,53	0
58	MG	2A	3397	1/1	0.87	0.26	65,65,65,65	0
58	MG	2a	1720	1/1	0.87	0.21	64,64,64,64	0
58	MG	1A	3707	1/1	0.87	0.09	34,34,34,34	0
58	MG	1a	1629	1/1	0.87	0.13	52,52,52,52	0
58	MG	1A	3457	1/1	0.87	0.10	51,51,51,51	0
58	MG	2A	3740	1/1	0.87	0.09	45,45,45,45	0
58	MG	2A	3438	1/1	0.87	0.19	64,64,64,64	0
58	MG	2A	3445	1/1	0.87	0.15	48,48,48,48	0
58	MG	2A	3755	1/1	0.87	0.09	40,40,40,40	0
58	MG	2A	3472	1/1	0.87	0.30	63,63,63,63	0
58	MG	1a	1645	1/1	0.87	0.17	61,61,61,61	0
58	MG	2a	1788	1/1	0.87	0.16	57,57,57,57	0
58	MG	1B	207	1/1	0.87	0.15	50,50,50,50	0
58	MG	1a	1669	1/1	0.87	0.15	60,60,60,60	0
58	MG	2A	3066	1/1	0.87	0.17	50,50,50,50	0
58	MG	2A	3093	1/1	0.87	0.30	52,52,52,52	0
58	MG	1A	4003	1/1	0.87	0.13	49,49,49,49	0
58	MG	1A	3567	1/1	0.87	0.14	55,55,55,55	0
58	MG	2A	3804	1/1	0.87	0.15	66,66,66,66	0
58	MG	1a	1695	1/1	0.87	0.21	49,49,49,49	0
58	MG	2A	3542	1/1	0.87	0.18	53,53,53,53	0
58	MG	1A	3919	1/1	0.87	0.10	38,38,38,38	0
58	MG	2g	201	1/1	0.87	0.10	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3650	1/1	0.87	0.11	35,35,35,35	0
58	MG	1A	3211	1/1	0.87	0.10	60,60,60,60	0
58	MG	2A	3553	1/1	0.87	0.12	38,38,38,38	0
58	MG	2A	3207	1/1	0.87	0.11	53,53,53,53	0
58	MG	2A	3212	1/1	0.87	0.12	57,57,57,57	0
58	MG	2A	3573	1/1	0.87	0.09	30,30,30,30	0
58	MG	1V	203	1/1	0.88	0.08	39,39,39,39	0
58	MG	2V	202	1/1	0.88	0.10	55,55,55,55	0
58	MG	1A	3335	1/1	0.88	0.12	50,50,50,50	0
58	MG	25	101	1/1	0.88	0.27	67,67,67,67	0
58	MG	1A	3259	1/1	0.88	0.14	58,58,58,58	0
58	MG	1Z	301	1/1	0.88	0.20	59,59,59,59	0
58	MG	1Z	302	1/1	0.88	0.11	62,62,62,62	0
58	MG	1A	3160	1/1	0.88	0.09	49,49,49,49	0
58	MG	2A	3338	1/1	0.88	0.12	43,43,43,43	0
58	MG	1A	3020	1/1	0.88	0.13	37,37,37,37	0
58	MG	1A	3959	1/1	0.88	0.10	56,56,56,56	0
58	MG	1A	3311	1/1	0.88	0.14	47,47,47,47	0
58	MG	1A	3548	1/1	0.88	0.17	52,52,52,52	0
58	MG	1A	3867	1/1	0.88	0.08	23,23,23,23	0
58	MG	1a	1813	1/1	0.88	0.18	53,53,53,53	0
58	MG	2a	1616	1/1	0.88	0.29	64,64,64,64	0
58	MG	1d	301	1/1	0.88	0.20	59,59,59,59	0
58	MG	1a	1636	1/1	0.88	0.20	62,62,62,62	0
58	MG	2a	1620	1/1	0.88	0.16	58,58,58,58	0
58	MG	1A	3555	1/1	0.88	0.14	66,66,66,66	0
58	MG	1A	3417	1/1	0.88	0.12	45,45,45,45	0
58	MG	2a	1626	1/1	0.88	0.12	55,55,55,55	0
58	MG	2A	3420	1/1	0.88	0.15	48,48,48,48	0
58	MG	2A	3041	1/1	0.88	0.16	49,49,49,49	0
58	MG	1a	1649	1/1	0.88	0.13	56,56,56,56	0
58	MG	2a	1642	1/1	0.88	0.27	62,62,62,62	0
58	MG	1A	3436	1/1	0.88	0.24	50,50,50,50	0
58	MG	2A	3449	1/1	0.88	0.14	56,56,56,56	0
58	MG	2A	3724	1/1	0.88	0.10	53,53,53,53	0
58	MG	2a	1653	1/1	0.88	0.23	61,61,61,61	0
58	MG	2a	1657	1/1	0.88	0.16	66,66,66,66	0
58	MG	2A	3729	1/1	0.88	0.15	46,46,46,46	0
58	MG	1a	1666	1/1	0.88	0.15	57,57,57,57	0
58	MG	2A	3073	1/1	0.88	0.12	54,54,54,54	0
58	MG	2a	1674	1/1	0.88	0.14	59,59,59,59	0
58	MG	2A	3481	1/1	0.88	0.10	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3750	1/1	0.88	0.14	65,65,65,65	0
58	MG	1A	3251	1/1	0.88	0.10	47,47,47,47	0
58	MG	2A	3105	1/1	0.88	0.20	64,64,64,64	0
58	MG	1A	4108	1/1	0.88	0.24	55,55,55,55	0
58	MG	1A	3890	1/1	0.88	0.13	24,24,24,24	0
58	MG	2A	3117	1/1	0.88	0.15	49,49,49,49	0
58	MG	2A	3123	1/1	0.88	0.24	62,62,62,62	0
58	MG	2A	3780	1/1	0.88	0.08	44,44,44,44	0
58	MG	1a	1678	1/1	0.88	0.18	49,49,49,49	0
58	MG	2A	3171	1/1	0.88	0.14	59,59,59,59	0
58	MG	1a	1679	1/1	0.88	0.19	55,55,55,55	0
58	MG	2A	3187	1/1	0.88	0.21	59,59,59,59	0
58	MG	2A	3191	1/1	0.88	0.30	69,69,69,69	0
58	MG	1a	1682	1/1	0.88	0.19	58,58,58,58	0
58	MG	1a	1692	1/1	0.88	0.30	60,60,60,60	0
58	MG	2A	3817	1/1	0.88	0.10	35,35,35,35	0
58	MG	1A	3725	1/1	0.88	0.16	52,52,52,52	0
58	MG	1A	3314	1/1	0.88	0.19	50,50,50,50	0
58	MG	1A	3748	1/1	0.88	0.18	37,37,37,37	0
58	MG	2A	3243	1/1	0.88	0.13	63,63,63,63	0
58	MG	1A	3825	1/1	0.88	0.11	56,56,56,56	0
58	MG	1A	4021	1/1	0.88	0.08	30,30,30,30	0
58	MG	2A	3846	1/1	0.88	0.11	48,48,48,48	0
58	MG	2a	1818	1/1	0.88	0.12	61,61,61,61	0
58	MG	2a	1820	1/1	0.88	0.19	56,56,56,56	0
58	MG	1A	3258	1/1	0.88	0.13	49,49,49,49	0
58	MG	2A	3605	1/1	0.88	0.10	30,30,30,30	0
58	MG	2d	302	1/1	0.88	0.12	58,58,58,58	0
58	MG	1A	4035	1/1	0.88	0.12	35,35,35,35	0
58	MG	1A	3751	1/1	0.88	0.10	45,45,45,45	0
58	MG	1A	3675	1/1	0.88	0.08	33,33,33,33	0
58	MG	2A	3297	1/1	0.88	0.09	38,38,38,38	0
58	MG	2n	101	1/1	0.88	0.17	60,60,60,60	0
58	MG	2q	202	1/1	0.88	0.12	57,57,57,57	0
58	MG	2A	3304	1/1	0.88	0.11	57,57,57,57	0
58	MG	2w	101	1/1	0.88	0.19	44,44,44,44	0
58	MG	1A	4041	1/1	0.88	0.13	50,50,50,50	0
58	MG	2G	201	1/1	0.88	0.12	61,61,61,61	0
58	MG	2A	3218	1/1	0.89	0.15	58,58,58,58	0
58	MG	2A	3229	1/1	0.89	0.10	44,44,44,44	0
58	MG	1A	3542	1/1	0.89	0.21	54,54,54,54	0
58	MG	1A	3173	1/1	0.89	0.16	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2F	302	1/1	0.89	0.09	56,56,56,56	0
58	MG	1A	3911	1/1	0.89	0.16	45,45,45,45	0
58	MG	2A	3593	1/1	0.89	0.14	58,58,58,58	0
58	MG	2Q	202	1/1	0.89	0.14	46,46,46,46	0
58	MG	2A	3596	1/1	0.89	0.09	60,60,60,60	0
58	MG	2T	202	1/1	0.89	0.21	70,70,70,70	0
58	MG	2A	3257	1/1	0.89	0.13	61,61,61,61	0
58	MG	2A	3258	1/1	0.89	0.11	51,51,51,51	0
58	MG	2A	3606	1/1	0.89	0.10	66,66,66,66	0
58	MG	2A	3262	1/1	0.89	0.16	59,59,59,59	0
58	MG	1A	3661	1/1	0.89	0.10	54,54,54,54	0
58	MG	2A	3266	1/1	0.89	0.12	50,50,50,50	0
58	MG	2A	3271	1/1	0.89	0.19	64,64,64,64	0
58	MG	1A	3344	1/1	0.89	0.14	51,51,51,51	0
58	MG	1A	3931	1/1	0.89	0.09	24,24,24,24	0
58	MG	1a	1780	1/1	0.89	0.09	62,62,62,62	0
58	MG	11	104	1/1	0.89	0.10	34,34,34,34	0
58	MG	2A	3301	1/1	0.89	0.14	67,67,67,67	0
58	MG	16	101	1/1	0.89	0.15	60,60,60,60	0
58	MG	2A	3305	1/1	0.89	0.22	53,53,53,53	0
58	MG	2A	3309	1/1	0.89	0.11	53,53,53,53	0
58	MG	2a	1617	1/1	0.89	0.13	67,67,67,67	0
58	MG	1A	3452	1/1	0.89	0.17	48,48,48,48	0
58	MG	2A	3665	1/1	0.89	0.09	59,59,59,59	0
58	MG	1a	1800	1/1	0.89	0.11	61,61,61,61	0
58	MG	2A	3670	1/1	0.89	0.12	51,51,51,51	0
58	MG	2A	3671	1/1	0.89	0.11	50,50,50,50	0
58	MG	1A	4066	1/1	0.89	0.12	46,46,46,46	0
58	MG	1A	3265	1/1	0.89	0.15	50,50,50,50	0
58	MG	1a	1625	1/1	0.89	0.19	48,48,48,48	0
58	MG	1A	3353	1/1	0.89	0.18	48,48,48,48	0
58	MG	2a	1637	1/1	0.89	0.19	57,57,57,57	0
58	MG	2a	1641	1/1	0.89	0.13	62,62,62,62	0
58	MG	1a	1630	1/1	0.89	0.21	58,58,58,58	0
58	MG	2a	1643	1/1	0.89	0.24	73,73,73,73	0
58	MG	1A	3460	1/1	0.89	0.10	44,44,44,44	0
58	MG	1A	3235	1/1	0.89	0.14	53,53,53,53	0
58	MG	2a	1647	1/1	0.89	0.14	50,50,50,50	0
58	MG	1A	3853	1/1	0.89	0.17	51,51,51,51	0
58	MG	1x	104	1/1	0.89	0.09	43,43,43,43	0
58	MG	2a	1655	1/1	0.89	0.15	58,58,58,58	0
58	MG	2A	3357	1/1	0.89	0.12	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3706	1/1	0.89	0.09	52,52,52,52	0
58	MG	2A	3359	1/1	0.89	0.11	50,50,50,50	0
58	MG	1x	108	1/1	0.89	0.08	20,20,20,20	0
58	MG	2A	3369	1/1	0.89	0.11	51,51,51,51	0
58	MG	2a	1680	1/1	0.89	0.16	50,50,50,50	0
58	MG	2a	1681	1/1	0.89	0.25	57,57,57,57	0
58	MG	1A	3965	1/1	0.89	0.15	31,31,31,31	0
58	MG	1A	3978	1/1	0.89	0.20	49,49,49,49	0
58	MG	2A	3042	1/1	0.89	0.24	53,53,53,53	0
58	MG	2A	3045	1/1	0.89	0.09	61,61,61,61	0
58	MG	1A	4102	1/1	0.89	0.14	42,42,42,42	0
58	MG	2a	1719	1/1	0.89	0.24	68,68,68,68	0
58	MG	2A	3404	1/1	0.89	0.08	53,53,53,53	0
58	MG	1A	3617	1/1	0.89	0.09	23,23,23,23	0
58	MG	2a	1725	1/1	0.89	0.18	59,59,59,59	0
58	MG	2a	1737	1/1	0.89	0.15	53,53,53,53	0
58	MG	2a	1739	1/1	0.89	0.16	56,56,56,56	0
58	MG	1A	3690	1/1	0.89	0.12	44,44,44,44	0
58	MG	1A	3271	1/1	0.89	0.17	47,47,47,47	0
58	MG	2a	1755	1/1	0.89	0.16	51,51,51,51	0
58	MG	1A	3697	1/1	0.89	0.17	62,62,62,62	0
58	MG	2A	3104	1/1	0.89	0.10	52,52,52,52	0
58	MG	2A	3759	1/1	0.89	0.12	56,56,56,56	0
58	MG	1A	3386	1/1	0.89	0.11	52,52,52,52	0
58	MG	2a	1774	1/1	0.89	0.12	61,61,61,61	0
58	MG	1A	3784	1/1	0.89	0.13	34,34,34,34	0
58	MG	1a	1686	1/1	0.89	0.09	49,49,49,49	0
58	MG	2a	1783	1/1	0.89	0.20	60,60,60,60	0
58	MG	2A	3786	1/1	0.89	0.09	63,63,63,63	0
58	MG	2a	1793	1/1	0.89	0.22	59,59,59,59	0
58	MG	1A	3319	1/1	0.89	0.12	43,43,43,43	0
58	MG	2a	1798	1/1	0.89	0.18	51,51,51,51	0
58	MG	2A	3792	1/1	0.89	0.09	53,53,53,53	0
58	MG	2A	3797	1/1	0.89	0.12	46,46,46,46	0
58	MG	2A	3492	1/1	0.89	0.09	46,46,46,46	0
58	MG	1A	3702	1/1	0.89	0.10	25,25,25,25	0
58	MG	1A	3889	1/1	0.89	0.19	35,35,35,35	0
58	MG	1A	3296	1/1	0.89	0.12	53,53,53,53	0
58	MG	2A	3175	1/1	0.89	0.13	47,47,47,47	0
58	MG	2a	1817	1/1	0.89	0.14	65,65,65,65	0
58	MG	1A	3528	1/1	0.89	0.13	47,47,47,47	0
58	MG	2A	3812	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
58	MG	2a	1821	1/1	0.89	0.26	71,71,71,71	0
58	MG	1a	1737	1/1	0.89	0.15	57,57,57,57	0
58	MG	2A	3190	1/1	0.89	0.19	61,61,61,61	0
58	MG	2A	3541	1/1	0.89	0.20	59,59,59,59	0
58	MG	1a	1740	1/1	0.89	0.14	56,56,56,56	0
58	MG	2A	3194	1/1	0.89	0.09	52,52,52,52	0
58	MG	1F	313	1/1	0.89	0.21	34,34,34,34	0
58	MG	1A	3532	1/1	0.89	0.10	40,40,40,40	0
58	MG	2A	3551	1/1	0.89	0.07	37,37,37,37	0
58	MG	1A	3897	1/1	0.89	0.07	21,21,21,21	0
58	MG	2v	102	1/1	0.89	0.13	46,46,46,46	0
58	MG	2A	3859	1/1	0.89	0.15	62,62,62,62	0
58	MG	2A	3864	1/1	0.89	0.13	61,61,61,61	0
58	MG	1A	3812	1/1	0.89	0.10	54,54,54,54	0
58	MG	1a	1759	1/1	0.89	0.14	49,49,49,49	0
58	MG	2y	101	1/1	0.89	0.11	61,61,61,61	0
58	MG	1A	3549	1/1	0.90	0.15	52,52,52,52	0
58	MG	2A	3848	1/1	0.90	0.08	38,38,38,38	0
58	MG	2A	3852	1/1	0.90	0.09	41,41,41,41	0
58	MG	1A	3934	1/1	0.90	0.08	29,29,29,29	0
58	MG	1A	3655	1/1	0.90	0.14	64,64,64,64	0
58	MG	1A	3946	1/1	0.90	0.08	27,27,27,27	0
58	MG	2A	3866	1/1	0.90	0.14	40,40,40,40	0
58	MG	1A	4083	1/1	0.90	0.19	43,43,43,43	0
58	MG	2A	3869	1/1	0.90	0.17	57,57,57,57	0
58	MG	2A	3530	1/1	0.90	0.10	53,53,53,53	0
58	MG	2B	211	1/1	0.90	0.16	50,50,50,50	0
58	MG	1A	3551	1/1	0.90	0.10	46,46,46,46	0
58	MG	1A	4095	1/1	0.90	0.13	65,65,65,65	0
58	MG	1A	3731	1/1	0.90	0.09	32,32,32,32	0
58	MG	2D	307	1/1	0.90	0.12	54,54,54,54	0
58	MG	2E	303	1/1	0.90	0.21	59,59,59,59	0
58	MG	1a	1691	1/1	0.90	0.20	41,41,41,41	0
58	MG	1A	3955	1/1	0.90	0.10	45,45,45,45	0
58	MG	1a	1694	1/1	0.90	0.21	50,50,50,50	0
58	MG	2A	3201	1/1	0.90	0.14	51,51,51,51	0
58	MG	1A	3746	1/1	0.90	0.15	52,52,52,52	0
58	MG	1A	3006	1/1	0.90	0.14	50,50,50,50	0
58	MG	1A	4109	1/1	0.90	0.19	50,50,50,50	0
58	MG	2A	3566	1/1	0.90	0.13	47,47,47,47	0
58	MG	20	101	1/1	0.90	0.12	49,49,49,49	0
58	MG	1a	1728	1/1	0.90	0.15	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1a	1733	1/1	0.90	0.11	36,36,36,36	0
58	MG	1A	3002	1/1	0.90	0.12	56,56,56,56	0
58	MG	1A	3184	1/1	0.90	0.16	52,52,52,52	0
58	MG	1a	1739	1/1	0.90	0.13	57,57,57,57	0
58	MG	2A	3250	1/1	0.90	0.16	59,59,59,59	0
58	MG	2A	3595	1/1	0.90	0.10	59,59,59,59	0
58	MG	1A	3976	1/1	0.90	0.12	37,37,37,37	0
58	MG	1A	3250	1/1	0.90	0.15	48,48,48,48	0
58	MG	1A	3574	1/1	0.90	0.09	43,43,43,43	0
58	MG	1A	3770	1/1	0.90	0.07	15,15,15,15	0
58	MG	2A	3607	1/1	0.90	0.13	56,56,56,56	0
58	MG	2A	3608	1/1	0.90	0.17	50,50,50,50	0
58	MG	1A	3771	1/1	0.90	0.09	37,37,37,37	0
58	MG	1B	238	1/1	0.90	0.07	35,35,35,35	0
58	MG	1a	1761	1/1	0.90	0.13	50,50,50,50	0
58	MG	1D	310	1/1	0.90	0.17	39,39,39,39	0
58	MG	2A	3272	1/1	0.90	0.11	60,60,60,60	0
58	MG	1A	3598	1/1	0.90	0.20	39,39,39,39	0
58	MG	2a	1623	1/1	0.90	0.12	57,57,57,57	0
58	MG	2A	3626	1/1	0.90	0.18	57,57,57,57	0
58	MG	1A	3775	1/1	0.90	0.07	23,23,23,23	0
58	MG	2A	3633	1/1	0.90	0.11	61,61,61,61	0
58	MG	2A	3636	1/1	0.90	0.12	46,46,46,46	0
58	MG	2A	3638	1/1	0.90	0.17	43,43,43,43	0
58	MG	2A	3289	1/1	0.90	0.12	61,61,61,61	0
58	MG	2A	3293	1/1	0.90	0.12	66,66,66,66	0
58	MG	1A	3873	1/1	0.90	0.07	41,41,41,41	0
58	MG	1A	4000	1/1	0.90	0.13	53,53,53,53	0
58	MG	1O	203	1/1	0.90	0.12	58,58,58,58	0
58	MG	1A	3606	1/1	0.90	0.14	56,56,56,56	0
58	MG	1O	205	1/1	0.90	0.10	48,48,48,48	0
58	MG	1A	3678	1/1	0.90	0.07	34,34,34,34	0
58	MG	1A	3337	1/1	0.90	0.12	48,48,48,48	0
58	MG	1a	1792	1/1	0.90	0.09	64,64,64,64	0
58	MG	1A	3686	1/1	0.90	0.11	19,19,19,19	0
58	MG	2A	3678	1/1	0.90	0.12	56,56,56,56	0
58	MG	2A	3680	1/1	0.90	0.12	48,48,48,48	0
58	MG	2A	3681	1/1	0.90	0.10	32,32,32,32	0
58	MG	2A	3329	1/1	0.90	0.11	53,53,53,53	0
58	MG	1A	4007	1/1	0.90	0.07	13,13,13,13	0
58	MG	1A	3609	1/1	0.90	0.15	58,58,58,58	0
58	MG	1A	3892	1/1	0.90	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
58	MG	2a	1684	1/1	0.90	0.14	54,54,54,54	0
58	MG	1A	4022	1/1	0.90	0.10	40,40,40,40	0
58	MG	2a	1688	1/1	0.90	0.10	62,62,62,62	0
58	MG	2A	3336	1/1	0.90	0.10	66,66,66,66	0
58	MG	1A	4024	1/1	0.90	0.12	43,43,43,43	0
58	MG	1b	301	1/1	0.90	0.16	66,66,66,66	0
58	MG	2a	1714	1/1	0.90	0.09	66,66,66,66	0
58	MG	2a	1716	1/1	0.90	0.15	53,53,53,53	0
58	MG	2A	3700	1/1	0.90	0.10	41,41,41,41	0
58	MG	11	106	1/1	0.90	0.09	43,43,43,43	0
58	MG	13	106	1/1	0.90	0.09	42,42,42,42	0
58	MG	2A	3351	1/1	0.90	0.12	68,68,68,68	0
58	MG	2a	1727	1/1	0.90	0.12	53,53,53,53	0
58	MG	2a	1732	1/1	0.90	0.19	59,59,59,59	0
58	MG	2A	3710	1/1	0.90	0.18	62,62,62,62	0
58	MG	2A	3712	1/1	0.90	0.15	55,55,55,55	0
58	MG	2a	1740	1/1	0.90	0.23	38,38,38,38	0
58	MG	2a	1744	1/1	0.90	0.36	69,69,69,69	0
58	MG	2a	1746	1/1	0.90	0.12	69,69,69,69	0
58	MG	2A	3355	1/1	0.90	0.12	46,46,46,46	0
58	MG	14	101	1/1	0.90	0.13	58,58,58,58	0
58	MG	1A	3498	1/1	0.90	0.12	37,37,37,37	0
58	MG	1A	3499	1/1	0.90	0.08	41,41,41,41	0
58	MG	2A	3364	1/1	0.90	0.13	52,52,52,52	0
58	MG	2A	3365	1/1	0.90	0.12	55,55,55,55	0
58	MG	2A	3016	1/1	0.90	0.11	60,60,60,60	0
58	MG	1a	1604	1/1	0.90	0.11	54,54,54,54	0
58	MG	2A	3745	1/1	0.90	0.08	44,44,44,44	0
58	MG	1A	3300	1/1	0.90	0.19	51,51,51,51	0
58	MG	2A	3375	1/1	0.90	0.10	64,64,64,64	0
58	MG	2a	1787	1/1	0.90	0.11	59,59,59,59	0
58	MG	1a	1612	1/1	0.90	0.10	51,51,51,51	0
58	MG	2a	1789	1/1	0.90	0.20	66,66,66,66	0
58	MG	2a	1790	1/1	0.90	0.18	67,67,67,67	0
58	MG	1A	3186	1/1	0.90	0.15	62,62,62,62	0
58	MG	1A	3198	1/1	0.90	0.15	42,42,42,42	0
58	MG	2A	3403	1/1	0.90	0.14	49,49,49,49	0
58	MG	2A	3057	1/1	0.90	0.14	65,65,65,65	0
58	MG	1A	3809	1/1	0.90	0.07	13,13,13,13	0
58	MG	2a	1803	1/1	0.90	0.18	58,58,58,58	0
58	MG	1A	3905	1/1	0.90	0.08	21,21,21,21	0
58	MG	2A	3421	1/1	0.90	0.19	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	4049	1/1	0.90	0.09	56,56,56,56	0
58	MG	2A	3088	1/1	0.90	0.15	65,65,65,65	0
58	MG	2A	3795	1/1	0.90	0.10	38,38,38,38	0
58	MG	2A	3444	1/1	0.90	0.21	58,58,58,58	0
58	MG	1A	3208	1/1	0.90	0.10	51,51,51,51	0
58	MG	2a	1819	1/1	0.90	0.16	62,62,62,62	0
58	MG	2A	3448	1/1	0.90	0.12	58,58,58,58	0
58	MG	2A	3100	1/1	0.90	0.17	68,68,68,68	0
58	MG	2a	1822	1/1	0.90	0.16	44,44,44,44	0
58	MG	2A	3453	1/1	0.90	0.15	56,56,56,56	0
58	MG	2a	1831	1/1	0.90	0.14	55,55,55,55	0
58	MG	2A	3471	1/1	0.90	0.18	56,56,56,56	0
58	MG	1A	3546	1/1	0.90	0.15	48,48,48,48	0
58	MG	2A	3810	1/1	0.90	0.16	45,45,45,45	0
58	MG	2A	3811	1/1	0.90	0.14	47,47,47,47	0
58	MG	1A	3924	1/1	0.90	0.12	27,27,27,27	0
58	MG	1A	3458	1/1	0.90	0.13	41,41,41,41	0
58	MG	2A	3483	1/1	0.90	0.14	62,62,62,62	0
58	MG	2A	3487	1/1	0.90	0.08	54,54,54,54	0
58	MG	2t	201	1/1	0.90	0.15	48,48,48,48	0
58	MG	2A	3831	1/1	0.90	0.09	42,42,42,42	0
58	MG	2A	3833	1/1	0.90	0.08	25,25,25,25	0
58	MG	2A	3110	1/1	0.90	0.13	52,52,52,52	0
58	MG	2A	3498	1/1	0.90	0.17	71,71,71,71	0
58	MG	2A	3505	1/1	0.90	0.11	38,38,38,38	0
58	MG	2A	3114	1/1	0.90	0.24	55,55,55,55	0
58	MG	2A	3562	1/1	0.91	0.11	45,45,45,45	0
58	MG	1a	1718	1/1	0.91	0.08	49,49,49,49	0
58	MG	1a	1723	1/1	0.91	0.40	60,60,60,60	0
58	MG	2E	306	1/1	0.91	0.12	54,54,54,54	0
58	MG	1a	1725	1/1	0.91	0.10	42,42,42,42	0
58	MG	1A	3190	1/1	0.91	0.13	47,47,47,47	0
58	MG	2A	3224	1/1	0.91	0.11	52,52,52,52	0
58	MG	2O	201	1/1	0.91	0.13	57,57,57,57	0
58	MG	2A	3583	1/1	0.91	0.12	42,42,42,42	0
58	MG	2A	3225	1/1	0.91	0.08	57,57,57,57	0
58	MG	2T	201	1/1	0.91	0.11	59,59,59,59	0
58	MG	1a	1730	1/1	0.91	0.09	58,58,58,58	0
58	MG	2A	3231	1/1	0.91	0.11	38,38,38,38	0
58	MG	2A	3241	1/1	0.91	0.13	54,54,54,54	0
58	MG	1a	1732	1/1	0.91	0.09	41,41,41,41	0
58	MG	21	101	1/1	0.91	0.23	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3793	1/1	0.91	0.17	53,53,53,53	0
58	MG	1A	3894	1/1	0.91	0.06	33,33,33,33	0
58	MG	27	103	1/1	0.91	0.26	43,43,43,43	0
58	MG	2A	3254	1/1	0.91	0.09	50,50,50,50	0
58	MG	1E	306	1/1	0.91	0.12	53,53,53,53	0
58	MG	1A	3640	1/1	0.91	0.06	28,28,28,28	0
58	MG	1A	3229	1/1	0.91	0.08	42,42,42,42	0
58	MG	1A	4012	1/1	0.91	0.09	57,57,57,57	0
58	MG	2A	3264	1/1	0.91	0.26	59,59,59,59	0
58	MG	1A	3649	1/1	0.91	0.11	38,38,38,38	0
58	MG	1a	1747	1/1	0.91	0.08	46,46,46,46	0
58	MG	1G	205	1/1	0.91	0.18	57,57,57,57	0
58	MG	1N	201	1/1	0.91	0.33	51,51,51,51	0
58	MG	2A	3273	1/1	0.91	0.09	65,65,65,65	0
58	MG	2A	3280	1/1	0.91	0.10	46,46,46,46	0
58	MG	1A	3310	1/1	0.91	0.08	33,33,33,33	0
58	MG	1A	3808	1/1	0.91	0.14	22,22,22,22	0
58	MG	1A	3715	1/1	0.91	0.08	26,26,26,26	0
58	MG	1R	203	1/1	0.91	0.18	47,47,47,47	0
58	MG	2A	3648	1/1	0.91	0.13	36,36,36,36	0
58	MG	2A	3295	1/1	0.91	0.19	52,52,52,52	0
58	MG	2A	3654	1/1	0.91	0.10	43,43,43,43	0
58	MG	1A	3233	1/1	0.91	0.11	40,40,40,40	0
58	MG	2a	1628	1/1	0.91	0.13	64,64,64,64	0
58	MG	1A	3266	1/1	0.91	0.10	34,34,34,34	0
58	MG	2A	3663	1/1	0.91	0.14	50,50,50,50	0
58	MG	2a	1636	1/1	0.91	0.19	73,73,73,73	0
58	MG	1A	3917	1/1	0.91	0.10	37,37,37,37	0
58	MG	2a	1640	1/1	0.91	0.19	50,50,50,50	0
58	MG	1a	1772	1/1	0.91	0.13	68,68,68,68	0
58	MG	1X	106	1/1	0.91	0.08	55,55,55,55	0
58	MG	1Y	201	1/1	0.91	0.10	41,41,41,41	0
58	MG	1A	3360	1/1	0.91	0.08	43,43,43,43	0
58	MG	2A	3673	1/1	0.91	0.11	60,60,60,60	0
58	MG	2A	3319	1/1	0.91	0.12	49,49,49,49	0
58	MG	1A	3363	1/1	0.91	0.19	65,65,65,65	0
58	MG	1A	3824	1/1	0.91	0.10	52,52,52,52	0
58	MG	1A	3124	1/1	0.91	0.22	46,46,46,46	0
58	MG	11	103	1/1	0.91	0.07	33,33,33,33	0
58	MG	2a	1658	1/1	0.91	0.13	61,61,61,61	0
58	MG	1A	4047	1/1	0.91	0.09	25,25,25,25	0
58	MG	1A	4048	1/1	0.91	0.14	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	13	104	1/1	0.91	0.11	51,51,51,51	0
58	MG	2a	1666	1/1	0.91	0.14	65,65,65,65	0
58	MG	2a	1669	1/1	0.91	0.13	53,53,53,53	0
58	MG	1A	3744	1/1	0.91	0.14	70,70,70,70	0
58	MG	1a	1811	1/1	0.91	0.09	61,61,61,61	0
58	MG	1A	4052	1/1	0.91	0.10	26,26,26,26	0
58	MG	1A	3936	1/1	0.91	0.11	51,51,51,51	0
58	MG	1A	3745	1/1	0.91	0.08	53,53,53,53	0
58	MG	1l	202	1/1	0.91	0.20	64,64,64,64	0
58	MG	2A	3352	1/1	0.91	0.14	54,54,54,54	0
58	MG	2A	3708	1/1	0.91	0.12	29,29,29,29	0
58	MG	1v	101	1/1	0.91	0.16	60,60,60,60	0
58	MG	1a	1603	1/1	0.91	0.23	60,60,60,60	0
58	MG	1A	4062	1/1	0.91	0.12	44,44,44,44	0
58	MG	1a	1607	1/1	0.91	0.17	57,57,57,57	0
58	MG	2a	1717	1/1	0.91	0.18	56,56,56,56	0
58	MG	1x	105	1/1	0.91	0.17	53,53,53,53	0
58	MG	1x	107	1/1	0.91	0.15	53,53,53,53	0
58	MG	1A	4063	1/1	0.91	0.06	36,36,36,36	0
58	MG	1x	110	1/1	0.91	0.13	67,67,67,67	0
58	MG	2A	3006	1/1	0.91	0.17	51,51,51,51	0
58	MG	1A	4064	1/1	0.91	0.10	40,40,40,40	0
58	MG	1A	3836	1/1	0.91	0.09	30,30,30,30	0
58	MG	1A	3375	1/1	0.91	0.19	47,47,47,47	0
58	MG	2A	3749	1/1	0.91	0.09	53,53,53,53	0
58	MG	1A	3476	1/1	0.91	0.20	47,47,47,47	0
58	MG	1A	3846	1/1	0.91	0.10	27,27,27,27	0
58	MG	2A	3754	1/1	0.91	0.12	63,63,63,63	0
58	MG	2a	1750	1/1	0.91	0.11	79,79,79,79	0
58	MG	1A	3589	1/1	0.91	0.10	54,54,54,54	0
58	MG	1A	3958	1/1	0.91	0.07	39,39,39,39	0
58	MG	2A	3419	1/1	0.91	0.11	36,36,36,36	0
58	MG	1a	1642	1/1	0.91	0.16	60,60,60,60	0
58	MG	1A	3185	1/1	0.91	0.07	44,44,44,44	0
58	MG	2A	3424	1/1	0.91	0.14	54,54,54,54	0
58	MG	1A	4084	1/1	0.91	0.12	36,36,36,36	0
58	MG	2A	3785	1/1	0.91	0.10	40,40,40,40	0
58	MG	2A	3435	1/1	0.91	0.18	58,58,58,58	0
58	MG	1a	1658	1/1	0.91	0.10	49,49,49,49	0
58	MG	2A	3441	1/1	0.91	0.26	52,52,52,52	0
58	MG	2A	3090	1/1	0.91	0.11	59,59,59,59	0
58	MG	1A	3674	1/1	0.91	0.09	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3447	1/1	0.91	0.19	52,52,52,52	0
58	MG	1a	1663	1/1	0.91	0.24	53,53,53,53	0
58	MG	2A	3801	1/1	0.91	0.13	59,59,59,59	0
58	MG	1A	3497	1/1	0.91	0.13	45,45,45,45	0
58	MG	1A	3972	1/1	0.91	0.12	61,61,61,61	0
58	MG	1a	1671	1/1	0.91	0.12	50,50,50,50	0
58	MG	1A	4099	1/1	0.91	0.09	39,39,39,39	0
58	MG	1A	3080	1/1	0.91	0.11	55,55,55,55	0
58	MG	1A	3332	1/1	0.91	0.12	48,48,48,48	0
58	MG	2A	3116	1/1	0.91	0.10	40,40,40,40	0
58	MG	1A	3984	1/1	0.91	0.08	49,49,49,49	0
58	MG	1a	1681	1/1	0.91	0.12	61,61,61,61	0
58	MG	2A	3136	1/1	0.91	0.09	41,41,41,41	0
58	MG	1A	3525	1/1	0.91	0.13	53,53,53,53	0
58	MG	2A	3507	1/1	0.91	0.13	46,46,46,46	0
58	MG	2A	3510	1/1	0.91	0.17	59,59,59,59	0
58	MG	2A	3151	1/1	0.91	0.17	54,54,54,54	0
58	MG	2A	3162	1/1	0.91	0.12	59,59,59,59	0
58	MG	2A	3166	1/1	0.91	0.13	53,53,53,53	0
58	MG	1B	202	1/1	0.91	0.10	39,39,39,39	0
58	MG	2A	3173	1/1	0.91	0.18	66,66,66,66	0
58	MG	1A	3614	1/1	0.91	0.08	17,17,17,17	0
58	MG	1A	3419	1/1	0.91	0.09	52,52,52,52	0
58	MG	2A	3857	1/1	0.91	0.09	56,56,56,56	0
58	MG	1a	1693	1/1	0.91	0.24	52,52,52,52	0
58	MG	2l	203	1/1	0.91	0.10	60,60,60,60	0
58	MG	2A	3537	1/1	0.91	0.14	49,49,49,49	0
58	MG	2A	3865	1/1	0.91	0.10	64,64,64,64	0
58	MG	1A	3424	1/1	0.91	0.07	44,44,44,44	0
58	MG	1A	3695	1/1	0.91	0.07	31,31,31,31	0
58	MG	1A	3297	1/1	0.91	0.09	47,47,47,47	0
58	MG	2A	3197	1/1	0.91	0.11	48,48,48,48	0
58	MG	1A	3698	1/1	0.91	0.08	26,26,26,26	0
58	MG	1a	1711	1/1	0.91	0.14	50,50,50,50	0
58	MG	2A	3204	1/1	0.91	0.09	48,48,48,48	0
58	MG	1a	1713	1/1	0.91	0.24	57,57,57,57	0
58	MG	2A	3044	1/1	0.92	0.28	46,46,46,46	0
58	MG	1a	1635	1/1	0.92	0.11	48,48,48,48	0
58	MG	2A	3384	1/1	0.92	0.08	46,46,46,46	0
58	MG	2A	3046	1/1	0.92	0.08	48,48,48,48	0
58	MG	2A	3393	1/1	0.92	0.09	52,52,52,52	0
58	MG	1A	3117	1/1	0.92	0.10	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3398	1/1	0.92	0.10	51,51,51,51	0
58	MG	2A	3399	1/1	0.92	0.13	57,57,57,57	0
58	MG	2A	3056	1/1	0.92	0.15	60,60,60,60	0
58	MG	2A	3402	1/1	0.92	0.07	51,51,51,51	0
58	MG	1A	3379	1/1	0.92	0.09	29,29,29,29	0
58	MG	2A	3062	1/1	0.92	0.08	42,42,42,42	0
58	MG	2A	3813	1/1	0.92	0.12	53,53,53,53	0
58	MG	2A	3816	1/1	0.92	0.08	49,49,49,49	0
58	MG	2A	3409	1/1	0.92	0.07	58,58,58,58	0
58	MG	1A	3923	1/1	0.92	0.11	33,33,33,33	0
58	MG	2A	3414	1/1	0.92	0.13	59,59,59,59	0
58	MG	2A	3065	1/1	0.92	0.18	57,57,57,57	0
58	MG	1A	3063	1/1	0.92	0.17	49,49,49,49	0
58	MG	2A	3067	1/1	0.92	0.18	62,62,62,62	0
58	MG	2A	3422	1/1	0.92	0.15	35,35,35,35	0
58	MG	2A	3842	1/1	0.92	0.07	49,49,49,49	0
58	MG	2A	3423	1/1	0.92	0.14	37,37,37,37	0
58	MG	1A	3326	1/1	0.92	0.08	39,39,39,39	0
58	MG	1a	1655	1/1	0.92	0.10	39,39,39,39	0
58	MG	1A	3616	1/1	0.92	0.07	35,35,35,35	0
58	MG	2A	3851	1/1	0.92	0.13	53,53,53,53	0
58	MG	1A	3399	1/1	0.92	0.10	52,52,52,52	0
58	MG	1A	3813	1/1	0.92	0.07	43,43,43,43	0
58	MG	2A	3101	1/1	0.92	0.17	61,61,61,61	0
58	MG	1A	3500	1/1	0.92	0.17	48,48,48,48	0
58	MG	1A	3941	1/1	0.92	0.09	41,41,41,41	0
58	MG	1A	3944	1/1	0.92	0.07	52,52,52,52	0
58	MG	1A	3817	1/1	0.92	0.06	35,35,35,35	0
58	MG	2A	3112	1/1	0.92	0.09	47,47,47,47	0
58	MG	1a	1674	1/1	0.92	0.17	64,64,64,64	0
58	MG	1A	3506	1/1	0.92	0.10	32,32,32,32	0
58	MG	2A	3474	1/1	0.92	0.18	53,53,53,53	0
58	MG	2B	212	1/1	0.92	0.21	61,61,61,61	0
58	MG	1A	4091	1/1	0.92	0.16	46,46,46,46	0
58	MG	1A	3711	1/1	0.92	0.07	38,38,38,38	0
58	MG	2A	3118	1/1	0.92	0.08	45,45,45,45	0
58	MG	1A	3712	1/1	0.92	0.10	28,28,28,28	0
58	MG	2A	3127	1/1	0.92	0.06	30,30,30,30	0
58	MG	1A	4097	1/1	0.92	0.08	39,39,39,39	0
58	MG	2A	3137	1/1	0.92	0.11	31,31,31,31	0
58	MG	1A	3631	1/1	0.92	0.10	50,50,50,50	0
58	MG	1a	1690	1/1	0.92	0.27	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3152	1/1	0.92	0.18	54,54,54,54	0
58	MG	2A	3155	1/1	0.92	0.08	45,45,45,45	0
58	MG	1A	3508	1/1	0.92	0.06	44,44,44,44	0
58	MG	2R	201	1/1	0.92	0.14	60,60,60,60	0
58	MG	2A	3516	1/1	0.92	0.14	52,52,52,52	0
58	MG	1A	3719	1/1	0.92	0.11	31,31,31,31	0
58	MG	2A	3169	1/1	0.92	0.10	61,61,61,61	0
58	MG	2A	3526	1/1	0.92	0.08	49,49,49,49	0
58	MG	2W	201	1/1	0.92	0.11	59,59,59,59	0
58	MG	2W	202	1/1	0.92	0.13	47,47,47,47	0
58	MG	2Z	301	1/1	0.92	0.11	62,62,62,62	0
58	MG	1A	3960	1/1	0.92	0.08	58,58,58,58	0
58	MG	1A	3963	1/1	0.92	0.07	43,43,43,43	0
58	MG	1A	3327	1/1	0.92	0.14	31,31,31,31	0
58	MG	2A	3533	1/1	0.92	0.09	36,36,36,36	0
58	MG	2A	3536	1/1	0.92	0.09	45,45,45,45	0
58	MG	27	102	1/1	0.92	0.11	48,48,48,48	0
58	MG	2A	3178	1/1	0.92	0.12	44,44,44,44	0
58	MG	2A	3179	1/1	0.92	0.21	63,63,63,63	0
58	MG	1A	3129	1/1	0.92	0.06	45,45,45,45	0
58	MG	1A	3970	1/1	0.92	0.07	41,41,41,41	0
58	MG	1B	219	1/1	0.92	0.09	38,38,38,38	0
58	MG	1A	3971	1/1	0.92	0.07	28,28,28,28	0
58	MG	2A	3192	1/1	0.92	0.10	51,51,51,51	0
58	MG	2A	3193	1/1	0.92	0.11	46,46,46,46	0
58	MG	1A	3724	1/1	0.92	0.08	55,55,55,55	0
58	MG	1A	3648	1/1	0.92	0.09	40,40,40,40	0
58	MG	2A	3198	1/1	0.92	0.13	56,56,56,56	0
58	MG	1a	1724	1/1	0.92	0.25	53,53,53,53	0
58	MG	2A	3572	1/1	0.92	0.10	37,37,37,37	0
58	MG	1A	3423	1/1	0.92	0.10	43,43,43,43	0
58	MG	1a	1726	1/1	0.92	0.23	55,55,55,55	0
58	MG	2A	3578	1/1	0.92	0.07	39,39,39,39	0
58	MG	1A	3980	1/1	0.92	0.10	52,52,52,52	0
58	MG	1A	3289	1/1	0.92	0.07	33,33,33,33	0
58	MG	2A	3210	1/1	0.92	0.11	51,51,51,51	0
58	MG	2A	3586	1/1	0.92	0.08	27,27,27,27	0
58	MG	1A	3539	1/1	0.92	0.14	50,50,50,50	0
58	MG	2A	3590	1/1	0.92	0.14	51,51,51,51	0
58	MG	2A	3591	1/1	0.92	0.09	38,38,38,38	0
58	MG	2a	1633	1/1	0.92	0.26	54,54,54,54	0
58	MG	2A	3214	1/1	0.92	0.10	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3434	1/1	0.92	0.09	45,45,45,45	0
58	MG	1A	3860	1/1	0.92	0.10	49,49,49,49	0
58	MG	2A	3220	1/1	0.92	0.09	40,40,40,40	0
58	MG	2A	3222	1/1	0.92	0.19	50,50,50,50	0
58	MG	2A	3223	1/1	0.92	0.26	51,51,51,51	0
58	MG	1A	3993	1/1	0.92	0.16	36,36,36,36	0
58	MG	1A	3295	1/1	0.92	0.10	40,40,40,40	0
58	MG	2A	3228	1/1	0.92	0.10	47,47,47,47	0
58	MG	1A	3997	1/1	0.92	0.08	20,20,20,20	0
58	MG	2A	3613	1/1	0.92	0.10	37,37,37,37	0
58	MG	2A	3617	1/1	0.92	0.07	31,31,31,31	0
58	MG	1A	3866	1/1	0.92	0.08	47,47,47,47	0
58	MG	2A	3238	1/1	0.92	0.14	64,64,64,64	0
58	MG	1A	3099	1/1	0.92	0.10	43,43,43,43	0
58	MG	1O	201	1/1	0.92	0.09	58,58,58,58	0
58	MG	2A	3624	1/1	0.92	0.14	56,56,56,56	0
58	MG	2A	3625	1/1	0.92	0.08	36,36,36,36	0
58	MG	2A	3247	1/1	0.92	0.12	44,44,44,44	0
58	MG	1A	3443	1/1	0.92	0.08	52,52,52,52	0
58	MG	2a	1673	1/1	0.92	0.16	55,55,55,55	0
58	MG	1A	3662	1/1	0.92	0.13	48,48,48,48	0
58	MG	2A	3634	1/1	0.92	0.06	25,25,25,25	0
58	MG	1A	3876	1/1	0.92	0.09	45,45,45,45	0
58	MG	1A	3762	1/1	0.92	0.08	51,51,51,51	0
58	MG	2A	3640	1/1	0.92	0.09	30,30,30,30	0
58	MG	1T	201	1/1	0.92	0.07	39,39,39,39	0
58	MG	1T	203	1/1	0.92	0.12	42,42,42,42	0
58	MG	1A	3444	1/1	0.92	0.11	39,39,39,39	0
58	MG	2a	1699	1/1	0.92	0.13	52,52,52,52	0
58	MG	2a	1705	1/1	0.92	0.18	56,56,56,56	0
58	MG	1a	1768	1/1	0.92	0.10	46,46,46,46	0
58	MG	1A	3100	1/1	0.92	0.10	55,55,55,55	0
58	MG	1A	4009	1/1	0.92	0.09	18,18,18,18	0
58	MG	2A	3267	1/1	0.92	0.16	46,46,46,46	0
58	MG	2A	3662	1/1	0.92	0.10	62,62,62,62	0
58	MG	1W	202	1/1	0.92	0.09	45,45,45,45	0
58	MG	1A	4010	1/1	0.92	0.05	28,28,28,28	0
58	MG	1a	1779	1/1	0.92	0.09	56,56,56,56	0
58	MG	2a	1724	1/1	0.92	0.16	45,45,45,45	0
58	MG	2A	3277	1/1	0.92	0.20	56,56,56,56	0
58	MG	2A	3668	1/1	0.92	0.11	52,52,52,52	0
58	MG	2A	3669	1/1	0.92	0.09	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3885	1/1	0.92	0.11	24,24,24,24	0
58	MG	1A	4014	1/1	0.92	0.10	37,37,37,37	0
58	MG	2A	3286	1/1	0.92	0.11	49,49,49,49	0
58	MG	1A	3205	1/1	0.92	0.11	43,43,43,43	0
58	MG	2A	3676	1/1	0.92	0.13	45,45,45,45	0
58	MG	2a	1747	1/1	0.92	0.12	60,60,60,60	0
58	MG	1A	3306	1/1	0.92	0.11	34,34,34,34	0
58	MG	2A	3290	1/1	0.92	0.09	53,53,53,53	0
58	MG	2A	3291	1/1	0.92	0.08	58,58,58,58	0
58	MG	1A	3568	1/1	0.92	0.11	37,37,37,37	0
58	MG	1A	3893	1/1	0.92	0.09	31,31,31,31	0
58	MG	1A	4025	1/1	0.92	0.09	49,49,49,49	0
58	MG	1A	3256	1/1	0.92	0.14	39,39,39,39	0
58	MG	1A	3171	1/1	0.92	0.13	44,44,44,44	0
58	MG	1A	3361	1/1	0.92	0.09	56,56,56,56	0
58	MG	1A	3592	1/1	0.92	0.13	55,55,55,55	0
58	MG	2a	1781	1/1	0.92	0.12	49,49,49,49	0
58	MG	2A	3694	1/1	0.92	0.09	47,47,47,47	0
58	MG	1a	1812	1/1	0.92	0.20	58,58,58,58	0
58	MG	2a	1785	1/1	0.92	0.21	63,63,63,63	0
58	MG	2A	3314	1/1	0.92	0.17	37,37,37,37	0
58	MG	1A	4040	1/1	0.92	0.06	38,38,38,38	0
58	MG	2A	3317	1/1	0.92	0.11	50,50,50,50	0
58	MG	1A	3682	1/1	0.92	0.09	37,37,37,37	0
58	MG	2a	1791	1/1	0.92	0.14	63,63,63,63	0
58	MG	2a	1792	1/1	0.92	0.15	49,49,49,49	0
58	MG	1a	1601	1/1	0.92	0.11	48,48,48,48	0
58	MG	2A	3322	1/1	0.92	0.16	62,62,62,62	0
58	MG	2A	3711	1/1	0.92	0.14	59,59,59,59	0
58	MG	2a	1799	1/1	0.92	0.12	61,61,61,61	0
58	MG	2A	3323	1/1	0.92	0.12	57,57,57,57	0
58	MG	1a	1602	1/1	0.92	0.17	56,56,56,56	0
58	MG	1n	101	1/1	0.92	0.23	58,58,58,58	0
58	MG	2A	3719	1/1	0.92	0.09	44,44,44,44	0
58	MG	1A	4043	1/1	0.92	0.07	40,40,40,40	0
58	MG	2A	3721	1/1	0.92	0.12	58,58,58,58	0
58	MG	1A	3016	1/1	0.92	0.14	49,49,49,49	0
58	MG	1w	105	1/1	0.92	0.23	59,59,59,59	0
58	MG	2A	3732	1/1	0.92	0.09	49,49,49,49	0
58	MG	1w	107	1/1	0.92	0.08	57,57,57,57	0
58	MG	2A	3737	1/1	0.92	0.13	57,57,57,57	0
58	MG	1A	3688	1/1	0.92	0.06	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3742	1/1	0.92	0.15	46,46,46,46	0
58	MG	1A	3599	1/1	0.92	0.11	31,31,31,31	0
58	MG	1A	3909	1/1	0.92	0.10	40,40,40,40	0
58	MG	2a	1826	1/1	0.92	0.19	58,58,58,58	0
58	MG	2a	1827	1/1	0.92	0.13	49,49,49,49	0
58	MG	2A	3747	1/1	0.92	0.07	60,60,60,60	0
58	MG	1x	106	1/1	0.92	0.21	54,54,54,54	0
58	MG	2d	301	1/1	0.92	0.21	48,48,48,48	0
58	MG	2A	3344	1/1	0.92	0.07	51,51,51,51	0
58	MG	2f	202	1/1	0.92	0.13	58,58,58,58	0
58	MG	2A	3346	1/1	0.92	0.13	57,57,57,57	0
58	MG	2i	201	1/1	0.92	0.11	52,52,52,52	0
58	MG	1a	1613	1/1	0.92	0.09	62,62,62,62	0
58	MG	1a	1617	1/1	0.92	0.13	40,40,40,40	0
58	MG	1a	1620	1/1	0.92	0.09	46,46,46,46	0
58	MG	2A	3354	1/1	0.92	0.09	59,59,59,59	0
58	MG	2A	3001	1/1	0.92	0.14	45,45,45,45	0
58	MG	2p	101	1/1	0.92	0.09	58,58,58,58	0
58	MG	2q	201	1/1	0.92	0.09	63,63,63,63	0
58	MG	1A	3224	1/1	0.92	0.08	43,43,43,43	0
58	MG	1A	3912	1/1	0.92	0.08	28,28,28,28	0
58	MG	2A	3770	1/1	0.92	0.08	49,49,49,49	0
58	MG	1a	1627	1/1	0.92	0.18	51,51,51,51	0
58	MG	2A	3031	1/1	0.92	0.09	51,51,51,51	0
58	MG	1A	3914	1/1	0.92	0.10	41,41,41,41	0
58	MG	1A	4054	1/1	0.92	0.08	30,30,30,30	0
58	MG	2x	104	1/1	0.92	0.17	49,49,49,49	0
58	MG	2x	106	1/1	0.92	0.11	49,49,49,49	0
58	MG	2A	3043	1/1	0.92	0.15	61,61,61,61	0
58	MG	2A	3160	1/1	0.93	0.12	55,55,55,55	0
58	MG	1A	3870	1/1	0.93	0.09	41,41,41,41	0
58	MG	2A	3165	1/1	0.93	0.29	55,55,55,55	0
58	MG	1a	1722	1/1	0.93	0.19	59,59,59,59	0
58	MG	1A	3994	1/1	0.93	0.10	21,21,21,21	0
58	MG	2A	3815	1/1	0.93	0.07	31,31,31,31	0
58	MG	1A	3543	1/1	0.93	0.12	43,43,43,43	0
58	MG	2A	3451	1/1	0.93	0.19	51,51,51,51	0
58	MG	2A	3818	1/1	0.93	0.09	33,33,33,33	0
58	MG	1A	3996	1/1	0.93	0.10	30,30,30,30	0
58	MG	2A	3825	1/1	0.93	0.11	55,55,55,55	0
58	MG	2A	3455	1/1	0.93	0.20	47,47,47,47	0
58	MG	2A	3459	1/1	0.93	0.12	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3463	1/1	0.93	0.16	35,35,35,35	0
58	MG	2A	3468	1/1	0.93	0.20	58,58,58,58	0
58	MG	2A	3174	1/1	0.93	0.15	48,48,48,48	0
58	MG	1A	3433	1/1	0.93	0.06	36,36,36,36	0
58	MG	2A	3473	1/1	0.93	0.11	52,52,52,52	0
58	MG	1E	312	1/1	0.93	0.12	35,35,35,35	0
58	MG	2A	3845	1/1	0.93	0.07	36,36,36,36	0
58	MG	1F	309	1/1	0.93	0.10	22,22,22,22	0
58	MG	1A	3875	1/1	0.93	0.07	39,39,39,39	0
58	MG	2A	3850	1/1	0.93	0.08	49,49,49,49	0
58	MG	2A	3186	1/1	0.93	0.09	44,44,44,44	0
58	MG	1A	3753	1/1	0.93	0.07	15,15,15,15	0
58	MG	2A	3489	1/1	0.93	0.13	55,55,55,55	0
58	MG	1A	3758	1/1	0.93	0.09	55,55,55,55	0
58	MG	2A	3494	1/1	0.93	0.07	40,40,40,40	0
58	MG	2A	3861	1/1	0.93	0.08	50,50,50,50	0
58	MG	2A	3862	1/1	0.93	0.12	44,44,44,44	0
58	MG	1A	3879	1/1	0.93	0.13	30,30,30,30	0
58	MG	1A	3880	1/1	0.93	0.10	48,48,48,48	0
58	MG	1A	3011	1/1	0.93	0.08	37,37,37,37	0
58	MG	2A	3509	1/1	0.93	0.17	54,54,54,54	0
58	MG	1A	3666	1/1	0.93	0.06	34,34,34,34	0
58	MG	2B	201	1/1	0.93	0.15	60,60,60,60	0
58	MG	2B	205	1/1	0.93	0.13	53,53,53,53	0
58	MG	1A	3769	1/1	0.93	0.13	34,34,34,34	0
58	MG	2B	207	1/1	0.93	0.09	51,51,51,51	0
58	MG	1a	1746	1/1	0.93	0.07	49,49,49,49	0
58	MG	2A	3200	1/1	0.93	0.09	50,50,50,50	0
58	MG	1A	3333	1/1	0.93	0.12	37,37,37,37	0
58	MG	1A	3203	1/1	0.93	0.09	36,36,36,36	0
58	MG	2B	218	1/1	0.93	0.14	56,56,56,56	0
58	MG	1A	3017	1/1	0.93	0.15	46,46,46,46	0
58	MG	2D	306	1/1	0.93	0.12	48,48,48,48	0
58	MG	1A	3339	1/1	0.93	0.10	41,41,41,41	0
58	MG	1a	1760	1/1	0.93	0.10	64,64,64,64	0
58	MG	1A	3776	1/1	0.93	0.06	25,25,25,25	0
58	MG	1A	3027	1/1	0.93	0.12	56,56,56,56	0
58	MG	2E	307	1/1	0.93	0.10	46,46,46,46	0
58	MG	1A	3302	1/1	0.93	0.08	30,30,30,30	0
58	MG	2A	3535	1/1	0.93	0.05	28,28,28,28	0
58	MG	2F	304	1/1	0.93	0.06	47,47,47,47	0
58	MG	1A	4023	1/1	0.93	0.06	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3779	1/1	0.93	0.07	33,33,33,33	0
58	MG	1A	3095	1/1	0.93	0.09	55,55,55,55	0
58	MG	2A	3221	1/1	0.93	0.08	40,40,40,40	0
58	MG	1A	4026	1/1	0.93	0.07	57,57,57,57	0
58	MG	1A	4029	1/1	0.93	0.07	35,35,35,35	0
58	MG	1A	3680	1/1	0.93	0.10	35,35,35,35	0
58	MG	2T	203	1/1	0.93	0.07	47,47,47,47	0
58	MG	10	107	1/1	0.93	0.07	37,37,37,37	0
58	MG	2A	3227	1/1	0.93	0.14	54,54,54,54	0
58	MG	11	101	1/1	0.93	0.23	34,34,34,34	0
58	MG	1a	1782	1/1	0.93	0.09	64,64,64,64	0
58	MG	1A	4031	1/1	0.93	0.08	55,55,55,55	0
58	MG	2A	3235	1/1	0.93	0.18	49,49,49,49	0
58	MG	20	103	1/1	0.93	0.08	46,46,46,46	0
58	MG	2A	3569	1/1	0.93	0.06	36,36,36,36	0
58	MG	1A	3354	1/1	0.93	0.10	46,46,46,46	0
58	MG	25	102	1/1	0.93	0.10	48,48,48,48	0
58	MG	25	104	1/1	0.93	0.09	48,48,48,48	0
58	MG	25	105	1/1	0.93	0.07	45,45,45,45	0
58	MG	11	105	1/1	0.93	0.07	57,57,57,57	0
58	MG	1a	1791	1/1	0.93	0.07	39,39,39,39	0
58	MG	2A	3577	1/1	0.93	0.08	43,43,43,43	0
58	MG	2A	3246	1/1	0.93	0.11	56,56,56,56	0
58	MG	1A	3586	1/1	0.93	0.11	20,20,20,20	0
58	MG	2a	1603	1/1	0.93	0.12	56,56,56,56	0
58	MG	2A	3581	1/1	0.93	0.11	38,38,38,38	0
58	MG	1a	1799	1/1	0.93	0.08	59,59,59,59	0
58	MG	1A	3261	1/1	0.93	0.09	36,36,36,36	0
58	MG	1a	1803	1/1	0.93	0.08	57,57,57,57	0
58	MG	2A	3255	1/1	0.93	0.16	57,57,57,57	0
58	MG	1A	3309	1/1	0.93	0.25	54,54,54,54	0
58	MG	1A	3262	1/1	0.93	0.07	32,32,32,32	0
58	MG	15	107	1/1	0.93	0.08	41,41,41,41	0
58	MG	1A	3691	1/1	0.93	0.10	54,54,54,54	0
58	MG	1A	4044	1/1	0.93	0.07	43,43,43,43	0
58	MG	2A	3597	1/1	0.93	0.18	51,51,51,51	0
58	MG	1A	3692	1/1	0.93	0.07	24,24,24,24	0
58	MG	1A	3918	1/1	0.93	0.07	42,42,42,42	0
58	MG	1A	3467	1/1	0.93	0.11	51,51,51,51	0
58	MG	2A	3268	1/1	0.93	0.17	55,55,55,55	0
58	MG	1A	3469	1/1	0.93	0.08	45,45,45,45	0
58	MG	1A	3810	1/1	0.93	0.10	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1a	1609	1/1	0.93	0.16	44,44,44,44	0
58	MG	2A	3274	1/1	0.93	0.11	52,52,52,52	0
58	MG	2a	1629	1/1	0.93	0.10	48,48,48,48	0
58	MG	2a	1630	1/1	0.93	0.17	57,57,57,57	0
58	MG	2a	1631	1/1	0.93	0.09	44,44,44,44	0
58	MG	2A	3275	1/1	0.93	0.07	65,65,65,65	0
58	MG	1t	201	1/1	0.93	0.17	46,46,46,46	0
58	MG	2a	1634	1/1	0.93	0.08	57,57,57,57	0
58	MG	1A	3264	1/1	0.93	0.11	53,53,53,53	0
58	MG	1A	3930	1/1	0.93	0.17	47,47,47,47	0
58	MG	2A	3622	1/1	0.93	0.07	39,39,39,39	0
58	MG	2a	1638	1/1	0.93	0.13	45,45,45,45	0
58	MG	1A	3368	1/1	0.93	0.10	45,45,45,45	0
58	MG	1a	1614	1/1	0.93	0.15	52,52,52,52	0
58	MG	1a	1616	1/1	0.93	0.11	54,54,54,54	0
58	MG	1x	103	1/1	0.93	0.18	54,54,54,54	0
58	MG	2A	3628	1/1	0.93	0.06	38,38,38,38	0
58	MG	1A	3477	1/1	0.93	0.08	41,41,41,41	0
58	MG	1A	4060	1/1	0.93	0.06	9,9,9,9	0
58	MG	1a	1622	1/1	0.93	0.25	63,63,63,63	0
58	MG	2a	1650	1/1	0.93	0.23	55,55,55,55	0
58	MG	1A	4061	1/1	0.93	0.18	57,57,57,57	0
58	MG	1A	3481	1/1	0.93	0.07	35,35,35,35	0
58	MG	2A	3299	1/1	0.93	0.12	38,38,38,38	0
58	MG	2A	3642	1/1	0.93	0.07	42,42,42,42	0
58	MG	1A	3615	1/1	0.93	0.07	23,23,23,23	0
58	MG	1A	3128	1/1	0.93	0.15	33,33,33,33	0
58	MG	2A	3002	1/1	0.93	0.18	52,52,52,52	0
58	MG	2a	1665	1/1	0.93	0.19	55,55,55,55	0
58	MG	2A	3649	1/1	0.93	0.08	43,43,43,43	0
58	MG	2a	1667	1/1	0.93	0.11	55,55,55,55	0
58	MG	2A	3307	1/1	0.93	0.09	49,49,49,49	0
58	MG	2A	3651	1/1	0.93	0.09	49,49,49,49	0
58	MG	2A	3652	1/1	0.93	0.13	59,59,59,59	0
58	MG	2a	1677	1/1	0.93	0.11	41,41,41,41	0
58	MG	2A	3004	1/1	0.93	0.16	48,48,48,48	0
58	MG	2A	3313	1/1	0.93	0.11	46,46,46,46	0
58	MG	2A	3656	1/1	0.93	0.10	51,51,51,51	0
58	MG	2A	3658	1/1	0.93	0.09	46,46,46,46	0
58	MG	1A	3943	1/1	0.93	0.08	54,54,54,54	0
58	MG	2A	3661	1/1	0.93	0.16	51,51,51,51	0
58	MG	2A	3008	1/1	0.93	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1691	1/1	0.93	0.14	64,64,64,64	0
58	MG	2a	1695	1/1	0.93	0.12	61,61,61,61	0
58	MG	2a	1698	1/1	0.93	0.10	60,60,60,60	0
58	MG	1A	3821	1/1	0.93	0.13	37,37,37,37	0
58	MG	2a	1702	1/1	0.93	0.20	53,53,53,53	0
58	MG	1A	3313	1/1	0.93	0.11	40,40,40,40	0
58	MG	1a	1639	1/1	0.93	0.17	50,50,50,50	0
58	MG	2a	1709	1/1	0.93	0.11	54,54,54,54	0
58	MG	2A	3033	1/1	0.93	0.09	32,32,32,32	0
58	MG	2A	3039	1/1	0.93	0.09	48,48,48,48	0
58	MG	1A	3040	1/1	0.93	0.16	47,47,47,47	0
58	MG	1A	3828	1/1	0.93	0.10	43,43,43,43	0
58	MG	1A	3315	1/1	0.93	0.14	49,49,49,49	0
58	MG	2A	3331	1/1	0.93	0.14	46,46,46,46	0
58	MG	2a	1721	1/1	0.93	0.11	59,59,59,59	0
58	MG	1a	1647	1/1	0.93	0.09	47,47,47,47	0
58	MG	2a	1723	1/1	0.93	0.20	61,61,61,61	0
58	MG	1A	3626	1/1	0.93	0.10	23,23,23,23	0
58	MG	1A	3137	1/1	0.93	0.11	48,48,48,48	0
58	MG	2A	3047	1/1	0.93	0.21	51,51,51,51	0
58	MG	2a	1728	1/1	0.93	0.08	49,49,49,49	0
58	MG	1A	3325	1/1	0.93	0.08	46,46,46,46	0
58	MG	2a	1733	1/1	0.93	0.13	42,42,42,42	0
58	MG	2a	1734	1/1	0.93	0.13	53,53,53,53	0
58	MG	2a	1735	1/1	0.93	0.17	47,47,47,47	0
58	MG	2A	3340	1/1	0.93	0.09	45,45,45,45	0
58	MG	1a	1660	1/1	0.93	0.08	44,44,44,44	0
58	MG	1A	3639	1/1	0.93	0.10	56,56,56,56	0
58	MG	2a	1741	1/1	0.93	0.07	52,52,52,52	0
58	MG	2A	3060	1/1	0.93	0.11	42,42,42,42	0
58	MG	2A	3345	1/1	0.93	0.10	57,57,57,57	0
58	MG	1A	4094	1/1	0.93	0.09	38,38,38,38	0
58	MG	2A	3692	1/1	0.93	0.19	51,51,51,51	0
58	MG	1a	1664	1/1	0.93	0.10	47,47,47,47	0
58	MG	2A	3064	1/1	0.93	0.11	60,60,60,60	0
58	MG	2A	3695	1/1	0.93	0.12	30,30,30,30	0
58	MG	1A	3406	1/1	0.93	0.06	37,37,37,37	0
58	MG	1a	1667	1/1	0.93	0.20	58,58,58,58	0
58	MG	2A	3703	1/1	0.93	0.14	53,53,53,53	0
58	MG	1A	3848	1/1	0.93	0.08	47,47,47,47	0
58	MG	2A	3356	1/1	0.93	0.24	54,54,54,54	0
58	MG	2A	3707	1/1	0.93	0.15	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1779	1/1	0.93	0.10	40,40,40,40	0
58	MG	2A	3070	1/1	0.93	0.11	49,49,49,49	0
58	MG	1A	3517	1/1	0.93	0.09	46,46,46,46	0
58	MG	2A	3361	1/1	0.93	0.21	54,54,54,54	0
58	MG	2A	3082	1/1	0.93	0.12	51,51,51,51	0
58	MG	1A	3150	1/1	0.93	0.26	35,35,35,35	0
58	MG	2A	3715	1/1	0.93	0.09	32,32,32,32	0
58	MG	1A	3526	1/1	0.93	0.11	39,39,39,39	0
58	MG	1A	4103	1/1	0.93	0.22	51,51,51,51	0
58	MG	2A	3096	1/1	0.93	0.12	48,48,48,48	0
58	MG	2A	3372	1/1	0.93	0.20	49,49,49,49	0
58	MG	1A	3735	1/1	0.93	0.09	39,39,39,39	0
58	MG	2A	3723	1/1	0.93	0.07	43,43,43,43	0
58	MG	1A	4105	1/1	0.93	0.07	42,42,42,42	0
58	MG	2A	3727	1/1	0.93	0.17	71,71,71,71	0
58	MG	2A	3379	1/1	0.93	0.21	55,55,55,55	0
58	MG	1A	4106	1/1	0.93	0.09	40,40,40,40	0
58	MG	2A	3385	1/1	0.93	0.19	45,45,45,45	0
58	MG	1A	3974	1/1	0.93	0.06	41,41,41,41	0
58	MG	2A	3389	1/1	0.93	0.15	55,55,55,55	0
58	MG	2a	1810	1/1	0.93	0.21	50,50,50,50	0
58	MG	2A	3391	1/1	0.93	0.13	48,48,48,48	0
58	MG	2A	3107	1/1	0.93	0.14	52,52,52,52	0
58	MG	1a	1683	1/1	0.93	0.09	55,55,55,55	0
58	MG	1A	3272	1/1	0.93	0.07	45,45,45,45	0
58	MG	1a	1687	1/1	0.93	0.24	58,58,58,58	0
58	MG	2A	3400	1/1	0.93	0.14	43,43,43,43	0
58	MG	1a	1688	1/1	0.93	0.09	51,51,51,51	0
58	MG	2A	3753	1/1	0.93	0.14	58,58,58,58	0
58	MG	1A	3328	1/1	0.93	0.08	35,35,35,35	0
58	MG	1A	3864	1/1	0.93	0.13	34,34,34,34	0
58	MG	2A	3756	1/1	0.93	0.11	45,45,45,45	0
58	MG	1A	3196	1/1	0.93	0.13	24,24,24,24	0
58	MG	2a	1828	1/1	0.93	0.21	58,58,58,58	0
58	MG	2a	1829	1/1	0.93	0.11	46,46,46,46	0
58	MG	1A	3427	1/1	0.93	0.12	51,51,51,51	0
58	MG	1A	3986	1/1	0.93	0.07	60,60,60,60	0
58	MG	2A	3763	1/1	0.93	0.12	40,40,40,40	0
58	MG	2A	3412	1/1	0.93	0.14	39,39,39,39	0
58	MG	2A	3766	1/1	0.93	0.09	51,51,51,51	0
58	MG	2A	3413	1/1	0.93	0.09	54,54,54,54	0
58	MG	1A	3987	1/1	0.93	0.07	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1a	1696	1/1	0.93	0.10	44,44,44,44	0
58	MG	2l	201	1/1	0.93	0.12	53,53,53,53	0
58	MG	2A	3783	1/1	0.93	0.11	61,61,61,61	0
58	MG	1A	3989	1/1	0.93	0.07	51,51,51,51	0
58	MG	2A	3141	1/1	0.93	0.19	50,50,50,50	0
58	MG	1A	3430	1/1	0.93	0.07	36,36,36,36	0
58	MG	2A	3791	1/1	0.93	0.11	57,57,57,57	0
58	MG	1a	1703	1/1	0.93	0.08	57,57,57,57	0
58	MG	2A	3793	1/1	0.93	0.09	58,58,58,58	0
58	MG	1A	3868	1/1	0.93	0.07	19,19,19,19	0
58	MG	2A	3429	1/1	0.93	0.13	30,30,30,30	0
58	MG	2A	3154	1/1	0.93	0.10	54,54,54,54	0
58	MG	1B	237	1/1	0.93	0.08	33,33,33,33	0
58	MG	2w	102	1/1	0.93	0.16	54,54,54,54	0
58	MG	2A	3436	1/1	0.93	0.15	48,48,48,48	0
58	MG	2A	3802	1/1	0.93	0.07	64,64,64,64	0
58	MG	2x	103	1/1	0.93	0.18	53,53,53,53	0
58	MG	2A	3158	1/1	0.93	0.10	64,64,64,64	0
58	MG	2A	3439	1/1	0.93	0.17	45,45,45,45	0
58	MG	2A	3440	1/1	0.93	0.14	53,53,53,53	0
58	MG	1A	3590	1/1	0.94	0.09	36,36,36,36	0
58	MG	1A	3412	1/1	0.94	0.10	43,43,43,43	0
58	MG	2A	3860	1/1	0.94	0.07	42,42,42,42	0
58	MG	2A	3518	1/1	0.94	0.06	25,25,25,25	0
58	MG	2A	3520	1/1	0.94	0.09	16,16,16,16	0
58	MG	1A	3478	1/1	0.94	0.16	42,42,42,42	0
58	MG	1a	1789	1/1	0.94	0.07	40,40,40,40	0
58	MG	1A	4042	1/1	0.94	0.10	39,39,39,39	0
58	MG	1A	3921	1/1	0.94	0.08	45,45,45,45	0
58	MG	1A	3479	1/1	0.94	0.11	51,51,51,51	0
58	MG	1a	1793	1/1	0.94	0.08	54,54,54,54	0
58	MG	1a	1795	1/1	0.94	0.07	64,64,64,64	0
58	MG	1A	3480	1/1	0.94	0.10	45,45,45,45	0
58	MG	1A	3413	1/1	0.94	0.07	37,37,37,37	0
58	MG	2A	3232	1/1	0.94	0.14	39,39,39,39	0
58	MG	16	102	1/1	0.94	0.18	46,46,46,46	0
58	MG	2A	3236	1/1	0.94	0.07	39,39,39,39	0
58	MG	2A	3237	1/1	0.94	0.18	46,46,46,46	0
58	MG	1A	3928	1/1	0.94	0.07	25,25,25,25	0
58	MG	2A	3550	1/1	0.94	0.09	41,41,41,41	0
58	MG	2D	301	1/1	0.94	0.11	31,31,31,31	0
58	MG	1A	3415	1/1	0.94	0.08	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3243	1/1	0.94	0.15	37,37,37,37	0
58	MG	2E	301	1/1	0.94	0.08	51,51,51,51	0
58	MG	1A	3613	1/1	0.94	0.09	33,33,33,33	0
58	MG	1a	1810	1/1	0.94	0.09	46,46,46,46	0
58	MG	2A	3248	1/1	0.94	0.12	46,46,46,46	0
58	MG	1A	3935	1/1	0.94	0.06	45,45,45,45	0
58	MG	2A	3251	1/1	0.94	0.12	46,46,46,46	0
58	MG	2A	3570	1/1	0.94	0.10	51,51,51,51	0
58	MG	1a	1605	1/1	0.94	0.09	41,41,41,41	0
58	MG	1A	3270	1/1	0.94	0.10	49,49,49,49	0
58	MG	2A	3575	1/1	0.94	0.07	42,42,42,42	0
58	MG	1A	3703	1/1	0.94	0.06	25,25,25,25	0
58	MG	1A	4059	1/1	0.94	0.10	41,41,41,41	0
58	MG	1A	3938	1/1	0.94	0.06	34,34,34,34	0
58	MG	1m	3001	1/1	0.94	0.09	54,54,54,54	0
58	MG	2A	3259	1/1	0.94	0.08	43,43,43,43	0
58	MG	2A	3582	1/1	0.94	0.09	43,43,43,43	0
58	MG	1A	3939	1/1	0.94	0.10	43,43,43,43	0
58	MG	1A	3248	1/1	0.94	0.14	52,52,52,52	0
58	MG	1a	1615	1/1	0.94	0.11	46,46,46,46	0
58	MG	2X	101	1/1	0.94	0.09	47,47,47,47	0
58	MG	1A	3179	1/1	0.94	0.05	24,24,24,24	0
58	MG	1w	104	1/1	0.94	0.17	63,63,63,63	0
58	MG	1A	3710	1/1	0.94	0.09	22,22,22,22	0
58	MG	2A	3270	1/1	0.94	0.11	54,54,54,54	0
58	MG	1A	3826	1/1	0.94	0.12	61,61,61,61	0
58	MG	23	101	1/1	0.94	0.09	51,51,51,51	0
58	MG	1a	1621	1/1	0.94	0.10	46,46,46,46	0
58	MG	1x	102	1/1	0.94	0.14	52,52,52,52	0
58	MG	1A	3947	1/1	0.94	0.07	35,35,35,35	0
58	MG	1A	3948	1/1	0.94	0.07	58,58,58,58	0
58	MG	1A	3502	1/1	0.94	0.25	39,39,39,39	0
58	MG	1A	4073	1/1	0.94	0.07	9,9,9,9	0
58	MG	2A	3281	1/1	0.94	0.08	48,48,48,48	0
58	MG	28	102	1/1	0.94	0.21	51,51,51,51	0
58	MG	2A	3609	1/1	0.94	0.09	50,50,50,50	0
58	MG	1a	1628	1/1	0.94	0.18	46,46,46,46	0
58	MG	1A	3619	1/1	0.94	0.11	24,24,24,24	0
58	MG	2A	3612	1/1	0.94	0.07	54,54,54,54	0
58	MG	1A	4079	1/1	0.94	0.10	45,45,45,45	0
58	MG	1x	111	1/1	0.94	0.12	56,56,56,56	0
58	MG	1x	112	1/1	0.94	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
58	MG	1A	3504	1/1	0.94	0.15	30,30,30,30	0
58	MG	2A	3620	1/1	0.94	0.07	43,43,43,43	0
58	MG	1A	3019	1/1	0.94	0.14	33,33,33,33	0
58	MG	2A	3294	1/1	0.94	0.14	54,54,54,54	0
58	MG	2a	1614	1/1	0.94	0.09	54,54,54,54	0
58	MG	2a	1615	1/1	0.94	0.13	54,54,54,54	0
58	MG	2A	3003	1/1	0.94	0.13	45,45,45,45	0
58	MG	1A	3355	1/1	0.94	0.10	46,46,46,46	0
58	MG	1A	3840	1/1	0.94	0.12	43,43,43,43	0
58	MG	1A	4087	1/1	0.94	0.10	40,40,40,40	0
58	MG	2A	3011	1/1	0.94	0.09	39,39,39,39	0
58	MG	2a	1621	1/1	0.94	0.08	51,51,51,51	0
58	MG	2A	3629	1/1	0.94	0.11	55,55,55,55	0
58	MG	2A	3303	1/1	0.94	0.11	56,56,56,56	0
58	MG	1A	3843	1/1	0.94	0.11	46,46,46,46	0
58	MG	2a	1625	1/1	0.94	0.09	56,56,56,56	0
58	MG	1A	4093	1/1	0.94	0.08	42,42,42,42	0
58	MG	2A	3306	1/1	0.94	0.13	52,52,52,52	0
58	MG	2A	3637	1/1	0.94	0.07	32,32,32,32	0
58	MG	2A	3025	1/1	0.94	0.10	50,50,50,50	0
58	MG	1A	3961	1/1	0.94	0.06	53,53,53,53	0
58	MG	2A	3641	1/1	0.94	0.06	38,38,38,38	0
58	MG	2A	3032	1/1	0.94	0.07	37,37,37,37	0
58	MG	1A	3627	1/1	0.94	0.08	29,29,29,29	0
58	MG	2A	3315	1/1	0.94	0.10	57,57,57,57	0
58	MG	2A	3647	1/1	0.94	0.10	42,42,42,42	0
58	MG	2A	3036	1/1	0.94	0.09	50,50,50,50	0
58	MG	1a	1657	1/1	0.94	0.24	54,54,54,54	0
58	MG	2A	3318	1/1	0.94	0.09	44,44,44,44	0
58	MG	1A	3630	1/1	0.94	0.07	28,28,28,28	0
58	MG	1A	3847	1/1	0.94	0.06	30,30,30,30	0
58	MG	1A	4098	1/1	0.94	0.09	45,45,45,45	0
58	MG	1A	3510	1/1	0.94	0.07	39,39,39,39	0
58	MG	2A	3326	1/1	0.94	0.08	45,45,45,45	0
58	MG	1A	3632	1/1	0.94	0.09	29,29,29,29	0
58	MG	1A	3514	1/1	0.94	0.09	45,45,45,45	0
58	MG	2A	3660	1/1	0.94	0.10	40,40,40,40	0
58	MG	1A	3638	1/1	0.94	0.07	19,19,19,19	0
58	MG	1a	1668	1/1	0.94	0.15	51,51,51,51	0
58	MG	2A	3054	1/1	0.94	0.12	55,55,55,55	0
58	MG	1A	3743	1/1	0.94	0.08	19,19,19,19	0
58	MG	1A	3290	1/1	0.94	0.06	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3058	1/1	0.94	0.09	46,46,46,46	0
58	MG	2a	1660	1/1	0.94	0.08	52,52,52,52	0
58	MG	2a	1661	1/1	0.94	0.09	52,52,52,52	0
58	MG	2A	3059	1/1	0.94	0.06	47,47,47,47	0
58	MG	2A	3339	1/1	0.94	0.11	48,48,48,48	0
58	MG	2a	1664	1/1	0.94	0.06	58,58,58,58	0
58	MG	1A	3518	1/1	0.94	0.07	46,46,46,46	0
58	MG	1A	3861	1/1	0.94	0.07	37,37,37,37	0
58	MG	1A	3862	1/1	0.94	0.07	34,34,34,34	0
58	MG	1A	3520	1/1	0.94	0.14	29,29,29,29	0
58	MG	1B	210	1/1	0.94	0.11	53,53,53,53	0
58	MG	2A	3677	1/1	0.94	0.09	48,48,48,48	0
58	MG	2a	1675	1/1	0.94	0.16	40,40,40,40	0
58	MG	1a	1680	1/1	0.94	0.18	60,60,60,60	0
58	MG	1A	3524	1/1	0.94	0.10	42,42,42,42	0
58	MG	2A	3350	1/1	0.94	0.14	53,53,53,53	0
58	MG	2A	3682	1/1	0.94	0.07	46,46,46,46	0
58	MG	1A	3357	1/1	0.94	0.15	60,60,60,60	0
58	MG	2a	1686	1/1	0.94	0.10	52,52,52,52	0
58	MG	2A	3071	1/1	0.94	0.07	43,43,43,43	0
58	MG	2A	3353	1/1	0.94	0.14	44,44,44,44	0
58	MG	2A	3072	1/1	0.94	0.06	35,35,35,35	0
58	MG	1A	3292	1/1	0.94	0.07	42,42,42,42	0
58	MG	1B	227	1/1	0.94	0.10	49,49,49,49	0
58	MG	1B	228	1/1	0.94	0.06	35,35,35,35	0
58	MG	1A	3750	1/1	0.94	0.08	53,53,53,53	0
58	MG	2A	3360	1/1	0.94	0.25	57,57,57,57	0
58	MG	2a	1703	1/1	0.94	0.11	52,52,52,52	0
58	MG	2A	3091	1/1	0.94	0.08	44,44,44,44	0
58	MG	1A	3651	1/1	0.94	0.09	53,53,53,53	0
58	MG	1B	232	1/1	0.94	0.07	50,50,50,50	0
58	MG	1B	233	1/1	0.94	0.08	42,42,42,42	0
58	MG	2a	1711	1/1	0.94	0.18	59,59,59,59	0
58	MG	2a	1713	1/1	0.94	0.12	51,51,51,51	0
58	MG	2A	3368	1/1	0.94	0.11	58,58,58,58	0
58	MG	1A	3437	1/1	0.94	0.11	38,38,38,38	0
58	MG	2A	3102	1/1	0.94	0.12	40,40,40,40	0
58	MG	1A	3438	1/1	0.94	0.14	30,30,30,30	0
58	MG	1A	3759	1/1	0.94	0.08	46,46,46,46	0
58	MG	2A	3106	1/1	0.94	0.08	37,37,37,37	0
58	MG	1A	3530	1/1	0.94	0.08	45,45,45,45	0
58	MG	1A	3766	1/1	0.94	0.10	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1a	1698	1/1	0.94	0.17	50,50,50,50	0
58	MG	2A	3716	1/1	0.94	0.09	39,39,39,39	0
58	MG	2A	3111	1/1	0.94	0.13	39,39,39,39	0
58	MG	1A	3151	1/1	0.94	0.18	22,22,22,22	0
58	MG	1A	3216	1/1	0.94	0.12	41,41,41,41	0
58	MG	2A	3392	1/1	0.94	0.16	56,56,56,56	0
58	MG	1a	1707	1/1	0.94	0.10	48,48,48,48	0
58	MG	2A	3394	1/1	0.94	0.14	58,58,58,58	0
58	MG	1a	1710	1/1	0.94	0.06	41,41,41,41	0
58	MG	2A	3726	1/1	0.94	0.14	40,40,40,40	0
58	MG	1A	3364	1/1	0.94	0.10	45,45,45,45	0
58	MG	1a	1712	1/1	0.94	0.15	46,46,46,46	0
58	MG	2a	1742	1/1	0.94	0.22	55,55,55,55	0
58	MG	2A	3121	1/1	0.94	0.10	59,59,59,59	0
58	MG	1A	3447	1/1	0.94	0.13	41,41,41,41	0
58	MG	1a	1714	1/1	0.94	0.09	42,42,42,42	0
58	MG	2A	3739	1/1	0.94	0.08	53,53,53,53	0
58	MG	2A	3131	1/1	0.94	0.09	42,42,42,42	0
58	MG	2A	3741	1/1	0.94	0.10	47,47,47,47	0
58	MG	2a	1752	1/1	0.94	0.08	59,59,59,59	0
58	MG	1a	1717	1/1	0.94	0.12	55,55,55,55	0
58	MG	2A	3408	1/1	0.94	0.08	53,53,53,53	0
58	MG	1A	3884	1/1	0.94	0.07	41,41,41,41	0
58	MG	2a	1760	1/1	0.94	0.10	62,62,62,62	0
58	MG	2A	3410	1/1	0.94	0.22	60,60,60,60	0
58	MG	2a	1764	1/1	0.94	0.10	50,50,50,50	0
58	MG	1a	1721	1/1	0.94	0.12	57,57,57,57	0
58	MG	2a	1772	1/1	0.94	0.13	61,61,61,61	0
58	MG	1F	311	1/1	0.94	0.12	44,44,44,44	0
58	MG	2A	3751	1/1	0.94	0.12	56,56,56,56	0
58	MG	2a	1777	1/1	0.94	0.18	53,53,53,53	0
58	MG	2A	3147	1/1	0.94	0.13	32,32,32,32	0
58	MG	2A	3149	1/1	0.94	0.14	50,50,50,50	0
58	MG	2A	3418	1/1	0.94	0.20	39,39,39,39	0
58	MG	1A	4004	1/1	0.94	0.07	44,44,44,44	0
58	MG	1A	4005	1/1	0.94	0.06	42,42,42,42	0
58	MG	1A	3366	1/1	0.94	0.08	48,48,48,48	0
58	MG	1A	3217	1/1	0.94	0.06	48,48,48,48	0
58	MG	2A	3156	1/1	0.94	0.09	26,26,26,26	0
58	MG	1A	3156	1/1	0.94	0.17	33,33,33,33	0
58	MG	1O	202	1/1	0.94	0.19	47,47,47,47	0
58	MG	1A	3301	1/1	0.94	0.33	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3164	1/1	0.94	0.07	33,33,33,33	0
58	MG	2a	1794	1/1	0.94	0.11	51,51,51,51	0
58	MG	1A	3553	1/1	0.94	0.10	41,41,41,41	0
58	MG	2a	1797	1/1	0.94	0.09	50,50,50,50	0
58	MG	2A	3771	1/1	0.94	0.07	50,50,50,50	0
58	MG	2A	3778	1/1	0.94	0.12	46,46,46,46	0
58	MG	2A	3779	1/1	0.94	0.05	45,45,45,45	0
58	MG	1A	3377	1/1	0.94	0.12	35,35,35,35	0
58	MG	2A	3167	1/1	0.94	0.09	36,36,36,36	0
58	MG	1Q	202	1/1	0.94	0.24	31,31,31,31	0
58	MG	2a	1805	1/1	0.94	0.15	52,52,52,52	0
58	MG	2a	1806	1/1	0.94	0.09	47,47,47,47	0
58	MG	2a	1808	1/1	0.94	0.14	48,48,48,48	0
58	MG	2A	3170	1/1	0.94	0.06	53,53,53,53	0
58	MG	1a	1738	1/1	0.94	0.09	48,48,48,48	0
58	MG	1Q	208	1/1	0.94	0.07	33,33,33,33	0
58	MG	1A	4016	1/1	0.94	0.06	21,21,21,21	0
58	MG	1A	3024	1/1	0.94	0.12	50,50,50,50	0
58	MG	1A	4020	1/1	0.94	0.05	38,38,38,38	0
58	MG	1A	3462	1/1	0.94	0.07	43,43,43,43	0
58	MG	2A	3452	1/1	0.94	0.22	41,41,41,41	0
58	MG	2A	3182	1/1	0.94	0.19	51,51,51,51	0
58	MG	2A	3183	1/1	0.94	0.09	41,41,41,41	0
58	MG	2A	3456	1/1	0.94	0.13	44,44,44,44	0
58	MG	2A	3457	1/1	0.94	0.19	45,45,45,45	0
58	MG	1A	3382	1/1	0.94	0.08	41,41,41,41	0
58	MG	1a	1748	1/1	0.94	0.07	44,44,44,44	0
58	MG	1A	3130	1/1	0.94	0.07	26,26,26,26	0
58	MG	2A	3469	1/1	0.94	0.08	46,46,46,46	0
58	MG	1W	201	1/1	0.94	0.17	41,41,41,41	0
58	MG	1a	1754	1/1	0.94	0.15	64,64,64,64	0
58	MG	1A	3787	1/1	0.94	0.07	43,43,43,43	0
58	MG	1X	105	1/1	0.94	0.07	32,32,32,32	0
58	MG	2A	3475	1/1	0.94	0.08	52,52,52,52	0
58	MG	1A	3788	1/1	0.94	0.06	34,34,34,34	0
58	MG	2A	3196	1/1	0.94	0.13	36,36,36,36	0
58	MG	1A	3334	1/1	0.94	0.08	37,37,37,37	0
58	MG	2k	201	1/1	0.94	0.13	55,55,55,55	0
58	MG	1A	4027	1/1	0.94	0.10	61,61,61,61	0
58	MG	1A	3907	1/1	0.94	0.07	16,16,16,16	0
58	MG	1A	3795	1/1	0.94	0.08	49,49,49,49	0
58	MG	2A	3493	1/1	0.94	0.09	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3836	1/1	0.94	0.11	37,37,37,37	0
58	MG	2A	3837	1/1	0.94	0.06	47,47,47,47	0
58	MG	2A	3202	1/1	0.94	0.16	55,55,55,55	0
58	MG	10	104	1/1	0.94	0.10	45,45,45,45	0
58	MG	2A	3501	1/1	0.94	0.08	50,50,50,50	0
58	MG	1A	3089	1/1	0.94	0.11	41,41,41,41	0
58	MG	10	106	1/1	0.94	0.12	57,57,57,57	0
58	MG	1a	1773	1/1	0.94	0.08	57,57,57,57	0
58	MG	1a	1774	1/1	0.94	0.08	63,63,63,63	0
58	MG	1A	4033	1/1	0.94	0.11	54,54,54,54	0
58	MG	2A	3512	1/1	0.94	0.08	65,65,65,65	0
58	MG	2A	3513	1/1	0.94	0.07	47,47,47,47	0
58	MG	1A	3799	1/1	0.94	0.07	34,34,34,34	0
58	MG	2A	3853	1/1	0.94	0.07	55,55,55,55	0
58	MG	1A	3141	1/1	0.94	0.08	37,37,37,37	0
58	MG	1a	1788	1/1	0.95	0.09	46,46,46,46	0
58	MG	2A	3488	1/1	0.95	0.11	51,51,51,51	0
58	MG	1A	3122	1/1	0.95	0.08	32,32,32,32	0
58	MG	2A	3490	1/1	0.95	0.06	34,34,34,34	0
58	MG	2A	3491	1/1	0.95	0.07	43,43,43,43	0
58	MG	2A	3206	1/1	0.95	0.12	44,44,44,44	0
58	MG	12	102	1/1	0.95	0.09	38,38,38,38	0
58	MG	2A	3849	1/1	0.95	0.09	48,48,48,48	0
58	MG	2A	3209	1/1	0.95	0.06	37,37,37,37	0
58	MG	2A	3495	1/1	0.95	0.22	57,57,57,57	0
58	MG	1A	3062	1/1	0.95	0.07	44,44,44,44	0
58	MG	2A	3500	1/1	0.95	0.06	47,47,47,47	0
58	MG	2A	3211	1/1	0.95	0.07	41,41,41,41	0
58	MG	1A	3910	1/1	0.95	0.15	29,29,29,29	0
58	MG	2A	3858	1/1	0.95	0.08	53,53,53,53	0
58	MG	2A	3213	1/1	0.95	0.11	56,56,56,56	0
58	MG	1A	3435	1/1	0.95	0.10	40,40,40,40	0
58	MG	1A	3064	1/1	0.95	0.14	45,45,45,45	0
58	MG	1a	1797	1/1	0.95	0.06	67,67,67,67	0
58	MG	2A	3863	1/1	0.95	0.17	44,44,44,44	0
58	MG	1a	1798	1/1	0.95	0.07	54,54,54,54	0
58	MG	1A	3780	1/1	0.95	0.09	22,22,22,22	0
58	MG	1A	3915	1/1	0.95	0.09	44,44,44,44	0
58	MG	1A	3273	1/1	0.95	0.15	28,28,28,28	0
58	MG	1a	1804	1/1	0.95	0.17	43,43,43,43	0
58	MG	18	105	1/1	0.95	0.10	52,52,52,52	0
58	MG	1A	4050	1/1	0.95	0.07	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3316	1/1	0.95	0.12	46,46,46,46	0
58	MG	1A	3362	1/1	0.95	0.08	33,33,33,33	0
58	MG	2A	3522	1/1	0.95	0.13	37,37,37,37	0
58	MG	2A	3523	1/1	0.95	0.08	36,36,36,36	0
58	MG	2B	213	1/1	0.95	0.24	57,57,57,57	0
58	MG	1A	3920	1/1	0.95	0.10	33,33,33,33	0
58	MG	1A	4057	1/1	0.95	0.04	22,22,22,22	0
58	MG	2B	217	1/1	0.95	0.06	46,46,46,46	0
58	MG	2A	3233	1/1	0.95	0.17	44,44,44,44	0
58	MG	1A	3536	1/1	0.95	0.07	46,46,46,46	0
58	MG	1A	3165	1/1	0.95	0.07	42,42,42,42	0
58	MG	2D	302	1/1	0.95	0.17	55,55,55,55	0
58	MG	2A	3534	1/1	0.95	0.07	45,45,45,45	0
58	MG	1A	3320	1/1	0.95	0.06	22,22,22,22	0
58	MG	1A	3791	1/1	0.95	0.10	27,27,27,27	0
58	MG	1e	202	1/1	0.95	0.09	54,54,54,54	0
58	MG	2A	3538	1/1	0.95	0.05	27,27,27,27	0
58	MG	2A	3540	1/1	0.95	0.13	58,58,58,58	0
58	MG	1f	202	1/1	0.95	0.09	47,47,47,47	0
58	MG	2A	3245	1/1	0.95	0.07	35,35,35,35	0
58	MG	1A	3323	1/1	0.95	0.07	31,31,31,31	0
58	MG	1A	3673	1/1	0.95	0.07	16,16,16,16	0
58	MG	2F	306	1/1	0.95	0.19	40,40,40,40	0
58	MG	1A	3449	1/1	0.95	0.12	35,35,35,35	0
58	MG	2A	3249	1/1	0.95	0.14	58,58,58,58	0
58	MG	1A	3450	1/1	0.95	0.25	31,31,31,31	0
58	MG	1A	3451	1/1	0.95	0.13	26,26,26,26	0
58	MG	2A	3554	1/1	0.95	0.06	49,49,49,49	0
58	MG	2A	3557	1/1	0.95	0.10	29,29,29,29	0
58	MG	2A	3252	1/1	0.95	0.12	64,64,64,64	0
58	MG	2A	3561	1/1	0.95	0.12	43,43,43,43	0
58	MG	2U	201	1/1	0.95	0.15	38,38,38,38	0
58	MG	1a	1619	1/1	0.95	0.08	48,48,48,48	0
58	MG	1A	3067	1/1	0.95	0.04	23,23,23,23	0
58	MG	2A	3565	1/1	0.95	0.07	25,25,25,25	0
58	MG	1A	3804	1/1	0.95	0.09	43,43,43,43	0
58	MG	2Y	201	1/1	0.95	0.10	45,45,45,45	0
58	MG	2A	3567	1/1	0.95	0.09	53,53,53,53	0
58	MG	1A	3679	1/1	0.95	0.05	21,21,21,21	0
58	MG	1w	108	1/1	0.95	0.07	33,33,33,33	0
58	MG	1A	3092	1/1	0.95	0.06	47,47,47,47	0
58	MG	1A	3255	1/1	0.95	0.06	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3574	1/1	0.95	0.10	42,42,42,42	0
58	MG	2A	3260	1/1	0.95	0.06	44,44,44,44	0
58	MG	2A	3261	1/1	0.95	0.10	42,42,42,42	0
58	MG	25	103	1/1	0.95	0.08	57,57,57,57	0
58	MG	1A	3557	1/1	0.95	0.10	33,33,33,33	0
58	MG	1A	3683	1/1	0.95	0.08	21,21,21,21	0
58	MG	2A	3579	1/1	0.95	0.10	48,48,48,48	0
58	MG	1A	3685	1/1	0.95	0.06	15,15,15,15	0
58	MG	1A	3558	1/1	0.95	0.09	18,18,18,18	0
58	MG	28	101	1/1	0.95	0.11	52,52,52,52	0
58	MG	1a	1633	1/1	0.95	0.15	45,45,45,45	0
58	MG	1A	3559	1/1	0.95	0.11	42,42,42,42	0
58	MG	1A	4090	1/1	0.95	0.16	50,50,50,50	0
58	MG	1a	1638	1/1	0.95	0.21	45,45,45,45	0
58	MG	1A	3951	1/1	0.95	0.07	53,53,53,53	0
58	MG	2A	3588	1/1	0.95	0.15	53,53,53,53	0
58	MG	2A	3589	1/1	0.95	0.06	37,37,37,37	0
58	MG	1a	1640	1/1	0.95	0.19	47,47,47,47	0
58	MG	1A	3952	1/1	0.95	0.05	39,39,39,39	0
58	MG	1A	3562	1/1	0.95	0.14	29,29,29,29	0
58	MG	2A	3276	1/1	0.95	0.09	52,52,52,52	0
58	MG	1a	1643	1/1	0.95	0.07	55,55,55,55	0
58	MG	2A	3278	1/1	0.95	0.08	58,58,58,58	0
58	MG	1A	3819	1/1	0.95	0.19	17,17,17,17	0
58	MG	1a	1646	1/1	0.95	0.09	33,33,33,33	0
58	MG	2A	3010	1/1	0.95	0.17	54,54,54,54	0
58	MG	1A	3563	1/1	0.95	0.11	34,34,34,34	0
58	MG	2A	3014	1/1	0.95	0.06	36,36,36,36	0
58	MG	1A	3376	1/1	0.95	0.10	41,41,41,41	0
58	MG	2A	3017	1/1	0.95	0.20	48,48,48,48	0
58	MG	2A	3020	1/1	0.95	0.14	55,55,55,55	0
58	MG	1a	1650	1/1	0.95	0.09	42,42,42,42	0
58	MG	1A	3823	1/1	0.95	0.06	27,27,27,27	0
58	MG	2A	3029	1/1	0.95	0.11	41,41,41,41	0
58	MG	1A	3132	1/1	0.95	0.10	36,36,36,36	0
58	MG	1A	4101	1/1	0.95	0.10	46,46,46,46	0
58	MG	2A	3298	1/1	0.95	0.06	41,41,41,41	0
58	MG	1A	3378	1/1	0.95	0.21	39,39,39,39	0
58	MG	2A	3035	1/1	0.95	0.07	31,31,31,31	0
58	MG	2A	3302	1/1	0.95	0.10	62,62,62,62	0
58	MG	1a	1661	1/1	0.95	0.17	58,58,58,58	0
58	MG	1A	3696	1/1	0.95	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
58	MG	1A	3104	1/1	0.95	0.07	26,26,26,26	0
58	MG	2A	3627	1/1	0.95	0.07	34,34,34,34	0
58	MG	1A	3571	1/1	0.95	0.08	27,27,27,27	0
58	MG	1A	3573	1/1	0.95	0.04	11,11,11,11	0
58	MG	2A	3308	1/1	0.95	0.07	40,40,40,40	0
58	MG	1A	4107	1/1	0.95	0.23	51,51,51,51	0
58	MG	2A	3311	1/1	0.95	0.09	35,35,35,35	0
58	MG	1A	3966	1/1	0.95	0.07	44,44,44,44	0
58	MG	1A	3381	1/1	0.95	0.07	39,39,39,39	0
58	MG	1a	1670	1/1	0.95	0.10	45,45,45,45	0
58	MG	1B	201	1/1	0.95	0.13	45,45,45,45	0
58	MG	1A	3577	1/1	0.95	0.09	35,35,35,35	0
58	MG	2a	1648	1/1	0.95	0.08	56,56,56,56	0
58	MG	1A	3839	1/1	0.95	0.09	29,29,29,29	0
58	MG	1B	208	1/1	0.95	0.07	48,48,48,48	0
58	MG	1A	3183	1/1	0.95	0.15	49,49,49,49	0
58	MG	2a	1654	1/1	0.95	0.13	54,54,54,54	0
58	MG	1B	212	1/1	0.95	0.10	33,33,33,33	0
58	MG	2a	1656	1/1	0.95	0.16	50,50,50,50	0
58	MG	1A	3975	1/1	0.95	0.09	16,16,16,16	0
58	MG	2A	3324	1/1	0.95	0.09	61,61,61,61	0
58	MG	2A	3325	1/1	0.95	0.12	46,46,46,46	0
58	MG	1A	3841	1/1	0.95	0.10	40,40,40,40	0
58	MG	1B	222	1/1	0.95	0.06	52,52,52,52	0
58	MG	2A	3653	1/1	0.95	0.14	38,38,38,38	0
58	MG	1B	223	1/1	0.95	0.08	40,40,40,40	0
58	MG	1a	1684	1/1	0.95	0.06	37,37,37,37	0
58	MG	1A	3842	1/1	0.95	0.08	50,50,50,50	0
58	MG	2A	3657	1/1	0.95	0.10	46,46,46,46	0
58	MG	1B	226	1/1	0.95	0.07	36,36,36,36	0
58	MG	2A	3068	1/1	0.95	0.05	34,34,34,34	0
58	MG	2a	1671	1/1	0.95	0.11	53,53,53,53	0
58	MG	1A	3704	1/1	0.95	0.07	48,48,48,48	0
58	MG	2A	3335	1/1	0.95	0.07	32,32,32,32	0
58	MG	1A	3982	1/1	0.95	0.05	49,49,49,49	0
58	MG	2A	3337	1/1	0.95	0.10	56,56,56,56	0
58	MG	2a	1678	1/1	0.95	0.19	52,52,52,52	0
58	MG	1B	229	1/1	0.95	0.07	37,37,37,37	0
58	MG	1A	3468	1/1	0.95	0.06	25,25,25,25	0
58	MG	2A	3074	1/1	0.95	0.14	58,58,58,58	0
58	MG	2A	3075	1/1	0.95	0.10	35,35,35,35	0
58	MG	2A	3079	1/1	0.95	0.07	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3343	1/1	0.95	0.10	50,50,50,50	0
58	MG	2A	3080	1/1	0.95	0.11	41,41,41,41	0
58	MG	2A	3672	1/1	0.95	0.09	51,51,51,51	0
58	MG	2A	3081	1/1	0.95	0.06	42,42,42,42	0
58	MG	2a	1692	1/1	0.95	0.25	55,55,55,55	0
58	MG	1A	3220	1/1	0.95	0.08	49,49,49,49	0
58	MG	2a	1697	1/1	0.95	0.20	57,57,57,57	0
58	MG	2A	3084	1/1	0.95	0.13	48,48,48,48	0
58	MG	2A	3349	1/1	0.95	0.10	60,60,60,60	0
58	MG	2a	1700	1/1	0.95	0.16	34,34,34,34	0
58	MG	1A	3473	1/1	0.95	0.12	53,53,53,53	0
58	MG	2A	3089	1/1	0.95	0.07	45,45,45,45	0
58	MG	1A	3596	1/1	0.95	0.12	37,37,37,37	0
58	MG	1B	234	1/1	0.95	0.07	33,33,33,33	0
58	MG	2a	1707	1/1	0.95	0.10	51,51,51,51	0
58	MG	1A	3988	1/1	0.95	0.05	32,32,32,32	0
58	MG	1A	3849	1/1	0.95	0.08	54,54,54,54	0
58	MG	1A	3223	1/1	0.95	0.07	31,31,31,31	0
58	MG	1a	1700	1/1	0.95	0.28	52,52,52,52	0
58	MG	2A	3358	1/1	0.95	0.10	55,55,55,55	0
58	MG	2a	1715	1/1	0.95	0.08	53,53,53,53	0
58	MG	1a	1702	1/1	0.95	0.25	52,52,52,52	0
58	MG	1A	3713	1/1	0.95	0.08	19,19,19,19	0
58	MG	1a	1704	1/1	0.95	0.09	37,37,37,37	0
58	MG	1A	3392	1/1	0.95	0.15	22,22,22,22	0
58	MG	2A	3363	1/1	0.95	0.08	52,52,52,52	0
58	MG	1a	1708	1/1	0.95	0.09	55,55,55,55	0
58	MG	1A	3855	1/1	0.95	0.08	52,52,52,52	0
58	MG	2A	3367	1/1	0.95	0.10	52,52,52,52	0
58	MG	1A	3396	1/1	0.95	0.20	29,29,29,29	0
58	MG	2a	1726	1/1	0.95	0.14	46,46,46,46	0
58	MG	1A	3303	1/1	0.95	0.09	22,22,22,22	0
58	MG	1A	3402	1/1	0.95	0.15	30,30,30,30	0
58	MG	2a	1729	1/1	0.95	0.18	43,43,43,43	0
58	MG	2a	1730	1/1	0.95	0.22	60,60,60,60	0
58	MG	2a	1731	1/1	0.95	0.14	53,53,53,53	0
58	MG	2A	3371	1/1	0.95	0.14	51,51,51,51	0
58	MG	1E	314	1/1	0.95	0.07	34,34,34,34	0
58	MG	1a	1716	1/1	0.95	0.14	39,39,39,39	0
58	MG	1F	303	1/1	0.95	0.10	23,23,23,23	0
58	MG	1F	305	1/1	0.95	0.08	34,34,34,34	0
58	MG	2a	1738	1/1	0.95	0.25	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3713	1/1	0.95	0.18	53,53,53,53	0
58	MG	2A	3383	1/1	0.95	0.08	45,45,45,45	0
58	MG	1A	3405	1/1	0.95	0.10	37,37,37,37	0
58	MG	1A	3723	1/1	0.95	0.07	40,40,40,40	0
58	MG	1F	312	1/1	0.95	0.09	44,44,44,44	0
58	MG	2A	3388	1/1	0.95	0.08	51,51,51,51	0
58	MG	2A	3124	1/1	0.95	0.14	44,44,44,44	0
58	MG	2A	3126	1/1	0.95	0.06	58,58,58,58	0
58	MG	2A	3722	1/1	0.95	0.07	49,49,49,49	0
58	MG	1A	3305	1/1	0.95	0.16	38,38,38,38	0
58	MG	2A	3130	1/1	0.95	0.09	44,44,44,44	0
58	MG	2a	1754	1/1	0.95	0.09	60,60,60,60	0
58	MG	1G	203	1/1	0.95	0.06	50,50,50,50	0
58	MG	2A	3395	1/1	0.95	0.08	42,42,42,42	0
58	MG	1A	3487	1/1	0.95	0.09	30,30,30,30	0
58	MG	2a	1759	1/1	0.95	0.06	59,59,59,59	0
58	MG	1A	3730	1/1	0.95	0.09	41,41,41,41	0
58	MG	2A	3139	1/1	0.95	0.07	53,53,53,53	0
58	MG	1A	3490	1/1	0.95	0.07	33,33,33,33	0
58	MG	2A	3142	1/1	0.95	0.24	47,47,47,47	0
58	MG	2a	1767	1/1	0.95	0.06	59,59,59,59	0
58	MG	2a	1770	1/1	0.95	0.11	48,48,48,48	0
58	MG	2a	1771	1/1	0.95	0.12	57,57,57,57	0
58	MG	2A	3145	1/1	0.95	0.09	43,43,43,43	0
58	MG	1a	1731	1/1	0.95	0.07	48,48,48,48	0
58	MG	1N	204	1/1	0.95	0.16	37,37,37,37	0
58	MG	2A	3407	1/1	0.95	0.07	54,54,54,54	0
58	MG	1A	3491	1/1	0.95	0.06	30,30,30,30	0
58	MG	1a	1735	1/1	0.95	0.06	42,42,42,42	0
58	MG	1A	3737	1/1	0.95	0.08	41,41,41,41	0
58	MG	1A	3493	1/1	0.95	0.12	43,43,43,43	0
58	MG	2a	1784	1/1	0.95	0.07	53,53,53,53	0
58	MG	1A	3410	1/1	0.95	0.09	37,37,37,37	0
58	MG	1A	3338	1/1	0.95	0.13	46,46,46,46	0
58	MG	1A	3263	1/1	0.95	0.06	40,40,40,40	0
58	MG	2A	3415	1/1	0.95	0.14	58,58,58,58	0
58	MG	2A	3417	1/1	0.95	0.06	48,48,48,48	0
58	MG	2A	3159	1/1	0.95	0.07	42,42,42,42	0
58	MG	1a	1742	1/1	0.95	0.09	40,40,40,40	0
58	MG	1Q	205	1/1	0.95	0.09	61,61,61,61	0
58	MG	1A	3622	1/1	0.95	0.08	42,42,42,42	0
58	MG	2A	3761	1/1	0.95	0.07	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3762	1/1	0.95	0.07	46,46,46,46	0
58	MG	1A	3340	1/1	0.95	0.06	36,36,36,36	0
58	MG	1S	201	1/1	0.95	0.08	35,35,35,35	0
58	MG	1A	3140	1/1	0.95	0.09	29,29,29,29	0
58	MG	2A	3768	1/1	0.95	0.10	37,37,37,37	0
58	MG	2A	3428	1/1	0.95	0.13	33,33,33,33	0
58	MG	1A	4017	1/1	0.95	0.04	16,16,16,16	0
58	MG	1A	3629	1/1	0.95	0.05	28,28,28,28	0
58	MG	2A	3776	1/1	0.95	0.12	55,55,55,55	0
58	MG	1A	3111	1/1	0.95	0.06	34,34,34,34	0
58	MG	1A	3420	1/1	0.95	0.10	43,43,43,43	0
58	MG	2A	3437	1/1	0.95	0.19	51,51,51,51	0
58	MG	2A	3782	1/1	0.95	0.08	38,38,38,38	0
58	MG	1A	3757	1/1	0.95	0.15	47,47,47,47	0
58	MG	2a	1813	1/1	0.95	0.16	59,59,59,59	0
58	MG	2a	1814	1/1	0.95	0.07	49,49,49,49	0
58	MG	2A	3784	1/1	0.95	0.12	48,48,48,48	0
58	MG	1A	3505	1/1	0.95	0.11	39,39,39,39	0
58	MG	2A	3176	1/1	0.95	0.08	47,47,47,47	0
58	MG	2A	3787	1/1	0.95	0.09	58,58,58,58	0
58	MG	1a	1762	1/1	0.95	0.05	41,41,41,41	0
58	MG	2A	3442	1/1	0.95	0.07	42,42,42,42	0
58	MG	1A	3421	1/1	0.95	0.10	31,31,31,31	0
58	MG	2A	3180	1/1	0.95	0.14	55,55,55,55	0
58	MG	2A	3181	1/1	0.95	0.06	37,37,37,37	0
58	MG	1A	3347	1/1	0.95	0.06	39,39,39,39	0
58	MG	2A	3798	1/1	0.95	0.07	46,46,46,46	0
58	MG	1A	3764	1/1	0.95	0.10	39,39,39,39	0
58	MG	2A	3184	1/1	0.95	0.10	35,35,35,35	0
58	MG	1A	3509	1/1	0.95	0.10	52,52,52,52	0
58	MG	2a	1834	1/1	0.95	0.14	62,62,62,62	0
58	MG	1a	1769	1/1	0.95	0.05	35,35,35,35	0
58	MG	1A	3350	1/1	0.95	0.16	54,54,54,54	0
58	MG	2A	3189	1/1	0.95	0.09	48,48,48,48	0
58	MG	1A	3426	1/1	0.95	0.06	37,37,37,37	0
58	MG	2A	3458	1/1	0.95	0.22	51,51,51,51	0
58	MG	10	101	1/1	0.95	0.14	32,32,32,32	0
58	MG	2A	3460	1/1	0.95	0.18	40,40,40,40	0
58	MG	1A	3516	1/1	0.95	0.10	42,42,42,42	0
58	MG	2A	3464	1/1	0.95	0.10	31,31,31,31	0
58	MG	1A	3227	1/1	0.95	0.05	32,32,32,32	0
58	MG	1A	3093	1/1	0.95	0.06	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3195	1/1	0.95	0.08	62,62,62,62	0
58	MG	1A	4036	1/1	0.95	0.05	28,28,28,28	0
58	MG	2A	3819	1/1	0.95	0.08	43,43,43,43	0
58	MG	2A	3821	1/1	0.95	0.09	40,40,40,40	0
58	MG	2r	101	1/1	0.95	0.06	44,44,44,44	0
58	MG	2A	3822	1/1	0.95	0.06	29,29,29,29	0
58	MG	1A	3900	1/1	0.95	0.05	20,20,20,20	0
58	MG	1a	1781	1/1	0.95	0.08	36,36,36,36	0
58	MG	2v	104	1/1	0.95	0.13	59,59,59,59	0
58	MG	1A	3901	1/1	0.95	0.09	46,46,46,46	0
58	MG	2A	3476	1/1	0.95	0.11	38,38,38,38	0
58	MG	1A	3774	1/1	0.95	0.10	26,26,26,26	0
58	MG	2A	3835	1/1	0.95	0.11	57,57,57,57	0
58	MG	1A	3431	1/1	0.95	0.07	41,41,41,41	0
58	MG	2A	3482	1/1	0.95	0.28	43,43,43,43	0
58	MG	2x	105	1/1	0.95	0.07	59,59,59,59	0
58	MG	2A	3838	1/1	0.95	0.07	63,63,63,63	0
58	MG	2x	107	1/1	0.95	0.14	45,45,45,45	0
58	MG	1a	1785	1/1	0.95	0.07	48,48,48,48	0
58	MG	2A	3022	1/1	0.96	0.14	35,35,35,35	0
58	MG	2A	3556	1/1	0.96	0.14	41,41,41,41	0
58	MG	2B	210	1/1	0.96	0.09	49,49,49,49	0
58	MG	2A	3023	1/1	0.96	0.07	49,49,49,49	0
58	MG	2A	3558	1/1	0.96	0.09	35,35,35,35	0
58	MG	1a	1654	1/1	0.96	0.14	46,46,46,46	0
58	MG	2B	214	1/1	0.96	0.07	48,48,48,48	0
58	MG	2A	3560	1/1	0.96	0.09	55,55,55,55	0
58	MG	1A	3513	1/1	0.96	0.09	50,50,50,50	0
58	MG	2A	3026	1/1	0.96	0.13	40,40,40,40	0
58	MG	2A	3027	1/1	0.96	0.05	32,32,32,32	0
58	MG	1a	1656	1/1	0.96	0.16	47,47,47,47	0
58	MG	2A	3285	1/1	0.96	0.08	47,47,47,47	0
58	MG	1A	4100	1/1	0.96	0.15	50,50,50,50	0
58	MG	2D	305	1/1	0.96	0.11	45,45,45,45	0
58	MG	1A	3647	1/1	0.96	0.05	15,15,15,15	0
58	MG	1a	1659	1/1	0.96	0.05	40,40,40,40	0
58	MG	2A	3571	1/1	0.96	0.07	30,30,30,30	0
58	MG	2E	302	1/1	0.96	0.08	45,45,45,45	0
58	MG	1A	3213	1/1	0.96	0.08	33,33,33,33	0
58	MG	1A	3288	1/1	0.96	0.09	27,27,27,27	0
58	MG	2A	3292	1/1	0.96	0.17	53,53,53,53	0
58	MG	2A	3037	1/1	0.96	0.15	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3341	1/1	0.96	0.11	48,48,48,48	0
58	MG	2A	3040	1/1	0.96	0.06	40,40,40,40	0
58	MG	1A	3342	1/1	0.96	0.08	44,44,44,44	0
58	MG	2F	305	1/1	0.96	0.10	33,33,33,33	0
58	MG	1A	3789	1/1	0.96	0.07	30,30,30,30	0
58	MG	1A	3519	1/1	0.96	0.10	23,23,23,23	0
58	MG	1A	3215	1/1	0.96	0.05	40,40,40,40	0
58	MG	2P	201	1/1	0.96	0.06	46,46,46,46	0
58	MG	1A	3521	1/1	0.96	0.06	26,26,26,26	0
58	MG	1A	3796	1/1	0.96	0.08	35,35,35,35	0
58	MG	1A	3797	1/1	0.96	0.05	22,22,22,22	0
58	MG	2A	3585	1/1	0.96	0.19	62,62,62,62	0
58	MG	2A	3048	1/1	0.96	0.07	45,45,45,45	0
58	MG	1B	206	1/1	0.96	0.14	39,39,39,39	0
58	MG	2A	3051	1/1	0.96	0.06	38,38,38,38	0
58	MG	2U	202	1/1	0.96	0.04	36,36,36,36	0
58	MG	2V	201	1/1	0.96	0.11	45,45,45,45	0
58	MG	2A	3052	1/1	0.96	0.19	55,55,55,55	0
58	MG	1A	3657	1/1	0.96	0.08	22,22,22,22	0
58	MG	1a	1673	1/1	0.96	0.17	54,54,54,54	0
58	MG	2A	3310	1/1	0.96	0.07	55,55,55,55	0
58	MG	1A	3345	1/1	0.96	0.08	45,45,45,45	0
58	MG	2A	3312	1/1	0.96	0.10	55,55,55,55	0
58	MG	1A	3432	1/1	0.96	0.07	43,43,43,43	0
58	MG	1B	211	1/1	0.96	0.07	43,43,43,43	0
58	MG	2A	3604	1/1	0.96	0.09	47,47,47,47	0
58	MG	1A	3801	1/1	0.96	0.04	17,17,17,17	0
58	MG	1B	213	1/1	0.96	0.10	46,46,46,46	0
58	MG	1B	215	1/1	0.96	0.05	39,39,39,39	0
58	MG	1A	3145	1/1	0.96	0.06	44,44,44,44	0
58	MG	1B	217	1/1	0.96	0.06	58,58,58,58	0
58	MG	1B	218	1/1	0.96	0.08	42,42,42,42	0
58	MG	2A	3321	1/1	0.96	0.06	45,45,45,45	0
58	MG	1a	1685	1/1	0.96	0.07	46,46,46,46	0
58	MG	1A	3803	1/1	0.96	0.10	49,49,49,49	0
58	MG	2A	3614	1/1	0.96	0.07	61,61,61,61	0
58	MG	2A	3615	1/1	0.96	0.11	50,50,50,50	0
58	MG	1A	3025	1/1	0.96	0.09	34,34,34,34	0
58	MG	1A	3294	1/1	0.96	0.05	25,25,25,25	0
58	MG	1B	224	1/1	0.96	0.07	34,34,34,34	0
58	MG	1A	3962	1/1	0.96	0.06	38,38,38,38	0
58	MG	1A	3529	1/1	0.96	0.12	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3668	1/1	0.96	0.08	43,43,43,43	0
58	MG	2A	3078	1/1	0.96	0.06	20,20,20,20	0
58	MG	1A	3669	1/1	0.96	0.06	19,19,19,19	0
58	MG	1A	3670	1/1	0.96	0.04	21,21,21,21	0
58	MG	1A	3968	1/1	0.96	0.10	43,43,43,43	0
58	MG	2a	1610	1/1	0.96	0.10	47,47,47,47	0
58	MG	2a	1611	1/1	0.96	0.14	51,51,51,51	0
58	MG	1A	3005	1/1	0.96	0.08	30,30,30,30	0
58	MG	1A	3154	1/1	0.96	0.08	33,33,33,33	0
58	MG	2A	3085	1/1	0.96	0.06	38,38,38,38	0
58	MG	2A	3630	1/1	0.96	0.06	33,33,33,33	0
58	MG	2A	3086	1/1	0.96	0.09	45,45,45,45	0
58	MG	2A	3632	1/1	0.96	0.12	32,32,32,32	0
58	MG	1A	3155	1/1	0.96	0.09	34,34,34,34	0
58	MG	1A	3537	1/1	0.96	0.09	31,31,31,31	0
58	MG	1a	1701	1/1	0.96	0.15	44,44,44,44	0
58	MG	1A	3538	1/1	0.96	0.17	36,36,36,36	0
58	MG	1A	3065	1/1	0.96	0.08	27,27,27,27	0
58	MG	2A	3094	1/1	0.96	0.06	31,31,31,31	0
58	MG	2A	3095	1/1	0.96	0.07	37,37,37,37	0
58	MG	1A	3441	1/1	0.96	0.11	39,39,39,39	0
58	MG	2A	3644	1/1	0.96	0.10	50,50,50,50	0
58	MG	2A	3097	1/1	0.96	0.07	60,60,60,60	0
58	MG	1a	1705	1/1	0.96	0.06	46,46,46,46	0
58	MG	1a	1706	1/1	0.96	0.13	49,49,49,49	0
58	MG	1A	3013	1/1	0.96	0.05	22,22,22,22	0
58	MG	1D	301	1/1	0.96	0.13	47,47,47,47	0
58	MG	1a	1709	1/1	0.96	0.07	52,52,52,52	0
58	MG	1D	308	1/1	0.96	0.07	26,26,26,26	0
58	MG	1A	3228	1/1	0.96	0.09	39,39,39,39	0
58	MG	1A	3547	1/1	0.96	0.13	40,40,40,40	0
58	MG	1A	3445	1/1	0.96	0.17	31,31,31,31	0
58	MG	1A	3105	1/1	0.96	0.13	35,35,35,35	0
58	MG	1A	3829	1/1	0.96	0.14	22,22,22,22	0
58	MG	1A	3550	1/1	0.96	0.10	39,39,39,39	0
58	MG	1A	3448	1/1	0.96	0.08	35,35,35,35	0
58	MG	1A	3990	1/1	0.96	0.05	43,43,43,43	0
58	MG	1A	3832	1/1	0.96	0.04	18,18,18,18	0
58	MG	1A	3833	1/1	0.96	0.06	25,25,25,25	0
58	MG	2a	1645	1/1	0.96	0.20	57,57,57,57	0
58	MG	2A	3119	1/1	0.96	0.05	28,28,28,28	0
58	MG	2A	3366	1/1	0.96	0.08	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3120	1/1	0.96	0.07	47,47,47,47	0
58	MG	1A	3552	1/1	0.96	0.09	40,40,40,40	0
58	MG	1A	3068	1/1	0.96	0.05	23,23,23,23	0
58	MG	2a	1651	1/1	0.96	0.08	38,38,38,38	0
58	MG	2a	1652	1/1	0.96	0.07	49,49,49,49	0
58	MG	1F	314	1/1	0.96	0.10	40,40,40,40	0
58	MG	1A	3554	1/1	0.96	0.06	48,48,48,48	0
58	MG	1a	1729	1/1	0.96	0.08	47,47,47,47	0
58	MG	2A	3128	1/1	0.96	0.16	45,45,45,45	0
58	MG	2A	3129	1/1	0.96	0.11	40,40,40,40	0
58	MG	2A	3377	1/1	0.96	0.13	56,56,56,56	0
58	MG	2A	3378	1/1	0.96	0.06	52,52,52,52	0
58	MG	1A	3169	1/1	0.96	0.05	23,23,23,23	0
58	MG	2A	3380	1/1	0.96	0.09	47,47,47,47	0
58	MG	2A	3382	1/1	0.96	0.21	53,53,53,53	0
58	MG	1A	3236	1/1	0.96	0.07	35,35,35,35	0
58	MG	2A	3132	1/1	0.96	0.07	59,59,59,59	0
58	MG	1A	3365	1/1	0.96	0.06	36,36,36,36	0
58	MG	1N	202	1/1	0.96	0.06	48,48,48,48	0
58	MG	1A	3241	1/1	0.96	0.04	29,29,29,29	0
58	MG	2a	1668	1/1	0.96	0.11	58,58,58,58	0
58	MG	1A	3455	1/1	0.96	0.06	38,38,38,38	0
58	MG	2A	3687	1/1	0.96	0.10	50,50,50,50	0
58	MG	2a	1672	1/1	0.96	0.07	59,59,59,59	0
58	MG	2A	3390	1/1	0.96	0.07	43,43,43,43	0
58	MG	1A	3367	1/1	0.96	0.09	27,27,27,27	0
58	MG	1A	3170	1/1	0.96	0.09	38,38,38,38	0
58	MG	2a	1676	1/1	0.96	0.06	44,44,44,44	0
58	MG	1A	3115	1/1	0.96	0.07	32,32,32,32	0
58	MG	1A	3371	1/1	0.96	0.08	37,37,37,37	0
58	MG	1A	3373	1/1	0.96	0.09	26,26,26,26	0
58	MG	1A	3069	1/1	0.96	0.06	36,36,36,36	0
58	MG	1Q	207	1/1	0.96	0.18	36,36,36,36	0
58	MG	2a	1683	1/1	0.96	0.08	39,39,39,39	0
58	MG	1A	3852	1/1	0.96	0.04	34,34,34,34	0
58	MG	2a	1685	1/1	0.96	0.06	56,56,56,56	0
58	MG	2A	3702	1/1	0.96	0.09	50,50,50,50	0
58	MG	1A	3572	1/1	0.96	0.12	20,20,20,20	0
58	MG	1A	3706	1/1	0.96	0.05	35,35,35,35	0
58	MG	2A	3705	1/1	0.96	0.06	51,51,51,51	0
58	MG	1S	202	1/1	0.96	0.05	38,38,38,38	0
58	MG	1a	1751	1/1	0.96	0.07	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2a	1693	1/1	0.96	0.13	48,48,48,48	0
58	MG	1S	203	1/1	0.96	0.05	54,54,54,54	0
58	MG	2A	3405	1/1	0.96	0.09	54,54,54,54	0
58	MG	1A	4011	1/1	0.96	0.07	55,55,55,55	0
58	MG	1a	1757	1/1	0.96	0.10	43,43,43,43	0
58	MG	1T	202	1/1	0.96	0.06	37,37,37,37	0
58	MG	2a	1701	1/1	0.96	0.27	54,54,54,54	0
58	MG	1A	3466	1/1	0.96	0.07	50,50,50,50	0
58	MG	1U	207	1/1	0.96	0.12	25,25,25,25	0
58	MG	2a	1704	1/1	0.96	0.12	62,62,62,62	0
58	MG	1A	4013	1/1	0.96	0.07	43,43,43,43	0
58	MG	1A	3708	1/1	0.96	0.04	28,28,28,28	0
58	MG	1A	3709	1/1	0.96	0.08	20,20,20,20	0
58	MG	2a	1708	1/1	0.96	0.11	52,52,52,52	0
58	MG	2A	3172	1/1	0.96	0.05	39,39,39,39	0
58	MG	1A	3118	1/1	0.96	0.15	19,19,19,19	0
58	MG	1a	1767	1/1	0.96	0.11	41,41,41,41	0
58	MG	1A	3575	1/1	0.96	0.07	37,37,37,37	0
58	MG	1A	3253	1/1	0.96	0.09	46,46,46,46	0
58	MG	1A	3579	1/1	0.96	0.10	30,30,30,30	0
58	MG	1A	3581	1/1	0.96	0.09	35,35,35,35	0
58	MG	1A	3716	1/1	0.96	0.06	22,22,22,22	0
58	MG	2a	1718	1/1	0.96	0.12	57,57,57,57	0
58	MG	2A	3728	1/1	0.96	0.07	35,35,35,35	0
58	MG	1A	3584	1/1	0.96	0.10	31,31,31,31	0
58	MG	2A	3731	1/1	0.96	0.07	32,32,32,32	0
58	MG	1A	3869	1/1	0.96	0.05	31,31,31,31	0
58	MG	2A	3733	1/1	0.96	0.08	55,55,55,55	0
58	MG	2A	3734	1/1	0.96	0.10	36,36,36,36	0
58	MG	1A	3254	1/1	0.96	0.05	35,35,35,35	0
58	MG	2A	3736	1/1	0.96	0.08	44,44,44,44	0
58	MG	2A	3430	1/1	0.96	0.07	38,38,38,38	0
58	MG	2A	3431	1/1	0.96	0.20	49,49,49,49	0
58	MG	2A	3432	1/1	0.96	0.23	46,46,46,46	0
58	MG	1a	1777	1/1	0.96	0.10	58,58,58,58	0
58	MG	2A	3434	1/1	0.96	0.15	50,50,50,50	0
58	MG	2A	3743	1/1	0.96	0.06	55,55,55,55	0
58	MG	1A	3588	1/1	0.96	0.25	29,29,29,29	0
58	MG	1A	3120	1/1	0.96	0.09	38,38,38,38	0
58	MG	1A	3474	1/1	0.96	0.09	41,41,41,41	0
58	MG	2A	3748	1/1	0.96	0.11	38,38,38,38	0
58	MG	2A	3188	1/1	0.96	0.06	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3380	1/1	0.96	0.12	23,23,23,23	0
58	MG	1A	3318	1/1	0.96	0.10	39,39,39,39	0
58	MG	11	102	1/1	0.96	0.07	36,36,36,36	0
58	MG	1A	4034	1/1	0.96	0.05	32,32,32,32	0
58	MG	1a	1786	1/1	0.96	0.11	50,50,50,50	0
58	MG	1A	3878	1/1	0.96	0.05	20,20,20,20	0
58	MG	2A	3446	1/1	0.96	0.18	42,42,42,42	0
58	MG	1A	3726	1/1	0.96	0.08	9,9,9,9	0
58	MG	1A	3727	1/1	0.96	0.09	42,42,42,42	0
58	MG	1A	3035	1/1	0.96	0.05	31,31,31,31	0
58	MG	2A	3760	1/1	0.96	0.10	57,57,57,57	0
58	MG	2A	3450	1/1	0.96	0.06	48,48,48,48	0
58	MG	13	101	1/1	0.96	0.05	40,40,40,40	0
58	MG	1A	3385	1/1	0.96	0.08	36,36,36,36	0
58	MG	2A	3764	1/1	0.96	0.06	43,43,43,43	0
58	MG	1A	3734	1/1	0.96	0.09	43,43,43,43	0
58	MG	1A	3600	1/1	0.96	0.06	34,34,34,34	0
58	MG	15	102	1/1	0.96	0.05	30,30,30,30	0
58	MG	2a	1763	1/1	0.96	0.06	42,42,42,42	0
58	MG	15	103	1/1	0.96	0.10	23,23,23,23	0
58	MG	2a	1765	1/1	0.96	0.06	48,48,48,48	0
58	MG	15	106	1/1	0.96	0.13	27,27,27,27	0
58	MG	1a	1801	1/1	0.96	0.06	52,52,52,52	0
58	MG	2A	3773	1/1	0.96	0.08	46,46,46,46	0
58	MG	2A	3774	1/1	0.96	0.06	44,44,44,44	0
58	MG	1a	1802	1/1	0.96	0.06	51,51,51,51	0
58	MG	2a	1773	1/1	0.96	0.13	50,50,50,50	0
58	MG	2A	3208	1/1	0.96	0.06	45,45,45,45	0
58	MG	1A	3603	1/1	0.96	0.07	37,37,37,37	0
58	MG	2A	3465	1/1	0.96	0.09	58,58,58,58	0
58	MG	2A	3466	1/1	0.96	0.07	47,47,47,47	0
58	MG	2a	1780	1/1	0.96	0.06	45,45,45,45	0
58	MG	1A	3738	1/1	0.96	0.11	50,50,50,50	0
58	MG	1A	3891	1/1	0.96	0.07	28,28,28,28	0
58	MG	18	101	1/1	0.96	0.12	39,39,39,39	0
58	MG	1A	3605	1/1	0.96	0.27	53,53,53,53	0
58	MG	1A	3015	1/1	0.96	0.08	26,26,26,26	0
58	MG	2a	1786	1/1	0.96	0.09	43,43,43,43	0
58	MG	2A	3215	1/1	0.96	0.14	53,53,53,53	0
58	MG	19	101	1/1	0.96	0.08	39,39,39,39	0
58	MG	1A	3607	1/1	0.96	0.08	53,53,53,53	0
58	MG	2A	3219	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
58	MG	1A	3322	1/1	0.96	0.05	43,43,43,43	0
58	MG	1A	3084	1/1	0.96	0.05	24,24,24,24	0
58	MG	1A	3485	1/1	0.96	0.08	37,37,37,37	0
58	MG	2A	3484	1/1	0.96	0.13	52,52,52,52	0
58	MG	1A	3324	1/1	0.96	0.08	38,38,38,38	0
58	MG	1A	3488	1/1	0.96	0.06	48,48,48,48	0
58	MG	1A	4055	1/1	0.96	0.07	36,36,36,36	0
58	MG	2A	3226	1/1	0.96	0.20	38,38,38,38	0
58	MG	2a	1800	1/1	0.96	0.17	52,52,52,52	0
58	MG	1l	201	1/1	0.96	0.06	49,49,49,49	0
58	MG	1A	3489	1/1	0.96	0.06	41,41,41,41	0
58	MG	1A	3752	1/1	0.96	0.07	46,46,46,46	0
58	MG	2A	3230	1/1	0.96	0.07	40,40,40,40	0
58	MG	1A	3903	1/1	0.96	0.08	21,21,21,21	0
58	MG	2A	3497	1/1	0.96	0.08	42,42,42,42	0
58	MG	2a	1807	1/1	0.96	0.20	47,47,47,47	0
58	MG	1A	3397	1/1	0.96	0.07	47,47,47,47	0
58	MG	1A	3086	1/1	0.96	0.08	25,25,25,25	0
58	MG	1w	101	1/1	0.96	0.06	35,35,35,35	0
58	MG	1A	3906	1/1	0.96	0.04	27,27,27,27	0
58	MG	1w	103	1/1	0.96	0.09	46,46,46,46	0
58	MG	1A	3618	1/1	0.96	0.05	28,28,28,28	0
58	MG	2A	3239	1/1	0.96	0.09	46,46,46,46	0
58	MG	2a	1815	1/1	0.96	0.06	50,50,50,50	0
58	MG	1A	3908	1/1	0.96	0.09	56,56,56,56	0
58	MG	1A	3492	1/1	0.96	0.15	36,36,36,36	0
58	MG	1A	3760	1/1	0.96	0.08	28,28,28,28	0
58	MG	1A	3761	1/1	0.96	0.11	33,33,33,33	0
58	MG	1A	3192	1/1	0.96	0.08	27,27,27,27	0
58	MG	2A	3832	1/1	0.96	0.06	48,48,48,48	0
58	MG	1A	3763	1/1	0.96	0.06	27,27,27,27	0
58	MG	2A	3834	1/1	0.96	0.05	24,24,24,24	0
58	MG	2a	1825	1/1	0.96	0.06	44,44,44,44	0
58	MG	1a	1626	1/1	0.96	0.17	53,53,53,53	0
58	MG	1A	4075	1/1	0.96	0.07	46,46,46,46	0
58	MG	2A	3519	1/1	0.96	0.08	33,33,33,33	0
58	MG	1A	3042	1/1	0.96	0.10	21,21,21,21	0
58	MG	1A	3197	1/1	0.96	0.18	27,27,27,27	0
58	MG	2A	3840	1/1	0.96	0.08	22,22,22,22	0
58	MG	1A	3624	1/1	0.96	0.06	29,29,29,29	0
58	MG	2a	1835	1/1	0.96	0.14	52,52,52,52	0
58	MG	1x	109	1/1	0.96	0.05	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3524	1/1	0.96	0.10	61,61,61,61	0
58	MG	2A	3525	1/1	0.96	0.11	46,46,46,46	0
58	MG	1A	4082	1/1	0.96	0.07	31,31,31,31	0
58	MG	1A	3091	1/1	0.96	0.06	42,42,42,42	0
58	MG	2A	3847	1/1	0.96	0.05	29,29,29,29	0
58	MG	1A	3411	1/1	0.96	0.08	31,31,31,31	0
58	MG	1a	1637	1/1	0.96	0.07	43,43,43,43	0
58	MG	1A	3330	1/1	0.96	0.09	43,43,43,43	0
58	MG	1A	3133	1/1	0.96	0.07	23,23,23,23	0
58	MG	1A	3414	1/1	0.96	0.10	45,45,45,45	0
58	MG	1A	3055	1/1	0.96	0.09	34,34,34,34	0
58	MG	2A	3854	1/1	0.96	0.07	45,45,45,45	0
58	MG	2A	3263	1/1	0.96	0.08	40,40,40,40	0
58	MG	1A	4092	1/1	0.96	0.09	38,38,38,38	0
58	MG	2A	3539	1/1	0.96	0.09	40,40,40,40	0
58	MG	1A	3635	1/1	0.96	0.06	36,36,36,36	0
58	MG	1A	3268	1/1	0.96	0.09	29,29,29,29	0
58	MG	2A	3012	1/1	0.96	0.06	39,39,39,39	0
58	MG	1A	3058	1/1	0.96	0.04	13,13,13,13	0
58	MG	1A	3933	1/1	0.96	0.08	29,29,29,29	0
58	MG	2A	3545	1/1	0.96	0.05	33,33,33,33	0
58	MG	2A	3546	1/1	0.96	0.07	35,35,35,35	0
58	MG	2A	3547	1/1	0.96	0.14	51,51,51,51	0
58	MG	2x	102	1/1	0.96	0.18	38,38,38,38	0
58	MG	1A	3210	1/1	0.96	0.05	44,44,44,44	0
58	MG	2A	3019	1/1	0.96	0.08	34,34,34,34	0
58	MG	1A	3001	1/1	0.96	0.08	36,36,36,36	0
58	MG	2B	202	1/1	0.96	0.05	37,37,37,37	0
58	MG	2B	203	1/1	0.96	0.15	60,60,60,60	0
58	MG	2A	3021	1/1	0.96	0.06	22,22,22,22	0
59	K	2x	101	1/1	0.96	0.06	43,43,43,43	0
60	ZN	2Y	202	1/1	0.96	0.06	86,86,86,86	0
58	MG	1A	3278	1/1	0.97	0.06	40,40,40,40	0
58	MG	2A	3555	1/1	0.97	0.05	34,34,34,34	0
58	MG	1A	3279	1/1	0.97	0.05	23,23,23,23	0
58	MG	2A	3269	1/1	0.97	0.06	43,43,43,43	0
58	MG	1A	3718	1/1	0.97	0.07	34,34,34,34	0
58	MG	1A	4056	1/1	0.97	0.07	34,34,34,34	0
58	MG	2A	3005	1/1	0.97	0.16	51,51,51,51	0
58	MG	1A	3883	1/1	0.97	0.21	33,33,33,33	0
58	MG	2A	3007	1/1	0.97	0.11	34,34,34,34	0
58	MG	1A	3456	1/1	0.97	0.08	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3009	1/1	0.97	0.07	40,40,40,40	0
58	MG	1A	3282	1/1	0.97	0.19	33,33,33,33	0
58	MG	2D	303	1/1	0.97	0.09	46,46,46,46	0
58	MG	1A	3886	1/1	0.97	0.10	22,22,22,22	0
58	MG	2A	3568	1/1	0.97	0.05	39,39,39,39	0
58	MG	2A	3279	1/1	0.97	0.10	47,47,47,47	0
58	MG	1A	3283	1/1	0.97	0.10	24,24,24,24	0
58	MG	1A	3459	1/1	0.97	0.14	38,38,38,38	0
58	MG	1A	3578	1/1	0.97	0.28	25,25,25,25	0
58	MG	2A	3283	1/1	0.97	0.11	40,40,40,40	0
58	MG	2A	3284	1/1	0.97	0.09	55,55,55,55	0
58	MG	1A	3286	1/1	0.97	0.05	37,37,37,37	0
58	MG	2A	3018	1/1	0.97	0.09	48,48,48,48	0
58	MG	1a	1624	1/1	0.97	0.15	56,56,56,56	0
58	MG	1A	4065	1/1	0.97	0.07	30,30,30,30	0
58	MG	1A	3287	1/1	0.97	0.05	34,34,34,34	0
58	MG	1A	3582	1/1	0.97	0.18	26,26,26,26	0
58	MG	1A	3050	1/1	0.97	0.06	34,34,34,34	0
58	MG	1A	4071	1/1	0.97	0.05	34,34,34,34	0
58	MG	1A	3585	1/1	0.97	0.14	25,25,25,25	0
58	MG	2Q	201	1/1	0.97	0.04	46,46,46,46	0
58	MG	1a	1631	1/1	0.97	0.14	44,44,44,44	0
58	MG	1A	3732	1/1	0.97	0.07	33,33,33,33	0
58	MG	2A	3028	1/1	0.97	0.08	45,45,45,45	0
58	MG	1a	1634	1/1	0.97	0.09	22,22,22,22	0
58	MG	1A	3463	1/1	0.97	0.11	44,44,44,44	0
58	MG	2A	3300	1/1	0.97	0.24	52,52,52,52	0
58	MG	1A	3587	1/1	0.97	0.09	18,18,18,18	0
58	MG	1A	4077	1/1	0.97	0.04	15,15,15,15	0
58	MG	1A	3464	1/1	0.97	0.06	38,38,38,38	0
58	MG	2A	3594	1/1	0.97	0.06	51,51,51,51	0
58	MG	1A	3073	1/1	0.97	0.03	9,9,9,9	0
58	MG	1A	3902	1/1	0.97	0.05	33,33,33,33	0
58	MG	2A	3038	1/1	0.97	0.04	14,14,14,14	0
58	MG	2A	3600	1/1	0.97	0.06	43,43,43,43	0
58	MG	2A	3601	1/1	0.97	0.07	42,42,42,42	0
58	MG	2A	3602	1/1	0.97	0.08	41,41,41,41	0
58	MG	1A	3740	1/1	0.97	0.07	41,41,41,41	0
58	MG	1A	3741	1/1	0.97	0.05	37,37,37,37	0
58	MG	1A	3212	1/1	0.97	0.12	23,23,23,23	0
58	MG	1A	3054	1/1	0.97	0.07	32,32,32,32	0
58	MG	23	103	1/1	0.97	0.05	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	4088	1/1	0.97	0.06	26,26,26,26	0
58	MG	1A	3593	1/1	0.97	0.06	39,39,39,39	0
58	MG	1A	3595	1/1	0.97	0.08	21,21,21,21	0
58	MG	1A	3103	1/1	0.97	0.08	28,28,28,28	0
58	MG	1a	1651	1/1	0.97	0.07	43,43,43,43	0
58	MG	1a	1652	1/1	0.97	0.06	32,32,32,32	0
58	MG	27	101	1/1	0.97	0.10	40,40,40,40	0
58	MG	2A	3049	1/1	0.97	0.07	18,18,18,18	0
58	MG	1A	3597	1/1	0.97	0.07	42,42,42,42	0
58	MG	1A	3077	1/1	0.97	0.14	42,42,42,42	0
58	MG	1A	3470	1/1	0.97	0.18	28,28,28,28	0
58	MG	2A	3053	1/1	0.97	0.07	47,47,47,47	0
58	MG	1A	3472	1/1	0.97	0.06	49,49,49,49	0
58	MG	2a	1602	1/1	0.97	0.12	51,51,51,51	0
58	MG	2A	3055	1/1	0.97	0.07	38,38,38,38	0
58	MG	1A	3601	1/1	0.97	0.06	47,47,47,47	0
58	MG	1A	3916	1/1	0.97	0.13	24,24,24,24	0
58	MG	1A	3602	1/1	0.97	0.15	20,20,20,20	0
58	MG	2A	3327	1/1	0.97	0.06	34,34,34,34	0
58	MG	1A	3754	1/1	0.97	0.04	25,25,25,25	0
58	MG	1A	3152	1/1	0.97	0.11	26,26,26,26	0
58	MG	2A	3061	1/1	0.97	0.06	30,30,30,30	0
58	MG	1A	3604	1/1	0.97	0.13	25,25,25,25	0
58	MG	1A	3372	1/1	0.97	0.07	38,38,38,38	0
58	MG	1A	3218	1/1	0.97	0.09	31,31,31,31	0
58	MG	1A	3374	1/1	0.97	0.07	41,41,41,41	0
58	MG	1A	3298	1/1	0.97	0.08	35,35,35,35	0
58	MG	1A	3028	1/1	0.97	0.08	28,28,28,28	0
58	MG	1A	3929	1/1	0.97	0.10	22,22,22,22	0
58	MG	2A	3635	1/1	0.97	0.05	54,54,54,54	0
58	MG	1A	3222	1/1	0.97	0.06	37,37,37,37	0
58	MG	1A	3106	1/1	0.97	0.06	32,32,32,32	0
58	MG	1A	3932	1/1	0.97	0.05	49,49,49,49	0
58	MG	1B	204	1/1	0.97	0.20	52,52,52,52	0
58	MG	1B	205	1/1	0.97	0.05	40,40,40,40	0
58	MG	1A	3110	1/1	0.97	0.10	23,23,23,23	0
58	MG	2A	3076	1/1	0.97	0.12	32,32,32,32	0
58	MG	2A	3077	1/1	0.97	0.05	49,49,49,49	0
58	MG	1A	3768	1/1	0.97	0.07	41,41,41,41	0
58	MG	2A	3347	1/1	0.97	0.15	58,58,58,58	0
58	MG	1A	3482	1/1	0.97	0.05	30,30,30,30	0
58	MG	1B	209	1/1	0.97	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
58	MG	1A	3484	1/1	0.97	0.10	30,30,30,30	0
58	MG	1A	3304	1/1	0.97	0.06	16,16,16,16	0
58	MG	2A	3083	1/1	0.97	0.06	43,43,43,43	0
58	MG	1A	3225	1/1	0.97	0.08	32,32,32,32	0
58	MG	1A	3157	1/1	0.97	0.06	33,33,33,33	0
58	MG	1B	214	1/1	0.97	0.09	48,48,48,48	0
58	MG	2A	3087	1/1	0.97	0.09	41,41,41,41	0
58	MG	1A	3383	1/1	0.97	0.11	28,28,28,28	0
58	MG	2a	1639	1/1	0.97	0.23	48,48,48,48	0
58	MG	1A	3082	1/1	0.97	0.10	34,34,34,34	0
58	MG	1A	3112	1/1	0.97	0.17	24,24,24,24	0
58	MG	1A	3945	1/1	0.97	0.07	31,31,31,31	0
58	MG	1A	3623	1/1	0.97	0.09	23,23,23,23	0
58	MG	1A	3388	1/1	0.97	0.06	31,31,31,31	0
58	MG	1A	3113	1/1	0.97	0.07	28,28,28,28	0
58	MG	1A	3949	1/1	0.97	0.05	36,36,36,36	0
58	MG	1A	3390	1/1	0.97	0.13	33,33,33,33	0
58	MG	2A	3098	1/1	0.97	0.10	39,39,39,39	0
58	MG	2A	3667	1/1	0.97	0.06	48,48,48,48	0
58	MG	2A	3099	1/1	0.97	0.07	34,34,34,34	0
58	MG	1A	3628	1/1	0.97	0.08	10,10,10,10	0
58	MG	1A	3495	1/1	0.97	0.10	39,39,39,39	0
58	MG	1A	3496	1/1	0.97	0.21	25,25,25,25	0
58	MG	1A	3785	1/1	0.97	0.09	31,31,31,31	0
58	MG	1A	3786	1/1	0.97	0.04	33,33,33,33	0
58	MG	2A	3373	1/1	0.97	0.06	39,39,39,39	0
58	MG	1A	3957	1/1	0.97	0.04	39,39,39,39	0
58	MG	1A	3167	1/1	0.97	0.10	36,36,36,36	0
58	MG	2A	3376	1/1	0.97	0.08	42,42,42,42	0
58	MG	2A	3108	1/1	0.97	0.05	47,47,47,47	0
58	MG	1A	3393	1/1	0.97	0.08	29,29,29,29	0
58	MG	1A	3394	1/1	0.97	0.06	36,36,36,36	0
58	MG	1A	3114	1/1	0.97	0.07	26,26,26,26	0
58	MG	1A	3083	1/1	0.97	0.13	27,27,27,27	0
58	MG	1A	3794	1/1	0.97	0.09	23,23,23,23	0
58	MG	2A	3686	1/1	0.97	0.09	38,38,38,38	0
58	MG	1A	3503	1/1	0.97	0.08	21,21,21,21	0
58	MG	1A	3398	1/1	0.97	0.10	40,40,40,40	0
58	MG	1D	302	1/1	0.97	0.04	37,37,37,37	0
58	MG	2a	1670	1/1	0.97	0.13	36,36,36,36	0
58	MG	2A	3387	1/1	0.97	0.15	55,55,55,55	0
58	MG	1D	305	1/1	0.97	0.05	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1D	307	1/1	0.97	0.08	34,34,34,34	0
58	MG	1A	3641	1/1	0.97	0.08	37,37,37,37	0
58	MG	1D	309	1/1	0.97	0.14	30,30,30,30	0
58	MG	2A	3696	1/1	0.97	0.06	56,56,56,56	0
58	MG	2A	3697	1/1	0.97	0.12	28,28,28,28	0
58	MG	1A	3967	1/1	0.97	0.06	35,35,35,35	0
58	MG	2a	1679	1/1	0.97	0.07	42,42,42,42	0
58	MG	2A	3699	1/1	0.97	0.05	50,50,50,50	0
58	MG	1E	303	1/1	0.97	0.08	40,40,40,40	0
58	MG	2A	3701	1/1	0.97	0.05	35,35,35,35	0
58	MG	1a	1720	1/1	0.97	0.05	27,27,27,27	0
58	MG	1E	305	1/1	0.97	0.11	17,17,17,17	0
58	MG	1A	3644	1/1	0.97	0.04	18,18,18,18	0
58	MG	1A	3239	1/1	0.97	0.16	31,31,31,31	0
58	MG	1A	3646	1/1	0.97	0.07	25,25,25,25	0
58	MG	1A	3240	1/1	0.97	0.11	21,21,21,21	0
58	MG	2a	1689	1/1	0.97	0.18	58,58,58,58	0
58	MG	1A	3507	1/1	0.97	0.05	40,40,40,40	0
58	MG	2A	3133	1/1	0.97	0.10	46,46,46,46	0
58	MG	2A	3135	1/1	0.97	0.06	38,38,38,38	0
58	MG	1a	1727	1/1	0.97	0.10	47,47,47,47	0
58	MG	1A	3403	1/1	0.97	0.07	30,30,30,30	0
58	MG	2A	3406	1/1	0.97	0.12	46,46,46,46	0
58	MG	1F	304	1/1	0.97	0.05	21,21,21,21	0
58	MG	1A	3404	1/1	0.97	0.07	39,39,39,39	0
58	MG	1F	306	1/1	0.97	0.21	27,27,27,27	0
58	MG	1F	308	1/1	0.97	0.05	35,35,35,35	0
58	MG	1A	3036	1/1	0.97	0.07	22,22,22,22	0
58	MG	1A	3979	1/1	0.97	0.07	37,37,37,37	0
58	MG	1A	3807	1/1	0.97	0.06	15,15,15,15	0
58	MG	2A	3150	1/1	0.97	0.11	34,34,34,34	0
58	MG	1A	3981	1/1	0.97	0.06	47,47,47,47	0
58	MG	2A	3416	1/1	0.97	0.16	38,38,38,38	0
58	MG	2A	3725	1/1	0.97	0.09	35,35,35,35	0
58	MG	1A	3511	1/1	0.97	0.07	41,41,41,41	0
58	MG	1G	202	1/1	0.97	0.07	45,45,45,45	0
58	MG	1A	3983	1/1	0.97	0.06	54,54,54,54	0
58	MG	2a	1712	1/1	0.97	0.10	58,58,58,58	0
58	MG	1a	1741	1/1	0.97	0.04	35,35,35,35	0
58	MG	2A	3730	1/1	0.97	0.06	39,39,39,39	0
58	MG	1A	3512	1/1	0.97	0.07	42,42,42,42	0
58	MG	1A	3317	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
58	MG	1I	201	1/1	0.97	0.04	35,35,35,35	0
58	MG	2A	3161	1/1	0.97	0.15	37,37,37,37	0
58	MG	2A	3425	1/1	0.97	0.18	38,38,38,38	0
58	MG	2A	3427	1/1	0.97	0.15	43,43,43,43	0
58	MG	1a	1745	1/1	0.97	0.12	59,59,59,59	0
58	MG	2A	3738	1/1	0.97	0.05	46,46,46,46	0
58	MG	1A	3407	1/1	0.97	0.05	36,36,36,36	0
58	MG	1A	3658	1/1	0.97	0.04	15,15,15,15	0
58	MG	1N	203	1/1	0.97	0.04	27,27,27,27	0
58	MG	1A	3515	1/1	0.97	0.05	15,15,15,15	0
58	MG	2A	3168	1/1	0.97	0.11	55,55,55,55	0
58	MG	1N	205	1/1	0.97	0.04	35,35,35,35	0
58	MG	1a	1752	1/1	0.97	0.09	48,48,48,48	0
58	MG	1A	3408	1/1	0.97	0.12	41,41,41,41	0
58	MG	1A	3815	1/1	0.97	0.04	15,15,15,15	0
58	MG	1a	1755	1/1	0.97	0.05	43,43,43,43	0
58	MG	1A	3172	1/1	0.97	0.07	8,8,8,8	0
58	MG	1a	1758	1/1	0.97	0.06	49,49,49,49	0
58	MG	1A	3818	1/1	0.97	0.06	20,20,20,20	0
58	MG	1A	3246	1/1	0.97	0.08	38,38,38,38	0
58	MG	2A	3443	1/1	0.97	0.11	41,41,41,41	0
58	MG	1A	3665	1/1	0.97	0.06	38,38,38,38	0
58	MG	1A	3085	1/1	0.97	0.09	26,26,26,26	0
58	MG	1Q	206	1/1	0.97	0.08	41,41,41,41	0
58	MG	1A	3321	1/1	0.97	0.10	19,19,19,19	0
58	MG	2a	1743	1/1	0.97	0.27	54,54,54,54	0
58	MG	1A	3249	1/1	0.97	0.08	44,44,44,44	0
58	MG	2a	1745	1/1	0.97	0.12	44,44,44,44	0
58	MG	1A	3174	1/1	0.97	0.07	36,36,36,36	0
58	MG	1A	3416	1/1	0.97	0.10	30,30,30,30	0
58	MG	1A	3029	1/1	0.97	0.05	23,23,23,23	0
58	MG	2a	1749	1/1	0.97	0.09	54,54,54,54	0
58	MG	1A	3418	1/1	0.97	0.12	36,36,36,36	0
58	MG	1A	3087	1/1	0.97	0.07	22,22,22,22	0
58	MG	1A	3088	1/1	0.97	0.07	24,24,24,24	0
58	MG	2a	1753	1/1	0.97	0.07	56,56,56,56	0
58	MG	1A	3126	1/1	0.97	0.18	22,22,22,22	0
58	MG	2A	3767	1/1	0.97	0.07	33,33,33,33	0
58	MG	2a	1756	1/1	0.97	0.05	57,57,57,57	0
58	MG	1U	202	1/1	0.97	0.17	31,31,31,31	0
58	MG	1U	204	1/1	0.97	0.06	33,33,33,33	0
58	MG	1U	205	1/1	0.97	0.17	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3676	1/1	0.97	0.08	33,33,33,33	0
58	MG	2A	3461	1/1	0.97	0.19	45,45,45,45	0
58	MG	2a	1762	1/1	0.97	0.17	56,56,56,56	0
58	MG	2A	3462	1/1	0.97	0.10	45,45,45,45	0
58	MG	2A	3775	1/1	0.97	0.05	34,34,34,34	0
58	MG	1V	201	1/1	0.97	0.08	19,19,19,19	0
58	MG	1A	3034	1/1	0.97	0.15	23,23,23,23	0
58	MG	1A	3533	1/1	0.97	0.10	32,32,32,32	0
58	MG	2a	1769	1/1	0.97	0.09	42,42,42,42	0
58	MG	1A	3838	1/1	0.97	0.06	28,28,28,28	0
58	MG	2A	3781	1/1	0.97	0.06	51,51,51,51	0
58	MG	2A	3199	1/1	0.97	0.05	37,37,37,37	0
58	MG	1A	3535	1/1	0.97	0.12	33,33,33,33	0
58	MG	1A	3257	1/1	0.97	0.10	21,21,21,21	0
58	MG	1W	203	1/1	0.97	0.05	23,23,23,23	0
58	MG	1a	1787	1/1	0.97	0.08	46,46,46,46	0
58	MG	1W	204	1/1	0.97	0.05	28,28,28,28	0
58	MG	1X	102	1/1	0.97	0.10	37,37,37,37	0
58	MG	2A	3789	1/1	0.97	0.06	32,32,32,32	0
58	MG	2A	3790	1/1	0.97	0.06	52,52,52,52	0
58	MG	1A	3044	1/1	0.97	0.12	28,28,28,28	0
58	MG	2A	3477	1/1	0.97	0.09	34,34,34,34	0
58	MG	2A	3479	1/1	0.97	0.18	38,38,38,38	0
58	MG	2A	3794	1/1	0.97	0.09	47,47,47,47	0
58	MG	1A	3045	1/1	0.97	0.04	29,29,29,29	0
58	MG	2A	3796	1/1	0.97	0.09	33,33,33,33	0
58	MG	1A	3260	1/1	0.97	0.05	29,29,29,29	0
58	MG	1Y	202	1/1	0.97	0.06	55,55,55,55	0
58	MG	1A	3844	1/1	0.97	0.09	42,42,42,42	0
58	MG	1a	1796	1/1	0.97	0.05	51,51,51,51	0
58	MG	1A	3540	1/1	0.97	0.13	32,32,32,32	0
58	MG	1A	3541	1/1	0.97	0.10	40,40,40,40	0
58	MG	2a	1795	1/1	0.97	0.09	41,41,41,41	0
58	MG	1A	4019	1/1	0.97	0.09	20,20,20,20	0
58	MG	10	102	1/1	0.97	0.10	44,44,44,44	0
58	MG	1A	3687	1/1	0.97	0.05	23,23,23,23	0
58	MG	2A	3806	1/1	0.97	0.05	47,47,47,47	0
58	MG	2A	3807	1/1	0.97	0.08	40,40,40,40	0
58	MG	2A	3808	1/1	0.97	0.04	36,36,36,36	0
58	MG	2A	3217	1/1	0.97	0.07	40,40,40,40	0
58	MG	1A	3193	1/1	0.97	0.12	21,21,21,21	0
58	MG	1A	3194	1/1	0.97	0.05	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3544	1/1	0.97	0.19	44,44,44,44	0
58	MG	2A	3496	1/1	0.97	0.04	42,42,42,42	0
58	MG	1a	1805	1/1	0.97	0.15	52,52,52,52	0
58	MG	1A	3545	1/1	0.97	0.09	21,21,21,21	0
58	MG	2A	3499	1/1	0.97	0.13	51,51,51,51	0
58	MG	1A	3336	1/1	0.97	0.07	35,35,35,35	0
58	MG	1A	3694	1/1	0.97	0.10	16,16,16,16	0
58	MG	2A	3820	1/1	0.97	0.07	43,43,43,43	0
58	MG	2A	3502	1/1	0.97	0.06	33,33,33,33	0
58	MG	2A	3504	1/1	0.97	0.10	32,32,32,32	0
58	MG	1A	3131	1/1	0.97	0.12	56,56,56,56	0
58	MG	1A	4028	1/1	0.97	0.05	35,35,35,35	0
58	MG	2A	3828	1/1	0.97	0.09	51,51,51,51	0
58	MG	1A	3857	1/1	0.97	0.08	36,36,36,36	0
58	MG	1A	3046	1/1	0.97	0.05	17,17,17,17	0
58	MG	1A	3048	1/1	0.97	0.08	33,33,33,33	0
58	MG	13	103	1/1	0.97	0.14	34,34,34,34	0
58	MG	1A	4032	1/1	0.97	0.05	34,34,34,34	0
58	MG	1e	201	1/1	0.97	0.08	53,53,53,53	0
58	MG	13	105	1/1	0.97	0.04	37,37,37,37	0
58	MG	2A	3234	1/1	0.97	0.10	37,37,37,37	0
58	MG	1f	201	1/1	0.97	0.19	43,43,43,43	0
58	MG	1A	3199	1/1	0.97	0.06	39,39,39,39	0
58	MG	1k	201	1/1	0.97	0.11	41,41,41,41	0
58	MG	2a	1830	1/1	0.97	0.07	50,50,50,50	0
58	MG	1A	3699	1/1	0.97	0.03	19,19,19,19	0
58	MG	15	101	1/1	0.97	0.13	24,24,24,24	0
58	MG	2A	3240	1/1	0.97	0.07	40,40,40,40	0
58	MG	1A	3200	1/1	0.97	0.07	21,21,21,21	0
58	MG	2A	3242	1/1	0.97	0.12	42,42,42,42	0
58	MG	1A	3863	1/1	0.97	0.07	14,14,14,14	0
58	MG	2e	201	1/1	0.97	0.06	47,47,47,47	0
58	MG	2f	201	1/1	0.97	0.07	38,38,38,38	0
58	MG	2A	3244	1/1	0.97	0.07	43,43,43,43	0
58	MG	2A	3527	1/1	0.97	0.06	32,32,32,32	0
58	MG	15	104	1/1	0.97	0.17	24,24,24,24	0
58	MG	15	105	1/1	0.97	0.09	23,23,23,23	0
58	MG	2A	3531	1/1	0.97	0.09	36,36,36,36	0
58	MG	1A	3202	1/1	0.97	0.10	23,23,23,23	0
58	MG	1A	3343	1/1	0.97	0.18	24,24,24,24	0
58	MG	1A	3442	1/1	0.97	0.07	45,45,45,45	0
58	MG	2A	3855	1/1	0.97	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3269	1/1	0.97	0.07	46,46,46,46	0
58	MG	17	101	1/1	0.97	0.04	23,23,23,23	0
58	MG	17	104	1/1	0.97	0.09	44,44,44,44	0
58	MG	1A	3096	1/1	0.97	0.07	31,31,31,31	0
58	MG	1A	3138	1/1	0.97	0.05	18,18,18,18	0
58	MG	1x	101	1/1	0.97	0.16	50,50,50,50	0
58	MG	2v	101	1/1	0.97	0.18	52,52,52,52	0
58	MG	1A	3446	1/1	0.97	0.14	48,48,48,48	0
58	MG	1A	3139	1/1	0.97	0.22	32,32,32,32	0
58	MG	1A	3209	1/1	0.97	0.13	27,27,27,27	0
58	MG	1A	3564	1/1	0.97	0.09	26,26,26,26	0
58	MG	1A	3352	1/1	0.97	0.07	30,30,30,30	0
58	MG	2A	3867	1/1	0.97	0.06	38,38,38,38	0
58	MG	1A	3274	1/1	0.97	0.19	32,32,32,32	0
58	MG	1A	3275	1/1	0.97	0.10	17,17,17,17	0
58	MG	1a	1606	1/1	0.97	0.11	41,41,41,41	0
58	MG	2A	3549	1/1	0.97	0.04	41,41,41,41	0
58	MG	1A	4051	1/1	0.97	0.06	26,26,26,26	0
58	MG	1a	1608	1/1	0.97	0.06	43,43,43,43	0
58	MG	2A	3552	1/1	0.97	0.06	40,40,40,40	0
58	MG	1A	3276	1/1	0.97	0.05	32,32,32,32	0
59	K	1A	3569	1/1	0.97	0.05	37,37,37,37	0
58	MG	2B	208	1/1	0.97	0.13	48,48,48,48	0
58	MG	2B	209	1/1	0.97	0.07	49,49,49,49	0
60	ZN	2n	102	1/1	0.97	0.05	77,77,77,77	0
58	MG	1A	3108	1/1	0.98	0.08	30,30,30,30	0
58	MG	2A	3714	1/1	0.98	0.06	30,30,30,30	0
58	MG	1A	3721	1/1	0.98	0.03	29,29,29,29	0
58	MG	1A	4008	1/1	0.98	0.07	16,16,16,16	0
58	MG	2A	3478	1/1	0.98	0.09	51,51,51,51	0
58	MG	1A	3159	1/1	0.98	0.07	29,29,29,29	0
58	MG	1F	307	1/1	0.98	0.06	32,32,32,32	0
58	MG	1A	3400	1/1	0.98	0.06	29,29,29,29	0
58	MG	1A	3401	1/1	0.98	0.04	20,20,20,20	0
58	MG	1F	310	1/1	0.98	0.10	21,21,21,21	0
58	MG	1A	3230	1/1	0.98	0.04	25,25,25,25	0
58	MG	2A	3485	1/1	0.98	0.09	43,43,43,43	0
58	MG	2A	3486	1/1	0.98	0.05	22,22,22,22	0
58	MG	1A	3231	1/1	0.98	0.10	19,19,19,19	0
58	MG	1A	3232	1/1	0.98	0.07	21,21,21,21	0
58	MG	1a	1689	1/1	0.98	0.17	30,30,30,30	0
58	MG	1A	4015	1/1	0.98	0.03	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1G	201	1/1	0.98	0.10	32,32,32,32	0
58	MG	1A	3728	1/1	0.98	0.05	21,21,21,21	0
58	MG	1A	3109	1/1	0.98	0.12	24,24,24,24	0
58	MG	1A	3234	1/1	0.98	0.07	33,33,33,33	0
58	MG	1A	3501	1/1	0.98	0.05	46,46,46,46	0
58	MG	1H	201	1/1	0.98	0.15	40,40,40,40	0
58	MG	1A	3733	1/1	0.98	0.10	19,19,19,19	0
58	MG	1A	3871	1/1	0.98	0.20	27,27,27,27	0
58	MG	1A	3610	1/1	0.98	0.17	34,34,34,34	0
58	MG	1A	3611	1/1	0.98	0.05	30,30,30,30	0
58	MG	1A	3736	1/1	0.98	0.07	51,51,51,51	0
58	MG	1A	3161	1/1	0.98	0.05	28,28,28,28	0
58	MG	1A	3078	1/1	0.98	0.07	22,22,22,22	0
58	MG	1A	3739	1/1	0.98	0.05	54,54,54,54	0
58	MG	2A	3506	1/1	0.98	0.07	51,51,51,51	0
58	MG	1A	3409	1/1	0.98	0.12	34,34,34,34	0
58	MG	2A	3746	1/1	0.98	0.09	31,31,31,31	0
58	MG	2A	3508	1/1	0.98	0.08	55,55,55,55	0
58	MG	1A	3237	1/1	0.98	0.10	32,32,32,32	0
58	MG	1A	3742	1/1	0.98	0.06	26,26,26,26	0
58	MG	1P	204	1/1	0.98	0.08	34,34,34,34	0
58	MG	1Q	201	1/1	0.98	0.17	29,29,29,29	0
58	MG	2A	3069	1/1	0.98	0.06	27,27,27,27	0
58	MG	2A	3287	1/1	0.98	0.18	48,48,48,48	0
58	MG	1A	3079	1/1	0.98	0.08	27,27,27,27	0
58	MG	1Q	203	1/1	0.98	0.04	25,25,25,25	0
58	MG	1Q	204	1/1	0.98	0.05	37,37,37,37	0
58	MG	1A	3051	1/1	0.98	0.05	15,15,15,15	0
58	MG	1A	3168	1/1	0.98	0.11	24,24,24,24	0
58	MG	1a	1715	1/1	0.98	0.06	37,37,37,37	0
58	MG	1A	3242	1/1	0.98	0.08	15,15,15,15	0
58	MG	1A	3081	1/1	0.98	0.11	28,28,28,28	0
58	MG	1R	201	1/1	0.98	0.16	36,36,36,36	0
58	MG	1a	1719	1/1	0.98	0.09	33,33,33,33	0
58	MG	1R	202	1/1	0.98	0.04	26,26,26,26	0
58	MG	1A	3887	1/1	0.98	0.09	16,16,16,16	0
58	MG	1A	3245	1/1	0.98	0.08	34,34,34,34	0
58	MG	1A	3052	1/1	0.98	0.06	17,17,17,17	0
58	MG	2A	3529	1/1	0.98	0.04	37,37,37,37	0
58	MG	1A	4039	1/1	0.98	0.04	19,19,19,19	0
58	MG	1A	3247	1/1	0.98	0.04	31,31,31,31	0
58	MG	1A	3023	1/1	0.98	0.04	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3772	1/1	0.98	0.09	46,46,46,46	0
58	MG	1A	3625	1/1	0.98	0.06	31,31,31,31	0
58	MG	1A	3004	1/1	0.98	0.03	16,16,16,16	0
58	MG	1U	203	1/1	0.98	0.15	26,26,26,26	0
58	MG	1A	3331	1/1	0.98	0.03	29,29,29,29	0
58	MG	2A	3777	1/1	0.98	0.11	40,40,40,40	0
58	MG	1A	3755	1/1	0.98	0.06	17,17,17,17	0
58	MG	1U	206	1/1	0.98	0.09	20,20,20,20	0
58	MG	1A	3756	1/1	0.98	0.05	11,11,11,11	0
58	MG	1a	1734	1/1	0.98	0.05	37,37,37,37	0
58	MG	1U	208	1/1	0.98	0.13	25,25,25,25	0
58	MG	1U	209	1/1	0.98	0.12	25,25,25,25	0
58	MG	1U	211	1/1	0.98	0.08	28,28,28,28	0
58	MG	1A	3422	1/1	0.98	0.14	36,36,36,36	0
58	MG	1A	3056	1/1	0.98	0.06	32,32,32,32	0
58	MG	1V	204	1/1	0.98	0.04	27,27,27,27	0
58	MG	1A	3119	1/1	0.98	0.06	27,27,27,27	0
58	MG	2A	3103	1/1	0.98	0.04	26,26,26,26	0
58	MG	1A	3425	1/1	0.98	0.06	33,33,33,33	0
58	MG	2a	1696	1/1	0.98	0.11	43,43,43,43	0
58	MG	1A	3176	1/1	0.98	0.15	26,26,26,26	0
58	MG	1A	3633	1/1	0.98	0.03	19,19,19,19	0
58	MG	1A	3634	1/1	0.98	0.03	21,21,21,21	0
58	MG	1A	3522	1/1	0.98	0.12	23,23,23,23	0
58	MG	1X	101	1/1	0.98	0.07	37,37,37,37	0
58	MG	1A	3636	1/1	0.98	0.04	36,36,36,36	0
58	MG	1X	103	1/1	0.98	0.09	30,30,30,30	0
58	MG	1A	3523	1/1	0.98	0.06	21,21,21,21	0
58	MG	2A	3113	1/1	0.98	0.10	50,50,50,50	0
58	MG	1A	3177	1/1	0.98	0.09	23,23,23,23	0
58	MG	1A	3428	1/1	0.98	0.06	31,31,31,31	0
58	MG	1A	3429	1/1	0.98	0.07	34,34,34,34	0
58	MG	1Y	203	1/1	0.98	0.10	31,31,31,31	0
58	MG	1A	3178	1/1	0.98	0.07	22,22,22,22	0
58	MG	2A	3564	1/1	0.98	0.05	36,36,36,36	0
58	MG	1A	3772	1/1	0.98	0.07	34,34,34,34	0
58	MG	1A	3913	1/1	0.98	0.04	44,44,44,44	0
58	MG	1A	3642	1/1	0.98	0.03	16,16,16,16	0
58	MG	2A	3122	1/1	0.98	0.10	46,46,46,46	0
58	MG	1A	3643	1/1	0.98	0.02	21,21,21,21	0
58	MG	10	103	1/1	0.98	0.07	30,30,30,30	0
58	MG	2A	3125	1/1	0.98	0.05	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3037	1/1	0.98	0.07	16,16,16,16	0
58	MG	1A	3180	1/1	0.98	0.03	16,16,16,16	0
58	MG	1A	4068	1/1	0.98	0.04	11,11,11,11	0
58	MG	1A	3181	1/1	0.98	0.04	27,27,27,27	0
58	MG	1A	3531	1/1	0.98	0.07	41,41,41,41	0
58	MG	1A	3121	1/1	0.98	0.04	28,28,28,28	0
58	MG	1A	3059	1/1	0.98	0.07	30,30,30,30	0
58	MG	1A	3123	1/1	0.98	0.09	32,32,32,32	0
58	MG	2A	3134	1/1	0.98	0.06	43,43,43,43	0
58	MG	1A	4074	1/1	0.98	0.06	21,21,21,21	0
58	MG	2A	3824	1/1	0.98	0.04	41,41,41,41	0
58	MG	1A	3060	1/1	0.98	0.04	33,33,33,33	0
58	MG	2A	3827	1/1	0.98	0.07	54,54,54,54	0
58	MG	12	101	1/1	0.98	0.08	40,40,40,40	0
58	MG	1A	3926	1/1	0.98	0.03	22,22,22,22	0
58	MG	2A	3140	1/1	0.98	0.10	30,30,30,30	0
58	MG	1a	1776	1/1	0.98	0.06	40,40,40,40	0
58	MG	2a	1736	1/1	0.98	0.22	49,49,49,49	0
58	MG	1A	3187	1/1	0.98	0.04	28,28,28,28	0
58	MG	2A	3143	1/1	0.98	0.07	32,32,32,32	0
58	MG	2A	3144	1/1	0.98	0.13	41,41,41,41	0
58	MG	1a	1778	1/1	0.98	0.05	46,46,46,46	0
58	MG	13	102	1/1	0.98	0.07	25,25,25,25	0
58	MG	2A	3592	1/1	0.98	0.09	36,36,36,36	0
58	MG	1A	4078	1/1	0.98	0.04	45,45,45,45	0
58	MG	2A	3148	1/1	0.98	0.09	36,36,36,36	0
58	MG	1A	3439	1/1	0.98	0.05	31,31,31,31	0
58	MG	1A	3188	1/1	0.98	0.13	40,40,40,40	0
58	MG	1A	3656	1/1	0.98	0.06	15,15,15,15	0
58	MG	2A	3598	1/1	0.98	0.08	36,36,36,36	0
58	MG	2A	3599	1/1	0.98	0.04	32,32,32,32	0
58	MG	1A	3189	1/1	0.98	0.14	40,40,40,40	0
58	MG	2A	3153	1/1	0.98	0.04	40,40,40,40	0
58	MG	1A	3125	1/1	0.98	0.12	25,25,25,25	0
58	MG	1A	3191	1/1	0.98	0.16	32,32,32,32	0
58	MG	1A	3790	1/1	0.98	0.03	27,27,27,27	0
58	MG	2A	3157	1/1	0.98	0.06	43,43,43,43	0
58	MG	1A	3660	1/1	0.98	0.04	25,25,25,25	0
58	MG	1A	4089	1/1	0.98	0.08	48,48,48,48	0
58	MG	1A	3792	1/1	0.98	0.06	34,34,34,34	0
58	MG	1A	3012	1/1	0.98	0.04	24,24,24,24	0
58	MG	1A	3127	1/1	0.98	0.04	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	2A	3163	1/1	0.98	0.04	54,54,54,54	0
58	MG	1A	3090	1/1	0.98	0.06	28,28,28,28	0
58	MG	2A	3381	1/1	0.98	0.06	28,28,28,28	0
58	MG	1A	3940	1/1	0.98	0.03	23,23,23,23	0
58	MG	17	102	1/1	0.98	0.09	23,23,23,23	0
58	MG	2A	3616	1/1	0.98	0.05	43,43,43,43	0
58	MG	17	103	1/1	0.98	0.05	31,31,31,31	0
58	MG	2a	1768	1/1	0.98	0.05	57,57,57,57	0
58	MG	1A	3664	1/1	0.98	0.07	37,37,37,37	0
58	MG	17	105	1/1	0.98	0.03	28,28,28,28	0
58	MG	1A	3942	1/1	0.98	0.03	9,9,9,9	0
58	MG	18	102	1/1	0.98	0.12	40,40,40,40	0
58	MG	1A	3195	1/1	0.98	0.15	25,25,25,25	0
58	MG	1A	3041	1/1	0.98	0.05	26,26,26,26	0
58	MG	1A	3018	1/1	0.98	0.09	17,17,17,17	0
58	MG	2a	1776	1/1	0.98	0.07	49,49,49,49	0
58	MG	1A	3358	1/1	0.98	0.07	24,24,24,24	0
58	MG	2a	1778	1/1	0.98	0.04	38,38,38,38	0
58	MG	1A	3359	1/1	0.98	0.06	48,48,48,48	0
58	MG	2B	204	1/1	0.98	0.05	54,54,54,54	0
58	MG	1A	3007	1/1	0.98	0.05	20,20,20,20	0
58	MG	1A	3094	1/1	0.98	0.04	31,31,31,31	0
58	MG	2A	3396	1/1	0.98	0.10	32,32,32,32	0
58	MG	1A	3066	1/1	0.98	0.07	34,34,34,34	0
58	MG	1A	3805	1/1	0.98	0.06	41,41,41,41	0
58	MG	1A	3277	1/1	0.98	0.13	34,34,34,34	0
58	MG	1A	3201	1/1	0.98	0.06	34,34,34,34	0
58	MG	1A	3556	1/1	0.98	0.07	46,46,46,46	0
58	MG	1A	3134	1/1	0.98	0.15	25,25,25,25	0
58	MG	1A	3281	1/1	0.98	0.07	24,24,24,24	0
58	MG	1A	3135	1/1	0.98	0.05	33,33,33,33	0
58	MG	1A	3560	1/1	0.98	0.09	24,24,24,24	0
58	MG	1A	3561	1/1	0.98	0.09	15,15,15,15	0
58	MG	1A	3204	1/1	0.98	0.10	27,27,27,27	0
58	MG	1A	3284	1/1	0.98	0.11	27,27,27,27	0
58	MG	2A	3643	1/1	0.98	0.05	37,37,37,37	0
58	MG	1A	3816	1/1	0.98	0.03	11,11,11,11	0
58	MG	1A	3136	1/1	0.98	0.03	29,29,29,29	0
58	MG	2D	304	1/1	0.98	0.04	31,31,31,31	0
58	MG	1A	3565	1/1	0.98	0.07	24,24,24,24	0
58	MG	1A	3207	1/1	0.98	0.05	27,27,27,27	0
58	MG	1n	102	1/1	0.98	0.08	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3010	1/1	0.98	0.03	17,17,17,17	0
58	MG	1A	3097	1/1	0.98	0.03	22,22,22,22	0
58	MG	1A	3969	1/1	0.98	0.04	32,32,32,32	0
58	MG	2E	304	1/1	0.98	0.07	32,32,32,32	0
58	MG	1A	3822	1/1	0.98	0.04	22,22,22,22	0
58	MG	1A	3098	1/1	0.98	0.12	14,14,14,14	0
58	MG	1A	3291	1/1	0.98	0.04	44,44,44,44	0
58	MG	2E	308	1/1	0.98	0.12	32,32,32,32	0
58	MG	2F	301	1/1	0.98	0.09	36,36,36,36	0
58	MG	1A	3973	1/1	0.98	0.08	26,26,26,26	0
58	MG	1w	106	1/1	0.98	0.10	43,43,43,43	0
58	MG	1A	3021	1/1	0.98	0.07	11,11,11,11	0
58	MG	1B	221	1/1	0.98	0.05	25,25,25,25	0
58	MG	1a	1632	1/1	0.98	0.16	49,49,49,49	0
58	MG	1A	3293	1/1	0.98	0.17	27,27,27,27	0
58	MG	2A	3426	1/1	0.98	0.23	48,48,48,48	0
58	MG	1A	3471	1/1	0.98	0.05	20,20,20,20	0
58	MG	1A	3977	1/1	0.98	0.05	41,41,41,41	0
58	MG	1A	3047	1/1	0.98	0.04	25,25,25,25	0
58	MG	1A	3576	1/1	0.98	0.10	39,39,39,39	0
58	MG	2a	1823	1/1	0.98	0.10	39,39,39,39	0
58	MG	1A	3143	1/1	0.98	0.06	9,9,9,9	0
58	MG	1A	3101	1/1	0.98	0.04	38,38,38,38	0
58	MG	1A	3146	1/1	0.98	0.06	29,29,29,29	0
58	MG	1A	3834	1/1	0.98	0.05	21,21,21,21	0
58	MG	1A	3580	1/1	0.98	0.07	27,27,27,27	0
58	MG	1A	3148	1/1	0.98	0.10	24,24,24,24	0
58	MG	1a	1644	1/1	0.98	0.14	51,51,51,51	0
58	MG	1A	3149	1/1	0.98	0.03	25,25,25,25	0
58	MG	2A	3674	1/1	0.98	0.05	32,32,32,32	0
58	MG	1A	3583	1/1	0.98	0.08	40,40,40,40	0
58	MG	1A	3219	1/1	0.98	0.08	28,28,28,28	0
58	MG	2X	102	1/1	0.98	0.07	32,32,32,32	0
58	MG	1a	1648	1/1	0.98	0.11	40,40,40,40	0
58	MG	1A	3387	1/1	0.98	0.09	24,24,24,24	0
58	MG	2A	3679	1/1	0.98	0.07	35,35,35,35	0
58	MG	1A	3071	1/1	0.98	0.06	9,9,9,9	0
58	MG	1A	3221	1/1	0.98	0.07	31,31,31,31	0
58	MG	1A	3072	1/1	0.98	0.10	20,20,20,20	0
58	MG	1A	3483	1/1	0.98	0.06	36,36,36,36	0
58	MG	23	102	1/1	0.98	0.04	40,40,40,40	0
58	MG	1D	303	1/1	0.98	0.07	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1D	304	1/1	0.98	0.05	36,36,36,36	0
58	MG	1A	3391	1/1	0.98	0.10	23,23,23,23	0
58	MG	1A	3030	1/1	0.98	0.12	24,24,24,24	0
58	MG	2A	3015	1/1	0.98	0.08	42,42,42,42	0
58	MG	1A	3486	1/1	0.98	0.14	27,27,27,27	0
58	MG	2A	3690	1/1	0.98	0.13	53,53,53,53	0
58	MG	1A	3594	1/1	0.98	0.05	34,34,34,34	0
58	MG	2A	3454	1/1	0.98	0.17	33,33,33,33	0
58	MG	1A	3714	1/1	0.98	0.04	10,10,10,10	0
58	MG	1E	302	1/1	0.98	0.09	28,28,28,28	0
58	MG	1A	3153	1/1	0.98	0.15	27,27,27,27	0
58	MG	1A	3049	1/1	0.98	0.06	15,15,15,15	0
58	MG	1a	1665	1/1	0.98	0.05	51,51,51,51	0
58	MG	1A	3395	1/1	0.98	0.23	28,28,28,28	0
58	MG	1E	307	1/1	0.98	0.05	29,29,29,29	0
58	MG	1A	3854	1/1	0.98	0.04	33,33,33,33	0
58	MG	1E	310	1/1	0.98	0.09	16,16,16,16	0
58	MG	1A	3022	1/1	0.98	0.05	33,33,33,33	0
58	MG	1A	3856	1/1	0.98	0.05	43,43,43,43	0
58	MG	1E	313	1/1	0.98	0.07	36,36,36,36	0
58	MG	2A	3467	1/1	0.98	0.10	47,47,47,47	0
58	MG	2A	3030	1/1	0.98	0.10	37,37,37,37	0
58	MG	1A	3107	1/1	0.98	0.03	17,17,17,17	0
58	MG	2A	3470	1/1	0.98	0.10	22,22,22,22	0
58	MG	1F	301	1/1	0.98	0.07	26,26,26,26	0
58	MG	1F	302	1/1	0.98	0.04	24,24,24,24	0
58	MG	1a	1676	1/1	0.98	0.12	43,43,43,43	0
60	ZN	24	501	1/1	0.98	0.07	99,99,99,99	0
60	ZN	25	107	1/1	0.98	0.05	51,51,51,51	0
58	MG	1a	1677	1/1	0.98	0.07	37,37,37,37	0
61	SF4	2d	303	8/8	0.98	0.06	56,63,69,75	0
58	MG	1V	202	1/1	0.99	0.09	21,21,21,21	0
58	MG	2A	3138	1/1	0.99	0.03	31,31,31,31	0
58	MG	1A	3075	1/1	0.99	0.02	22,22,22,22	0
58	MG	1A	3142	1/1	0.99	0.04	20,20,20,20	0
58	MG	1A	3076	1/1	0.99	0.02	15,15,15,15	0
58	MG	1a	1756	1/1	0.99	0.10	45,45,45,45	0
58	MG	1a	1611	1/1	0.99	0.05	18,18,18,18	0
58	MG	1A	3144	1/1	0.99	0.05	42,42,42,42	0
58	MG	1A	3384	1/1	0.99	0.05	23,23,23,23	0
58	MG	1B	203	1/1	0.99	0.08	38,38,38,38	0
58	MG	1A	3950	1/1	0.99	0.07	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3280	1/1	0.99	0.09	19,19,19,19	0
58	MG	1A	3348	1/1	0.99	0.15	25,25,25,25	0
58	MG	1a	1618	1/1	0.99	0.04	40,40,40,40	0
58	MG	2A	3639	1/1	0.99	0.07	34,34,34,34	0
58	MG	1a	1765	1/1	0.99	0.05	38,38,38,38	0
58	MG	1A	3349	1/1	0.99	0.05	25,25,25,25	0
58	MG	1A	3061	1/1	0.99	0.05	24,24,24,24	0
58	MG	1X	104	1/1	0.99	0.03	38,38,38,38	0
58	MG	1A	3351	1/1	0.99	0.06	29,29,29,29	0
58	MG	1A	3039	1/1	0.99	0.11	28,28,28,28	0
58	MG	1A	3252	1/1	0.99	0.09	24,24,24,24	0
58	MG	1A	3031	1/1	0.99	0.04	22,22,22,22	0
58	MG	2A	3814	1/1	0.99	0.09	43,43,43,43	0
58	MG	1A	3285	1/1	0.99	0.18	29,29,29,29	0
58	MG	1A	3591	1/1	0.99	0.03	24,24,24,24	0
58	MG	1A	4067	1/1	0.99	0.03	31,31,31,31	0
58	MG	1A	3032	1/1	0.99	0.04	18,18,18,18	0
58	MG	1A	3765	1/1	0.99	0.07	17,17,17,17	0
58	MG	1A	3033	1/1	0.99	0.20	25,25,25,25	0
58	MG	1A	3053	1/1	0.99	0.07	32,32,32,32	0
58	MG	1B	220	1/1	0.99	0.06	33,33,33,33	0
58	MG	1A	3175	1/1	0.99	0.07	19,19,19,19	0
58	MG	1A	3043	1/1	0.99	0.11	23,23,23,23	0
58	MG	1A	3116	1/1	0.99	0.05	29,29,29,29	0
58	MG	2A	3826	1/1	0.99	0.04	49,49,49,49	0
58	MG	1A	3008	1/1	0.99	0.08	15,15,15,15	0
58	MG	2A	3013	1/1	0.99	0.09	32,32,32,32	0
58	MG	2A	3092	1/1	0.99	0.06	31,31,31,31	0
58	MG	2A	3830	1/1	0.99	0.04	53,53,53,53	0
58	MG	1A	3009	1/1	0.99	0.04	19,19,19,19	0
58	MG	1A	3070	1/1	0.99	0.05	11,11,11,11	0
58	MG	1A	3684	1/1	0.99	0.03	16,16,16,16	0
58	MG	2a	1832	1/1	0.99	0.05	56,56,56,56	0
58	MG	1A	3729	1/1	0.99	0.07	25,25,25,25	0
58	MG	2A	3177	1/1	0.99	0.07	39,39,39,39	0
58	MG	1A	4080	1/1	0.99	0.08	30,30,30,30	0
58	MG	2A	3503	1/1	0.99	0.07	42,42,42,42	0
58	MG	1A	3206	1/1	0.99	0.07	16,16,16,16	0
58	MG	1A	3057	1/1	0.99	0.06	31,31,31,31	0
58	MG	1P	201	1/1	0.99	0.06	16,16,16,16	0
58	MG	1P	202	1/1	0.99	0.03	24,24,24,24	0
58	MG	1a	1794	1/1	0.99	0.03	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3922	1/1	0.99	0.05	30,30,30,30	0
58	MG	1A	3182	1/1	0.99	0.06	29,29,29,29	0
58	MG	1A	3158	1/1	0.99	0.11	21,21,21,21	0
58	MG	1A	4086	1/1	0.99	0.04	23,23,23,23	0
58	MG	1A	3925	1/1	0.99	0.07	31,31,31,31	0
58	MG	1A	3874	1/1	0.99	0.03	33,33,33,33	0
58	MG	1a	1653	1/1	0.99	0.06	39,39,39,39	0
58	MG	1A	3689	1/1	0.99	0.03	21,21,21,21	0
58	MG	1A	3827	1/1	0.99	0.03	16,16,16,16	0
58	MG	1A	3299	1/1	0.99	0.06	34,34,34,34	0
58	MG	2A	3034	1/1	0.99	0.04	35,35,35,35	0
58	MG	1A	3370	1/1	0.99	0.13	31,31,31,31	0
58	MG	1A	3003	1/1	0.99	0.09	26,26,26,26	0
58	MG	1A	3238	1/1	0.99	0.05	57,57,57,57	0
58	MG	1D	306	1/1	0.99	0.04	35,35,35,35	0
58	MG	1A	3014	1/1	0.99	0.04	18,18,18,18	0
58	MG	1A	3038	1/1	0.99	0.06	16,16,16,16	0
58	MG	1A	3162	1/1	0.99	0.04	19,19,19,19	0
58	MG	1A	3835	1/1	0.99	0.03	23,23,23,23	0
58	MG	1E	301	1/1	0.99	0.05	28,28,28,28	0
58	MG	1U	201	1/1	0.99	0.04	15,15,15,15	0
58	MG	1A	3653	1/1	0.99	0.04	10,10,10,10	0
58	MG	1A	3214	1/1	0.99	0.23	27,27,27,27	0
58	MG	18	103	1/1	0.99	0.04	30,30,30,30	0
58	MG	1E	304	1/1	0.99	0.06	20,20,20,20	0
58	MG	1A	3453	1/1	0.99	0.08	25,25,25,25	0
58	MG	1A	3888	1/1	0.99	0.15	28,28,28,28	0
58	MG	2a	1694	1/1	0.99	0.14	39,39,39,39	0
58	MG	1A	3163	1/1	0.99	0.04	18,18,18,18	0
58	MG	1E	308	1/1	0.99	0.04	26,26,26,26	0
60	ZN	1Y	204	1/1	0.99	0.02	54,54,54,54	0
60	ZN	14	102	1/1	0.99	0.09	80,80,80,80	0
60	ZN	15	108	1/1	0.99	0.02	35,35,35,35	0
60	ZN	19	102	1/1	0.99	0.03	38,38,38,38	0
60	ZN	1n	103	1/1	0.99	0.03	53,53,53,53	0
58	MG	1A	3244	1/1	0.99	0.07	28,28,28,28	0
58	MG	1U	210	1/1	0.99	0.07	26,26,26,26	0
58	MG	1A	3534	1/1	0.99	0.08	30,30,30,30	0
60	ZN	26	501	1/1	0.99	0.02	50,50,50,50	0
60	ZN	29	501	1/1	0.99	0.05	55,55,55,55	0
58	MG	1a	1750	1/1	0.99	0.13	36,36,36,36	0
61	SF4	1d	302	8/8	0.99	0.04	48,53,54,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
58	MG	1A	3164	1/1	0.99	0.22	23,23,23,23	0
58	MG	1P	203	1/1	1.00	0.10	23,23,23,23	0
60	ZN	16	103	1/1	1.00	0.03	35,35,35,35	0
58	MG	1A	3308	1/1	1.00	0.02	16,16,16,16	0
58	MG	1A	3147	1/1	1.00	0.14	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.