Full wwPDB X-ray Structure Validation Report (i)

Apr 26, 2026 – 08:28 AM EDT

PDB ID	:	8UD6 / pdb_00008ud6
Title	:	Crystal structure of the wild-type Thermus thermophilus 70S ribosome in complex with cresomycin, mRNA, deacylated A-site tRNAphe, aminoacylated P-site fMet-tRNAmet, and deacylated E-site tRNAphe at 2.70A resolution
Authors	:	Aleksandrova, E.V.; Syroegin, E.A.; Wu, K.J.Y.; Tresco, B.I.C.; Ramkissoon, A.; See, D.N.Y.; Liow, P.; Dittemore, G.A.; Yu, M.; Testolin, G.; Mitcheltree, M.J.; Liu, R.Y.; Svetlov, M.S.; Myers, A.G.; Polikanov, Y.S.
Deposited on	:	2023-09-28
Resolution	:	2.70 Å(reported)

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

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

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

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

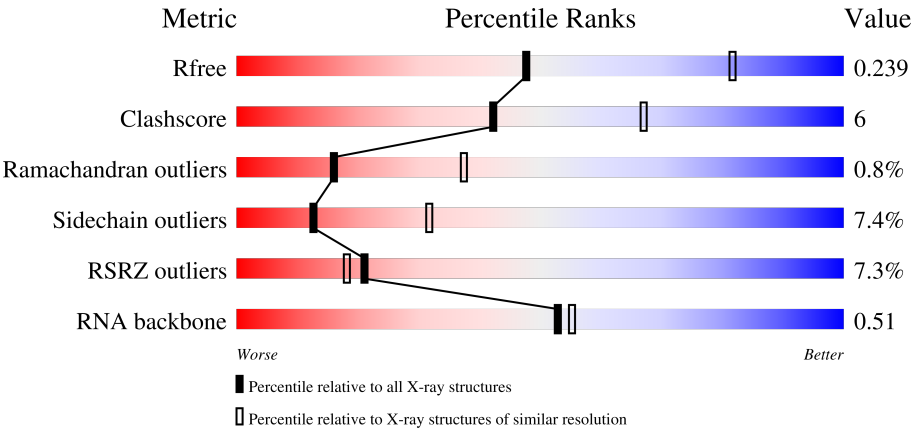
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	4% 70% 23% 5% •
1	2A	2915	4% 64% 27% 5% •

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	1B	121	82% 15%
2	2B	121	3% 60% 33% 7%
3	1D	276	% 82% 17%
3	2D	276	% 84% 15%
4	1E	206	84% 13%
4	2E	206	% 78% 18%
5	1F	210	76% 18%
5	2F	210	% 73% 21%
6	1G	182	6% 77% 20%
6	2G	182	22% 61% 30% 8%
7	1H	180	% 72% 23%
7	2H	180	17% 68% 24%
8	1I	148	5% 73% 20% 6%
8	2I	148	5% 78% 20%
9	1N	140	83% 15%
9	2N	140	4% 76% 23%
10	1O	122	93% 7%
10	2O	122	84% 15%
11	1P	150	% 85% 11%
11	2P	150	3% 77% 21%
12	1Q	141	% 81% 18%
12	2Q	141	13% 82% 18%
13	1R	118	86% 13%
13	2R	118	81% 18%
14	1S	112	2% 79% 14%

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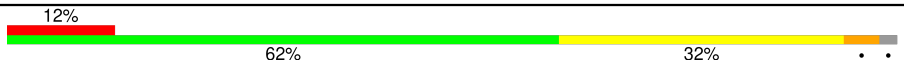
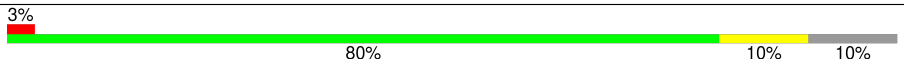
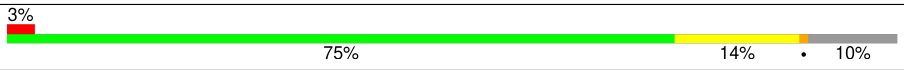
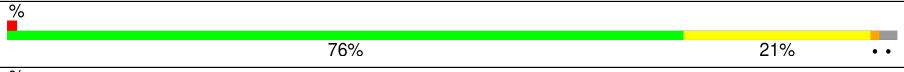
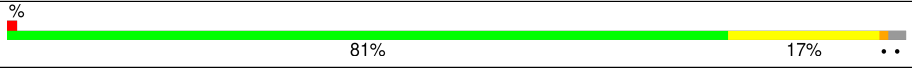
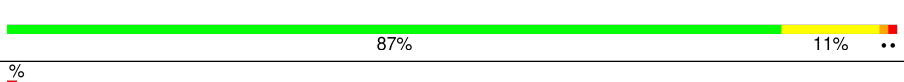
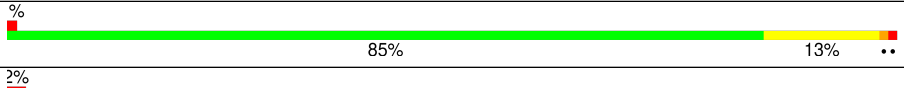
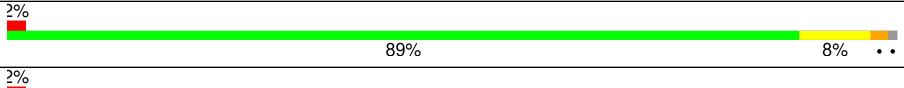
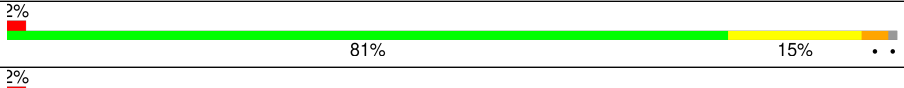
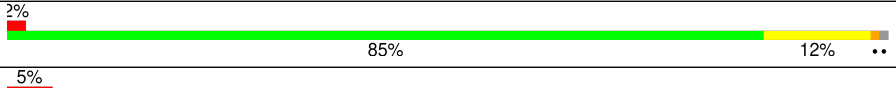
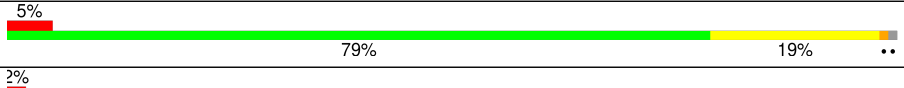
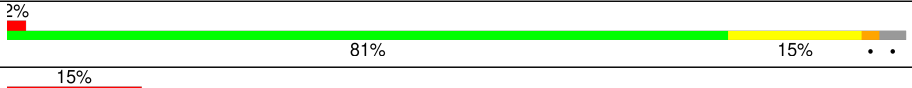
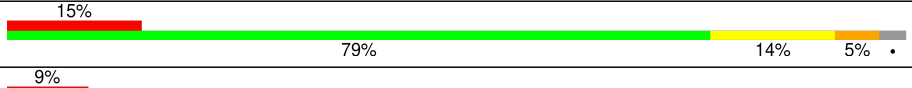
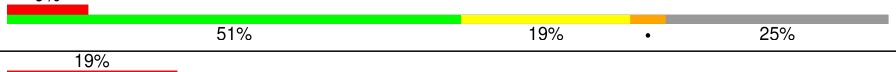
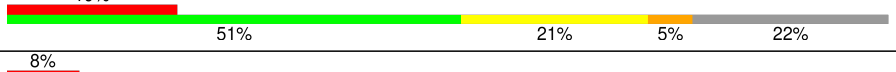
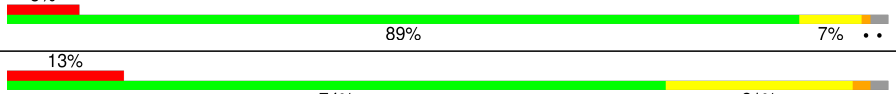
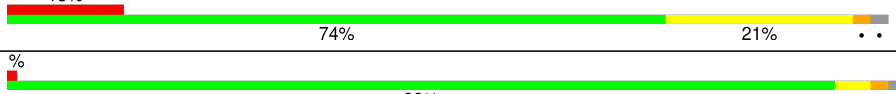
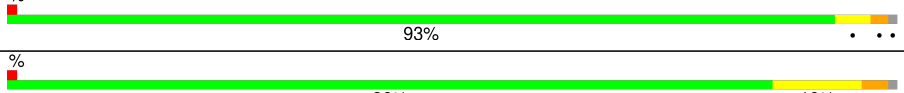
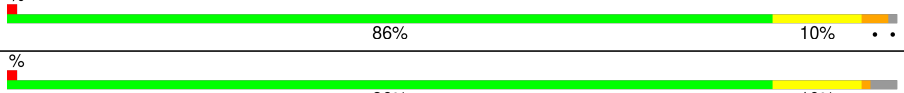
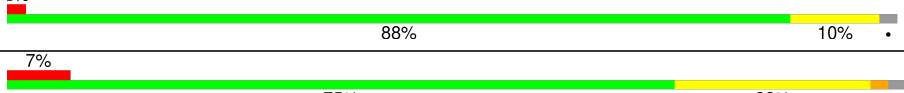
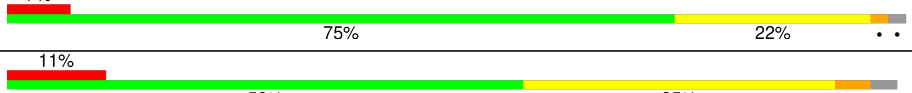
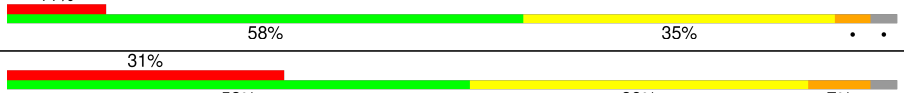
Mol	Chain	Length	Quality of chain
14	2S	112	
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	

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Mol	Chain	Length	Quality of chain
27	15	60	2% 82% 15%
27	25	60	2% 85% 13%
28	16	54	76% 20%
28	26	54	2% 85% 13%
29	17	49	4% 84% 12%
29	27	49	4% 82% 12%
30	18	65	71% 28%
30	28	65	2% 75% 23%
31	19	37	86% 14%
31	29	37	8% 86% 14%
32	1a	1521	4% 63% 31% 5%
32	2a	1521	11% 57% 35% 7%
33	1b	256	12% 58% 28% 10%
33	2b	256	28% 52% 31% 8% 10%
34	1c	239	5% 69% 16% 14%
34	2c	239	38% 56% 26% 14%
35	1d	209	7% 67% 28%
35	2d	209	5% 71% 24%
36	1e	162	% 68% 20% 9%
36	2e	162	12% 55% 32% 9%
37	1f	101	3% 79% 18%
37	2f	101	3% 77% 19%
38	1g	156	6% 84% 13%
38	2g	156	11% 72% 24%
39	1h	138	% 70% 25%

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Mol	Chain	Length	Quality of chain
39	2h	138	9% 71% 25%
40	1i	128	15% 66% 30%
40	2i	128	34% 60% 38%
41	1j	105	13% 64% 26% 8%
41	2j	105	52% 45% 42% 5% 9%
42	1k	129	3% 71% 16% 12%
42	2k	129	6% 70% 19% 12%
43	1l	132	4% 81% 10% 8%
43	2l	132	9% 69% 20% 8%
44	1m	126	6% 67% 27%
44	2m	126	37% 58% 36%
45	1n	61	5% 70% 26%
45	2n	61	77% 70% 26%
46	1o	89	4% 78% 19%
46	2o	89	3% 80% 17%
47	1p	88	11% 66% 22% 6% 7%
47	2p	88	8% 70% 22% 7%
48	1q	105	% 81% 11% 6%
48	2q	105	6% 77% 16% 6%
49	1r	88	% 60% 15% 23%
49	2r	88	% 55% 18% 5% 23%
50	1s	93	3% 67% 22% 11%
50	2s	93	40% 54% 31% 11%
51	1t	106	5% 61% 26% 9%
51	2t	106	8% 72% 16% 9%

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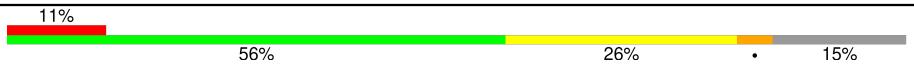
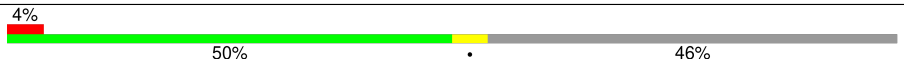
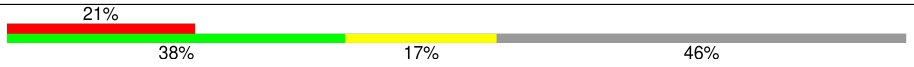
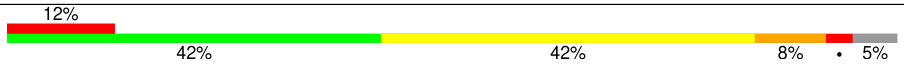
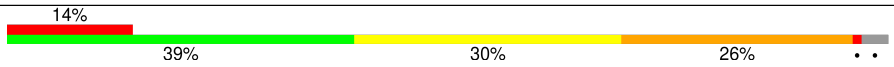
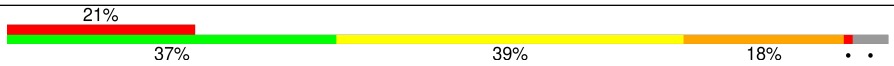
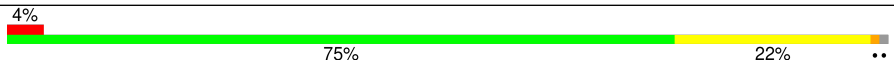
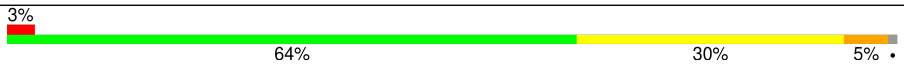
Mol	Chain	Length	Quality of chain
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	PSU	2y	55	-	-	X	-
56	MG	1a	1716	-	-	-	X
56	MG	2A	3155	-	-	-	X
56	MG	2A	3276	-	-	-	X
56	MG	2A	3340	-	-	-	X
56	MG	2A	3582	-	-	-	X
56	MG	2a	1630	-	-	-	X
56	MG	2a	1709	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 298872 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	2E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 54 is a RNA chain called A- and E-site Deacylated tRNAphe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	72	Total	C	N	O	P	S	0	0	0
			1550	694	277	505	72	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	70	Total	C	N	O	P	S	0	0	0
			1502	671	270	489	70	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1635	731	296	530	76	2			

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1059	Total	Mg	0	0
			1059	1059		
56	1B	34	Total	Mg	0	0
			34	34		
56	1D	12	Total	Mg	0	0
			12	12		
56	1E	17	Total	Mg	0	0
			17	17		
56	1F	12	Total	Mg	0	0
			12	12		
56	1G	5	Total	Mg	0	0
			5	5		
56	1I	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1N	5	Total Mg 5 5	0	0
56	1O	6	Total Mg 6 6	0	0
56	1P	6	Total Mg 6 6	0	0
56	1Q	6	Total Mg 6 6	0	0
56	1R	6	Total Mg 6 6	0	0
56	1S	2	Total Mg 2 2	0	0
56	1T	3	Total Mg 3 3	0	0
56	1U	10	Total Mg 10 10	0	0
56	1V	6	Total Mg 6 6	0	0
56	1W	7	Total Mg 7 7	0	0
56	1X	6	Total Mg 6 6	0	0
56	1Y	2	Total Mg 2 2	0	0
56	1Z	2	Total Mg 2 2	0	0
56	10	9	Total Mg 9 9	0	0
56	11	5	Total Mg 5 5	0	0
56	12	2	Total Mg 2 2	0	0
56	13	4	Total Mg 4 4	0	0
56	14	1	Total Mg 1 1	0	0
56	15	7	Total Mg 7 7	0	0
56	16	1	Total Mg 1 1	0	0
56	17	5	Total Mg 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	18	6	Total Mg 6 6	0	0
56	19	1	Total Mg 1 1	0	0
56	1a	208	Total Mg 208 208	0	0
56	1b	1	Total Mg 1 1	0	0
56	1d	1	Total Mg 1 1	0	0
56	1e	2	Total Mg 2 2	0	0
56	1f	1	Total Mg 1 1	0	0
56	1k	1	Total Mg 1 1	0	0
56	1l	2	Total Mg 2 2	0	0
56	1m	2	Total Mg 2 2	0	0
56	1n	1	Total Mg 1 1	0	0
56	1p	1	Total Mg 1 1	0	0
56	1r	1	Total Mg 1 1	0	0
56	1t	1	Total Mg 1 1	0	0
56	1w	3	Total Mg 3 3	0	0
56	1x	14	Total Mg 14 14	0	0
56	2A	771	Total Mg 771 771	0	0
56	2B	20	Total Mg 20 20	0	0
56	2D	8	Total Mg 8 8	0	0
56	2E	10	Total Mg 10 10	0	0
56	2F	5	Total Mg 5 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2G	1	Total Mg 1 1	0	0
56	2N	1	Total Mg 1 1	0	0
56	2O	1	Total Mg 1 1	0	0
56	2P	2	Total Mg 2 2	0	0
56	2Q	3	Total Mg 3 3	0	0
56	2R	2	Total Mg 2 2	0	0
56	2T	2	Total Mg 2 2	0	0
56	2U	1	Total Mg 1 1	0	0
56	2V	2	Total Mg 2 2	0	0
56	2W	2	Total Mg 2 2	0	0
56	2X	2	Total Mg 2 2	0	0
56	20	2	Total Mg 2 2	0	0
56	21	3	Total Mg 3 3	0	0
56	23	2	Total Mg 2 2	0	0
56	25	1	Total Mg 1 1	0	0
56	27	1	Total Mg 1 1	0	0
56	28	2	Total Mg 2 2	0	0
56	2a	214	Total Mg 214 214	0	0
56	2d	1	Total Mg 1 1	0	0
56	2e	1	Total Mg 1 1	0	0
56	2f	1	Total Mg 1 1	0	0

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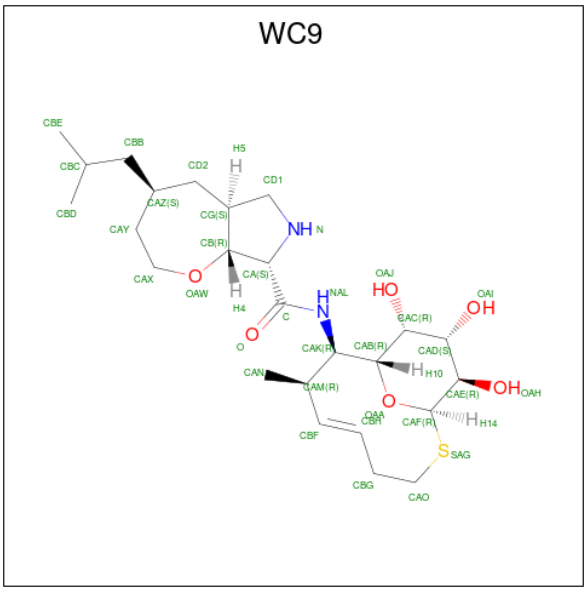
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2g	1	Total Mg 1 1	0	0
56	2i	2	Total Mg 2 2	0	0
56	2j	1	Total Mg 1 1	0	0
56	2k	1	Total Mg 1 1	0	0
56	2l	3	Total Mg 3 3	0	0
56	2q	3	Total Mg 3 3	0	0
56	2r	2	Total Mg 2 2	0	0
56	2t	1	Total Mg 1 1	0	0
56	2v	1	Total Mg 1 1	0	0
56	2w	1	Total Mg 1 1	0	0
56	2x	5	Total Mg 5 5	0	0
56	2y	2	Total Mg 2 2	0	0

- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1A	1	Total K 1 1	0	0
57	2x	1	Total K 1 1	0	0

- Molecule 58 is (4S,5aS,8S,8aR)-4-(2-methylpropyl)-N-[(1R,5Z,7R,8R,9R,10R,11S,12R)-10,11,12-trihydroxy-7-methyl-13-oxa-2-thiabicyclo[7.3.1]tridec-5-en-8-yl]octahydro-2H-oxepino[2,3-c]pyrrole-8-carboxamide (non-preferred name) (CCD ID: WC9) (formula: $C_{25}H_{42}N_2O_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total C N O S 34 25 2 6 1	0	0
58	2A	1	Total C N O S 34 25 2 6 1	0	0

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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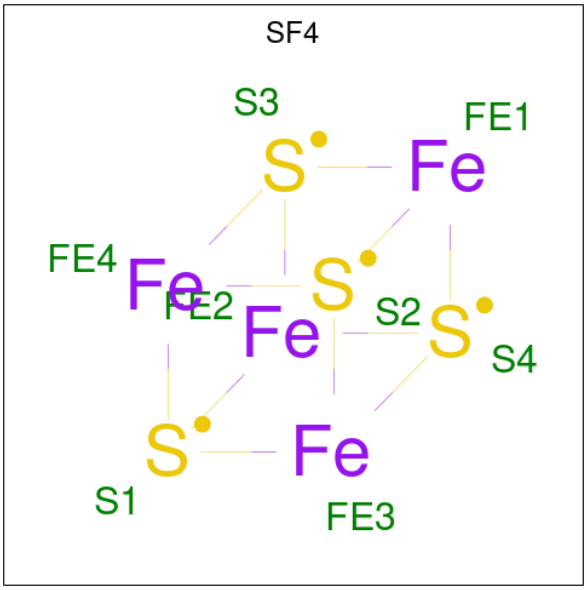
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	29	1	Total Zn 1 1	0	0
59	2n	1	Total Zn 1 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	1685	Total O 1685 1685	0	0
61	1B	54	Total O 54 54	0	0
61	1D	26	Total O 26 26	0	0
61	1E	25	Total O 25 25	0	0
61	1F	15	Total O 15 15	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1G	3	Total O 3 3	0	0
61	1H	1	Total O 1 1	0	0
61	1N	3	Total O 3 3	0	0
61	1O	5	Total O 5 5	0	0
61	1P	17	Total O 17 17	0	0
61	1Q	6	Total O 6 6	0	0
61	1R	9	Total O 9 9	0	0
61	1S	2	Total O 2 2	0	0
61	1T	7	Total O 7 7	0	0
61	1U	11	Total O 11 11	0	0
61	1V	5	Total O 5 5	0	0
61	1W	7	Total O 7 7	0	0
61	1X	3	Total O 3 3	0	0
61	1Y	1	Total O 1 1	0	0
61	10	12	Total O 12 12	0	0
61	11	8	Total O 8 8	0	0
61	12	2	Total O 2 2	0	0
61	13	3	Total O 3 3	0	0
61	14	1	Total O 1 1	0	0
61	15	6	Total O 6 6	0	0
61	16	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	17	8	Total O 8 8	0	0
61	18	11	Total O 11 11	0	0
61	1a	213	Total O 213 213	0	0
61	1b	1	Total O 1 1	0	0
61	1f	2	Total O 2 2	0	0
61	1g	1	Total O 1 1	0	0
61	1i	1	Total O 1 1	0	0
61	1j	1	Total O 1 1	0	0
61	1l	2	Total O 2 2	0	0
61	1q	1	Total O 1 1	0	0
61	1v	2	Total O 2 2	0	0
61	1w	4	Total O 4 4	0	0
61	1x	9	Total O 9 9	0	0
61	2A	848	Total O 848 848	0	0
61	2B	16	Total O 16 16	0	0
61	2D	16	Total O 16 16	0	0
61	2E	10	Total O 10 10	0	0
61	2F	11	Total O 11 11	0	0
61	2I	1	Total O 1 1	0	0
61	2O	3	Total O 3 3	0	0
61	2P	6	Total O 6 6	0	0

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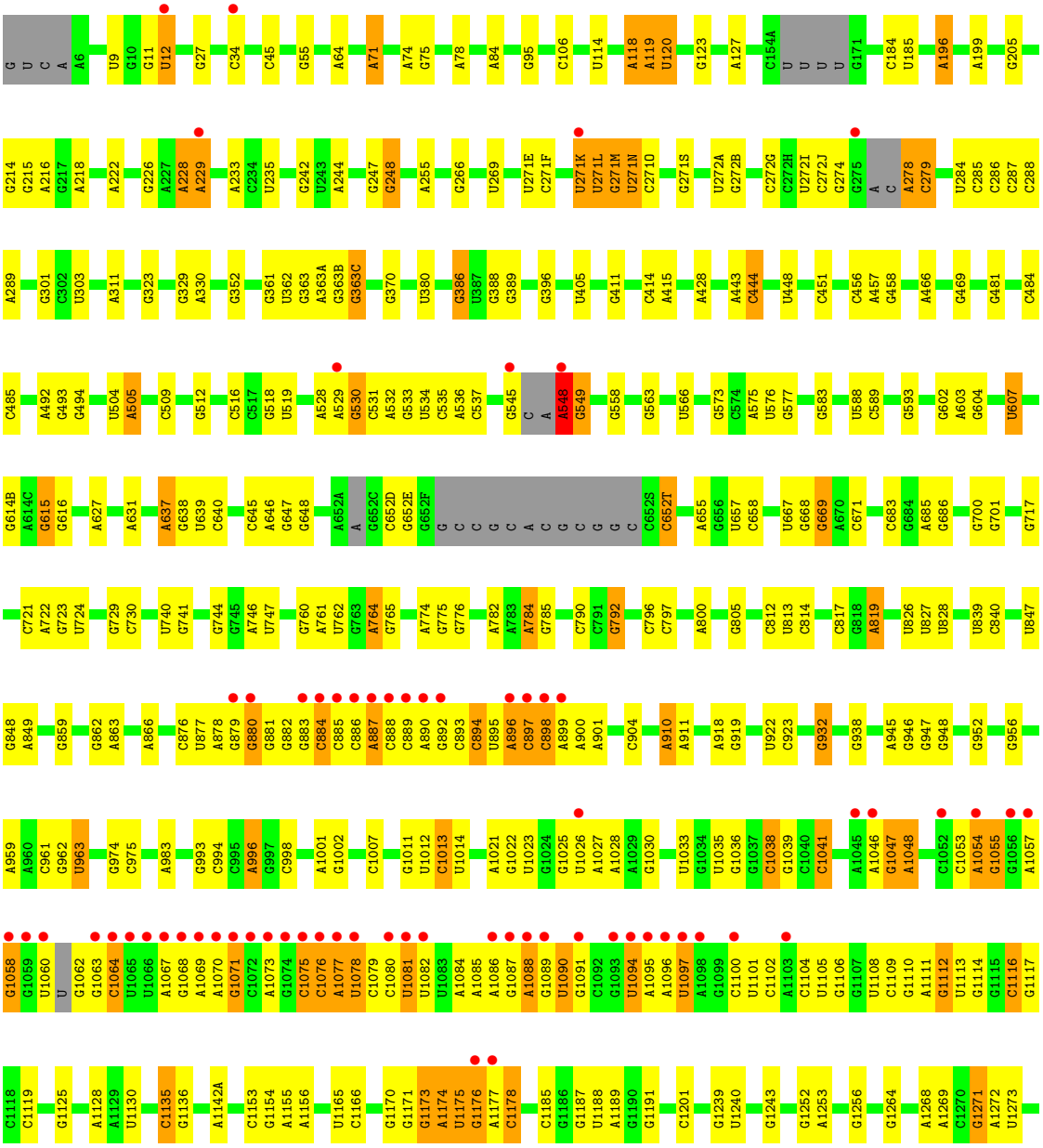
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2Q	1	Total O 1 1	0	0
61	2R	2	Total O 2 2	0	0
61	2T	4	Total O 4 4	0	0
61	2U	3	Total O 3 3	0	0
61	2V	1	Total O 1 1	0	0
61	2W	2	Total O 2 2	0	0
61	2X	1	Total O 1 1	0	0
61	2Y	1	Total O 1 1	0	0
61	20	1	Total O 1 1	0	0
61	21	7	Total O 7 7	0	0
61	27	4	Total O 4 4	0	0
61	28	5	Total O 5 5	0	0
61	29	1	Total O 1 1	0	0
61	2a	145	Total O 145 145	0	0
61	2d	3	Total O 3 3	0	0
61	2j	3	Total O 3 3	0	0
61	2l	3	Total O 3 3	0	0
61	2r	1	Total O 1 1	0	0
61	2t	1	Total O 1 1	0	0
61	2x	4	Total O 4 4	0	0
61	2y	4	Total O 4 4	0	0

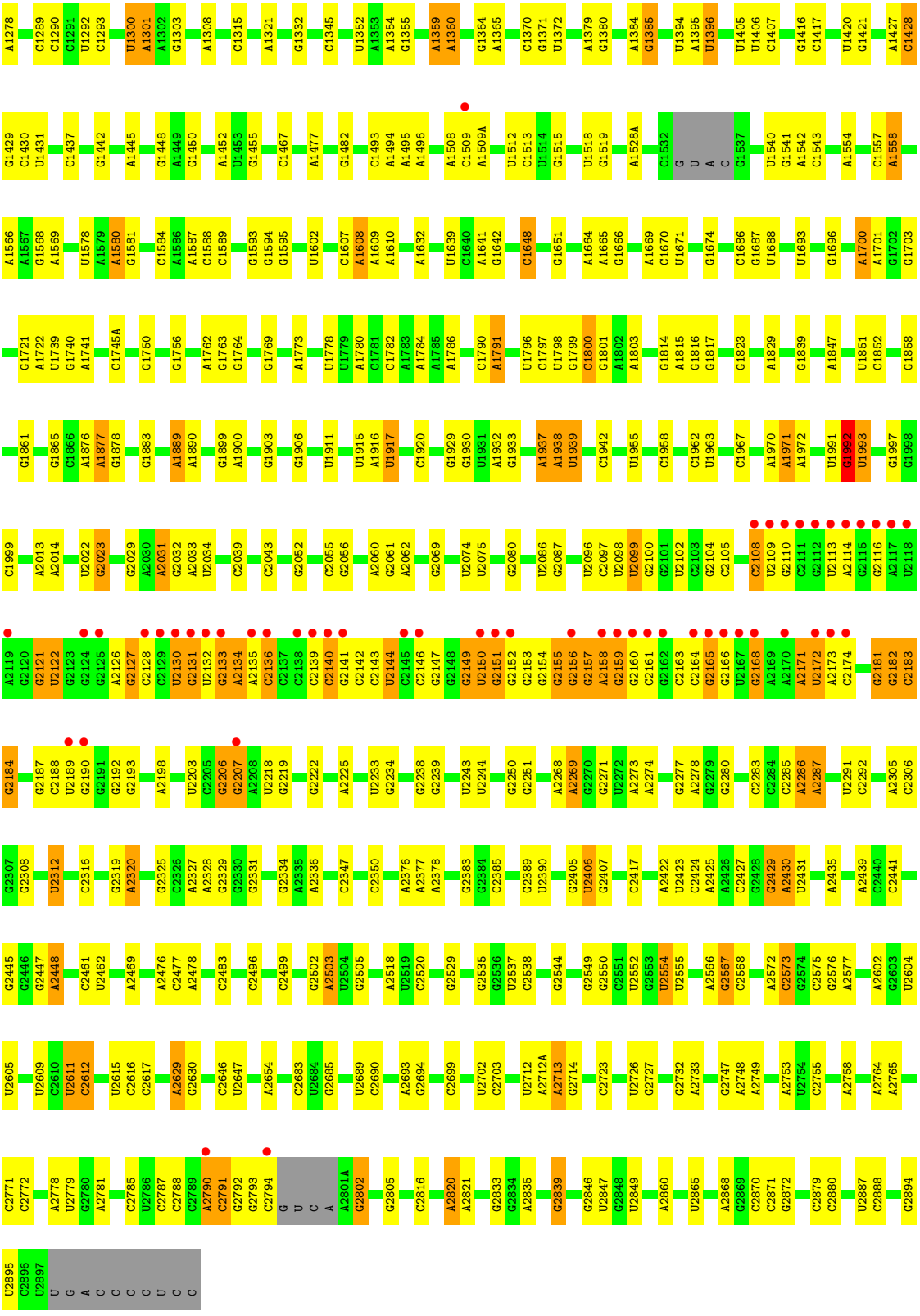
3 Residue-property plots (i)

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

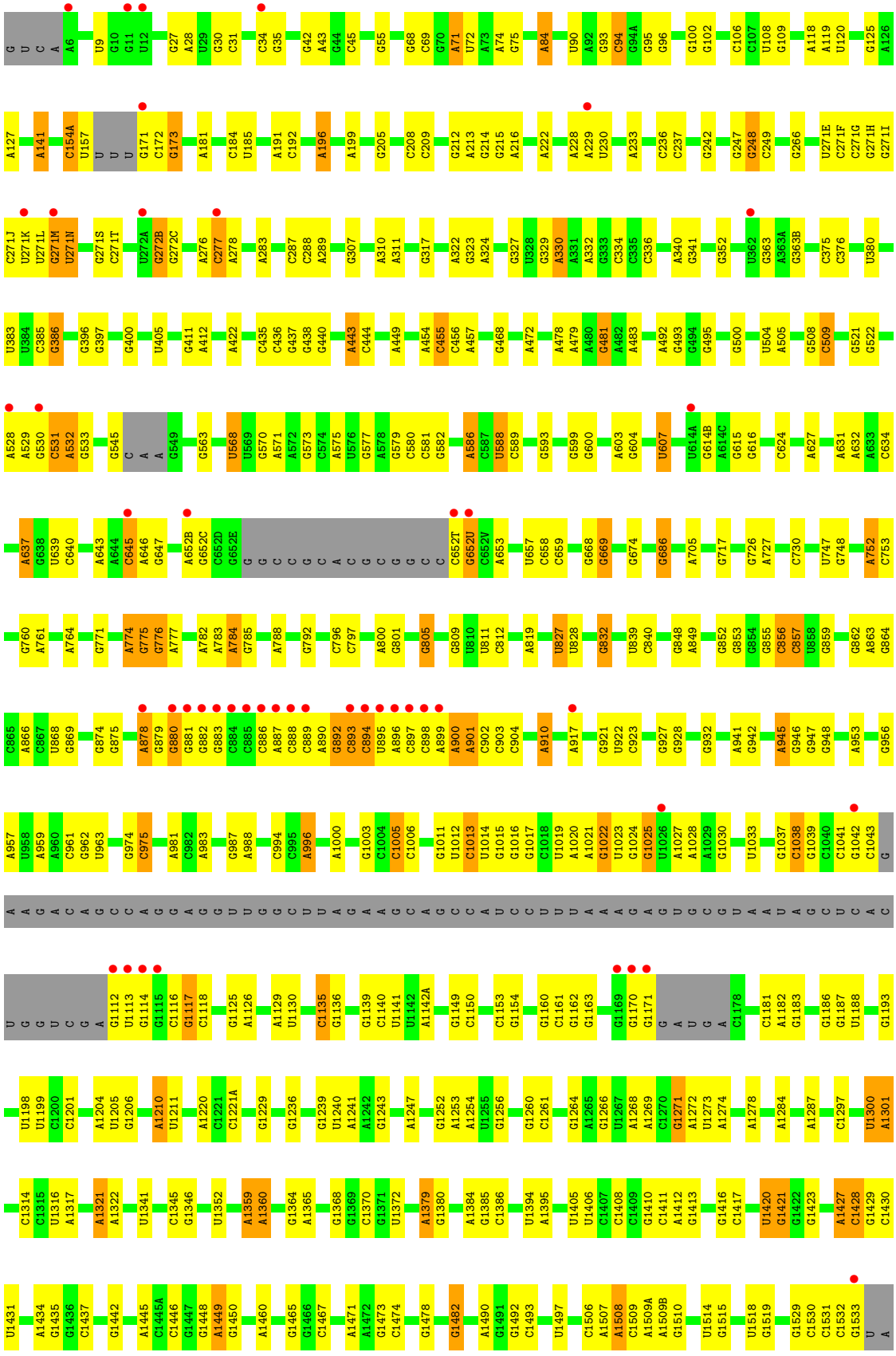
Chain 1A:

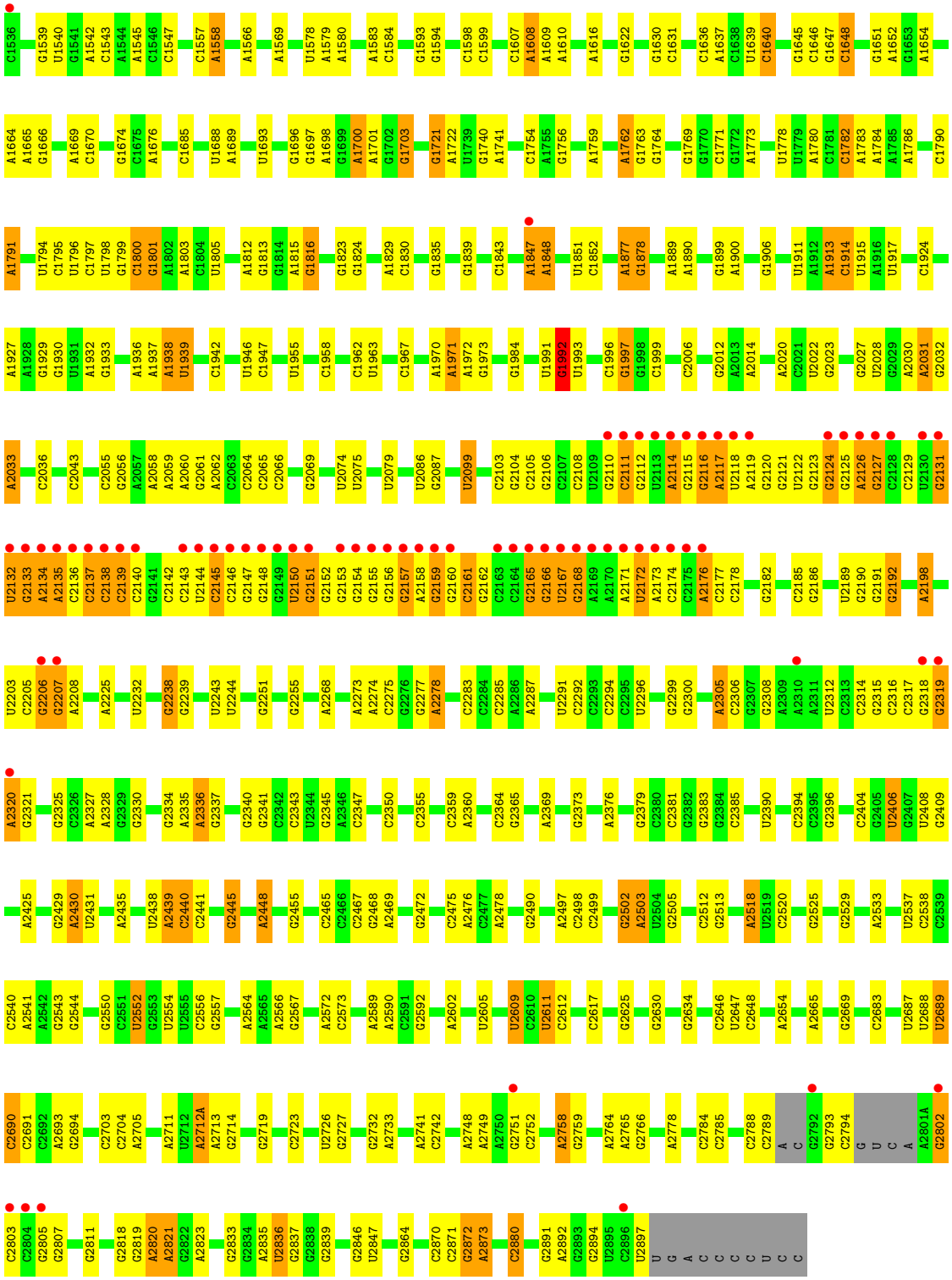




• Molecule 1: 23S Ribosomal RNA

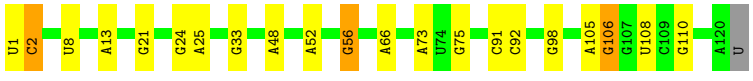
Chain 2A:





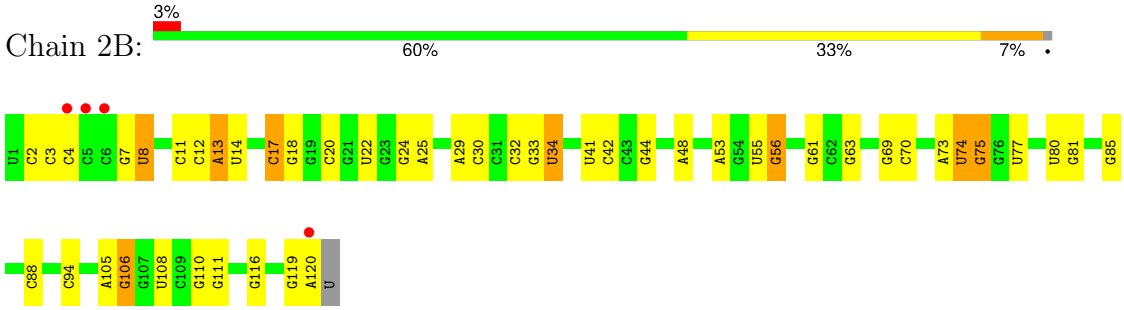
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



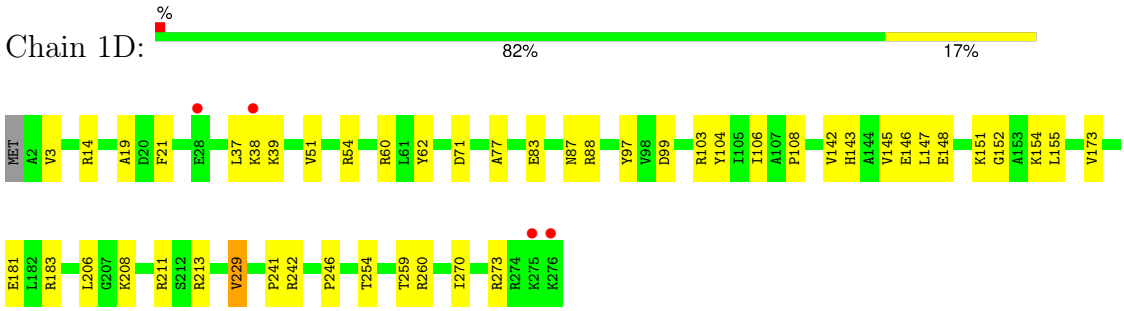
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



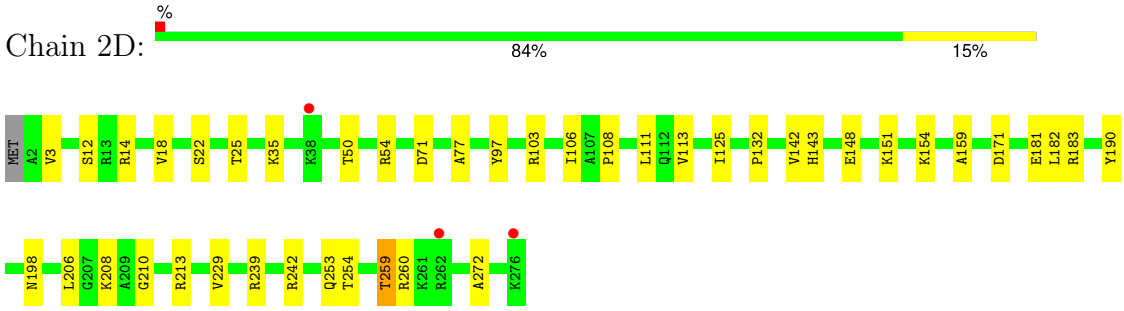
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



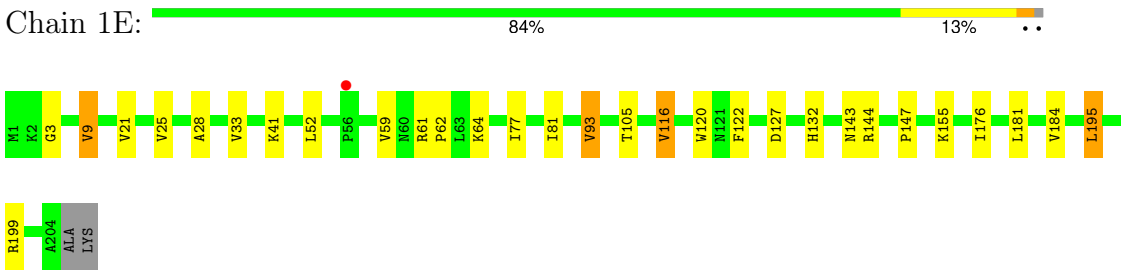
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



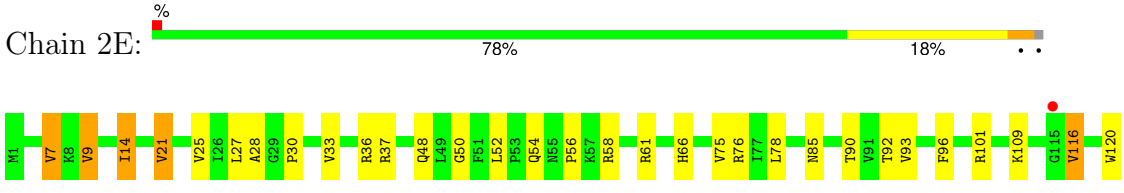
• Molecule 4: 50S ribosomal protein L3

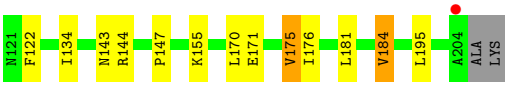
Chain 1E:



• Molecule 4: 50S ribosomal protein L3

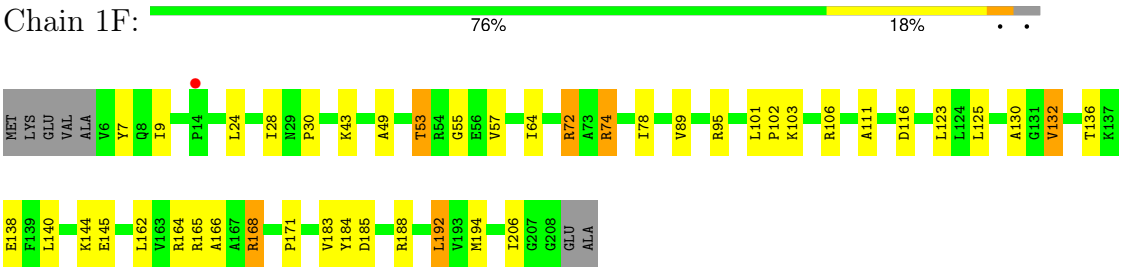
Chain 2E:





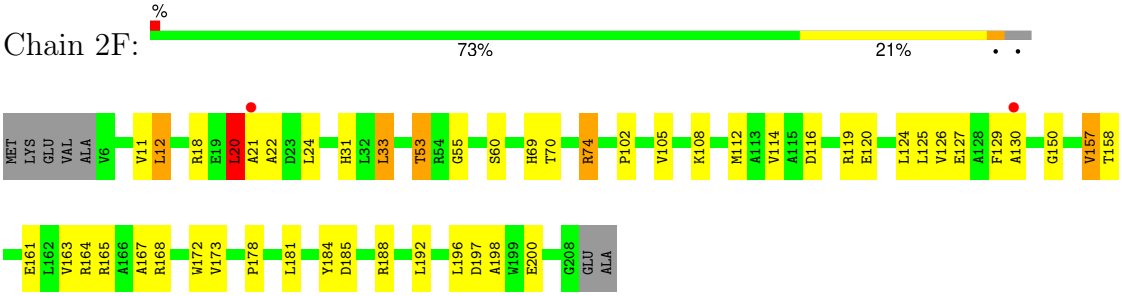
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



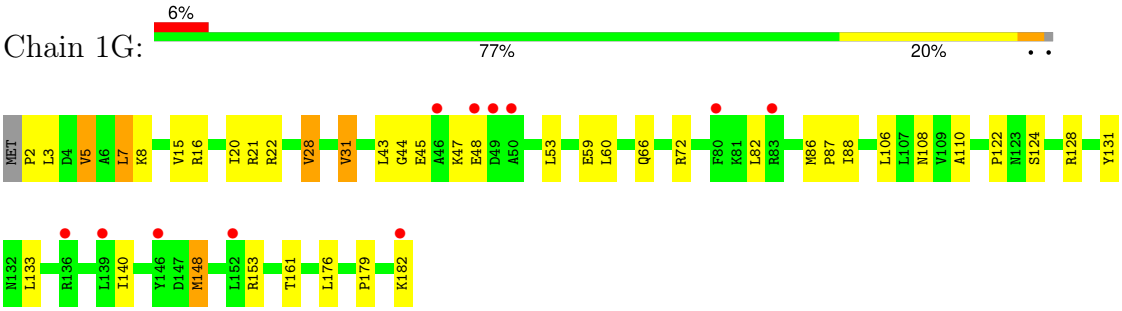
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



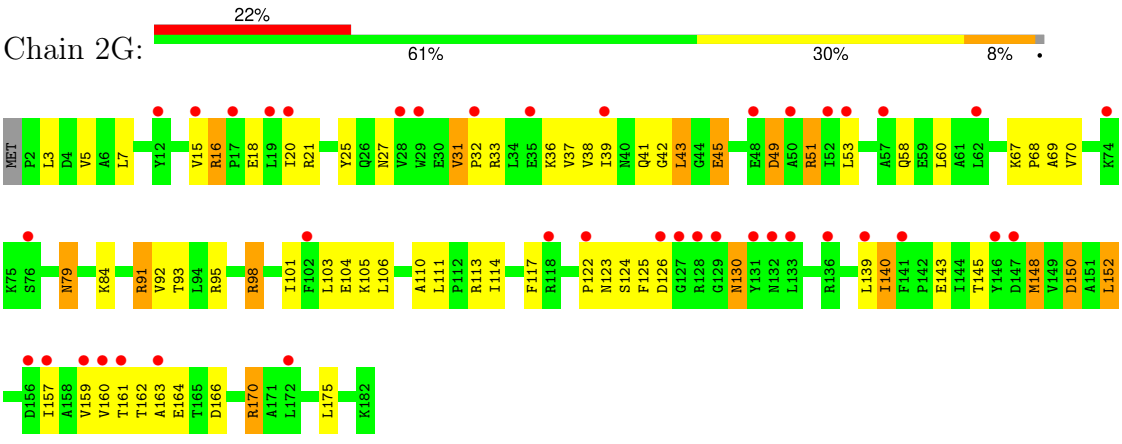
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



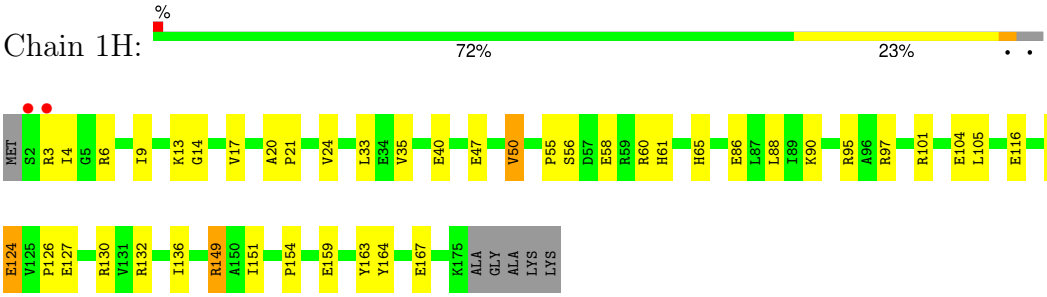
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



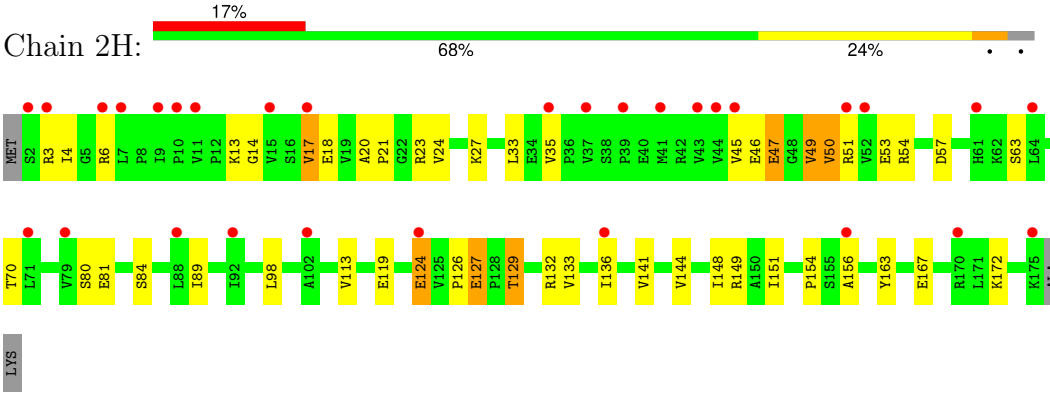
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



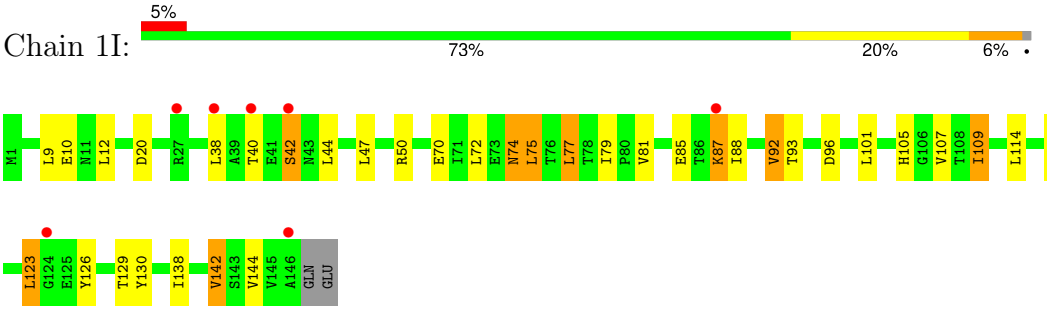
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



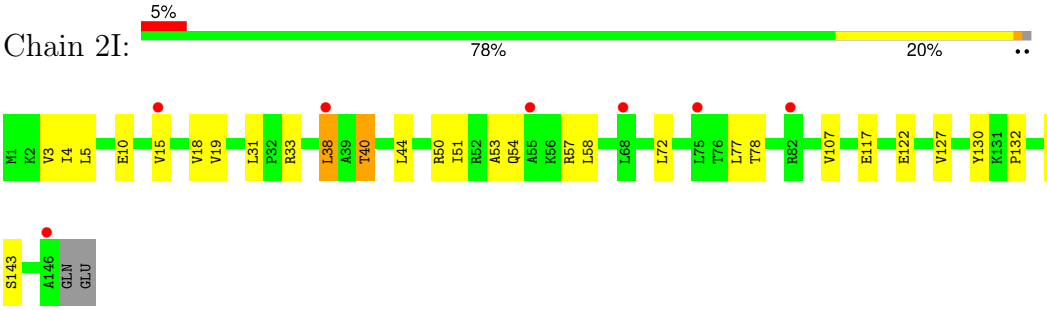
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



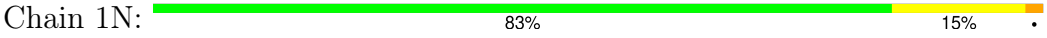
• Molecule 8: 50S ribosomal protein L9

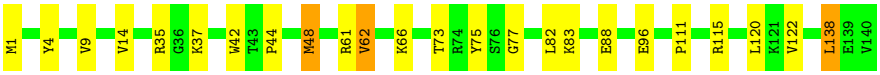
Chain 2I:



• Molecule 9: 50S ribosomal protein L13

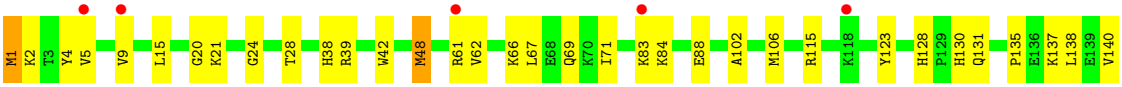
Chain 1N:





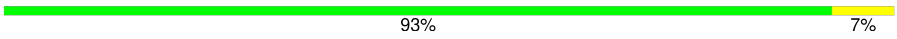
• Molecule 9: 50S ribosomal protein L13

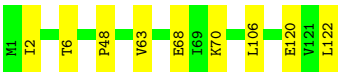
Chain 2N:



• Molecule 10: 50S ribosomal protein L14

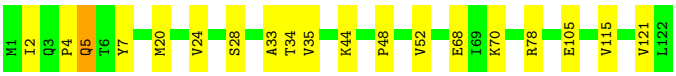
Chain 1O:





• Molecule 10: 50S ribosomal protein L14

Chain 2O:

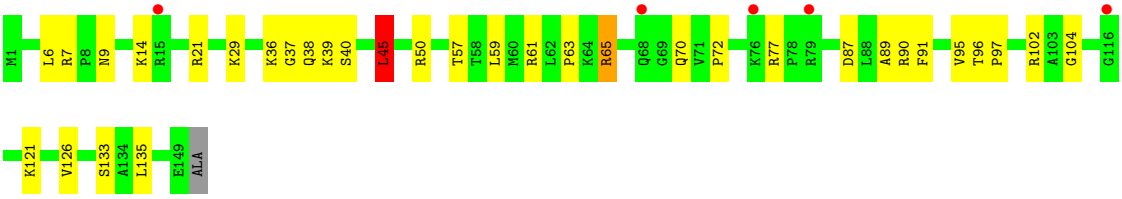


• Molecule 11: 50S ribosomal protein L15

Chain 1P:

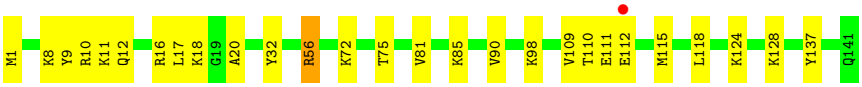
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



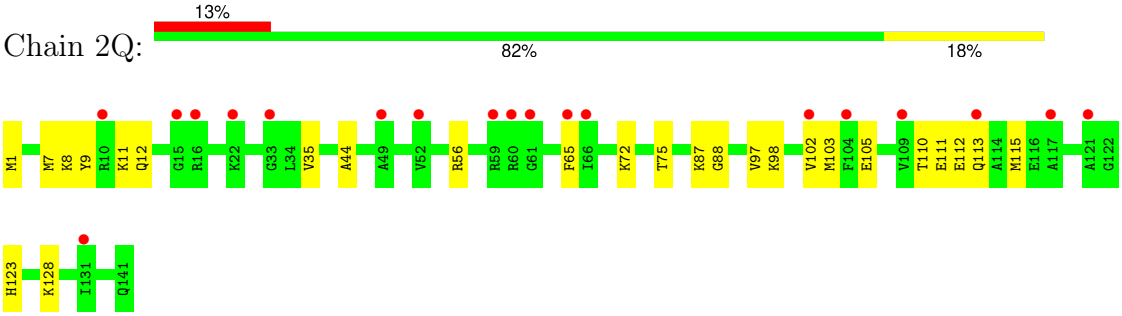
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



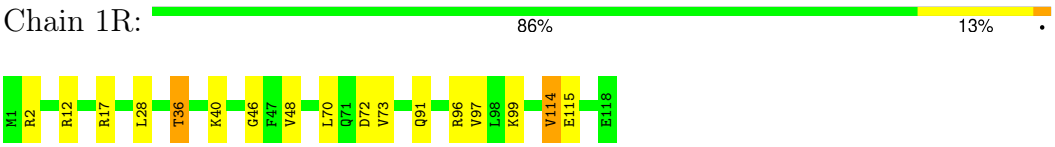
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



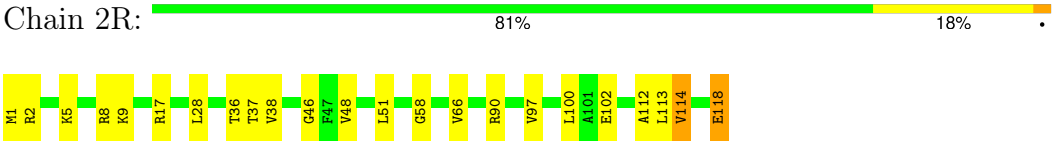
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



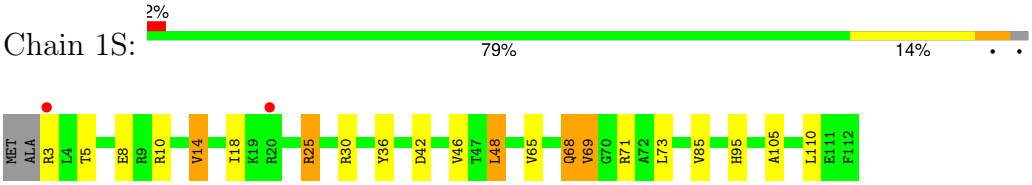
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



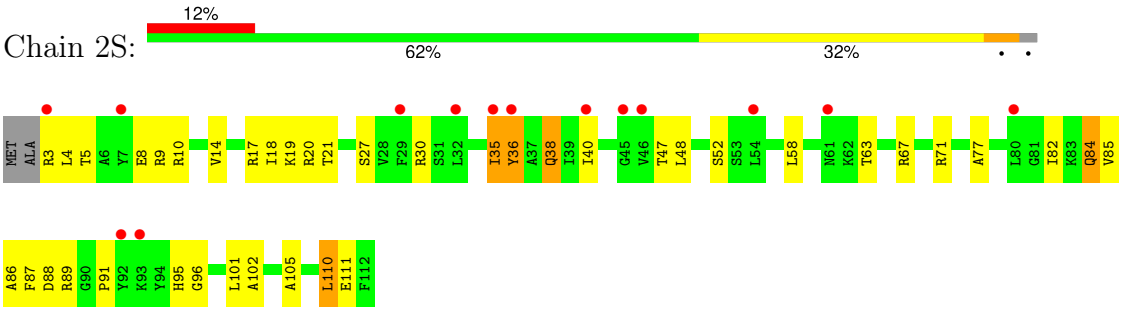
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



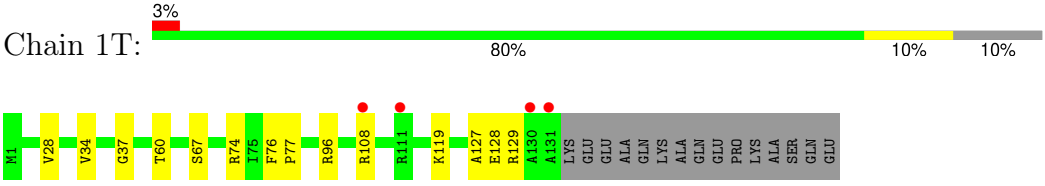
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



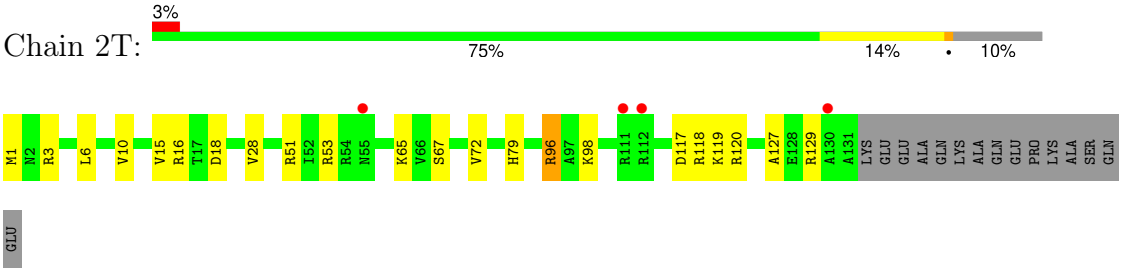
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



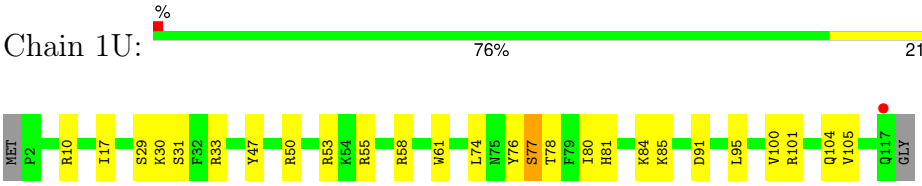
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



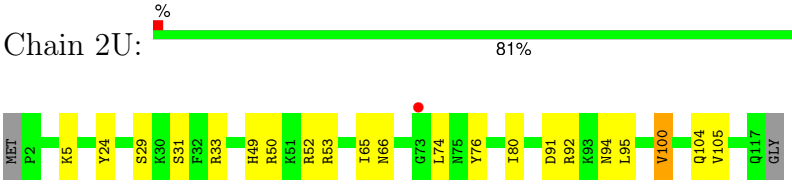
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



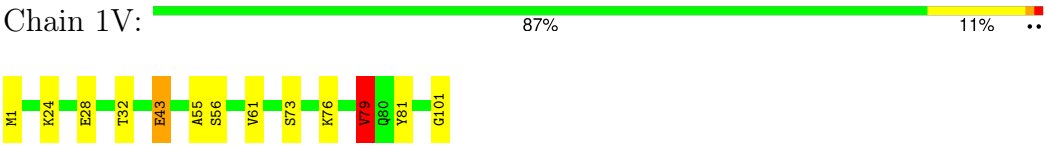
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



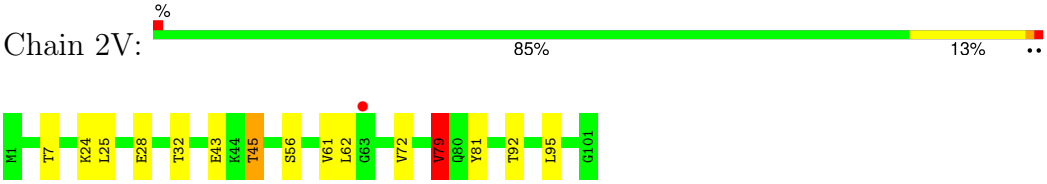
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



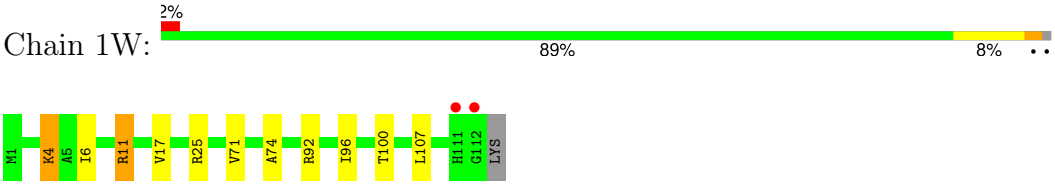
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



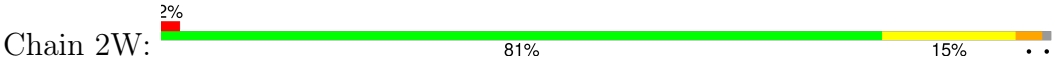
• Molecule 18: 50S ribosomal protein L22

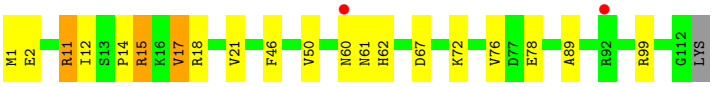
Chain 1W:



• Molecule 18: 50S ribosomal protein L22

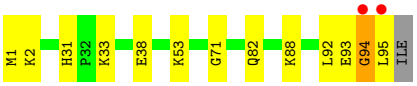
Chain 2W:





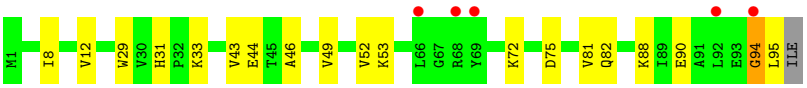
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



• Molecule 19: 50S ribosomal protein L23

Chain 2X:

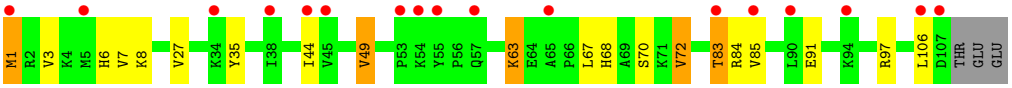


• Molecule 20: 50S ribosomal protein L24

Chain 1Y:

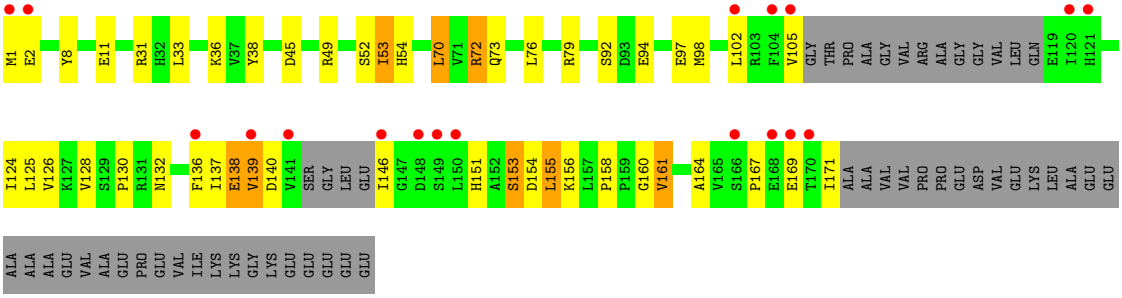
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



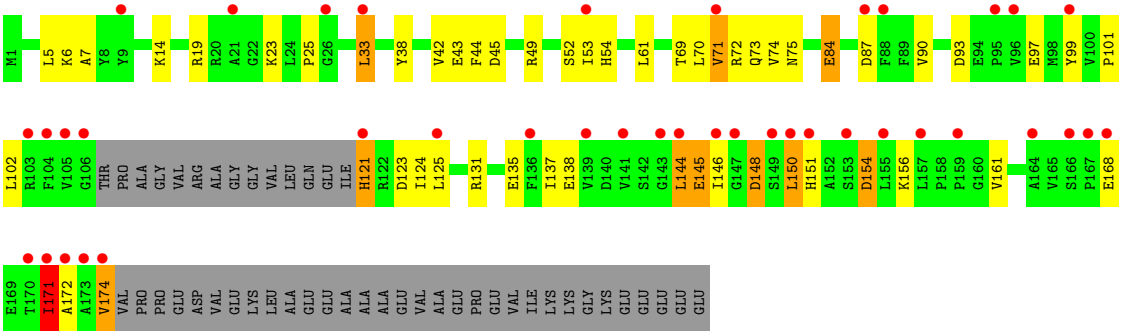
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:

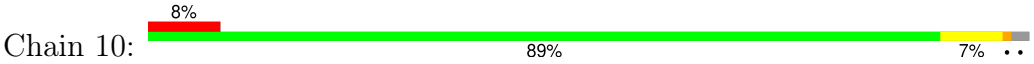


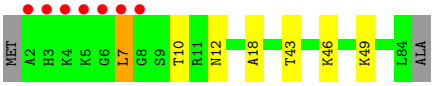
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:

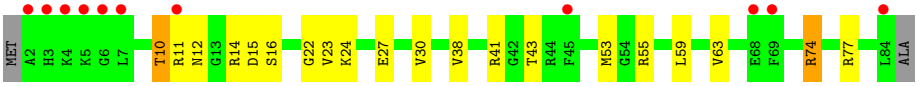


• Molecule 22: 50S ribosomal protein L27



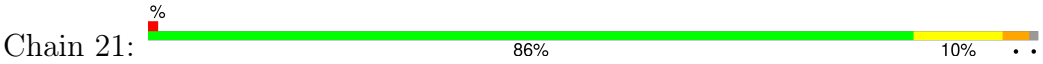


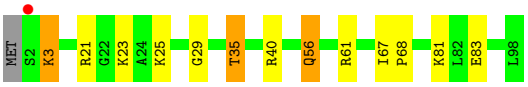
• Molecule 22: 50S ribosomal protein L27



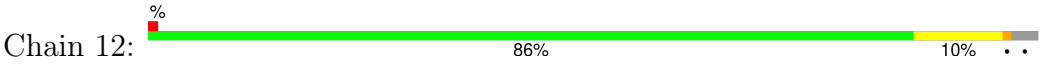
• Molecule 23: 50S ribosomal protein L28

• Molecule 23: 50S ribosomal protein L28



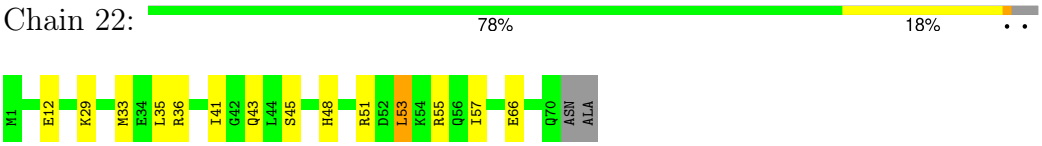


• Molecule 24: 50S ribosomal protein L29



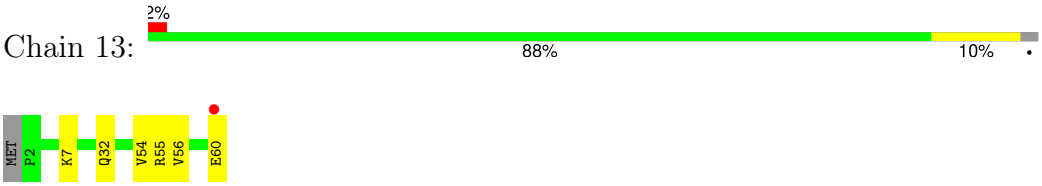
• Molecule 24: 50S ribosomal protein L29

Chain 22:



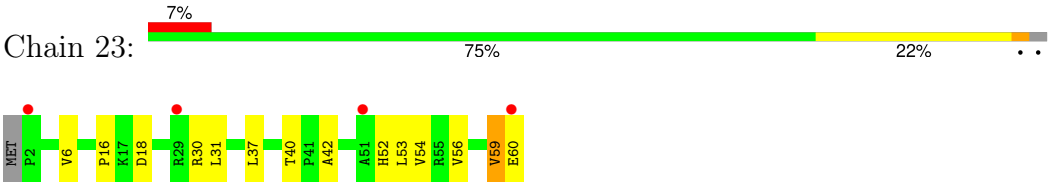
• Molecule 25: 50S ribosomal protein L30

Chain 13:



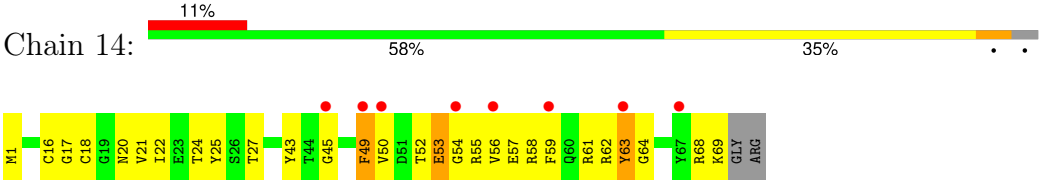
• Molecule 25: 50S ribosomal protein L30

Chain 23:



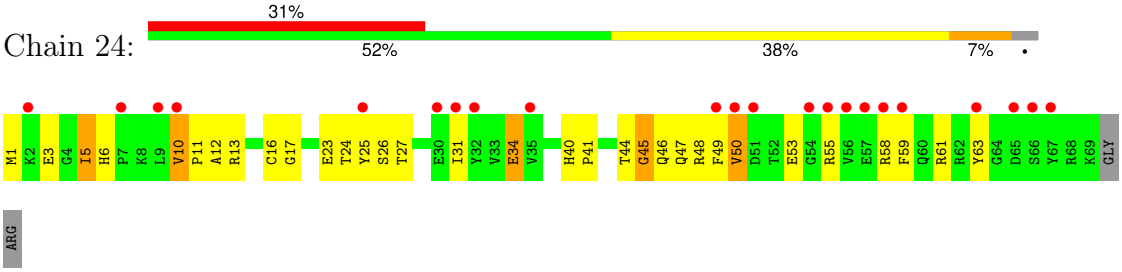
• Molecule 26: 50S ribosomal protein L31

Chain 14:



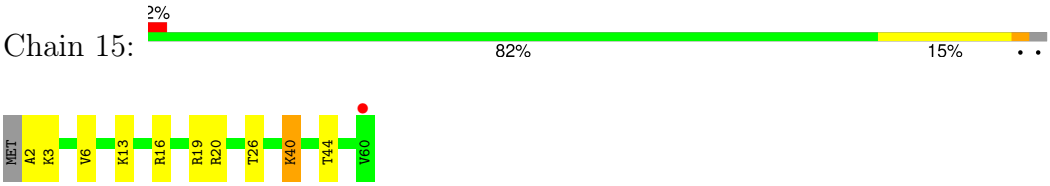
• Molecule 26: 50S ribosomal protein L31

Chain 24:



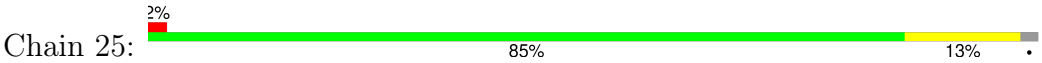
• Molecule 27: 50S ribosomal protein L32

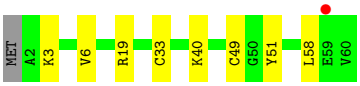
Chain 15:



• Molecule 27: 50S ribosomal protein L32

Chain 25:



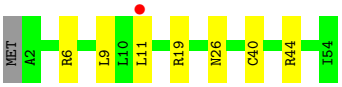


• Molecule 28: 50S ribosomal protein L33

Chain 16:

• Molecule 28: 50S ribosomal protein L33

Chain 26:

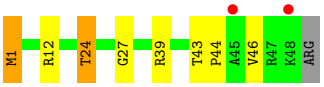


• Molecule 29: 50S ribosomal protein L34

Chain 17:

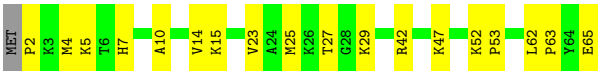
• Molecule 29: 50S ribosomal protein L34

Chain 27:



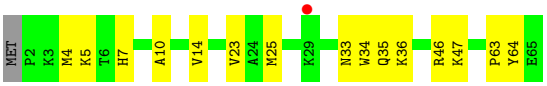
• Molecule 30: 50S ribosomal protein L35

Chain 18:



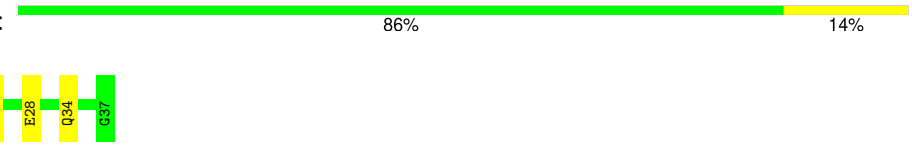
• Molecule 30: 50S ribosomal protein L35

Chain 28:



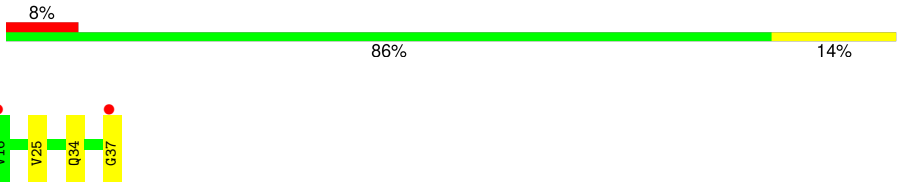
• Molecule 31: 50S ribosomal protein L36

Chain 19:



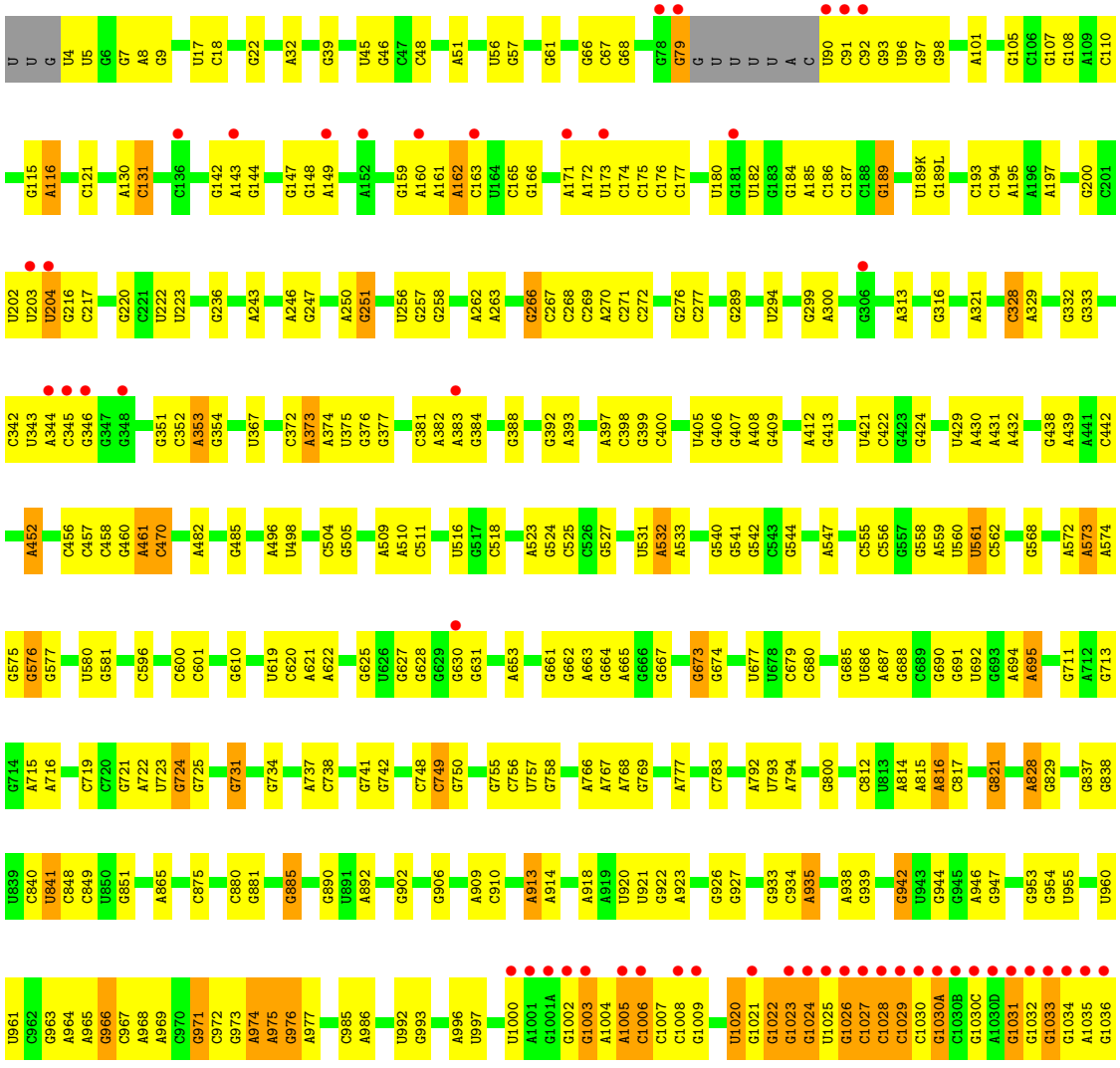
• Molecule 31: 50S ribosomal protein L36

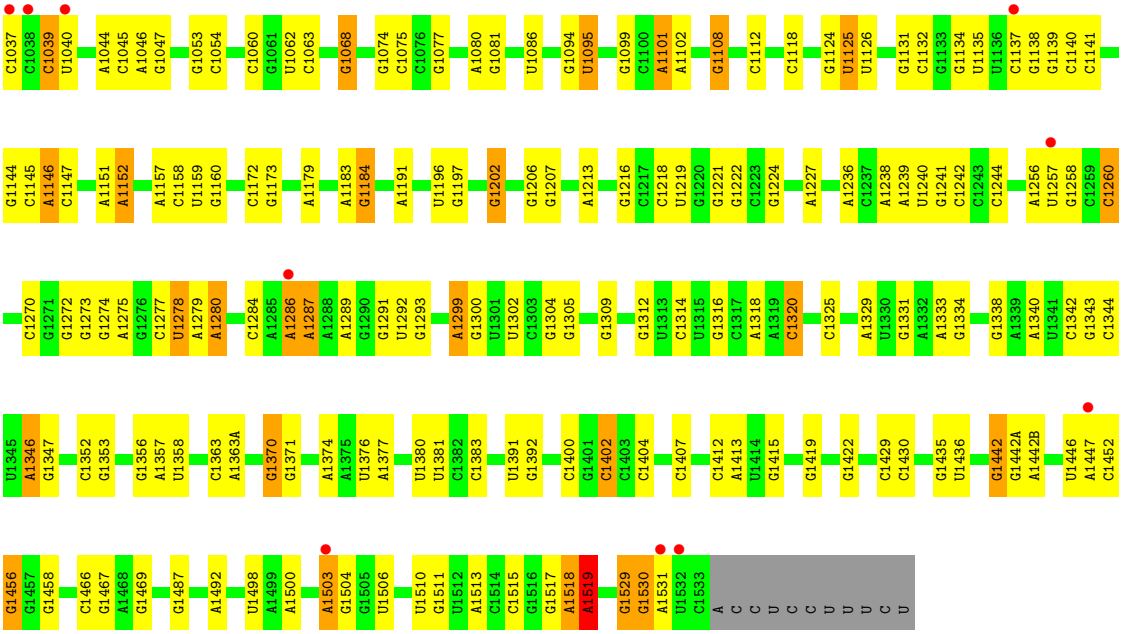
Chain 29:



• Molecule 32: 16S Ribosomal RNA

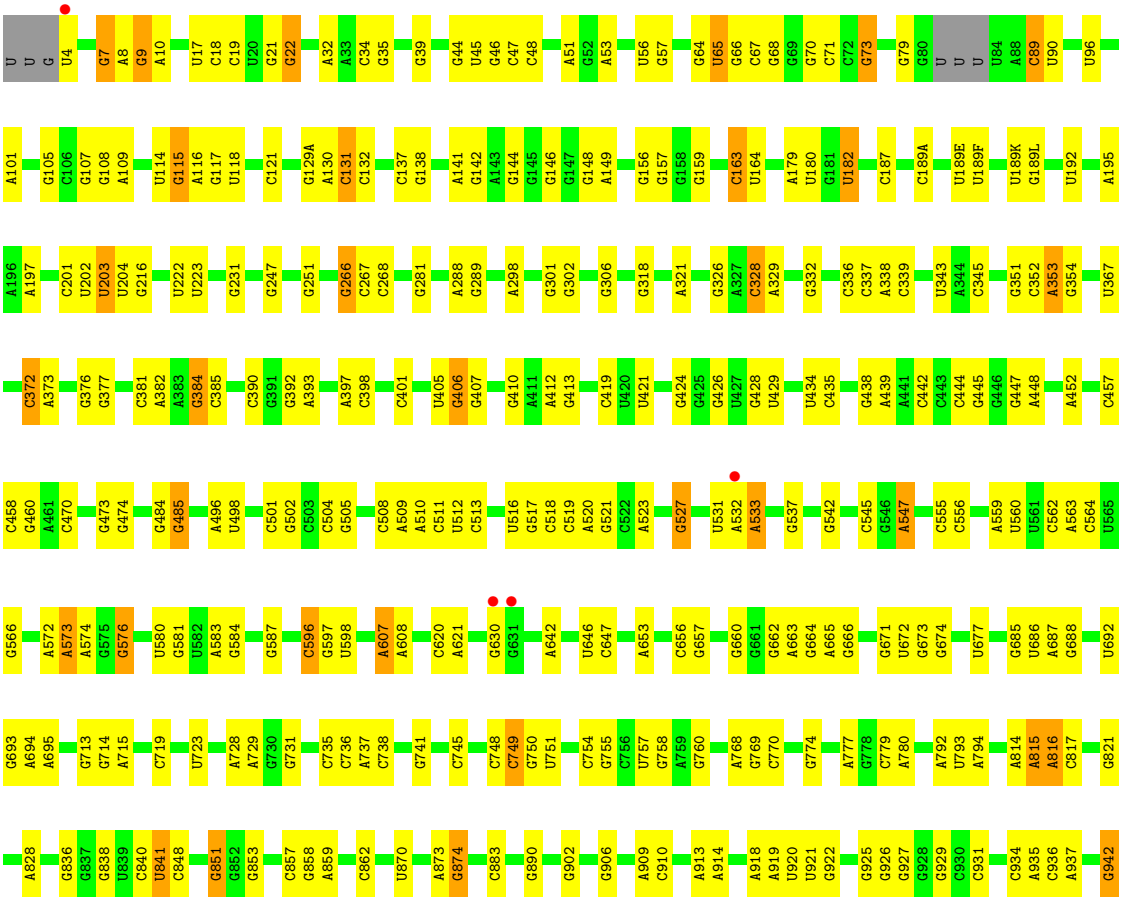
Chain 1a:

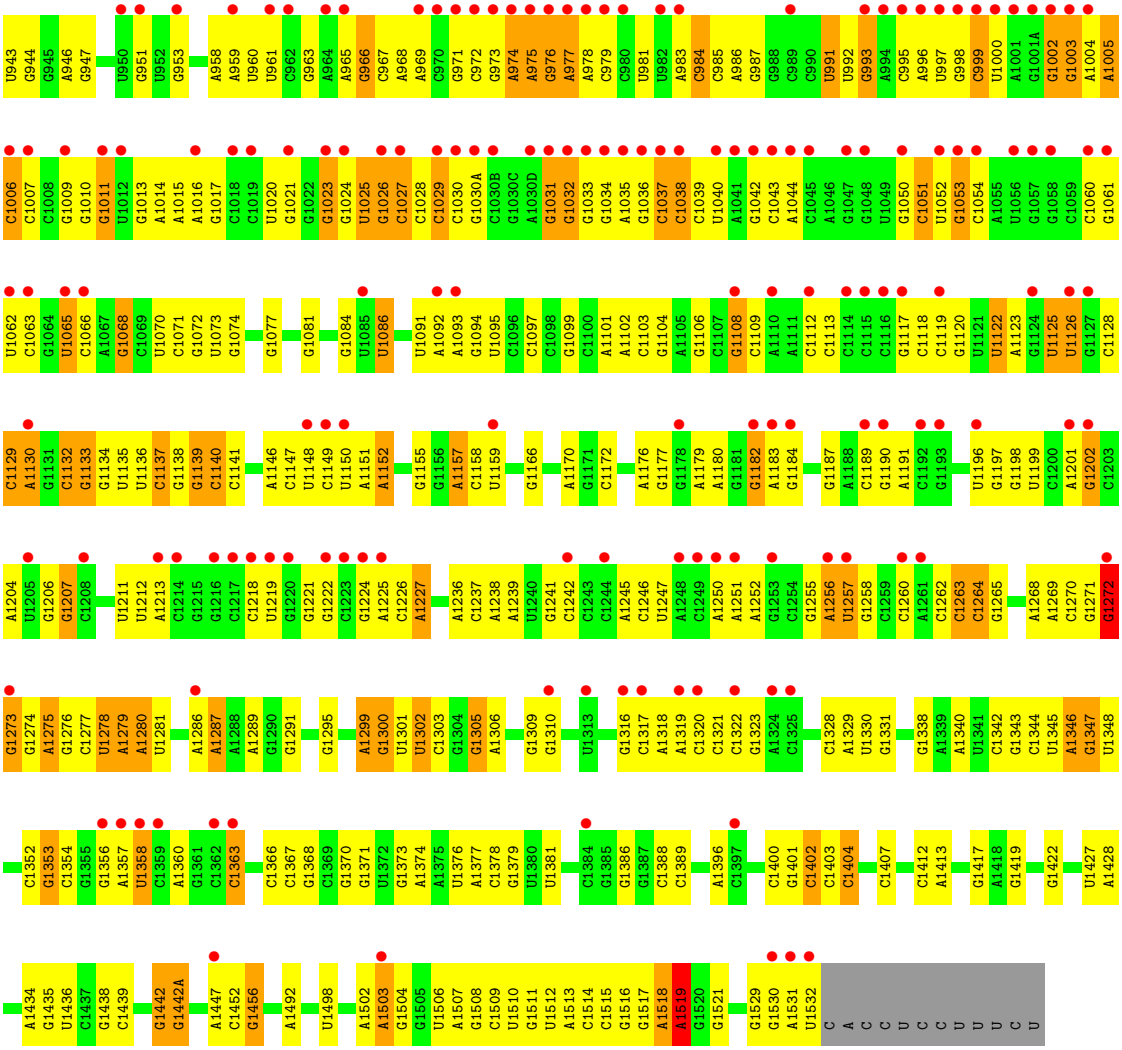




• Molecule 32: 16S Ribosomal RNA

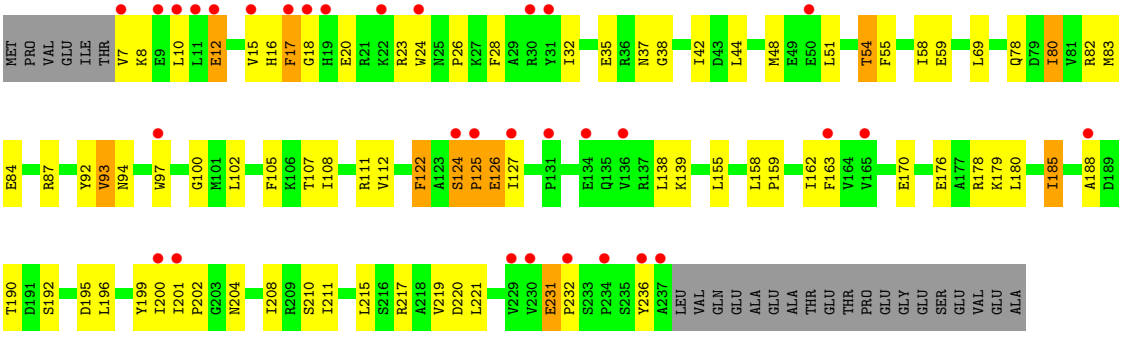
Chain 2a:





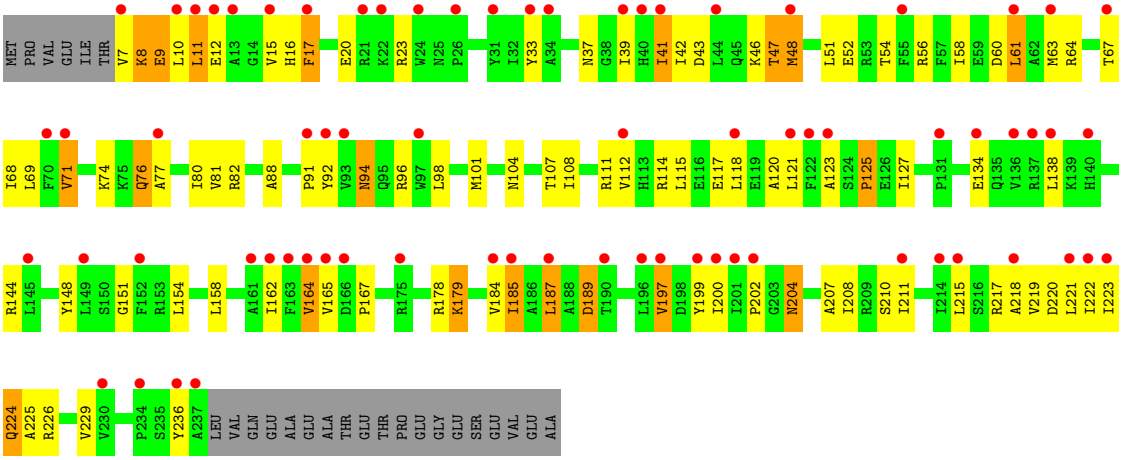
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



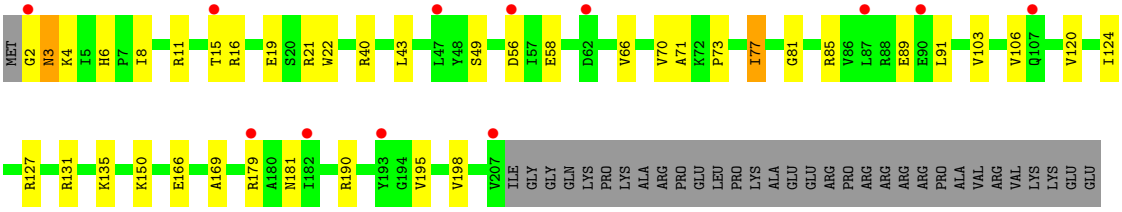
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



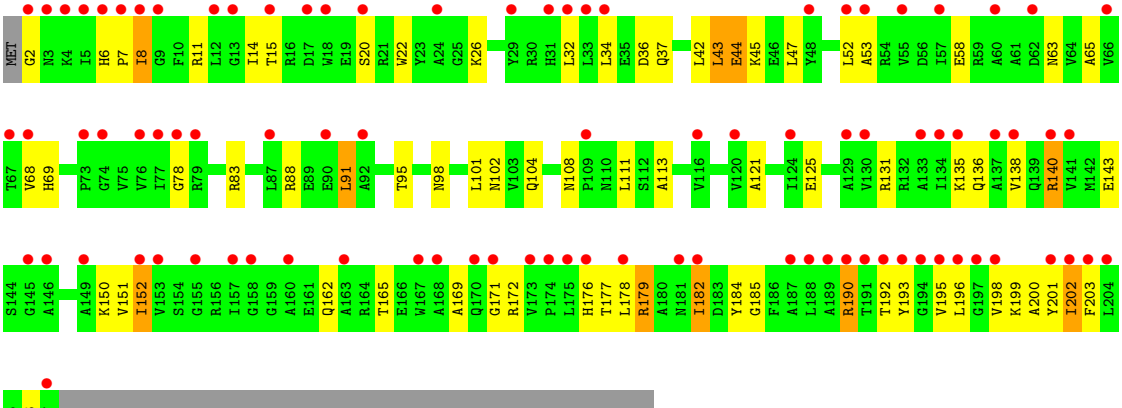
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



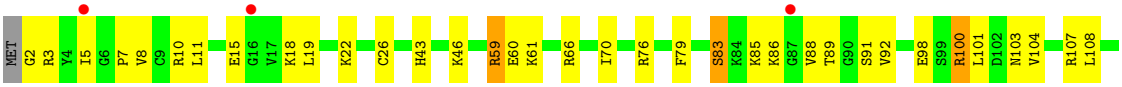
• Molecule 34: 30S ribosomal protein S3

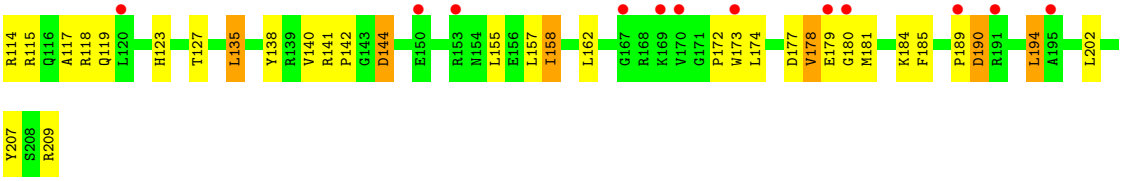
Chain 2c:



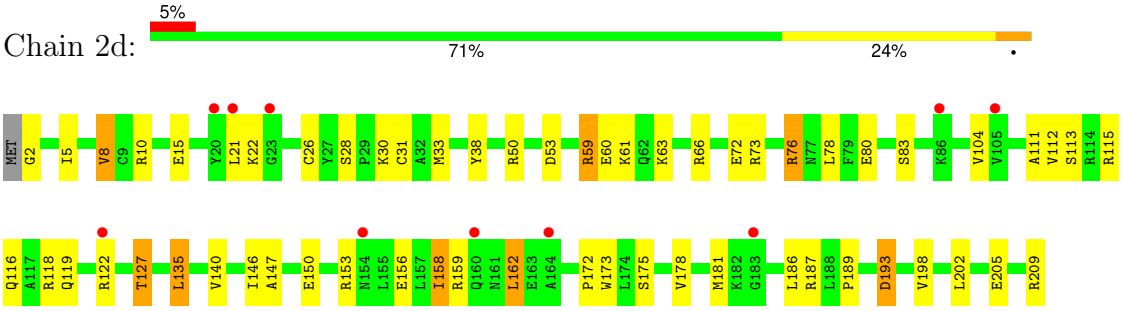
• Molecule 35: 30S ribosomal protein S4

Chain 1d:

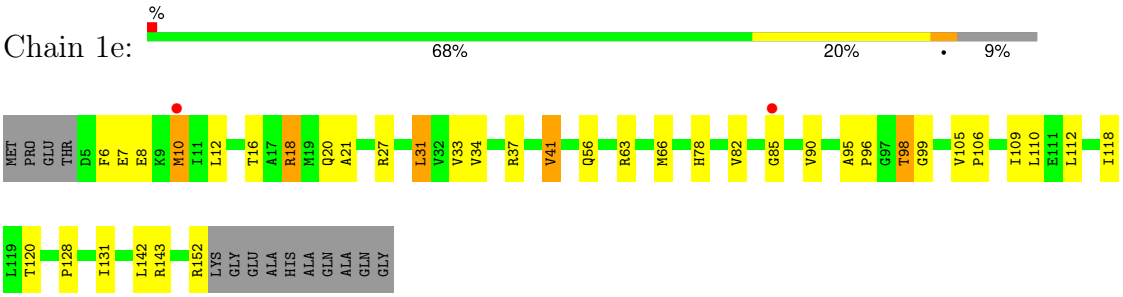




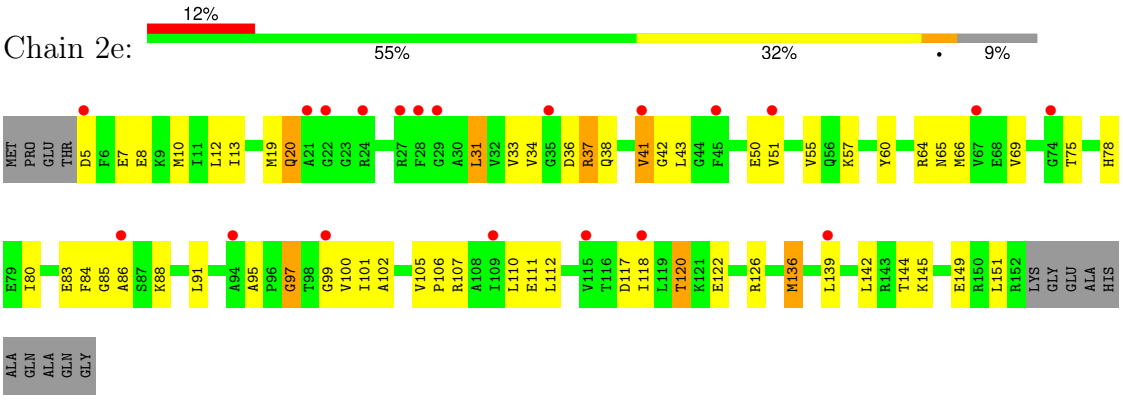
• Molecule 35: 30S ribosomal protein S4



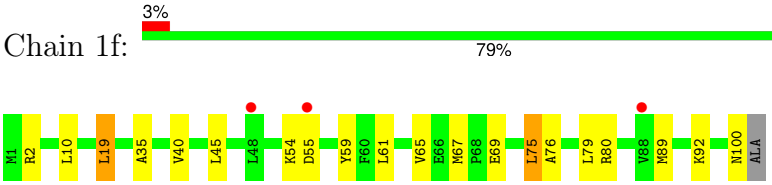
• Molecule 36: 30S ribosomal protein S5



• Molecule 36: 30S ribosomal protein S5

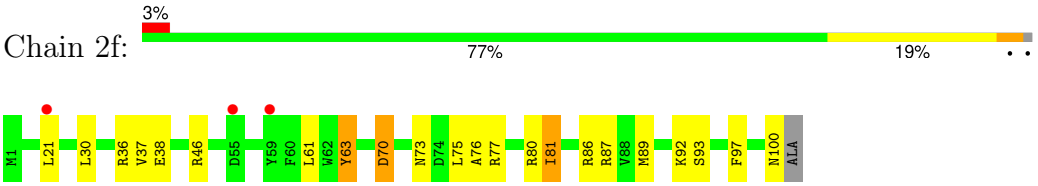


• Molecule 37: 30S ribosomal protein S6



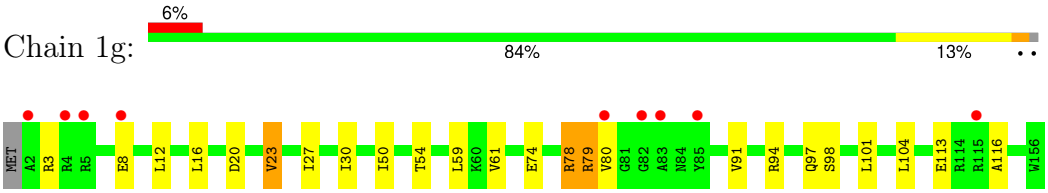
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



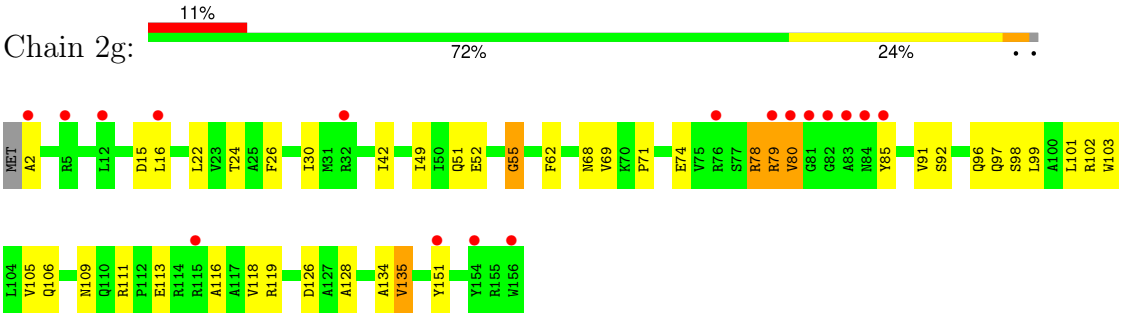
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



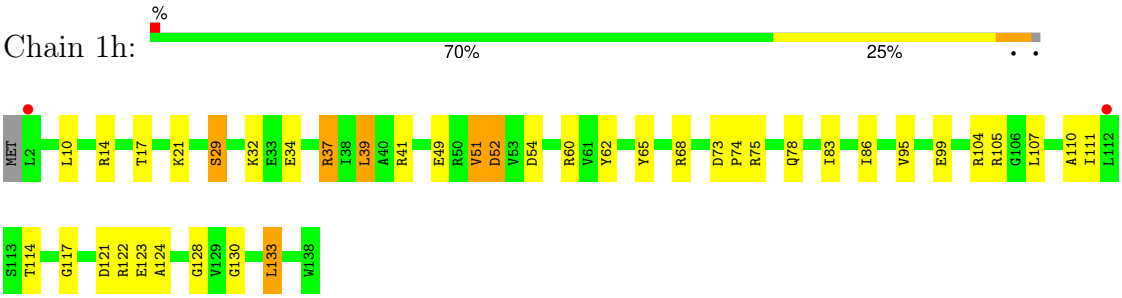
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



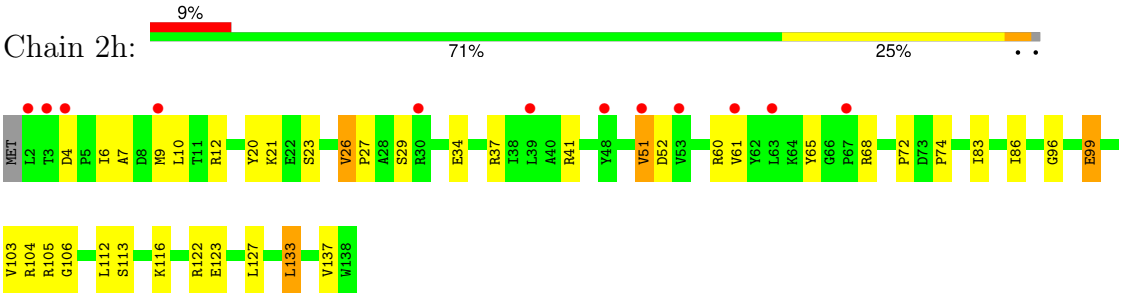
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



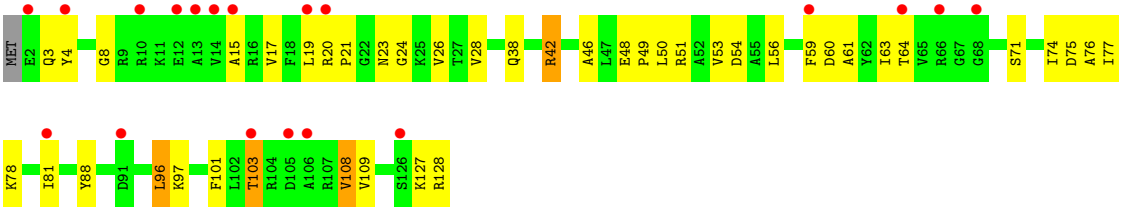
• Molecule 39: 30S ribosomal protein S8

Chain 2h:

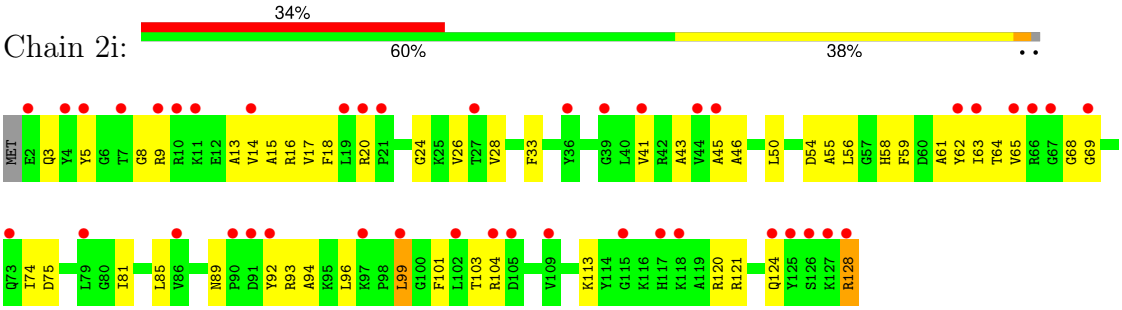


• Molecule 40: 30S ribosomal protein S9

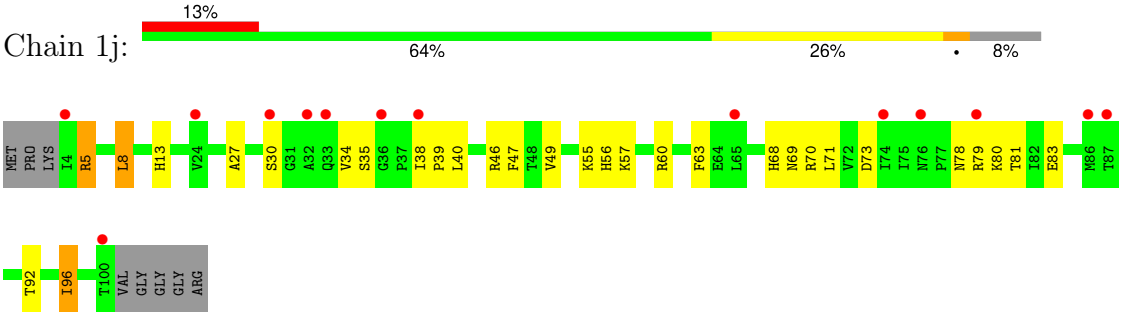
Chain 1i:



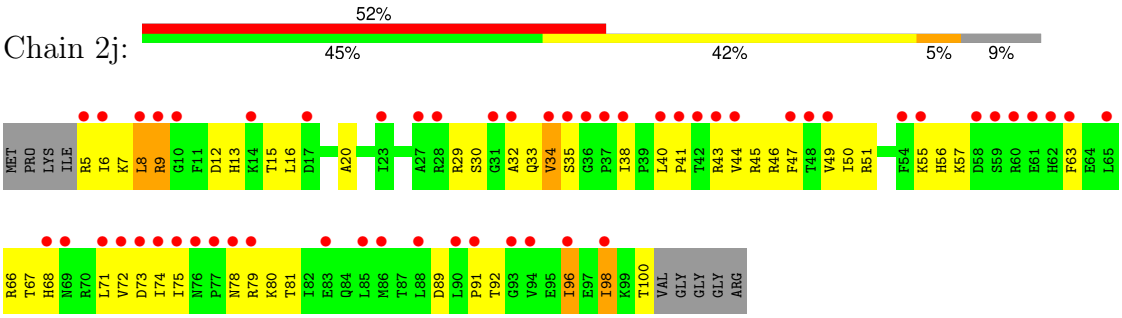
• Molecule 40: 30S ribosomal protein S9



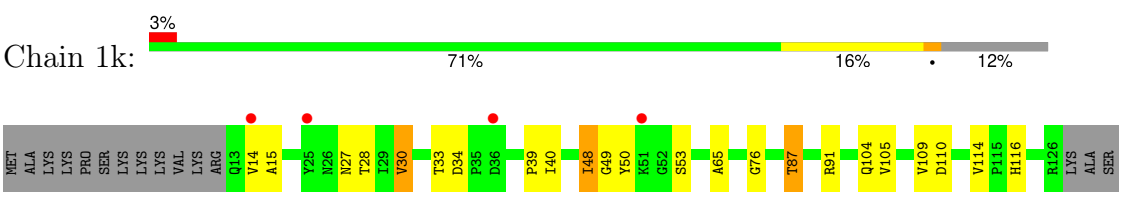
• Molecule 41: 30S ribosomal protein S10



• Molecule 41: 30S ribosomal protein S10

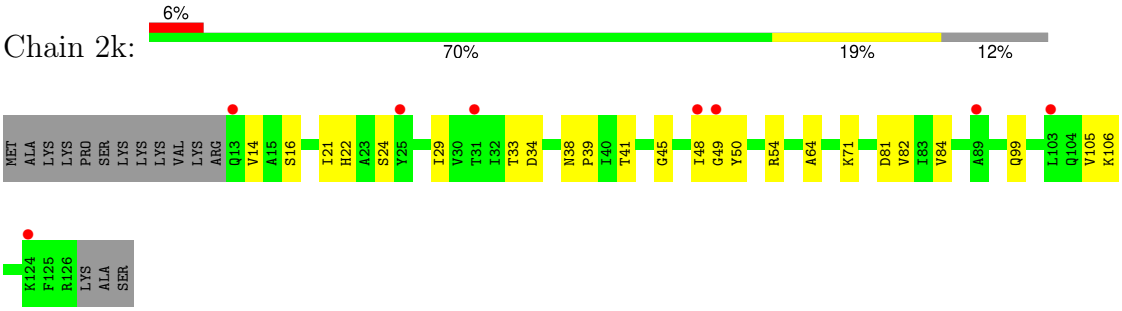


• Molecule 42: 30S ribosomal protein S11



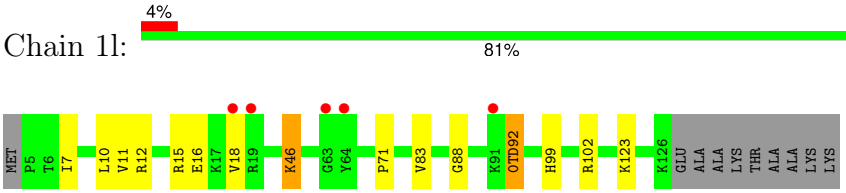
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



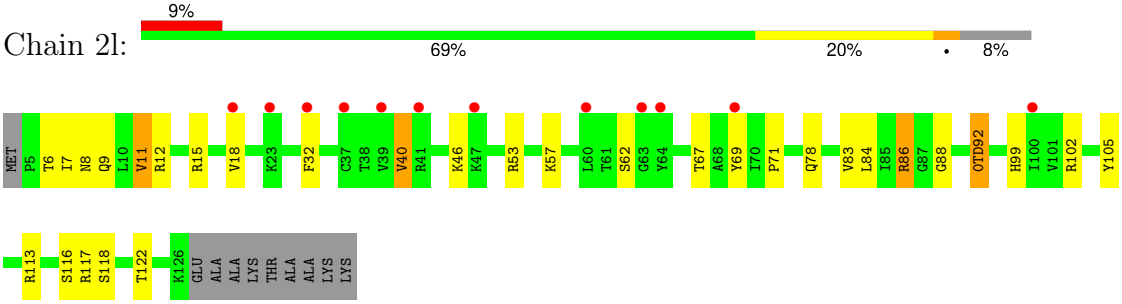
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



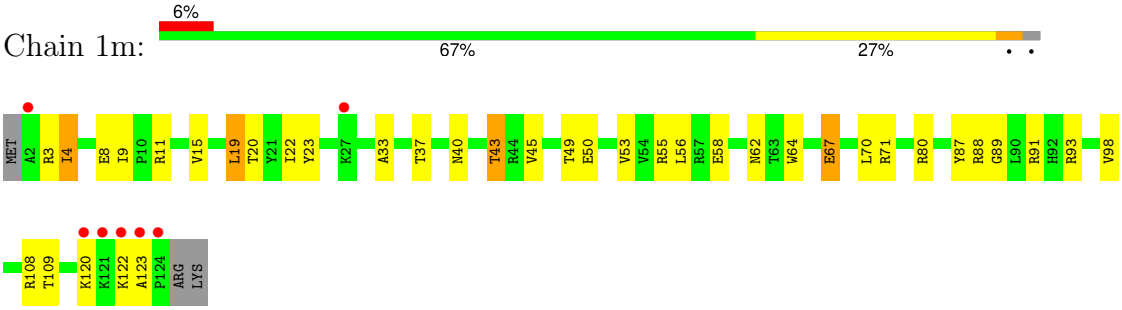
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



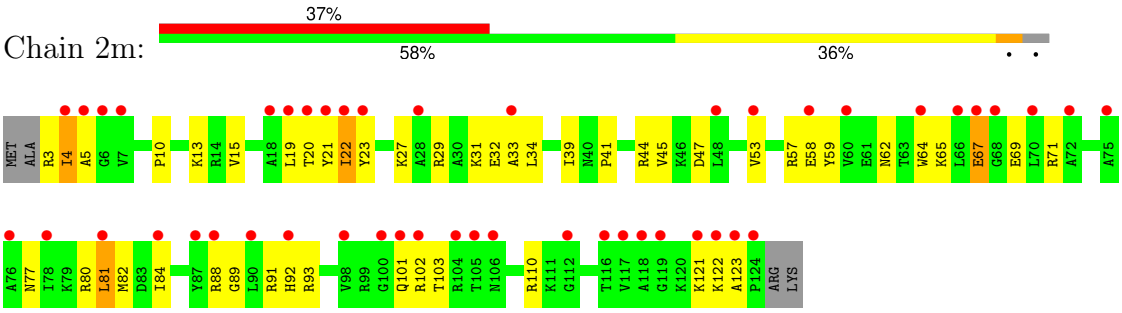
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



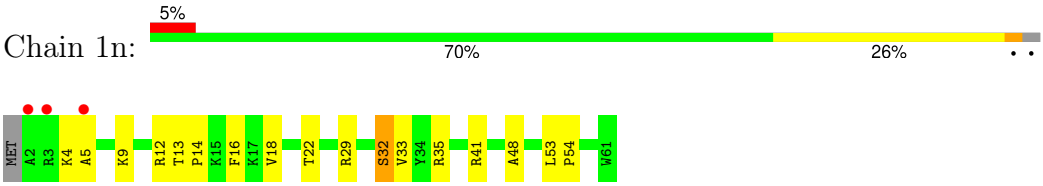
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



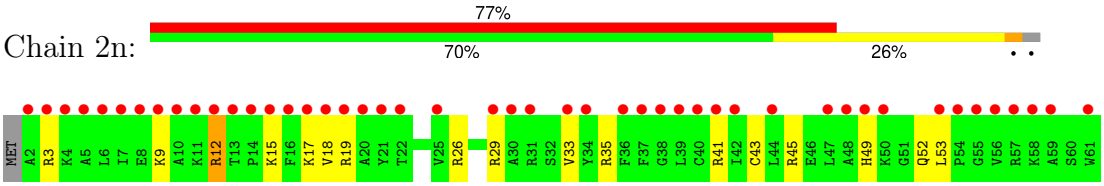
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



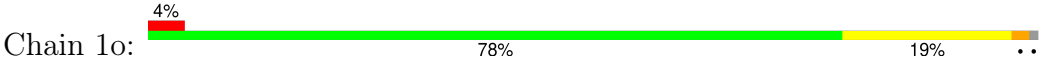
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



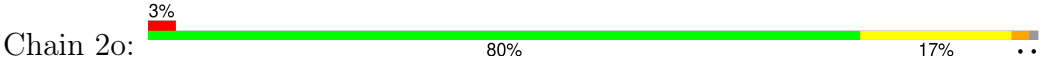
• Molecule 46: 30S ribosomal protein S15

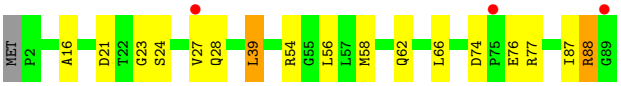
Chain 1o:



• Molecule 46: 30S ribosomal protein S15

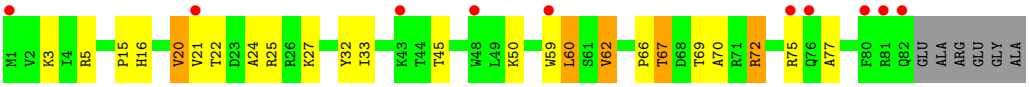
Chain 2o:





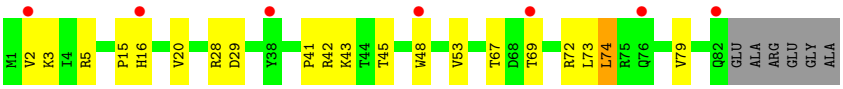
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



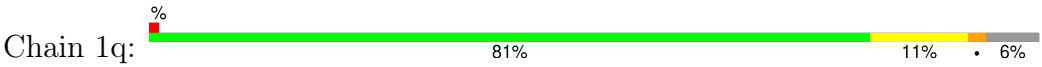
• Molecule 47: 30S ribosomal protein S16

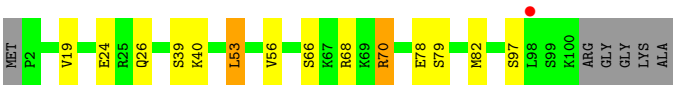
Chain 2p:



• Molecule 48: 30S ribosomal protein S17

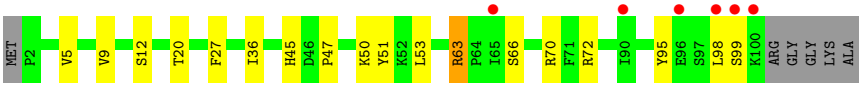
Chain 1q:





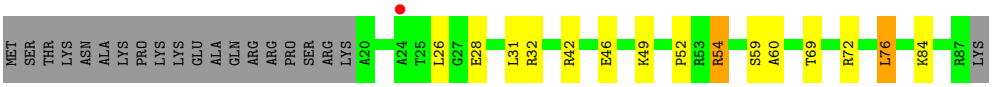
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



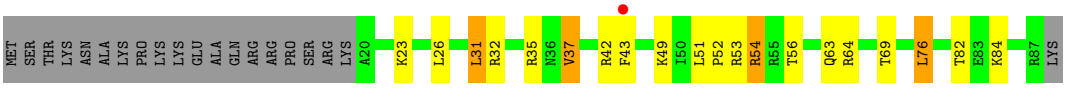
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



• Molecule 49: 30S ribosomal protein S18

Chain 2r:



• Molecule 50: 30S ribosomal protein S19

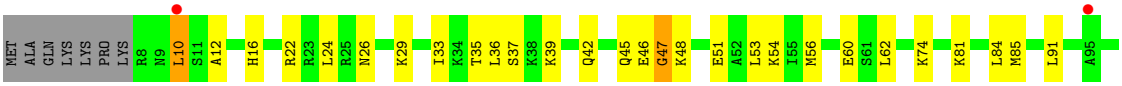
Chain 1s:

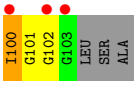
• Molecule 50: 30S ribosomal protein S19

Chain 2s:

• Molecule 51: 30S ribosomal protein S20

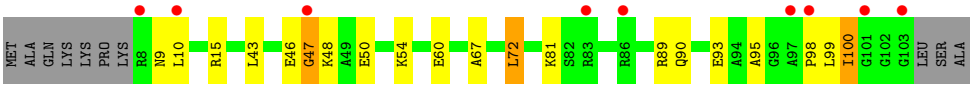
Chain 1t:





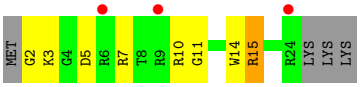
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



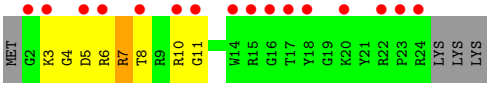
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



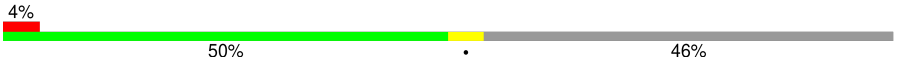
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



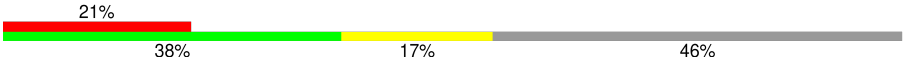
• Molecule 53: MF-mRNA

Chain 1v:



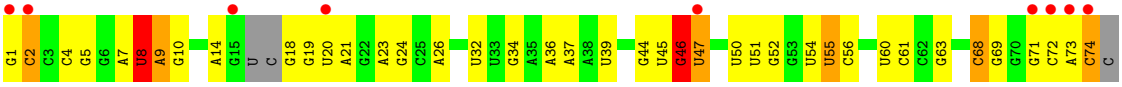
• Molecule 53: MF-mRNA

Chain 2v:



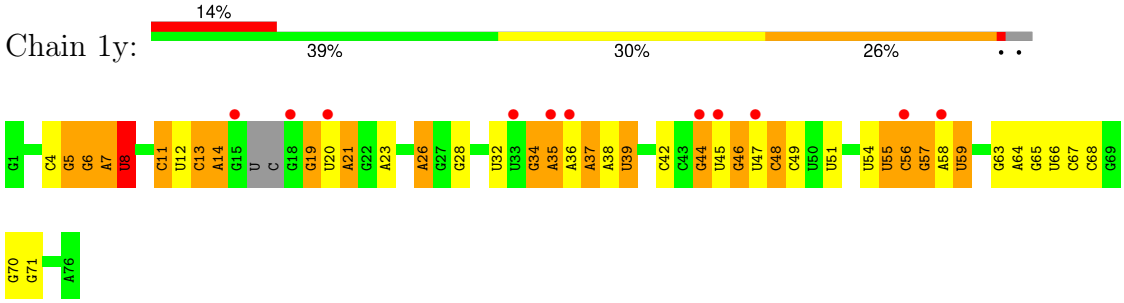
• Molecule 54: A- and E-site Deacylated tRNAphe

Chain 1w:



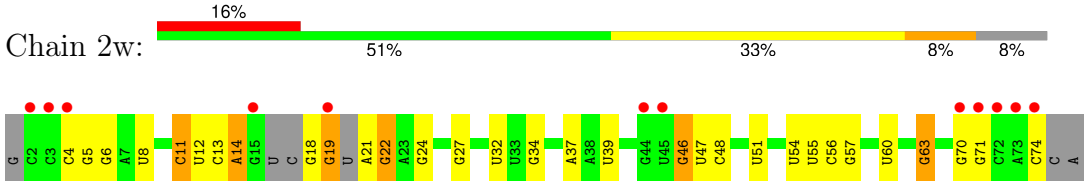
• Molecule 54: A- and E-site Deacylated tRNAphe

Chain 1y:



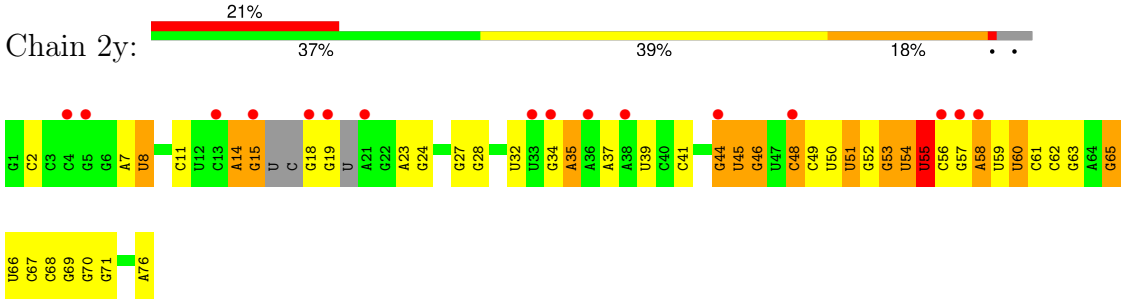
• Molecule 54: A- and E-site Deacylated tRNAphe

Chain 2w:



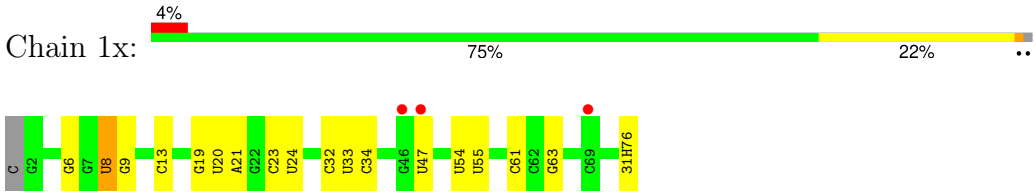
• Molecule 54: A- and E-site Deacylated tRNAphe

Chain 2y:



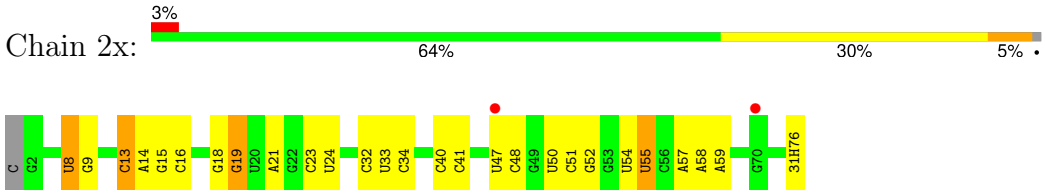
• Molecule 55: P-site Aminoacyl-tRNA fMet-tRNAmet

Chain 1x:



• Molecule 55: P-site Aminoacyl-tRNA fMet-tRNAmet

Chain 2x:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.00Å 449.39Å 623.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	182.26 – 2.70 182.26 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (182.26-2.70) 99.4 (182.26-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.201 , 0.241 0.200 , 0.239	Depositor DCC
R_{free} test set	79417 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	60.0	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 73.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	298872	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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: UR3, 4SU, 2MG, 31H, PSU, K, MG, MA6, OMG, OMC, 5MC, G7M, 0TD, SF4, OMU, ZN, 5MU, WC9, MIA, 2MA, M2G, 4OC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1A	0.27	0/69011	0.45	3/107720 (0.0%)
1	2A	0.21	0/67295	0.39	1/105042 (0.0%)
2	1B	0.20	0/2882	0.37	0/4494
2	2B	0.18	0/2879	0.35	0/4487
3	1D	0.27	0/2186	0.50	0/2944
3	2D	0.22	0/2186	0.45	0/2944
4	1E	0.26	0/1592	0.50	0/2149
4	2E	0.21	0/1592	0.45	0/2149
5	1F	0.25	0/1619	0.49	0/2193
5	2F	0.20	0/1615	0.45	0/2188
6	1G	0.21	0/1448	0.43	0/1957
6	2G	0.20	0/1453	0.41	0/1963
7	1H	0.21	0/1356	0.41	0/1834
7	2H	0.18	0/1356	0.35	0/1834
8	1I	0.20	0/1112	0.39	0/1514
8	2I	0.20	0/1079	0.41	0/1475
9	1N	0.24	0/1144	0.45	0/1543
9	2N	0.18	0/1144	0.38	0/1543
10	1O	0.24	0/943	0.43	0/1269
10	2O	0.20	0/943	0.43	0/1269
11	1P	0.25	0/1152	0.51	0/1533
11	2P	0.21	0/1152	0.51	0/1533
12	1Q	0.28	0/1143	0.46	0/1527
12	2Q	0.20	0/1143	0.42	0/1527
13	1R	0.26	0/982	0.49	0/1312
13	2R	0.19	0/982	0.43	0/1312
14	1S	0.21	0/883	0.47	0/1176
14	2S	0.21	0/880	0.45	0/1172
15	1T	0.23	0/1105	0.45	0/1477
15	2T	0.21	0/1097	0.43	0/1468
16	1U	0.26	0/977	0.45	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.19	0/977	0.38	0/1301
17	1V	0.24	0/782	0.45	0/1049
17	2V	0.17	0/782	0.37	0/1049
18	1W	0.27	0/897	0.45	0/1205
18	2W	0.21	0/897	0.40	0/1205
19	1X	0.27	0/764	0.50	2/1025 (0.2%)
19	2X	0.21	0/764	0.51	2/1025 (0.2%)
20	1Y	0.23	0/819	0.47	0/1095
20	2Y	0.18	0/819	0.41	0/1095
21	1Z	0.21	0/1267	0.43	0/1717
21	2Z	0.22	0/1299	0.47	1/1763 (0.1%)
22	10	0.25	0/662	0.46	0/881
22	20	0.21	0/662	0.49	1/881 (0.1%)
23	11	0.25	0/762	0.44	0/1014
23	21	0.23	0/762	0.44	0/1014
24	12	0.24	0/590	0.41	0/781
24	22	0.21	0/590	0.37	0/781
25	13	0.24	0/474	0.45	0/635
25	23	0.18	0/469	0.38	0/630
26	14	0.25	0/565	0.60	0/761
26	24	0.25	0/545	0.46	0/737
27	15	0.26	0/469	0.50	0/635
27	25	0.21	0/469	0.39	0/635
28	16	0.25	0/460	0.44	0/613
28	26	0.21	0/456	0.42	0/608
29	17	0.27	0/426	0.48	0/561
29	27	0.24	0/426	0.48	0/561
30	18	0.27	0/525	0.46	0/691
30	28	0.19	0/525	0.48	0/691
31	19	0.26	0/310	0.48	0/407
31	29	0.20	0/310	0.43	0/407
32	1a	0.20	0/35795	0.38	0/55864
32	2a	0.19	0/35886	0.37	3/56005 (0.0%)
33	1b	0.24	0/1881	0.46	0/2542
33	2b	0.23	0/1860	0.50	0/2518
34	1c	0.19	0/1572	0.39	0/2126
34	2c	0.22	0/1566	0.45	1/2119 (0.0%)
35	1d	0.19	0/1685	0.43	0/2262
35	2d	0.20	0/1704	0.46	0/2284
36	1e	0.21	0/1145	0.49	0/1543
36	2e	0.21	0/1149	0.44	0/1548
37	1f	0.18	0/823	0.40	0/1115
37	2f	0.20	0/829	0.41	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.18	0/1250	0.39	0/1679
38	2g	0.19	0/1254	0.39	0/1683
39	1h	0.20	0/1108	0.40	0/1494
39	2h	0.19	0/1108	0.42	0/1494
40	1i	0.20	0/1002	0.46	0/1346
40	2i	0.21	0/997	0.47	1/1343 (0.1%)
41	1j	0.20	0/722	0.45	0/982
41	2j	0.22	0/727	0.47	0/988
42	1k	0.17	0/844	0.40	0/1145
42	2k	0.18	0/848	0.38	0/1149
43	1l	0.21	0/937	0.44	0/1260
43	2l	0.18	0/937	0.41	0/1260
44	1m	0.19	0/969	0.46	0/1302
44	2m	0.21	0/961	0.49	0/1291
45	1n	0.18	0/501	0.42	0/664
45	2n	0.21	0/501	0.43	0/664
46	1o	0.19	0/739	0.40	0/985
46	2o	0.17	0/739	0.40	0/985
47	1p	0.19	0/697	0.45	0/939
47	2p	0.18	0/693	0.45	0/935
48	1q	0.19	0/836	0.41	0/1117
48	2q	0.18	0/836	0.37	0/1117
49	1r	0.19	0/560	0.40	0/746
49	2r	0.18	0/560	0.40	0/746
50	1s	0.18	0/667	0.44	0/900
50	2s	0.29	0/661	0.57	0/893
51	1t	0.20	0/730	0.48	0/965
51	2t	0.20	0/729	0.46	0/965
52	1u	0.17	0/203	0.41	0/266
52	2u	0.18	0/203	0.42	0/266
53	1v	0.19	0/310	0.35	0/480
53	2v	0.18	0/310	0.31	0/480
54	1w	0.28	0/1559	0.37	0/2424
54	1y	0.28	2/1606 (0.1%)	0.38	0/2497
54	2w	0.30	2/1509 (0.1%)	0.37	0/2345
54	2y	0.29	2/1583 (0.1%)	0.40	0/2459
55	1x	0.27	0/1700	0.40	0/2650
55	2x	0.24	0/1700	0.37	0/2650
All	All	0.22	6/316546 (0.0%)	0.41	15/473905 (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
5	2F	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	46	G7M	O3'-P	5.51	1.61	1.56
54	1y	8	4SU	O3'-P	5.35	1.61	1.56
54	2y	46	G7M	O3'-P	5.27	1.61	1.56
54	1y	46	G7M	O3'-P	5.16	1.61	1.56
54	2w	8	4SU	O3'-P	5.09	1.61	1.56
54	2y	8	4SU	O3'-P	5.07	1.61	1.56

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1992	G	C2'-C3'-O3'	7.42	120.63	109.50
19	2X	94	GLY	CA-C-N	6.56	133.50	121.70
19	2X	94	GLY	C-N-CA	6.56	133.50	121.70
1	2A	1992	G	C2'-C3'-O3'	6.53	119.30	109.50
21	2Z	135	GLU	N-CA-C	-5.87	107.93	114.62
32	2a	1272	G	N1-C2-N2	-5.39	100.04	116.20
34	2c	8	ILE	N-CA-C	-5.37	106.57	111.67
32	2a	1263	C	N1-C2-O2	5.33	134.90	118.90
1	1A	1992	G	P-O3'-C3'	5.24	128.06	120.20
19	1X	94	GLY	CA-C-N	5.18	131.03	121.70
19	1X	94	GLY	C-N-CA	5.18	131.03	121.70
40	2i	41	VAL	N-CA-C	-5.12	106.58	112.98
32	2a	1272	G	N3-C2-N2	5.09	135.19	119.90
1	1A	548	A	P-O3'-C3'	5.06	127.80	120.20
22	20	22	GLY	N-CA-C	5.03	118.11	111.52

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	2F	20	LEU	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	31197	432	0
1	2A	60322	0	30428	497	0
2	1B	2577	0	1305	14	0
2	2B	2575	0	1303	24	0
3	1D	2136	0	2218	37	0
3	2D	2136	0	2218	34	0
4	1E	1559	0	1618	17	0
4	2E	1559	0	1618	25	0
5	1F	1584	0	1625	26	0
5	2F	1580	0	1619	40	0
6	1G	1423	0	1436	25	0
6	2G	1428	0	1438	42	0
7	1H	1330	0	1407	26	0
7	2H	1330	0	1407	28	0
8	1I	1097	0	1140	25	0
8	2I	1064	0	1082	14	0
9	1N	1117	0	1184	17	0
9	2N	1117	0	1184	17	0
10	1O	933	0	996	7	0
10	2O	933	0	996	12	0
11	1P	1135	0	1212	17	0
11	2P	1135	0	1212	24	0
12	1Q	1122	0	1179	20	0
12	2Q	1122	0	1179	15	0
13	1R	968	0	1033	11	0
13	2R	968	0	1033	16	0
14	1S	873	0	927	12	0
14	2S	870	0	923	29	0
15	1T	1091	0	1151	5	0
15	2T	1083	0	1136	14	0
16	1U	959	0	1019	18	0
16	2U	959	0	1019	14	0
17	1V	771	0	830	7	0
17	2V	771	0	830	9	0
18	1W	886	0	940	4	0
18	2W	886	0	940	10	0
19	1X	750	0	814	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2X	750	0	814	14	0
20	1Y	806	0	881	8	0
20	2Y	806	0	881	10	0
21	1Z	1240	0	1240	31	0
21	2Z	1271	0	1273	42	0
22	10	653	0	674	9	0
22	20	653	0	674	15	0
23	11	755	0	826	6	0
23	21	755	0	826	13	0
24	12	588	0	643	5	0
24	22	588	0	643	8	0
25	13	469	0	518	1	0
25	23	464	0	514	6	0
26	14	552	0	533	21	0
26	24	532	0	503	24	0
27	15	455	0	465	7	0
27	25	455	0	465	4	0
28	16	453	0	473	6	0
28	26	449	0	469	4	0
29	17	418	0	467	1	0
29	27	418	0	467	4	0
30	18	517	0	582	13	0
30	28	517	0	582	11	0
31	19	307	0	335	3	0
31	29	307	0	335	3	0
32	1a	32246	0	16295	295	0
32	2a	32327	0	16338	397	0
33	1b	1846	0	1867	48	0
33	2b	1825	0	1828	63	0
34	1c	1548	0	1535	23	0
34	2c	1542	0	1517	51	0
35	1d	1655	0	1672	42	0
35	2d	1674	0	1714	43	0
36	1e	1129	0	1185	24	0
36	2e	1133	0	1191	36	0
37	1f	810	0	804	12	0
37	2f	816	0	808	14	0
38	1g	1231	0	1238	11	0
38	2g	1235	0	1249	27	0
39	1h	1088	0	1126	25	0
39	2h	1088	0	1126	23	0
40	1i	983	0	986	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	2i	978	0	966	39	0
41	1j	709	0	650	22	0
41	2j	714	0	672	36	0
42	1k	829	0	825	9	0
42	2k	833	0	836	13	0
43	1l	932	0	981	8	0
43	2l	932	0	981	17	0
44	1m	958	0	1002	25	0
44	2m	950	0	988	35	0
45	1n	492	0	529	12	0
45	2n	492	0	529	12	0
46	1o	728	0	760	12	0
46	2o	728	0	760	10	0
47	1p	681	0	697	16	0
47	2p	677	0	686	11	0
48	1q	823	0	891	9	0
48	2q	823	0	891	8	0
49	1r	555	0	618	9	0
49	2r	555	0	618	12	0
50	1s	652	0	662	18	0
50	2s	646	0	644	28	0
51	1t	728	0	798	19	0
51	2t	727	0	796	13	0
52	1u	199	0	208	7	0
52	2u	199	0	208	5	0
53	1v	277	0	140	1	0
53	2v	277	0	140	3	0
54	1w	1550	0	796	20	0
54	1y	1585	0	803	18	0
54	2w	1502	0	762	13	0
54	2y	1565	0	794	27	0
55	1x	1635	0	839	5	0
55	2x	1635	0	839	13	0
56	10	9	0	0	0	0
56	11	5	0	0	0	0
56	12	2	0	0	0	0
56	13	4	0	0	0	0
56	14	1	0	0	0	0
56	15	7	0	0	0	0
56	16	1	0	0	0	0
56	17	5	0	0	0	0
56	18	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	19	1	0	0	0	0
56	1A	1059	0	0	0	0
56	1B	34	0	0	0	0
56	1D	12	0	0	0	0
56	1E	17	0	0	0	0
56	1F	12	0	0	0	0
56	1G	5	0	0	0	0
56	1I	1	0	0	0	0
56	1N	5	0	0	0	0
56	1O	6	0	0	0	0
56	1P	6	0	0	0	0
56	1Q	6	0	0	0	0
56	1R	6	0	0	0	0
56	1S	2	0	0	0	0
56	1T	3	0	0	0	0
56	1U	10	0	0	0	0
56	1V	6	0	0	0	0
56	1W	7	0	0	0	0
56	1X	6	0	0	0	0
56	1Y	2	0	0	0	0
56	1Z	2	0	0	0	0
56	1a	208	0	0	0	0
56	1b	1	0	0	0	0
56	1d	1	0	0	0	0
56	1e	2	0	0	0	0
56	1f	1	0	0	0	0
56	1k	1	0	0	0	0
56	1l	2	0	0	0	0
56	1m	2	0	0	0	0
56	1n	1	0	0	0	0
56	1p	1	0	0	0	0
56	1r	1	0	0	0	0
56	1t	1	0	0	0	0
56	1w	3	0	0	0	0
56	1x	14	0	0	0	0
56	20	2	0	0	0	0
56	21	3	0	0	0	0
56	23	2	0	0	0	0
56	25	1	0	0	0	0
56	27	1	0	0	0	0
56	28	2	0	0	0	0
56	2A	771	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2B	20	0	0	0	0
56	2D	8	0	0	0	0
56	2E	10	0	0	0	0
56	2F	5	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	1	0	0	0	0
56	2P	2	0	0	0	0
56	2Q	3	0	0	0	0
56	2R	2	0	0	0	0
56	2T	2	0	0	0	0
56	2U	1	0	0	0	0
56	2V	2	0	0	0	0
56	2W	2	0	0	0	0
56	2X	2	0	0	0	0
56	2a	214	0	0	0	0
56	2d	1	0	0	0	0
56	2e	1	0	0	0	0
56	2f	1	0	0	0	0
56	2g	1	0	0	0	0
56	2i	2	0	0	0	0
56	2j	1	0	0	0	0
56	2k	1	0	0	0	0
56	2l	3	0	0	0	0
56	2q	3	0	0	0	0
56	2r	2	0	0	0	0
56	2t	1	0	0	0	0
56	2v	1	0	0	0	0
56	2w	1	0	0	0	0
56	2x	5	0	0	0	0
56	2y	2	0	0	0	0
57	1A	1	0	0	0	0
57	2x	1	0	0	0	0
58	1A	34	0	0	1	0
58	2A	34	0	0	1	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	1	0
61	10	12	0	0	1	0
61	11	8	0	0	0	0
61	12	2	0	0	0	0
61	13	3	0	0	0	0
61	14	1	0	0	0	0
61	15	6	0	0	0	0
61	16	1	0	0	0	0
61	17	8	0	0	0	0
61	18	11	0	0	1	0
61	1A	1685	0	0	48	0
61	1B	54	0	0	1	0
61	1D	26	0	0	0	0
61	1E	25	0	0	1	0
61	1F	15	0	0	1	0
61	1G	3	0	0	2	0
61	1H	1	0	0	0	0
61	1N	3	0	0	0	0
61	1O	5	0	0	0	0
61	1P	17	0	0	0	0
61	1Q	6	0	0	0	0
61	1R	9	0	0	0	0
61	1S	2	0	0	0	0
61	1T	7	0	0	0	0
61	1U	11	0	0	0	0
61	1V	5	0	0	0	0
61	1W	7	0	0	0	0
61	1X	3	0	0	0	0
61	1Y	1	0	0	1	0
61	1a	213	0	0	15	0
61	1b	1	0	0	0	0
61	1f	2	0	0	0	0
61	1g	1	0	0	0	0
61	1i	1	0	0	0	0
61	1j	1	0	0	0	0
61	1l	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1q	1	0	0	0	0
61	1v	2	0	0	0	0
61	1w	4	0	0	0	0
61	1x	9	0	0	0	0
61	20	1	0	0	0	0
61	21	7	0	0	0	0
61	27	4	0	0	0	0
61	28	5	0	0	0	0
61	29	1	0	0	0	0
61	2A	848	0	0	56	0
61	2B	16	0	0	0	0
61	2D	16	0	0	1	0
61	2E	10	0	0	0	0
61	2F	11	0	0	0	0
61	2I	1	0	0	0	0
61	2O	3	0	0	0	0
61	2P	6	0	0	0	0
61	2Q	1	0	0	0	0
61	2R	2	0	0	0	0
61	2T	4	0	0	0	0
61	2U	3	0	0	0	0
61	2V	1	0	0	0	0
61	2W	2	0	0	0	0
61	2X	1	0	0	0	0
61	2Y	1	0	0	0	0
61	2a	145	0	0	18	0
61	2d	3	0	0	0	0
61	2j	3	0	0	2	0
61	2l	3	0	0	1	0
61	2r	1	0	0	0	0
61	2t	1	0	0	0	0
61	2x	4	0	0	0	0
61	2y	4	0	0	0	0
All	All	298872	0	196667	3034	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 6.

All (3034) 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	1.25	1.34
1:1A:1082:U:O4	1:1A:1086:A:N1	1.92	1.03
10:2O:48:PRO:HB3	32:2a:1422:G:H5"	1.45	0.98
1:2A:784:A:OP2	61:2A:3801:HOH:O	1.84	0.95
54:2y:55:PSU:HN1	54:2y:57:G:H5"	1.29	0.94
1:2A:2589:A:OP1	61:2A:3801:HOH:O	1.88	0.92
41:1j:30:SER:HB3	41:1j:81:THR:HG23	1.53	0.90
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.54	0.89
10:1O:48:PRO:HB3	32:1a:1422:G:H5"	1.55	0.88
1:2A:1689:A:H62	1:2A:1698:A:H2	1.17	0.88
32:2a:1025:U:H3	32:2a:1036:G:H1	1.22	0.87
36:1e:78:HIS:HD2	39:1h:104:ARG:HD2	1.40	0.87
26:14:58:ARG:HE	50:1s:68:GLY:H	1.21	0.87
32:2a:1029:C:C4	32:2a:1032:G:N1	2.43	0.87
1:2A:783:A:OP2	61:2A:3801:HOH:O	1.91	0.86
32:2a:1286:A:H8	32:2a:1287:A:H4'	1.41	0.86
44:2m:23:TYR:HB3	44:2m:67:GLU:HA	1.57	0.85
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.09	0.85
32:2a:406:G:H21	35:2d:119:GLN:HE22	1.24	0.85
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.58	0.84
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.58	0.84
1:2A:1204:A:H2	1:2A:1241:A:H62	1.25	0.84
40:2i:28:VAL:HG12	40:2i:63:ILE:HB	1.60	0.84
1:1A:826:U:OP1	61:1A:4101:HOH:O	1.95	0.83
1:2A:2319:G:H22	14:2S:3:ARG:HH11	1.22	0.82
41:1j:8:LEU:HD22	41:1j:96:ILE:HG22	1.61	0.82
1:2A:2430:A:OP2	61:2A:3802:HOH:O	1.97	0.82
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.62	0.82
54:2y:18:G:N2	54:2y:55:PSU:N3	2.23	0.81
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	1.60	0.81
1:1A:2427:C:OP1	61:1A:4101:HOH:O	1.97	0.81
1:1A:1054:A:H61	1:1A:1105:U:H3	1.27	0.81
54:2y:18:G:H22	54:2y:55:PSU:HN3	1.25	0.80
1:1A:1053:C:H42	1:1A:1106:G:H1	1.30	0.80
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.14	0.80
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.15	0.79
26:14:16:CYS:SG	26:14:17:GLY:N	2.56	0.79
32:1a:116:A:OP1	61:1a:1901:HOH:O	2.00	0.79
32:2a:1278:U:H5'	32:2a:1279:A:H5'	1.64	0.79
32:1a:975:A:H4'	32:1a:976:G:H5"	1.64	0.79
32:2a:1264:C:H42	32:2a:1271:G:H1	1.30	0.79
32:2a:1310:G:H5'	44:2m:77:ASN:HD21	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:2s:49:ILE:HG22	50:2s:62:ILE:HD11	1.65	0.79
1:1A:1062:G:H1	1:1A:1077:A:H61	1.28	0.79
21:2Z:150:LEU:H	21:2Z:171:ILE:HD11	1.47	0.78
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.29	0.78
7:2H:3:ARG:HG2	7:2H:6:ARG:HE	1.49	0.78
49:2r:26:LEU:HD11	49:2r:42:ARG:HD3	1.63	0.78
1:1A:2499:C:OP1	61:1A:4102:HOH:O	2.01	0.78
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.17	0.77
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.63	0.77
26:24:53:GLU:HG2	26:24:55:ARG:H	1.48	0.77
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.64	0.77
34:2c:125:GLU:HB2	34:2c:190:ARG:HH21	1.49	0.77
1:1A:1865:G:OP1	61:1A:4103:HOH:O	2.04	0.76
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.67	0.76
32:1a:664:G:H22	32:1a:741:G:H1	1.34	0.75
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.18	0.75
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.31	0.75
29:27:24:THR:HG22	29:27:27:GLY:H	1.50	0.75
40:2i:128:ARG:NH2	55:2x:33:U:OP2	2.19	0.75
32:1a:1086:U:H3	32:1a:1099:G:H22	1.34	0.75
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.68	0.75
32:2a:953:G:H5'	32:2a:965:A:H61	1.49	0.75
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.20	0.75
6:1G:45:GLU:OE2	61:1G:301:HOH:O	2.03	0.75
32:1a:1030(A):G:O2'	32:1a:1031:G:N2	2.18	0.74
33:2b:178:ARG:HH12	39:2h:68:ARG:HH22	1.32	0.74
2:1B:21:G:N7	61:1B:301:HOH:O	2.19	0.74
1:1A:2447:G:OP2	61:1A:4106:HOH:O	2.06	0.74
1:2A:975:C:OP1	61:2A:3803:HOH:O	2.04	0.74
32:2a:504:C:OP1	61:2a:1901:HOH:O	2.05	0.74
32:2a:664:G:H22	32:2a:741:G:H1	1.34	0.74
46:2o:16:ALA:HB1	46:2o:21:ASP:HB3	1.69	0.74
34:2c:63:ASN:HB3	34:2c:98:ASN:HD22	1.50	0.74
38:2g:113:GLU:HG2	38:2g:119:ARG:HG2	1.67	0.74
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.18	0.74
32:1a:1108:G:O6	61:1a:1902:HOH:O	2.06	0.74
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.68	0.74
1:2A:962:G:OP1	61:2A:3805:HOH:O	2.06	0.74
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.68	0.74
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.23	0.74
1:1A:1602:U:O4	61:1A:4104:HOH:O	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1332:G:OP1	61:1A:4107:HOH:O	2.06	0.73
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.21	0.73
40:1i:50:LEU:HD13	40:1i:56:LEU:HA	1.70	0.73
40:2i:9:ARG:HG2	40:2i:14:VAL:HG12	1.70	0.73
1:1A:1264:G:OP1	27:15:19:ARG:NH2	2.17	0.73
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.36	0.73
1:2A:1830:C:OP2	61:2A:3804:HOH:O	2.06	0.73
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.71	0.73
1:2A:2292:C:OP1	14:2S:17:ARG:NH2	2.20	0.73
1:2A:2625:G:O6	61:2A:3806:HOH:O	2.07	0.73
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.21	0.73
1:1A:2550:G:OP1	61:1A:4105:HOH:O	2.05	0.73
32:2a:1271:G:N2	32:2a:1272:G:N7	2.37	0.72
32:1a:1027:C:C2	32:1a:1034:G:N2	2.56	0.72
32:2a:1224:G:OP1	61:2a:1902:HOH:O	2.07	0.72
1:1A:2573:C:OP1	61:1A:4108:HOH:O	2.06	0.72
33:1b:87:ARG:NH2	33:1b:220:ASP:OD1	2.22	0.72
39:1h:34:GLU:OE1	39:1h:37:ARG:NH1	2.23	0.72
41:2j:8:LEU:HB3	41:2j:96:ILE:HG23	1.70	0.72
32:2a:547:A:OP1	61:2a:1903:HOH:O	2.07	0.72
1:1A:884:C:H42	1:1A:892:G:H1	1.36	0.72
40:1i:48:GLU:HA	40:1i:51:ARG:HD3	1.70	0.72
1:2A:775:G:O3'	61:2A:3807:HOH:O	2.07	0.72
54:2w:18:G:O2'	54:2w:57:G:N2	2.20	0.72
1:1A:1669:A:OP2	61:1A:4105:HOH:O	2.06	0.72
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.72	0.72
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.72	0.71
1:1A:880:G:H2'	1:1A:881:G:H8	1.54	0.71
29:17:24:THR:HG22	29:17:27:GLY:H	1.53	0.71
54:1w:2:C:H42	54:1w:71:G:H1	1.38	0.71
1:2A:568:U:O4	61:2A:3808:HOH:O	2.07	0.71
1:2A:832:G:H5'	11:2P:45:LEU:HD11	1.72	0.71
1:2A:1812:A:OP2	61:2A:3809:HOH:O	2.08	0.71
32:1a:812:C:N3	61:1a:1911:HOH:O	2.22	0.71
36:1e:8:GLU:OE2	36:1e:63:ARG:NH2	2.23	0.71
32:2a:673:G:H2'	32:2a:674:G:C8	2.25	0.71
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.72	0.71
1:1A:2136:C:N3	1:1A:2155:G:N2	2.39	0.71
1:2A:248:G:OP1	61:2A:3812:HOH:O	2.09	0.71
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.55	0.71
54:1y:51:U:H3	54:1y:63:G:H1	1.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:558:G:OP1	61:1a:1904:HOH:O	2.08	0.70
32:1a:964:A:OP1	61:1a:1903:HOH:O	2.08	0.70
1:2A:2431:U:OP2	61:2A:3810:HOH:O	2.09	0.70
32:2a:1316:G:H22	32:2a:1319:A:H5"	1.55	0.70
1:1A:11:G:H2'	1:1A:12:U:H5"	1.72	0.70
1:2A:2143:C:H42	1:2A:2148:G:H1	1.38	0.70
41:2j:30:SER:O	41:2j:81:THR:OG1	2.09	0.70
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.39	0.70
44:1m:3:ARG:HG2	44:1m:8:GLU:HA	1.74	0.70
32:2a:1257:U:O4	45:2n:17:LYS:NZ	2.24	0.70
7:1H:86:GLU:OE2	7:1H:132:ARG:NH2	2.24	0.70
40:2i:16:ARG:HB2	40:2i:64:THR:HG22	1.73	0.70
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.74	0.70
1:1A:762:U:OP1	61:1A:4109:HOH:O	2.07	0.70
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.24	0.70
1:1A:602:G:O6	61:1A:4111:HOH:O	2.10	0.70
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.06	0.70
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.23	0.70
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.73	0.70
1:1A:1648:C:OP1	61:1A:4110:HOH:O	2.10	0.69
1:2A:1670:C:OP1	61:2A:3813:HOH:O	2.10	0.69
35:2d:156:GLU:HG3	35:2d:159:ARG:HH21	1.57	0.69
1:2A:805:G:OP1	61:2A:3815:HOH:O	2.10	0.69
1:2A:1024:G:OP2	61:2A:3811:HOH:O	2.09	0.69
1:2A:2058:A:N7	61:2A:3849:HOH:O	2.24	0.69
41:2j:38:ILE:HB	41:2j:71:LEU:HB3	1.74	0.69
1:1A:2306:C:O2	61:1G:301:HOH:O	2.08	0.69
1:1A:1055:G:H1	1:1A:1104:C:H42	1.40	0.69
1:1A:1670:C:OP2	61:1A:4105:HOH:O	2.10	0.69
1:1A:2702:U:OP2	61:1A:4112:HOH:O	2.10	0.69
32:2a:1189:C:OP1	41:2j:51:ARG:NH2	2.25	0.69
22:20:11:ARG:O	22:20:14:ARG:NH2	2.25	0.69
33:2b:185:ILE:HB	33:2b:199:TYR:HB2	1.73	0.69
1:1A:1993:U:OP2	61:1A:4113:HOH:O	2.10	0.69
1:2A:2151:G:H2'	1:2A:2152:G:C8	2.27	0.69
21:2Z:99:TYR:HB3	21:2Z:123:ASP:HB2	1.73	0.69
26:24:44:THR:O	26:24:46:GLN:N	2.26	0.69
1:1A:2100:G:H1	1:1A:2189:U:H3	1.39	0.69
1:1A:2575:C:OP2	61:1A:4108:HOH:O	2.11	0.69
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.75	0.69
1:2A:827:U:OP1	61:2A:3802:HOH:O	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1648:C:OP1	61:2A:3814:HOH:O	2.10	0.69
1:2A:2151:G:H2'	1:2A:2152:G:H8	1.57	0.69
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.27	0.69
32:2a:406:G:H5'	35:2d:5:ILE:HD11	1.74	0.69
33:2b:61:LEU:HD21	33:2b:68:ILE:HD11	1.75	0.69
33:2b:217:ARG:HA	33:2b:220:ASP:HB2	1.75	0.69
1:1A:882:G:H1	1:1A:894:C:H42	1.41	0.69
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.74	0.69
21:1Z:156:LYS:HD2	21:1Z:158:PRO:HD3	1.74	0.69
1:2A:2712(A):A:OP2	61:2A:3816:HOH:O	2.11	0.69
5:1F:89:VAL:O	61:1F:401:HOH:O	2.10	0.68
21:2Z:145:GLU:HB3	21:2Z:148:ASP:HB2	1.76	0.68
33:2b:98:LEU:HB2	33:2b:101:MET:HE3	1.75	0.68
8:1I:40:THR:HG22	8:1I:42:SER:H	1.57	0.68
33:1b:69:LEU:HB3	33:1b:162:ILE:HG22	1.75	0.68
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.27	0.68
1:1A:1054:A:N6	1:1A:1105:U:H3	1.90	0.68
1:2A:397:G:N7	61:2A:3861:HOH:O	2.27	0.68
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.75	0.68
21:2Z:53:ILE:HG22	21:2Z:71:VAL:HB	1.75	0.68
1:2A:878:A:H61	1:2A:899:A:H1'	1.58	0.68
21:1Z:72:ARG:NH2	21:1Z:97:GLU:O	2.26	0.68
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.27	0.68
33:2b:197:VAL:HG13	33:2b:200:ILE:HG22	1.75	0.68
1:1A:1664:A:OP1	61:1A:4114:HOH:O	2.11	0.68
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.26	0.68
1:1A:1693:U:O2'	3:1D:14:ARG:NH2	2.27	0.68
4:1E:77:ILE:HD13	4:1E:195:LEU:HD13	1.75	0.68
32:1a:504:C:OP1	61:1a:1905:HOH:O	2.11	0.68
32:1a:922:G:H4'	36:1e:20:GLN:HA	1.76	0.68
32:2a:1277:C:HO2'	32:2a:1279:A:H8	1.42	0.68
1:1A:1452:A:OP2	61:1A:4116:HOH:O	2.12	0.68
38:2g:111:ARG:NH1	38:2g:113:GLU:OE2	2.27	0.67
1:2A:1021:A:H62	1:2A:1141:U:H3	1.40	0.67
30:28:33:ASN:HA	30:28:36:LYS:HD2	1.75	0.67
34:2c:108:ASN:HB3	34:2c:111:LEU:HB2	1.75	0.67
41:2j:6:ILE:HG12	41:2j:98:ILE:HG22	1.75	0.67
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.28	0.67
32:1a:573:A:OP2	61:1a:1906:HOH:O	2.12	0.67
1:2A:2138:C:H42	1:2A:2153:G:H1	1.42	0.67
32:2a:1503:A:O2'	53:2v:13:A:N1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.30	0.67
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.28	0.67
42:2k:48:ILE:O	42:2k:50:TYR:N	2.28	0.67
21:1Z:138:GLU:H	21:1Z:156:LYS:HE3	1.60	0.67
32:1a:953:G:H5'	32:1a:965:A:H61	1.59	0.67
35:2d:175:SER:HB3	35:2d:186:LEU:HD11	1.77	0.67
42:2k:99:GLN:HG2	42:2k:105:VAL:HG21	1.77	0.67
1:1A:1315:C:OP2	61:1A:4107:HOH:O	2.13	0.67
1:2A:2116:G:N1	1:2A:2162:G:OP1	2.28	0.67
1:1A:602:G:O2'	1:1A:655:A:N6	2.28	0.67
1:2A:1647:G:OP1	61:2A:3814:HOH:O	2.13	0.67
1:2A:1973:G:OP1	61:2A:3817:HOH:O	2.12	0.67
12:2Q:35:VAL:HG22	12:2Q:102:VAL:HG22	1.77	0.67
33:2b:58:ILE:HA	33:2b:61:LEU:HB3	1.77	0.67
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.31	0.66
1:2A:1271:G:OP2	61:2A:3814:HOH:O	2.11	0.66
38:2g:80:VAL:HB	38:2g:85:TYR:HE2	1.60	0.66
1:1A:1014:U:OP2	61:1A:4117:HOH:O	2.13	0.66
32:1a:1006:C:H42	32:1a:1023:G:H1	1.42	0.66
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.20	0.66
1:1A:668:G:H5'	1:1A:669:G:OP2	1.95	0.66
1:2A:1163:G:OP1	17:2V:24:LYS:NZ	2.28	0.66
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.11	0.66
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.69	0.66
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.77	0.66
40:2i:3:GLN:HG3	40:2i:20:ARG:HE	1.60	0.66
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.28	0.66
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.11	0.66
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.60	0.66
10:1O:63:VAL:HG12	10:1O:106:LEU:HD11	1.78	0.66
35:1d:15:GLU:OE2	35:1d:59:ARG:NH1	2.29	0.66
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.28	0.66
44:1m:58:GLU:O	44:1m:62:ASN:ND2	2.26	0.66
23:21:83:GLU:OE1	23:21:83:GLU:N	2.29	0.66
32:2a:770:C:OP1	61:2a:1906:HOH:O	2.12	0.66
34:2c:47:LEU:HD12	34:2c:68:VAL:HG11	1.76	0.66
28:16:13:CYS:SG	28:16:47:THR:HG21	2.36	0.65
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	1.77	0.65
9:2N:20:GLY:HA2	9:2N:61:ARG:HE	1.61	0.65
1:2A:2499:C:OP2	61:2A:3818:HOH:O	2.13	0.65
32:2a:576:G:OP1	61:2a:1908:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1279:A:H4'	32:2a:1280:A:OP1	1.94	0.65
1:1A:744:G:OP1	61:1A:4118:HOH:O	2.13	0.65
1:1A:1060:U:H3	1:1A:1088:A:H8	1.45	0.65
1:2A:449:A:OP2	61:2A:3820:HOH:O	2.14	0.65
1:1A:1243:G:O2'	11:1P:7:ARG:NH2	2.30	0.65
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.79	0.65
11:1P:39:LYS:HB2	11:1P:45:LEU:HD13	1.77	0.65
33:2b:71:VAL:HB	33:2b:164:VAL:HG13	1.78	0.65
1:1A:1076:C:O2'	1:1A:1077:A:N7	2.30	0.65
12:1Q:110:THR:HG22	12:1Q:112:GLU:H	1.62	0.65
1:2A:900:A:O2'	1:2A:901:A:OP1	2.12	0.65
43:2l:57:LYS:HG3	43:2l:67:THR:HG22	1.77	0.65
32:1a:1009:G:O6	32:1a:1020:U:O2	2.15	0.65
1:2A:988:A:N7	61:2A:3868:HOH:O	2.29	0.65
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.29	0.65
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.61	0.65
1:1A:1185:C:OP2	61:1A:4119:HOH:O	2.15	0.65
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.77	0.65
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.32	0.65
1:1A:2222:G:O6	61:1A:4115:HOH:O	2.12	0.65
26:24:24:THR:OG1	26:24:25:TYR:N	2.24	0.65
32:2a:944:G:OP1	61:2a:1910:HOH:O	2.15	0.65
32:2a:986:A:N3	50:2s:52:TYR:OH	2.28	0.65
32:2a:1272:G:N2	32:2a:1273:G:N7	2.44	0.65
1:1A:1300:U:H4'	1:1A:1301:A:H5"	1.79	0.64
1:1A:2448:A:OP1	61:1A:4102:HOH:O	2.15	0.64
1:2A:752:A:H3'	29:27:1:MET:HE1	1.79	0.64
32:2a:1272:G:N2	32:2a:1273:G:C5	2.65	0.64
33:2b:165:VAL:HA	33:2b:187:LEU:HB3	1.79	0.64
1:1A:271(L):U:H4'	8:1I:50:ARG:HH22	1.61	0.64
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.79	0.64
36:1e:18:ARG:HD3	36:1e:27:ARG:HH12	1.62	0.64
4:2E:176:ILE:HB	4:2E:181:LEU:HB2	1.78	0.64
32:1a:711:G:OP1	37:1f:54:LYS:NZ	2.31	0.64
1:2A:963:U:OP2	61:2A:3805:HOH:O	2.14	0.64
43:2l:86:ARG:NH1	61:2l:301:HOH:O	2.27	0.64
1:1A:2131:G:H5'	1:1A:2133:G:C8	2.32	0.64
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.78	0.64
32:2a:533:A:OP1	61:2a:1907:HOH:O	2.14	0.64
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.15	0.64
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1503:A:O2'	53:1v:13:A:N1	2.30	0.64
32:2a:266:G:H5"	32:2a:268:C:H41	1.61	0.64
32:2a:975:A:H4'	32:2a:976:G:H5"	1.79	0.64
32:2a:1106:G:H5"	34:2c:172:ARG:HB3	1.79	0.64
7:1H:40:GLU:OE2	7:1H:60:ARG:NH1	2.31	0.64
1:2A:1676:A:OP2	61:2A:3822:HOH:O	2.15	0.64
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.11	0.64
44:2m:80:ARG:HH22	50:2s:69:HIS:HE1	1.46	0.64
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.79	0.64
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.80	0.64
8:2I:4:ILE:HD11	8:2I:44:LEU:HD12	1.80	0.64
8:2I:5:LEU:HD11	8:2I:19:VAL:HG22	1.79	0.64
8:2I:40:THR:O	8:2I:44:LEU:HB2	1.98	0.64
35:2d:150:GLU:HA	35:2d:153:ARG:HD2	1.79	0.64
1:1A:1082:U:N3	1:1A:1086:A:N6	2.05	0.63
7:1H:3:ARG:HG2	7:1H:6:ARG:HG2	1.80	0.63
32:1a:299:G:O6	61:1a:1904:HOH:O	2.10	0.63
9:2N:15:LEU:HB2	9:2N:135:PRO:HB2	1.80	0.63
32:2a:1108:G:O6	61:2a:1904:HOH:O	2.11	0.63
49:2r:52:PRO:HB2	49:2r:54:ARG:HG3	1.79	0.63
55:2x:8:4SU:O5'	55:2x:8:4SU:H6	1.99	0.63
20:1Y:34:LYS:NZ	61:1Y:301:HOH:O	2.19	0.63
24:12:1:MET:HE3	24:12:5:GLU:HB3	1.79	0.63
33:1b:8:LYS:O	33:1b:217:ARG:NH2	2.31	0.63
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.32	0.63
41:1j:49:VAL:HG23	45:1n:41:ARG:HB2	1.80	0.63
46:1o:87:ILE:HG22	46:1o:88:ARG:H	1.63	0.63
37:1f:89:MET:HE1	49:1r:72:ARG:HB3	1.80	0.63
6:2G:145:THR:HG23	6:2G:148:MET:HE3	1.79	0.63
33:2b:162:ILE:HD11	33:2b:184:VAL:HG22	1.78	0.63
34:2c:20:SER:HB3	34:2c:22:TRP:HE1	1.63	0.63
7:1H:124:GLU:HG2	7:1H:132:ARG:HB3	1.79	0.63
7:2H:3:ARG:HE	7:2H:54:ARG:HH12	1.45	0.63
32:2a:1129:C:H2'	32:2a:1139:G:N7	2.14	0.63
1:1A:998:C:OP1	61:1A:4120:HOH:O	2.15	0.63
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.32	0.63
44:1m:3:ARG:HD2	44:1m:9:ILE:HG12	1.80	0.63
33:1b:20:GLU:HA	33:1b:23:ARG:HH21	1.64	0.63
1:2A:2131:G:H4'	1:2A:2132:U:H3'	1.81	0.63
32:1a:165:C:H2'	32:1a:166:G:H8	1.64	0.63
1:2A:106:C:H1'	20:2Y:1:MET:HE2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1086:U:H3	32:2a:1099:G:H22	1.45	0.63
32:2a:1264:C:N4	32:2a:1271:G:H1	1.96	0.63
32:1a:544:G:OP1	35:1d:59:ARG:NH2	2.31	0.62
36:1e:20:GLN:NE2	36:1e:21:ALA:O	2.32	0.62
42:1k:48:ILE:O	42:1k:50:TYR:N	2.30	0.62
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.80	0.62
32:2a:1402:4OC:HM22	32:2a:1403:C:H5'	1.81	0.62
34:2c:37:GLN:NE2	45:2n:52:GLN:OE1	2.24	0.62
50:2s:77:THR:HG23	50:2s:78:ARG:HG3	1.80	0.62
1:1A:106:C:H1'	20:1Y:1:MET:HE2	1.82	0.62
32:1a:67:C:H2'	32:1a:68:G:C8	2.34	0.62
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.18	0.62
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.34	0.62
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.64	0.62
1:2A:2136:C:N4	1:2A:2155:G:H1	1.98	0.62
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.34	0.62
36:2e:12:LEU:HB3	36:2e:31:LEU:HB2	1.82	0.62
41:2j:35:SER:HB3	41:2j:73:ASP:HB2	1.81	0.62
54:2w:11:C:H42	54:2w:24:G:H1	1.47	0.62
1:1A:881:G:C2	1:1A:882:G:H1'	2.35	0.62
1:1A:1651:G:OP1	13:1R:40:LYS:NZ	2.33	0.62
32:2a:737:A:H1'	37:2f:73:ASN:HD21	1.64	0.62
1:1A:303:U:O4	61:1A:4122:HOH:O	2.15	0.62
1:2A:2079:U:OP1	23:21:21:ARG:NH2	2.27	0.62
3:2D:71:ASP:HB2	3:2D:103:ARG:HH12	1.64	0.62
6:2G:101:ILE:HG22	6:2G:105:LYS:HE2	1.81	0.62
32:2a:1118:C:OP1	40:2i:104:ARG:NH1	2.32	0.62
32:1a:1320:C:O2	50:1s:36:ARG:NH2	2.33	0.62
1:2A:893:C:H2'	1:2A:894:C:C4	2.35	0.62
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.80	0.62
32:2a:1129:C:OP1	40:2i:16:ARG:NH1	2.32	0.62
32:2a:1255:G:OP1	41:2j:45:ARG:NH2	2.26	0.62
32:2a:1417:G:O6	61:2a:1905:HOH:O	2.11	0.62
1:2A:2445:G:OP1	5:2F:74:ARG:NH2	2.33	0.62
1:1A:9:U:H3	1:1A:2629:A:H2	1.43	0.61
1:1A:2099:U:H3	1:1A:2190:G:H1	1.47	0.61
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.82	0.61
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.83	0.61
35:1d:85:LYS:HG3	35:1d:86:LYS:H	1.64	0.61
1:2A:1434:A:H61	1:2A:1558:A:H62	1.46	0.61
21:2Z:154:ASP:N	21:2Z:154:ASP:OD1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1010:G:N2	32:2a:1020:U:O2'	2.34	0.61
1:2A:2394:C:N3	54:2y:76:A:O2'	2.32	0.61
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.34	0.61
41:2j:44:VAL:HG13	41:2j:66:ARG:HG2	1.82	0.61
1:1A:847:U:OP2	61:1A:4123:HOH:O	2.16	0.61
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.36	0.61
33:1b:59:GLU:HB2	33:1b:221:LEU:HD11	1.82	0.61
1:2A:1693:U:O2'	3:2D:14:ARG:NH2	2.33	0.61
32:2a:1119:C:OP2	40:2i:9:ARG:NH2	2.34	0.61
1:1A:1271:G:OP2	61:1A:4110:HOH:O	2.16	0.61
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.65	0.61
26:14:58:ARG:HH21	50:1s:68:GLY:HA3	1.66	0.61
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.82	0.61
45:1n:48:ALA:HB2	45:1n:53:LEU:HD12	1.82	0.61
14:2S:67:ARG:HG2	14:2S:71:ARG:HD2	1.82	0.61
15:2T:127:ALA:C	15:2T:129:ARG:H	2.07	0.61
41:2j:47:PHE:N	41:2j:63:PHE:O	2.33	0.61
8:1I:126:TYR:HB2	8:1I:142:VAL:HG23	1.81	0.61
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.47	0.61
12:2Q:97:VAL:HG11	12:2Q:103:MET:HE3	1.83	0.61
26:24:16:CYS:SG	26:24:17:GLY:N	2.73	0.61
32:2a:67:C:H2'	32:2a:68:G:C8	2.35	0.61
40:2i:50:LEU:HD13	40:2i:56:LEU:HA	1.82	0.61
1:1A:2577:A:H5'	27:15:3:LYS:HD2	1.81	0.61
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.82	0.61
44:1m:19:LEU:HD21	44:1m:56:LEU:HD21	1.83	0.61
46:1o:39:LEU:HD13	46:1o:56:LEU:HB2	1.83	0.61
35:2d:112:VAL:H	35:2d:116:GLN:HE21	1.49	0.61
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.01	0.61
1:2A:852:G:H2'	1:2A:853:G:H8	1.66	0.61
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.28	0.61
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.35	0.60
32:1a:1352:C:OP1	52:1u:3:LYS:NZ	2.28	0.60
32:2a:407:G:H5"	35:2d:115:ARG:HB3	1.83	0.60
9:1N:73:THR:HB	9:1N:82:LEU:HD11	1.83	0.60
38:1g:20:ASP:HB3	38:1g:23:VAL:HG12	1.83	0.60
42:1k:91:ARG:NH1	42:1k:110:ASP:OD1	2.34	0.60
1:2A:947:G:O6	61:2A:3821:HOH:O	2.15	0.60
36:2e:36:ASP:O	36:2e:38:GLN:N	2.31	0.60
51:2t:43:LEU:O	51:2t:47:GLY:N	2.29	0.60
1:1A:530:G:N1	1:1A:2023:G:OP1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.01	0.60
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.36	0.60
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.82	0.60
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.08	0.60
36:1e:95:ALA:HB1	36:1e:96:PRO:HD2	1.84	0.60
1:2A:2125:G:H1'	1:2A:2173:A:H61	1.65	0.60
15:2T:118:ARG:HG2	32:2a:1442(A):G:C8	2.36	0.60
50:2s:64:GLU:CD	50:2s:64:GLU:H	2.09	0.60
32:1a:1036:G:H3'	32:1a:1037:C:C6	2.36	0.60
34:2c:185:GLY:O	34:2c:200:ALA:N	2.32	0.60
35:2d:15:GLU:OE2	35:2d:66:ARG:NH1	2.33	0.60
1:1A:363(A):A:H2'	1:1A:363(B):G:H8	1.66	0.60
32:2a:1226:C:OP2	44:2m:91:ARG:NH1	2.32	0.60
7:1H:3:ARG:HH21	7:1H:65:HIS:HB3	1.67	0.60
32:2a:1317:C:O2	50:2s:37:ARG:NH2	2.34	0.60
32:2a:1348:U:H4'	40:2i:120:ARG:HD2	1.83	0.60
1:1A:363(A):A:H2'	1:1A:363(B):G:C8	2.37	0.60
12:1Q:10:ARG:HH11	12:1Q:11:LYS:HE2	1.66	0.60
21:1Z:52:SER:O	21:1Z:54:HIS:N	2.34	0.60
1:2A:330:A:H2	1:2A:1210:A:HO2'	1.47	0.60
32:2a:560:U:H5'	32:2a:566:G:N2	2.16	0.60
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.84	0.60
5:1F:165:ARG:HA	5:1F:168:ARG:HD2	1.82	0.60
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.36	0.60
50:1s:22:LEU:HB3	50:1s:27:GLU:HB3	1.83	0.60
1:2A:880:G:N2	1:2A:898:C:O2	2.33	0.60
32:2a:1263:C:N3	32:2a:1272:G:O6	2.35	0.60
1:1A:1187:G:H5"	17:1V:81:TYR:CE1	2.36	0.60
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.83	0.60
32:1a:376:G:H5"	47:1p:5:ARG:HG2	1.84	0.60
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.83	0.60
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.31	0.60
33:2b:48:MET:HA	33:2b:51:LEU:HB2	1.84	0.60
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.82	0.60
42:1k:34:ASP:HB3	42:1k:40:ILE:HD11	1.84	0.60
33:1b:155:LEU:HD11	33:1b:159:PRO:HG3	1.82	0.59
44:1m:33:ALA:HB2	44:1m:64:TRP:HH2	1.67	0.59
1:2A:624:C:OP1	61:2A:3823:HOH:O	2.16	0.59
1:2A:2592:G:OP2	61:2A:3824:HOH:O	2.16	0.59
3:2D:12:SER:HB3	3:2D:208:LYS:HB3	1.83	0.59
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:91:PHE:O	11:2P:121:LYS:NZ	2.35	0.59
32:2a:17:U:H2'	32:2a:18:C:C6	2.37	0.59
40:2i:85:LEU:HB3	40:2i:92:TYR:HD2	1.67	0.59
7:2H:124:GLU:HG2	7:2H:132:ARG:HB3	1.83	0.59
26:24:46:GLN:C	26:24:48:ARG:H	2.11	0.59
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.35	0.59
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.00	0.59
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.84	0.59
39:2h:12:ARG:NH1	39:2h:27:PRO:HD3	2.18	0.59
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.02	0.59
1:2A:2115:G:O2'	1:2A:2117:A:N7	2.32	0.59
17:2V:25:LEU:H	17:2V:92:THR:HG1	1.51	0.59
32:2a:1135:U:H2'	32:2a:1137:C:C4	2.38	0.59
1:1A:1041:C:H42	1:1A:1114:G:H1	1.48	0.59
11:1P:91:PHE:O	11:1P:121:LYS:NZ	2.31	0.59
32:1a:1036:G:H5"	32:1a:1037:C:C5	2.38	0.59
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.84	0.59
1:2A:2206:G:H5"	1:2A:2207:G:N7	2.17	0.59
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.35	0.59
32:2a:598:U:O4	61:2a:1909:HOH:O	2.15	0.59
34:2c:11:ARG:NH2	34:2c:177:THR:O	2.33	0.59
3:1D:183:ARG:HG3	3:1D:270:ILE:HD13	1.84	0.59
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.84	0.59
1:2A:855:G:O2'	22:20:27:GLU:OE2	2.19	0.59
1:2A:1346:G:OP2	61:2A:3825:HOH:O	2.17	0.59
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	1.84	0.59
16:2U:49:HIS:HA	16:2U:52:ARG:HB2	1.83	0.59
22:20:23:VAL:HG22	22:20:38:VAL:HG22	1.85	0.59
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.38	0.59
1:1A:123:G:OP2	61:1A:4124:HOH:O	2.17	0.59
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.36	0.59
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.36	0.59
1:1A:2136:C:N4	1:1A:2155:G:N1	2.47	0.59
1:2A:2126:A:N6	1:2A:2162:G:O2'	2.36	0.59
6:2G:113:ARG:NH2	6:2G:139:LEU:O	2.36	0.59
7:2H:17:VAL:HG11	7:2H:50:VAL:HG21	1.83	0.59
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.01	0.59
1:1A:1053:C:N4	1:1A:1106:G:H1	1.98	0.59
8:1I:93:THR:HG22	8:1I:119:PRO:HB3	1.85	0.59
32:1a:560:U:O2'	32:1a:561:U:OP2	2.16	0.59
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:114:ILE:HB	6:2G:117:PHE:HD1	1.68	0.59
21:2Z:93:ASP:HA	21:2Z:131:ARG:NH1	2.17	0.59
32:2a:390:C:O3'	47:2p:28:ARG:NH2	2.36	0.59
32:2a:999:C:H42	32:2a:1042:G:H1	1.51	0.59
33:2b:114:ARG:O	33:2b:118:LEU:N	2.35	0.59
34:2c:58:GLU:HB2	34:2c:65:ALA:HB3	1.83	0.59
1:1A:2572:A:C8	4:1E:144:ARG:HD3	2.38	0.58
2:2B:22:U:H3	2:2B:61:G:H1	1.51	0.58
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.85	0.58
32:2a:966:M2G:HM22	55:2x:34:C:H5'	1.83	0.58
21:1Z:132:ASN:HD22	21:1Z:160:GLY:HA3	1.67	0.58
32:1a:966:M2G:O2'	40:1i:127:LYS:O	2.22	0.58
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.35	0.58
1:2A:637:A:OP1	11:2P:133:SER:OG	2.18	0.58
3:1D:71:ASP:HB3	3:1D:103:ARG:HH12	1.67	0.58
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.85	0.58
1:2A:141:A:H8	1:2A:1408:C:HO2'	1.47	0.58
14:2S:105:ALA:HB1	14:2S:110:LEU:HD23	1.86	0.58
41:2j:16:LEU:O	41:2j:20:ALA:N	2.29	0.58
1:1A:528:A:O2'	1:1A:529:A:H5'	2.04	0.58
1:1A:1823:G:OP1	3:1D:54:ARG:NH1	2.37	0.58
26:24:34:GLU:OE1	44:2m:3:ARG:N	2.36	0.58
48:2q:45:HIS:HB3	48:2q:72:ARG:HG2	1.85	0.58
32:1a:45:U:H2'	32:1a:46:G:C8	2.38	0.58
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.18	0.58
1:2A:1023:U:OP2	61:2A:3811:HOH:O	2.17	0.58
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.27	0.58
1:1A:1058:G:H1	1:1A:1080:C:H42	1.51	0.58
32:1a:405:U:OP2	35:1d:3:ARG:NH1	2.32	0.58
32:1a:1025:U:O2	32:1a:1036:G:O6	2.21	0.58
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.67	0.58
1:2A:2467:C:H4'	12:2Q:123:HIS:CD2	2.38	0.58
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.84	0.58
33:2b:77:ALA:HB2	33:2b:211:ILE:HD13	1.85	0.58
54:2y:11:C:H42	54:2y:24:G:H1	1.52	0.58
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.84	0.58
33:1b:93:VAL:HG11	33:1b:97:TRP:CD1	2.38	0.58
39:1h:29:SER:HB3	39:1h:32:LYS:HD2	1.85	0.58
26:24:58:ARG:HG3	50:2s:65:ASN:HA	1.85	0.58
9:1N:62:VAL:HG22	9:1N:66:LYS:HD2	1.86	0.58
32:1a:17:U:H2'	32:1a:18:C:C6	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:407:G:OP1	35:1d:115:ARG:NH2	2.37	0.58
32:1a:1224:G:OP1	61:1a:1907:HOH:O	2.17	0.58
7:2H:80:SER:OG	7:2H:81:GLU:OE1	2.19	0.58
40:1i:42:ARG:NH1	40:1i:71:SER:OG	2.37	0.58
46:1o:74:ASP:HB3	46:1o:77:ARG:HB2	1.85	0.58
1:2A:1762:A:N1	61:2A:3882:HOH:O	2.32	0.58
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.04	0.58
37:2f:36:ARG:NH2	37:2f:38:GLU:OE2	2.37	0.58
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.68	0.58
47:1p:60:LEU:HD11	47:1p:66:PRO:HD3	1.86	0.58
54:1y:19:G:O4'	54:1y:57:G:N2	2.37	0.58
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.39	0.58
54:1w:2:C:N4	54:1w:71:G:H1	2.02	0.57
1:2A:668:G:H5'	1:2A:669:G:OP2	2.03	0.57
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.19	0.57
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.86	0.57
33:2b:63:MET:HG3	33:2b:225:ALA:HB1	1.85	0.57
35:2d:112:VAL:H	35:2d:116:GLN:NE2	2.01	0.57
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.19	0.57
1:1A:2218:U:O4'	23:11:52:ARG:NH2	2.37	0.57
41:1j:38:ILE:HD11	41:1j:71:LEU:HD23	1.86	0.57
32:2a:1004:A:N6	32:2a:1037:C:H1'	2.19	0.57
32:2a:1345:U:OP2	61:2a:1911:HOH:O	2.18	0.57
34:2c:58:GLU:HB3	41:2j:92:THR:HG21	1.86	0.57
39:2h:86:ILE:HG21	39:2h:133:LEU:HD13	1.86	0.57
1:2A:646:A:H2'	1:2A:647:G:O4'	2.04	0.57
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.39	0.57
35:2d:153:ARG:HB3	35:2d:181:MET:HE3	1.86	0.57
36:1e:105:VAL:HG21	36:1e:128:PRO:HB3	1.86	0.57
40:1i:3:GLN:HE21	40:1i:20:ARG:HH21	1.52	0.57
49:1r:26:LEU:HD11	49:1r:42:ARG:HD3	1.85	0.57
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.22	0.57
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.22	0.57
12:2Q:12:GLN:NE2	12:2Q:72:LYS:HG3	2.19	0.57
32:2a:1029:C:C2	32:2a:1032:G:N2	2.71	0.57
40:2i:33:PHE:HE2	40:2i:43:ALA:HB1	1.69	0.57
54:2w:19:G:H1	54:2w:56:C:H42	1.51	0.57
32:1a:159:G:N2	32:1a:162:A:OP2	2.37	0.57
1:2A:1183:G:H5"	25:23:30:ARG:NH2	2.20	0.57
1:2A:1252:G:N3	16:2U:33:ARG:HG2	2.19	0.57
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.40	0.57
6:2G:114:ILE:HA	6:2G:140:ILE:HD11	1.84	0.57
21:2Z:171:ILE:HD12	21:2Z:172:ALA:H	1.69	0.57
32:2a:157:G:H1	32:2a:164:U:H3	1.53	0.57
33:2b:179:LYS:HA	39:2h:72:PRO:HG3	1.87	0.57
1:1A:248:G:OP1	61:1A:4126:HOH:O	2.17	0.57
1:1A:1071:G:H1	1:1A:1100:C:H42	1.52	0.57
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.03	0.57
6:2G:152:LEU:H	6:2G:152:LEU:HD12	1.69	0.57
32:2a:913:A:OP1	43:2l:46:LYS:NZ	2.37	0.57
1:1A:2136:C:N4	1:1A:2155:G:H1	2.02	0.57
1:1A:2336:A:H61	22:10:43:THR:HG22	1.70	0.57
35:1d:190:ASP:N	35:1d:190:ASP:OD1	2.37	0.57
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.37	0.57
26:24:40:HIS:HD2	26:24:41:PRO:HD2	1.68	0.57
32:2a:596:C:OP2	61:2a:1909:HOH:O	2.18	0.57
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.04	0.57
1:1A:2133:G:O2'	1:1A:2157:G:N2	2.36	0.57
1:1A:2316:C:O2'	6:1G:128:ARG:NH2	2.38	0.57
1:1A:2445:G:OP1	5:1F:74:ARG:NH2	2.38	0.57
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.38	0.57
38:2g:16:LEU:HG	40:2i:45:ALA:HB2	1.86	0.57
26:14:53:GLU:HB2	26:14:55:ARG:C	2.30	0.57
39:1h:86:ILE:HD12	39:1h:133:LEU:HD22	1.87	0.57
1:2A:2552:OMU:OP2	61:2A:3826:HOH:O	2.18	0.57
7:2H:18:GLU:OE2	7:2H:27:LYS:NZ	2.38	0.57
44:2m:122:LYS:HG3	44:2m:123:ALA:H	1.70	0.57
1:1A:2554:U:H3	54:1w:74:C:N4	2.03	0.57
33:1b:195:ASP:O	39:1h:68:ARG:NH2	2.37	0.57
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.04	0.57
7:2H:21:PRO:HD2	7:2H:23:ARG:HH21	1.70	0.57
32:2a:1029:C:N3	32:2a:1032:G:N2	2.53	0.57
33:2b:15:VAL:HG23	33:2b:16:HIS:HD2	1.70	0.57
1:1A:2611:U:C4	27:15:3:LYS:HG2	2.39	0.56
6:1G:122:PRO:HG3	6:1G:182:LYS:H	1.70	0.56
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.86	0.56
1:2A:890:A:H2'	1:2A:892:G:H8	1.71	0.56
2:2B:75:G:H22	21:2Z:73:GLN:HE21	1.52	0.56
23:21:3:LYS:HB2	23:21:61:ARG:HH22	1.70	0.56
1:1A:505:A:OP2	61:1A:4127:HOH:O	2.18	0.56
1:1A:741:G:OP2	61:1A:4125:HOH:O	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:972:C:O2'	41:1j:55:LYS:O	2.20	0.56
34:1c:22:TRP:CZ2	45:1n:54:PRO:HG2	2.39	0.56
8:2I:3:VAL:HG12	8:2I:38:LEU:HA	1.87	0.56
19:2X:72:LYS:NZ	19:2X:75:ASP:OD1	2.37	0.56
9:1N:14:VAL:HG11	9:1N:138:LEU:HD12	1.87	0.56
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.40	0.56
12:1Q:16:ARG:HG3	12:1Q:17:LEU:H	1.70	0.56
32:1a:269:C:H2'	32:1a:270:A:C8	2.41	0.56
32:1a:677:U:H3	32:1a:713:G:H22	1.53	0.56
32:1a:913:A:OP1	43:1l:46:LYS:NZ	2.35	0.56
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.89	0.56
41:1j:55:LYS:HE3	41:1j:56:HIS:CE1	2.40	0.56
1:2A:1125:G:H5'	31:29:37:GLY:HA2	1.87	0.56
21:2Z:93:ASP:HB3	21:2Z:131:ARG:HH22	1.70	0.56
24:22:29:LYS:HG2	24:22:57:ILE:HD13	1.88	0.56
24:22:41:ILE:HG13	24:22:43:GLN:HG3	1.87	0.56
32:2a:130:A:H5'	48:2q:63:ARG:HE	1.70	0.56
32:2a:662:G:H2'	32:2a:663:A:C8	2.40	0.56
32:2a:1255:G:N7	41:2j:43:ARG:NH2	2.53	0.56
32:2a:1346:A:H61	32:2a:1374:A:H3'	1.70	0.56
44:2m:31:LYS:HA	44:2m:34:LEU:HD12	1.87	0.56
46:2o:39:LEU:HD13	46:2o:56:LEU:HB2	1.85	0.56
26:14:55:ARG:N	26:14:56:VAL:HA	2.20	0.56
32:1a:946:A:H2'	32:1a:947:G:C8	2.41	0.56
32:2a:931:C:H42	32:2a:1386:G:H1	1.54	0.56
1:1A:272(J):C:H2'	1:1A:274:G:H8	1.70	0.56
43:1l:88:GLY:O	43:1l:99:HIS:HD2	1.89	0.56
47:1p:15:PRO:O	47:1p:16:HIS:ND1	2.39	0.56
2:2B:44:G:OP1	6:2G:98:ARG:NH2	2.37	0.56
6:2G:41:GLN:O	6:2G:43:LEU:N	2.39	0.56
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.88	0.56
32:2a:562:C:H1'	43:2l:15:ARG:HB3	1.86	0.56
15:1T:127:ALA:C	15:1T:129:ARG:H	2.13	0.56
54:1w:26:A:H61	54:1w:44:G:H1	1.54	0.56
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.21	0.56
36:1e:78:HIS:CD2	39:1h:104:ARG:HD2	2.31	0.56
1:2A:30:G:H2'	1:2A:31:C:C6	2.40	0.56
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.41	0.56
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.41	0.56
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.05	0.56
32:2a:929:G:H1	32:2a:1388:C:H42	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1002:G:N3	32:2a:1003:G:H1'	2.21	0.56
32:2a:1518:MA6:H93	32:2a:1519:MA6:H92	1.86	0.56
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	1.88	0.56
32:1a:458:C:H2'	32:1a:460:G:O4'	2.05	0.56
34:1c:58:GLU:HB3	41:1j:92:THR:HG21	1.88	0.56
50:1s:32:LYS:HA	50:1s:50:ALA:HB3	1.88	0.56
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.87	0.56
32:2a:187:C:O2'	51:2t:89:ARG:NH2	2.39	0.56
32:2a:1005:A:H5"	32:2a:1006:C:C5	2.40	0.56
37:2f:89:MET:HE3	49:2r:76:LEU:HD13	1.88	0.56
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.87	0.56
32:2a:1130:A:H5"	40:2i:18:PHE:CE2	2.41	0.56
1:1A:2503:2MA:H8	58:1A:4061:WC9:O	2.06	0.56
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.40	0.56
32:1a:1314:C:OP2	50:1s:4:SER:OG	2.12	0.56
35:1d:104:VAL:HG21	35:1d:140:VAL:HG21	1.88	0.56
6:2G:150:ASP:OD1	6:2G:150:ASP:N	2.39	0.56
33:2b:92:TYR:N	33:2b:151:GLY:O	2.29	0.56
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.88	0.55
32:1a:742:G:OP2	46:1o:35:ARG:NH2	2.28	0.55
43:1l:7:ILE:HA	43:1l:10:LEU:HD12	1.88	0.55
44:1m:50:GLU:HA	44:1m:53:VAL:HG22	1.88	0.55
5:2F:178:PRO:HB3	5:2F:198:ALA:HA	1.88	0.55
6:2G:69:ALA:HB3	6:2G:91:ARG:HH21	1.71	0.55
38:2g:74:GLU:HG2	38:2g:91:VAL:HG22	1.88	0.55
50:2s:12:ASP:OD2	50:2s:37:ARG:NH1	2.38	0.55
34:1c:8:ILE:HD12	34:1c:16:ARG:HG3	1.88	0.55
39:1h:17:THR:O	39:1h:78:GLN:NE2	2.34	0.55
54:1y:19:G:H1	54:1y:56:C:H42	1.52	0.55
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.21	0.55
18:2W:1:MET:HE2	18:2W:62:HIS:HB3	1.87	0.55
19:2X:94:GLY:N	19:2X:95:LEU:HB2	2.21	0.55
32:2a:56:U:H2'	32:2a:57:G:C8	2.42	0.55
32:2a:757:U:H2'	32:2a:758:G:O4'	2.07	0.55
32:2a:1263:C:C4	32:2a:1272:G:O6	2.58	0.55
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.06	0.55
1:1A:2794:C:H42	1:1A:2802:G:H22	1.53	0.55
33:1b:80:ILE:HD12	33:1b:211:ILE:HG22	1.88	0.55
2:2B:11:C:H3'	2:2B:12:C:C6	2.41	0.55
8:2I:130:TYR:HD2	8:2I:138:ILE:HD12	1.71	0.55
13:2R:38:VAL:HG22	13:2R:112:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2W:18:ARG:HG2	18:2W:76:VAL:HB	1.87	0.55
32:2a:959:A:HO2'	32:2a:984:C:HO2'	1.53	0.55
32:2a:1274:G:N2	32:2a:1275:A:N7	2.54	0.55
32:2a:1352:C:OP1	52:2u:3:LYS:NZ	2.32	0.55
32:2a:1521:G:N3	61:2a:1922:HOH:O	2.32	0.55
32:1a:200:G:H1	32:1a:217:C:H42	1.54	0.55
33:1b:122:PHE:HE2	33:1b:139:LYS:HB2	1.71	0.55
32:2a:1006:C:H42	32:2a:1023:G:H1	1.54	0.55
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.40	0.55
1:1A:1077:A:H2'	1:1A:1078:U:H4'	1.87	0.55
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.40	0.55
1:2A:400:G:N7	61:2A:3888:HOH:O	2.33	0.55
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.71	0.55
32:2a:1133:G:H1	32:2a:1141:C:H42	1.54	0.55
33:2b:134:GLU:O	33:2b:138:LEU:HG	2.06	0.55
38:2g:42:ILE:HD13	38:2g:116:ALA:HB3	1.89	0.55
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.88	0.55
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.42	0.55
32:1a:673:G:H2'	32:1a:674:G:C8	2.42	0.55
40:1i:96:LEU:HD22	40:1i:101:PHE:HD2	1.71	0.55
32:2a:1130:A:H5"	40:2i:18:PHE:HE2	1.71	0.55
33:2b:223:ILE:HA	33:2b:226:ARG:HD3	1.89	0.55
47:2p:15:PRO:HD2	47:2p:42:ARG:HD2	1.88	0.55
1:1A:2816:C:O3'	13:1R:99:LYS:NZ	2.39	0.55
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.71	0.55
32:1a:1047:G:H5"	45:1n:4:LYS:HD3	1.89	0.55
1:2A:1482:G:H1	1:2A:1506:C:H42	1.53	0.55
32:2a:1084:G:H5'	32:2a:1102:A:OP2	2.06	0.55
32:2a:1309:G:O3'	44:2m:77:ASN:ND2	2.39	0.55
1:1A:2417:C:OP1	11:1P:65:ARG:NH2	2.40	0.55
4:1E:127:ASP:OD2	61:1E:401:HOH:O	2.18	0.55
34:1c:71:ALA:HA	34:1c:106:VAL:HG21	1.89	0.55
35:1d:98:GLU:OE1	35:1d:103:ASN:ND2	2.39	0.55
41:1j:78:ASN:O	41:1j:80:LYS:N	2.39	0.55
42:1k:27:ASN:OD1	42:1k:28:THR:N	2.40	0.55
1:2A:184:C:H2'	1:2A:185:U:C6	2.42	0.55
1:2A:987:G:O2'	1:2A:1000:A:N3	2.35	0.55
8:1I:38:LEU:HD23	8:1I:38:LEU:H	1.70	0.55
30:18:23:VAL:HG22	30:18:47:LYS:HB3	1.89	0.55
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.42	0.55
32:1a:1530:G:H2'	32:1a:1531:A:C8	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:19:LEU:HD21	40:1i:81:ILE:HG13	1.87	0.55
1:2A:2278:A:OP2	22:20:12:ASN:ND2	2.39	0.55
7:2H:20:ALA:HB1	7:2H:23:ARG:HH21	1.72	0.55
19:2X:46:ALA:HB1	24:22:33:MET:HE1	1.89	0.55
36:2e:5:ASP:N	36:2e:5:ASP:OD1	2.40	0.55
1:1A:956:G:O6	61:1A:4121:HOH:O	2.15	0.55
12:1Q:18:LYS:O	12:1Q:98:LYS:NZ	2.33	0.55
32:1a:1191:A:OP1	34:1c:4:LYS:NZ	2.34	0.55
32:1a:1309:G:OP1	44:1m:88:ARG:NH2	2.40	0.55
50:1s:27:GLU:HB2	50:1s:28:LYS:HB3	1.88	0.55
1:2A:1971:A:OP2	3:2D:242:ARG:NH2	2.40	0.55
19:2X:94:GLY:H	19:2X:95:LEU:HB2	1.72	0.55
32:2a:920:U:H2'	32:2a:921:U:C6	2.42	0.55
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.21	0.54
32:1a:269:C:H2'	32:1a:270:A:H8	1.71	0.54
27:25:33:CYS:HB2	27:25:40:LYS:HD3	1.88	0.54
36:2e:33:VAL:HG13	36:2e:112:LEU:HD22	1.89	0.54
44:2m:81:LEU:HA	44:2m:84:ILE:HG12	1.88	0.54
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.42	0.54
1:1A:2285:C:OP2	28:16:6:ARG:NH1	2.39	0.54
37:1f:2:ARG:HD2	37:1f:69:GLU:HB3	1.89	0.54
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.72	0.54
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	1.88	0.54
1:2A:336:C:O2'	20:2Y:35:TYR:OH	2.24	0.54
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.25	0.54
1:2A:2138:C:N4	1:2A:2153:G:H1	2.05	0.54
32:2a:976:G:H5'	32:2a:1358:U:O2'	2.07	0.54
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.40	0.54
39:2h:34:GLU:OE1	39:2h:37:ARG:NH1	2.37	0.54
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.40	0.54
21:1Z:136:PHE:O	21:1Z:137:ILE:HG13	2.07	0.54
32:1a:1006:C:N4	32:1a:1023:G:H1	2.06	0.54
33:1b:16:HIS:HB2	33:1b:204:ASN:HB3	1.90	0.54
41:1j:5:ARG:HH21	41:1j:73:ASP:CG	2.14	0.54
54:1w:2:C:N3	54:1w:71:G:N2	2.56	0.54
1:2A:1721:G:H8	1:2A:1741:A:H62	1.55	0.54
11:2P:39:LYS:HB2	11:2P:45:LEU:HD13	1.87	0.54
16:2U:24:TYR:HB2	16:2U:29:SER:HB3	1.88	0.54
26:24:13:ARG:HD3	26:24:23:GLU:HG2	1.88	0.54
32:2a:646:U:H2'	32:2a:647:C:C6	2.42	0.54
18:1W:11:ARG:HA	18:1W:100:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.37	0.54
1:2A:2502:G:N7	61:2A:3886:HOH:O	2.33	0.54
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.43	0.54
21:2Z:45:ASP:OD1	21:2Z:49:ARG:NE	2.39	0.54
33:2b:81:VAL:HB	33:2b:94:ASN:HD21	1.73	0.54
44:2m:82:MET:O	44:2m:93:ARG:NH2	2.40	0.54
36:1e:7:GLU:OE2	36:1e:37:ARG:NH2	2.40	0.54
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.42	0.54
1:2A:2818:G:OP1	1:2A:2837:G:O2'	2.25	0.54
32:2a:406:G:H21	35:2d:119:GLN:NE2	2.01	0.54
32:2a:736:C:H2'	32:2a:737:A:C8	2.43	0.54
32:2a:1112:C:N3	34:2c:178:LEU:HD12	2.22	0.54
32:2a:1271:G:C2	32:2a:1272:G:N7	2.76	0.54
32:2a:1289:A:OP1	52:2u:10:ARG:NH2	2.41	0.54
44:2m:81:LEU:HD22	44:2m:88:ARG:HE	1.73	0.54
54:2y:34:G:H2'	54:2y:35:A:C8	2.42	0.54
61:1A:5125:HOH:O	11:1P:44:GLY:HA2	2.06	0.54
35:1d:107:ARG:HH22	35:1d:194:LEU:HG	1.73	0.54
1:2A:509:C:OP1	61:2A:3827:HOH:O	2.18	0.54
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.08	0.54
34:2c:44:GLU:HA	34:2c:52:LEU:HD23	1.88	0.54
1:1A:2312:U:H5'	6:1G:88:ILE:HD11	1.88	0.54
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.34	0.54
42:1k:87:THR:O	42:1k:87:THR:OG1	2.26	0.54
1:2A:882:G:H22	1:2A:894:C:N4	2.06	0.54
21:2Z:93:ASP:HA	21:2Z:131:ARG:HH12	1.72	0.54
32:2a:1147:C:O2	40:2i:16:ARG:NH1	2.41	0.54
33:2b:101:MET:HA	33:2b:108:ILE:HG13	1.90	0.54
36:2e:7:GLU:OE1	36:2e:37:ARG:NH2	2.36	0.54
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	1.90	0.54
1:1A:288:C:H2'	1:1A:289:A:H8	1.73	0.54
1:1A:813:U:H2'	1:1A:814:C:C6	2.42	0.54
4:1E:143:ASN:HD22	4:1E:147:PRO:HD3	1.73	0.54
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.08	0.54
1:2A:307:G:H21	1:2A:330:A:H62	1.54	0.54
4:2E:7:VAL:HG12	4:2E:27:LEU:HB3	1.90	0.54
32:2a:1202:G:O4'	45:2n:29:ARG:NH1	2.40	0.54
54:2w:51:U:H3	54:2w:63:G:H1	1.55	0.54
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.43	0.54
32:1a:79:G:O6	32:1a:90:U:C2	2.60	0.54
1:2A:1639:U:H2'	1:2A:1640:C:H5"	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.23	0.54
4:1E:9:VAL:HG22	4:1E:25:VAL:HB	1.90	0.54
54:1w:4:C:H2'	54:1w:5:G:H8	1.73	0.54
1:2A:1116:C:H2'	1:2A:1117:G:H8	1.70	0.54
32:2a:141:A:H1'	32:2a:182:U:O2	2.08	0.54
32:2a:984:C:H2'	32:2a:985:C:C6	2.43	0.54
32:2a:1006:C:N4	32:2a:1023:G:H1	2.06	0.54
55:2x:40:C:H2'	55:2x:41:C:H6	1.72	0.54
14:1S:68:GLN:HE21	14:1S:71:ARG:HH21	1.54	0.53
21:1Z:158:PRO:HG2	21:1Z:161:VAL:HG11	1.90	0.53
32:1a:176:C:OP1	51:1t:29:LYS:NZ	2.41	0.53
32:1a:1125:U:H4'	41:1j:5:ARG:HH22	1.73	0.53
39:1h:39:LEU:HD13	39:1h:111:ILE:HD11	1.88	0.53
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.34	0.53
11:2P:87:ASP:O	11:2P:90:ARG:NH1	2.41	0.53
26:24:58:ARG:HH11	50:2s:68:GLY:HA3	1.72	0.53
32:2a:838:G:H1	32:2a:848:C:H42	1.53	0.53
32:2a:1347:G:H22	32:2a:1373:G:H2'	1.72	0.53
34:2c:7:PRO:HG3	34:2c:201:TYR:HE1	1.73	0.53
35:2d:127:THR:HG23	35:2d:147:ALA:HB3	1.91	0.53
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.18	0.53
1:1A:1671:U:O4	61:1A:4105:HOH:O	2.17	0.53
32:1a:79:G:O6	32:1a:90:U:O2	2.26	0.53
1:2A:247:G:H4'	1:2A:386:G:C5	2.43	0.53
1:2A:2066:C:OP1	61:2A:3829:HOH:O	2.19	0.53
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.72	0.53
11:2P:89:ALA:HA	11:2P:121:LYS:HD3	1.89	0.53
33:2b:211:ILE:O	33:2b:215:LEU:HB2	2.08	0.53
3:1D:147:LEU:HD13	3:1D:155:LEU:HD11	1.88	0.53
32:1a:920:U:H2'	32:1a:921:U:C6	2.44	0.53
32:1a:1456:G:O3'	51:1t:39:LYS:NZ	2.41	0.53
34:1c:15:THR:HG21	34:1c:181:ASN:HA	1.91	0.53
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.24	0.53
16:2U:65:ILE:HD11	16:2U:95:LEU:HB3	1.89	0.53
32:2a:1029:C:N4	32:2a:1032:G:N1	2.57	0.53
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.89	0.53
7:1H:33:LEU:HD21	7:1H:136:ILE:HG13	1.91	0.53
49:1r:52:PRO:HB2	49:1r:54:ARG:HG3	1.90	0.53
18:2W:2:GLU:OE2	18:2W:72:LYS:NZ	2.32	0.53
32:2a:642:A:N3	39:2h:113:SER:OG	2.38	0.53
34:2c:88:ARG:HA	34:2c:91:LEU:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:2p:74:LEU:HD13	47:2p:79:VAL:HG21	1.91	0.53
1:1A:2096:U:H3	1:1A:2193:G:H1	1.56	0.53
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.91	0.53
3:1D:37:LEU:HD12	3:1D:62:TYR:HB2	1.90	0.53
21:1Z:8:TYR:HB2	21:1Z:38:TYR:CE2	2.44	0.53
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.41	0.53
1:2A:2343:C:HO2'	1:2A:2373:G:HO2'	1.55	0.53
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.91	0.53
26:24:61:ARG:HG2	50:2s:42:PRO:HG3	1.90	0.53
34:2c:32:LEU:O	34:2c:36:ASP:HB2	2.08	0.53
1:1A:1057:A:H61	1:1A:1081:U:H3	1.55	0.53
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.43	0.53
26:14:59:PHE:CD2	50:1s:64:GLU:HB3	2.43	0.53
32:1a:1531:A:H8	32:1a:1531:A:O5'	1.91	0.53
41:1j:81:THR:C	41:1j:83:GLU:H	2.17	0.53
6:2G:79:ASN:OD1	6:2G:79:ASN:N	2.39	0.53
34:2c:20:SER:HB3	34:2c:22:TRP:NE1	2.23	0.53
54:2y:14:A:H3'	54:2y:15:G:C8	2.44	0.53
32:1a:1036:G:H5"	32:1a:1037:C:H5	1.74	0.53
37:1f:10:LEU:HD11	37:1f:61:LEU:HD12	1.90	0.53
1:2A:2135:A:C8	1:2A:2136:C:H5	2.27	0.53
4:2E:14:ILE:HG13	4:2E:21:VAL:HG13	1.90	0.53
32:2a:118:U:H3'	32:2a:288:A:H61	1.74	0.53
32:2a:353:A:H5'	32:2a:353:A:H8	1.74	0.53
32:2a:1256:A:OP1	34:2c:26:LYS:NZ	2.40	0.53
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.44	0.53
54:2w:21:A:O2'	54:2w:22:G:OP1	2.27	0.53
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.44	0.53
32:1a:1218:C:OP2	45:1n:9:LYS:NZ	2.42	0.53
1:2A:882:G:H22	1:2A:894:C:H42	1.56	0.53
10:2O:68:GLU:OE1	10:2O:78:ARG:NH1	2.42	0.53
32:2a:419:C:OP1	32:2a:513:C:O2'	2.25	0.53
32:2a:1042:G:H2'	32:2a:1043:C:O4'	2.09	0.53
1:1A:1798:U:H5'	3:1D:259:THR:CG2	2.38	0.53
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.44	0.53
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.09	0.53
1:2A:1991:U:H2'	1:2A:1992:G:H5"	1.90	0.53
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.24	0.53
32:2a:1346:A:N1	32:2a:1374:A:H5"	2.22	0.53
39:2h:10:LEU:HG	39:2h:83:ILE:HD11	1.91	0.53
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:32:TYR:OH	12:1Q:111:GLU:OE2	2.28	0.53
32:1a:757:U:H2'	32:1a:758:G:O4'	2.08	0.53
54:1w:4:C:H2'	54:1w:5:G:C8	2.44	0.53
21:2Z:73:GLN:O	21:2Z:87:ASP:N	2.41	0.53
54:2y:18:G:N2	54:2y:55:PSU:HN3	1.99	0.53
1:1A:1090:U:C2	1:1A:1102:C:H1'	2.44	0.52
16:1U:104:GLN:HE21	16:1U:105:VAL:HG23	1.73	0.52
38:1g:27:ILE:HA	38:1g:30:ILE:HD12	1.91	0.52
1:2A:9:U:OP1	9:2N:115:ARG:NH2	2.42	0.52
1:2A:208:C:H2'	1:2A:209:C:C6	2.44	0.52
4:2E:9:VAL:HG13	4:2E:25:VAL:O	2.09	0.52
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.77	0.52
38:2g:111:ARG:NH2	38:2g:126:ASP:OD2	2.43	0.52
40:2i:15:ALA:HB2	40:2i:65:VAL:HG23	1.91	0.52
47:2p:28:ARG:HG2	47:2p:29:ASP:OD1	2.09	0.52
23:11:52:ARG:NH1	23:11:55:GLY:O	2.43	0.52
26:14:58:ARG:HD3	50:1s:67:VAL:H	1.74	0.52
32:1a:1002:G:N2	32:1a:1004:A:H1'	2.25	0.52
32:1a:1329:A:N7	52:1u:7:ARG:NH2	2.57	0.52
1:2A:2317:C:N4	1:2A:2318:G:O6	2.42	0.52
32:2a:1134:G:H1	32:2a:1140:C:H42	1.55	0.52
33:2b:82:ARG:HB2	33:2b:92:TYR:CZ	2.44	0.52
1:1A:800:A:H8	1:1A:800:A:OP1	1.92	0.52
1:1A:1890:A:OP2	61:1A:4128:HOH:O	2.19	0.52
1:2A:881:G:C2	1:2A:882:G:H1'	2.44	0.52
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.90	0.52
32:2a:1060:C:C5	34:2c:2:GLY:HA3	2.45	0.52
1:1A:1058:G:N2	1:1A:1081:U:O2	2.42	0.52
8:1I:109:ILE:HD12	8:1I:130:TYR:CZ	2.44	0.52
32:1a:1075:C:OP1	33:1b:179:LYS:NZ	2.33	0.52
32:1a:1278:U:H5'	32:1a:1279:A:O4'	2.10	0.52
36:1e:78:HIS:HE1	36:1e:142:LEU:HA	1.75	0.52
40:1i:3:GLN:HE21	40:1i:20:ARG:NH2	2.07	0.52
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.09	0.52
7:2H:20:ALA:HB3	7:2H:23:ARG:HB2	1.92	0.52
9:2N:21:LYS:NZ	9:2N:140:VAL:OXT	2.42	0.52
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.91	0.52
47:2p:53:VAL:HG13	47:2p:79:VAL:HG22	1.91	0.52
1:1A:897:C:N3	1:1A:898:C:N4	2.58	0.52
1:1A:1013:C:OP2	61:1A:4117:HOH:O	2.19	0.52
32:1a:971:G:N2	32:1a:1363(A):A:OP2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:764:A:H5'	3:2D:210:GLY:HA2	1.92	0.52
1:2A:996:A:H4'	16:2U:91:ASP:OD2	2.10	0.52
1:2A:2099:U:H3	1:2A:2190:G:H1	1.58	0.52
9:2N:38:HIS:CE1	9:2N:39:ARG:HG3	2.45	0.52
32:2a:9:G:H2'	32:2a:10:A:H8	1.75	0.52
8:1I:79:ILE:HB	8:1I:144:VAL:HG12	1.92	0.52
32:1a:1032:G:H2'	32:1a:1033:G:O4'	2.10	0.52
1:2A:2033:A:OP1	61:2A:3830:HOH:O	2.19	0.52
32:2a:890:G:O2'	32:2a:906:G:O6	2.27	0.52
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.45	0.52
33:2b:76:GLN:NE2	33:2b:76:GLN:H	2.07	0.52
50:2s:19:VAL:O	50:2s:23:ASN:ND2	2.43	0.52
1:1A:1055:G:H1	1:1A:1104:C:N4	2.06	0.52
3:2D:182:LEU:HB2	3:2D:272:ALA:HB3	1.91	0.52
32:2a:1002:G:H1	32:2a:1038:C:H42	1.58	0.52
32:2a:1006:C:H2'	32:2a:1007:C:O4'	2.10	0.52
36:2e:83:GLU:HA	36:2e:88:LYS:HA	1.91	0.52
1:1A:1075:C:H2'	1:1A:1076:C:H5'	1.91	0.52
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.43	0.52
32:1a:79:G:C6	32:1a:90:U:O2	2.63	0.52
32:1a:1036:G:H3'	32:1a:1037:C:H6	1.73	0.52
33:1b:17:PHE:HB3	33:1b:44:LEU:HD11	1.92	0.52
34:1c:19:GLU:O	34:1c:40:ARG:NH2	2.43	0.52
1:2A:1791:A:H5'	3:2D:206:LEU:HD12	1.91	0.52
1:2A:2143:C:N4	1:2A:2148:G:H1	2.05	0.52
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.91	0.52
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.43	0.52
26:24:45:GLY:C	26:24:47:GLN:H	2.18	0.52
32:2a:34:C:H2'	32:2a:35:G:H8	1.75	0.52
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.92	0.52
32:1a:333:G:H4'	51:1t:16:HIS:CE1	2.45	0.52
32:1a:1183:A:O2'	32:1a:1184:G:OP1	2.23	0.52
32:1a:1239:A:H62	32:1a:1299:A:N6	2.08	0.52
40:1i:21:PRO:HA	40:1i:59:PHE:HA	1.92	0.52
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.45	0.52
1:2A:2336:A:H61	22:20:43:THR:HG22	1.74	0.52
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.75	0.52
10:2O:24:VAL:HG13	10:2O:33:ALA:HB2	1.91	0.52
32:2a:501:C:H2'	32:2a:502:G:H8	1.74	0.52
32:2a:920:U:H2'	32:2a:921:U:H6	1.75	0.52
32:2a:1016:A:H2'	32:2a:1017:G:O4'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1328:C:O2'	44:2m:29:ARG:NE	2.40	0.52
1:1A:1058:G:H1	1:1A:1080:C:N4	2.07	0.52
1:1A:1252:G:N3	16:1U:33:ARG:HG2	2.25	0.52
37:1f:69:GLU:H	37:1f:69:GLU:CD	2.18	0.52
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.10	0.52
1:2A:1645:G:H5"	1:2A:1646:C:H5'	1.92	0.52
5:2F:18:ARG:NH1	5:2F:127:GLU:OE2	2.41	0.52
9:2N:67:LEU:HB3	9:2N:88:GLU:HG3	1.91	0.52
26:24:26:SER:OG	26:24:27:THR:N	2.43	0.52
29:27:12:ARG:NH2	29:27:44:PRO:HB3	2.25	0.52
1:1A:2139:C:H42	1:1A:2152:G:H1	1.57	0.51
1:1A:2429:G:OP1	61:1A:4101:HOH:O	2.18	0.51
33:1b:20:GLU:HB2	33:1b:190:THR:OG1	2.10	0.51
1:2A:2802:G:H2'	1:2A:2803:C:O4'	2.10	0.51
7:2H:24:VAL:HG22	7:2H:35:VAL:HB	1.90	0.51
8:2I:78:THR:HG22	8:2I:143:SER:HB3	1.92	0.51
9:2N:42:TRP:HA	9:2N:48:MET:SD	2.50	0.51
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.28	0.51
32:2a:1051:C:H2'	32:2a:1052:U:C6	2.45	0.51
8:1I:109:ILE:HD12	8:1I:130:TYR:CE2	2.45	0.51
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.93	0.51
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.11	0.51
33:1b:54:THR:HG21	33:1b:201:ILE:HG13	1.92	0.51
1:2A:774:A:H2'	1:2A:774:A:N3	2.25	0.51
1:2A:1783:A:OP2	61:2A:3831:HOH:O	2.19	0.51
32:2a:748:C:H4'	32:2a:749:C:O5'	2.11	0.51
32:2a:1003:G:H2'	32:2a:1004:A:O4'	2.11	0.51
32:2a:1330:U:H4'	44:2m:23:TYR:CE1	2.45	0.51
1:1A:1364:G:OP2	23:11:3:LYS:HG3	2.10	0.51
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.10	0.51
21:1Z:155:LEU:HD12	21:1Z:156:LYS:H	1.75	0.51
46:1o:87:ILE:HG22	46:1o:88:ARG:N	2.25	0.51
5:2F:126:VAL:HG21	5:2F:129:PHE:CZ	2.45	0.51
6:2G:106:LEU:HG	6:2G:111:LEU:HD13	1.93	0.51
24:22:51:ARG:O	24:22:55:ARG:HG2	2.11	0.51
32:2a:719:C:H1'	49:2r:49:LYS:HG2	1.92	0.51
32:2a:1239:A:H62	32:2a:1299:A:H62	1.58	0.51
33:2b:200:ILE:HD12	33:2b:202:PRO:HD3	1.92	0.51
43:2l:40:VAL:HG21	43:2l:78:GLN:HA	1.92	0.51
51:2t:50:GLU:O	51:2t:100:ILE:HD11	2.10	0.51
1:1A:1030:G:OP2	12:1Q:128:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:11:ARG:HB3	34:1c:15:THR:HB	1.92	0.51
1:2A:1364:G:P	23:21:3:LYS:HG3	2.50	0.51
1:2A:2155:G:C5	1:2A:2156:G:H1'	2.45	0.51
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.46	0.51
1:2A:2711:A:OP2	61:2A:3816:HOH:O	2.19	0.51
4:2E:50:GLY:HA3	4:2E:75:VAL:HG21	1.91	0.51
36:2e:8:GLU:HG2	36:2e:34:VAL:HG12	1.93	0.51
38:2g:51:GLN:O	38:2g:55:GLY:HA2	2.10	0.51
38:2g:78:ARG:HD3	38:2g:79:ARG:H	1.76	0.51
41:2j:98:ILE:O	61:2j:301:HOH:O	2.19	0.51
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.11	0.51
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.10	0.51
16:2U:104:GLN:NE2	16:2U:105:VAL:HG23	2.24	0.51
19:2X:94:GLY:CA	19:2X:95:LEU:HB2	2.40	0.51
32:2a:728:A:H2'	32:2a:729:A:C8	2.45	0.51
32:2a:1318:A:O2'	50:2s:37:ARG:HB2	2.10	0.51
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.46	0.51
1:1A:2136:C:N3	1:1A:2155:G:C2	2.78	0.51
54:1y:26:A:H61	54:1y:44:G:H1	1.58	0.51
14:2S:38:GLN:HB2	14:2S:40:ILE:HD11	1.93	0.51
32:2a:1157:A:H5'	32:2a:1158:C:C6	2.46	0.51
32:2a:1187:G:OP1	40:2i:113:LYS:NZ	2.43	0.51
33:2b:221:LEU:HA	33:2b:224:GLN:HG2	1.93	0.51
1:1A:1268:A:C2	1:1A:2013:A:C4	2.99	0.51
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.26	0.51
37:1f:67:MET:HE1	37:1f:75:LEU:HD12	1.91	0.51
1:2A:212:G:H2'	1:2A:213:A:O4'	2.11	0.51
32:2a:677:U:H3	32:2a:713:G:H22	1.57	0.51
32:2a:1005:A:H5"	32:2a:1006:C:H5	1.75	0.51
32:2a:1245:A:H2'	32:2a:1246:C:O4'	2.11	0.51
37:2f:70:ASP:OD1	37:2f:70:ASP:N	2.41	0.51
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.11	0.51
36:1e:152:ARG:NH2	39:1h:107:LEU:O	2.44	0.51
1:2A:947:G:H2'	1:2A:948:G:C8	2.45	0.51
1:2A:2268:A:OP1	61:2A:3828:HOH:O	2.19	0.51
1:2A:2404:C:O3'	11:2P:77:ARG:NH2	2.44	0.51
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.11	0.51
32:2a:1005:A:H3'	32:2a:1006:C:C6	2.45	0.51
35:2d:173:TRP:CD2	35:2d:189:PRO:HB3	2.46	0.51
38:2g:26:PHE:O	38:2g:30:ILE:HD12	2.10	0.51
51:2t:9:ASN:O	51:2t:10:LEU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2155:G:H2'	1:1A:2155:G:N3	2.25	0.51
32:1a:186:C:H2'	32:1a:187:C:C6	2.46	0.51
35:1d:173:TRP:CD2	35:1d:189:PRO:HG3	2.46	0.51
44:1m:67:GLU:HG3	44:1m:71:ARG:HH21	1.76	0.51
19:2X:31:HIS:HD2	19:2X:33:LYS:H	1.57	0.51
32:2a:34:C:H2'	32:2a:35:G:C8	2.46	0.51
44:2m:101:GLN:OE1	44:2m:101:GLN:N	2.44	0.51
54:2y:53:G:H3'	54:2y:54:5MU:H73	1.93	0.51
36:1e:33:VAL:HG13	36:1e:112:LEU:HD12	1.93	0.51
6:2G:3:LEU:HD12	6:2G:3:LEU:H	1.74	0.51
32:2a:1004:A:N6	32:2a:1037:C:O2	2.29	0.51
32:2a:1073:U:O2'	33:2b:104:ASN:OD1	2.27	0.51
36:2e:43:LEU:HB2	36:2e:136:MET:SD	2.51	0.51
44:2m:4:ILE:HG23	44:2m:5:ALA:H	1.75	0.51
26:14:58:ARG:O	26:14:61:ARG:N	2.44	0.50
36:1e:142:LEU:O	36:1e:143:ARG:NH1	2.44	0.50
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.77	0.50
32:2a:21:G:H2'	32:2a:22:G:C8	2.46	0.50
32:2a:545:C:OP1	35:2d:61:LYS:NZ	2.43	0.50
32:2a:1277:C:O2'	32:2a:1279:A:H8	1.93	0.50
30:18:42:ARG:HD2	61:18:203:HOH:O	2.10	0.50
32:1a:452:A:H4'	47:1p:72:ARG:CZ	2.41	0.50
32:1a:1500:A:OP1	61:1a:1908:HOH:O	2.18	0.50
33:1b:84:GLU:HB3	33:1b:219:VAL:HG21	1.92	0.50
35:1d:101:LEU:HB2	35:1d:138:TYR:HB3	1.92	0.50
36:1e:98:THR:HG22	36:1e:99:GLY:H	1.77	0.50
1:2A:764:A:H5'	3:2D:210:GLY:CA	2.41	0.50
1:2A:2064:C:H2'	1:2A:2065:C:C6	2.47	0.50
1:2A:2502:G:OP2	61:2A:3832:HOH:O	2.19	0.50
32:2a:936:C:H2'	32:2a:937:A:O4'	2.11	0.50
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.11	0.50
34:2c:69:HIS:CD2	34:2c:104:GLN:HG2	2.46	0.50
1:1A:2336:A:H61	22:10:43:THR:CG2	2.24	0.50
32:1a:316:G:OP2	32:1a:351:G:O2'	2.27	0.50
32:1a:456:C:H2'	32:1a:457:C:H6	1.77	0.50
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.47	0.50
33:1b:24:TRP:CD1	33:1b:24:TRP:H	2.28	0.50
34:1c:21:ARG:NH2	34:1c:56:ASP:OD2	2.35	0.50
54:1w:1:G:N1	54:1w:72:C:C2	2.79	0.50
1:2A:332:A:O2'	1:2A:334:C:OP2	2.26	0.50
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.41	0.50
14:2S:19:LYS:C	14:2S:21:THR:H	2.19	0.50
16:2U:105:VAL:HG22	17:2V:45:THR:HG23	1.92	0.50
32:2a:73:G:H1	32:2a:96:U:H3	1.60	0.50
54:2w:12:U:H2'	54:2w:13:C:H5"	1.93	0.50
1:1A:566:U:H5"	11:1P:29:LYS:HE3	1.93	0.50
8:1I:87:LYS:HD3	8:1I:87:LYS:H	1.76	0.50
32:1a:171:A:H2'	32:1a:172:A:C8	2.46	0.50
32:1a:405:U:O4	35:1d:2:GLY:N	2.44	0.50
32:1a:576:G:O6	32:1a:880:C:O2'	2.29	0.50
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.45	0.50
26:24:46:GLN:O	26:24:48:ARG:N	2.39	0.50
32:2a:951:G:N7	44:2m:102:ARG:NH2	2.60	0.50
32:2a:1148:U:H2'	32:2a:1149:C:O4'	2.11	0.50
33:2b:144:ARG:NH2	33:2b:148:TYR:OH	2.44	0.50
35:2d:150:GLU:H	35:2d:150:GLU:CD	2.20	0.50
43:2l:71:PRO:O	43:2l:102:ARG:NH1	2.42	0.50
49:2r:53:ARG:HG2	49:2r:63:GLN:HE21	1.77	0.50
55:2x:14:A:C2	55:2x:15:G:H1'	2.47	0.50
9:1N:14:VAL:HG13	9:1N:138:LEU:HB2	1.94	0.50
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.12	0.50
54:1y:55:PSU:N3	54:1y:57:G:H5'	2.27	0.50
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.47	0.50
3:2D:77:ALA:HB2	3:2D:97:TYR:CD1	2.46	0.50
32:2a:79:G:H1	32:2a:90:U:H3	1.59	0.50
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.27	0.50
42:2k:33:THR:HG22	42:2k:39:PRO:HA	1.92	0.50
48:2q:95:TYR:HA	48:2q:98:LEU:HG	1.92	0.50
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.47	0.50
21:1Z:151:HIS:HB3	21:1Z:169:GLU:O	2.12	0.50
54:1y:8:4SU:H4'	54:1y:48:C:H4'	1.94	0.50
6:2G:51:ARG:H	6:2G:51:ARG:HD3	1.76	0.50
32:2a:1029:C:N4	32:2a:1032:G:C6	2.80	0.50
34:2c:150:LYS:HG3	34:2c:169:ALA:HB2	1.92	0.50
41:2j:6:ILE:HB	41:2j:72:VAL:HG13	1.93	0.50
33:1b:200:ILE:HG22	33:1b:202:PRO:HD3	1.92	0.50
34:1c:15:THR:HG22	34:1c:16:ARG:HG2	1.94	0.50
46:1o:56:LEU:O	46:1o:60:VAL:HG23	2.11	0.50
1:2A:208:C:H2'	1:2A:209:C:H6	1.77	0.50
32:2a:1239:A:H62	32:2a:1299:A:N6	2.10	0.50
32:2a:1305:G:H5'	52:2u:4:GLY:HA3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:271(L):U:H4'	8:1I:50:ARG:NH2	2.26	0.50
1:1A:516:C:OP1	27:15:13:LYS:NZ	2.44	0.50
1:1A:796:C:H2'	1:1A:797:C:C6	2.46	0.50
1:1A:894:C:H2'	1:1A:895:U:O4'	2.12	0.50
1:1A:1011:G:OP1	16:1U:77:SER:OG	2.26	0.50
1:1A:2149:G:C2	1:1A:2150:U:H1'	2.47	0.50
22:10:10:THR:HA	61:10:207:HOH:O	2.12	0.50
32:1a:184:G:H2'	32:1a:185:A:H8	1.76	0.50
54:1w:46:G7M:H3'	54:1w:47:U:H5"	1.93	0.50
1:2A:942:G:OP2	11:2P:39:LYS:NZ	2.41	0.50
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.47	0.50
1:2A:2294:C:P	14:2S:89:ARG:HH22	2.34	0.50
2:2B:80:U:H2'	2:2B:81:G:C8	2.46	0.50
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.12	0.50
32:2a:1456:G:O6	51:2t:54:LYS:NZ	2.34	0.50
1:1A:887:A:H2	1:1A:889:C:H3'	1.77	0.50
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.27	0.50
41:1j:27:ALA:HA	41:1j:81:THR:HG21	1.94	0.50
1:2A:568:U:H5'	1:2A:945:A:N1	2.26	0.50
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.47	0.50
1:2A:1937:A:H1'	1:2A:1939:5MU:H72	1.94	0.50
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.94	0.50
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.94	0.50
33:2b:88:ALA:HB2	33:2b:219:VAL:HG23	1.93	0.50
45:2n:26:ARG:HD3	45:2n:43:CYS:HB3	1.93	0.50
1:1A:839:U:H1'	1:1A:1191:G:H1'	1.94	0.49
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.12	0.49
26:14:53:GLU:CD	26:14:54:GLY:H	2.20	0.49
40:1i:49:PRO:HG2	40:1i:81:ILE:HG23	1.93	0.49
44:1m:122:LYS:HG3	44:1m:123:ALA:H	1.77	0.49
54:1w:51:U:H2'	54:1w:52:G:C8	2.47	0.49
1:2A:1847:A:H3'	1:2A:1848:A:H5'	1.92	0.49
7:2H:51:ARG:NH1	7:2H:53:GLU:OE2	2.45	0.49
36:2e:43:LEU:HD22	36:2e:136:MET:HG3	1.94	0.49
36:2e:99:GLY:N	36:2e:117:ASP:OD1	2.45	0.49
41:2j:7:LYS:HG3	41:2j:71:LEU:HD23	1.93	0.49
55:2x:55:PSU:O2'	55:2x:57:A:N7	2.39	0.49
1:1A:615:G:OP2	5:1F:43:LYS:NZ	2.40	0.49
1:1A:2615:U:H2'	1:1A:2616:C:H6	1.76	0.49
12:1Q:81:VAL:HB	22:10:7:LEU:HD21	1.93	0.49
13:1R:12:ARG:O	13:1R:17:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:114:ARG:HA	35:1d:117:ALA:HB3	1.95	0.49
1:2A:1140:C:OP2	9:2N:66:LYS:NZ	2.41	0.49
4:2E:9:VAL:HB	15:2T:3:ARG:HG2	1.94	0.49
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	1.95	0.49
7:2H:149:ARG:NH1	7:2H:167:GLU:OE1	2.44	0.49
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.47	0.49
32:2a:1206:G:O2'	34:2c:193:TYR:HA	2.12	0.49
39:2h:116:LYS:HD3	39:2h:127:LEU:HD23	1.93	0.49
1:1A:1641:A:H2'	1:1A:1642:G:O4'	2.12	0.49
1:1A:1903:G:OP1	3:1D:241:PRO:HB2	2.12	0.49
1:1A:2126:A:N3	1:1A:2127:G:H1'	2.28	0.49
34:1c:150:LYS:HG3	34:1c:169:ALA:HB2	1.94	0.49
35:1d:79:PHE:O	35:1d:83:SER:OG	2.30	0.49
36:1e:6:PHE:HB3	36:1e:34:VAL:HG22	1.93	0.49
37:1f:75:LEU:HD22	37:1f:79:LEU:HG	1.94	0.49
12:2Q:11:LYS:NZ	12:2Q:88:GLY:O	2.36	0.49
27:25:49:CYS:SG	27:25:51:TYR:HB2	2.53	0.49
32:2a:381:C:H2'	32:2a:382:A:O4'	2.12	0.49
32:2a:1004:A:C6	32:2a:1037:C:H1'	2.47	0.49
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.48	0.49
33:2b:120:ALA:O	33:2b:125:PRO:HD2	2.12	0.49
1:1A:458:G:O2'	1:1A:469:G:O6	2.30	0.49
3:1D:242:ARG:HG2	3:1D:246:PRO:HG3	1.94	0.49
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	1.94	0.49
5:1F:192:LEU:HD13	5:1F:194:MET:HE2	1.94	0.49
12:1Q:16:ARG:HG2	12:1Q:18:LYS:HG3	1.93	0.49
32:1a:92:C:H2'	32:1a:93:G:C8	2.48	0.49
44:1m:80:ARG:NH1	50:1s:65:ASN:O	2.45	0.49
13:2R:100:LEU:HD21	13:2R:113:LEU:HD23	1.94	0.49
22:20:15:ASP:OD1	22:20:16:SER:N	2.45	0.49
32:2a:53:A:OP2	61:2a:1912:HOH:O	2.20	0.49
41:2j:13:HIS:HB3	41:2j:68:HIS:CE1	2.47	0.49
54:2y:18:G:N1	54:2y:55:PSU:C4	2.72	0.49
1:1A:1062:G:H1	1:1A:1077:A:N6	2.05	0.49
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.13	0.49
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.47	0.49
5:1F:28:ILE:O	5:1F:30:PRO:HD3	2.13	0.49
32:1a:574:A:OP2	61:1a:1906:HOH:O	2.19	0.49
51:1t:33:ILE:O	51:1t:37:SER:OG	2.22	0.49
1:2A:84:A:H5"	20:2Y:8:LYS:HE3	1.95	0.49
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1938:A:OP2	61:2A:3834:HOH:O	2.20	0.49
2:2B:3:C:H2'	2:2B:4:C:C6	2.47	0.49
21:2Z:138:GLU:H	21:2Z:156:LYS:HE3	1.77	0.49
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.94	0.49
32:2a:35:G:O2'	43:2l:118:SER:O	2.26	0.49
32:2a:1071:C:H2'	32:2a:1072:G:H8	1.77	0.49
34:2c:6:HIS:HD2	34:2c:8:ILE:H	1.58	0.49
41:2j:78:ASN:O	41:2j:80:LYS:N	2.45	0.49
51:2t:67:ALA:HA	51:2t:72:LEU:O	2.12	0.49
1:1A:729:G:C5	3:1D:208:LYS:HB2	2.48	0.49
1:1A:1058:G:N2	1:1A:1080:C:N3	2.57	0.49
1:1A:1580:A:OP2	1:1A:1580:A:H8	1.95	0.49
1:1A:2747:G:O6	1:1A:2755:C:H5"	2.12	0.49
32:1a:377:G:OP1	47:1p:3:LYS:HD3	2.12	0.49
36:1e:12:LEU:HB3	36:1e:31:LEU:HB2	1.94	0.49
54:1w:1:G:O6	54:1w:72:C:C4	2.65	0.49
1:2A:839:U:H2'	1:2A:840:C:C6	2.47	0.49
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.27	0.49
1:2A:2448:A:OP1	61:2A:3819:HOH:O	2.19	0.49
8:2I:50:ARG:HA	8:2I:53:ALA:HB3	1.94	0.49
12:2Q:8:LYS:HE2	12:2Q:9:TYR:CE2	2.48	0.49
32:2a:815:A:N7	32:2a:1509:C:O2'	2.41	0.49
32:2a:1360:A:H8	32:2a:1360:A:OP1	1.96	0.49
41:2j:74:ILE:HG22	61:2j:302:HOH:O	2.12	0.49
1:1A:184:C:H2'	1:1A:185:U:C6	2.47	0.49
1:1A:1359:A:C2	1:1A:1372:U:O4	2.65	0.49
1:1A:2153:G:H2'	1:1A:2154:G:C8	2.47	0.49
20:1Y:14:LEU:HB2	20:1Y:75:ILE:HD11	1.93	0.49
32:1a:1343:G:H2'	32:1a:1344:C:C6	2.47	0.49
37:1f:19:LEU:HD11	37:1f:59:TYR:CE1	2.48	0.49
54:1y:38:A:H2'	54:1y:39:PSU:O4'	2.12	0.49
1:2A:894:C:O2'	1:2A:895:U:H5"	2.13	0.49
1:2A:2255:G:OP2	61:2A:3833:HOH:O	2.19	0.49
1:2A:2497:A:H5"	61:2A:4135:HOH:O	2.12	0.49
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.13	0.49
1:2A:2741:A:H2'	1:2A:2742:C:O4'	2.12	0.49
2:2B:14:U:OP2	2:2B:70:C:O2'	2.20	0.49
32:2a:410:G:OP1	35:2d:30:LYS:NZ	2.35	0.49
34:2c:136:GLN:O	34:2c:140:ARG:HG3	2.13	0.49
40:2i:26:VAL:HG13	40:2i:61:ALA:HB3	1.93	0.49
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2131:G:N2	1:1A:2158:A:N1	2.60	0.49
32:1a:236:G:OP1	48:1q:40:LYS:NZ	2.45	0.49
1:2A:1243:G:O2'	11:2P:7:ARG:NH2	2.46	0.49
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.13	0.49
35:2d:22:LYS:O	35:2d:113:SER:HB3	2.13	0.49
40:2i:3:GLN:HE21	40:2i:20:ARG:HE	1.61	0.49
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.25	0.49
9:1N:96:GLU:H	9:1N:96:GLU:CD	2.21	0.49
13:1R:96:ARG:NH1	13:1R:115:GLU:OE2	2.44	0.49
32:1a:204:U:H4'	32:1a:216:G:H5"	1.93	0.49
35:1d:173:TRP:CE3	35:1d:174:LEU:HG	2.47	0.49
10:2O:2:ILE:HB	10:2O:33:ALA:HB3	1.95	0.49
25:23:6:VAL:HA	25:23:56:VAL:HG22	1.93	0.49
26:24:50:VAL:HG11	44:2m:64:TRP:C	2.38	0.49
54:2y:55:PSU:N1	54:2y:57:G:H5"	2.11	0.49
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.78	0.49
33:1b:93:VAL:HG11	33:1b:97:TRP:HD1	1.78	0.49
34:1c:73:PRO:HB3	34:1c:103:VAL:HG11	1.95	0.49
34:1c:131:ARG:HH21	34:1c:135:LYS:HE3	1.78	0.49
51:1t:36:LEU:HD12	51:1t:62:LEU:HD12	1.95	0.49
51:1t:45:GLN:HB2	51:1t:91:LEU:HD13	1.95	0.49
54:1y:4:C:H2'	54:1y:5:G:O4'	2.13	0.49
1:2A:271(G):C:H2'	1:2A:271(H):G:H8	1.77	0.49
25:23:59:VAL:HG12	25:23:60:GLU:H	1.78	0.49
26:24:34:GLU:HB2	44:2m:57:ARG:HE	1.78	0.49
32:2a:714:G:H2'	32:2a:715:A:C8	2.48	0.49
32:2a:1071:C:H2'	32:2a:1072:G:C8	2.48	0.49
33:2b:178:ARG:HH12	39:2h:68:ARG:NH2	2.07	0.49
54:2y:65:G:H2'	54:2y:66:U:C6	2.48	0.49
1:1A:288:C:H2'	1:1A:289:A:C8	2.46	0.48
1:1A:1176:G:N2	1:1A:1178:C:OP2	2.44	0.48
1:1A:2128:C:N4	1:1A:2160:G:H1	2.11	0.48
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.95	0.48
32:1a:841:U:C4	32:1a:848:C:H1'	2.47	0.48
44:1m:11:ARG:HA	44:1m:45:VAL:HB	1.95	0.48
44:1m:40:ASN:O	44:1m:43:THR:OG1	2.25	0.48
1:2A:2136:C:H42	1:2A:2155:G:H1	1.60	0.48
2:2B:17:C:H2'	2:2B:18:G:O4'	2.12	0.48
4:2E:7:VAL:HG11	15:2T:1:MET:HE1	1.95	0.48
5:2F:108:LYS:O	5:2F:112:MET:HG3	2.13	0.48
33:2b:96:ARG:HG2	33:2b:98:LEU:HD12	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:125:GLU:HB2	34:2c:190:ARG:NH2	2.24	0.48
1:1A:878:A:H61	1:1A:899:A:H1'	1.76	0.48
1:1A:2182:G:H2'	1:1A:2183:C:C6	2.48	0.48
2:1B:8:U:O3'	14:1S:25:ARG:NH2	2.46	0.48
32:2a:563:A:O2'	61:2a:1913:HOH:O	2.20	0.48
32:2a:1002:G:C2	32:2a:1003:G:H1'	2.47	0.48
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.48	0.48
47:2p:15:PRO:O	47:2p:16:HIS:ND1	2.46	0.48
55:2x:23:C:H2'	55:2x:24:U:C6	2.47	0.48
1:1A:1155:A:OP1	16:1U:55:ARG:HD2	2.13	0.48
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.46	0.48
1:1A:2753:A:N3	31:19:15:LYS:NZ	2.54	0.48
5:1F:101:LEU:HD12	5:1F:102:PRO:HD2	1.95	0.48
9:1N:42:TRP:HA	9:1N:48:MET:HE1	1.94	0.48
32:1a:1145:C:H4'	32:1a:1146:A:H5'	1.96	0.48
32:1a:1244:C:H42	32:1a:1293:G:H1	1.62	0.48
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.41	0.48
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.95	0.48
32:2a:130:A:O2'	32:2a:131:C:O5'	2.28	0.48
32:2a:1273:G:H3'	32:2a:1274:G:H8	1.77	0.48
34:2c:69:HIS:HA	34:2c:104:GLN:HB3	1.96	0.48
1:1A:639:U:H2'	1:1A:640:C:C6	2.49	0.48
1:1A:657:U:H2'	1:1A:658:C:C6	2.49	0.48
1:1A:774:A:N3	1:1A:774:A:H2'	2.29	0.48
32:1a:954:G:H5"	44:1m:120:LYS:HE2	1.95	0.48
32:1a:1289:A:OP1	52:1u:10:ARG:NH2	2.46	0.48
47:1p:59:TRP:HA	47:1p:62:VAL:HG12	1.95	0.48
1:2A:1011:G:OP2	16:2U:66:ASN:ND2	2.41	0.48
6:2G:122:PRO:HB3	6:2G:170:ARG:HH21	1.79	0.48
7:2H:144:VAL:O	7:2H:148:ILE:HG13	2.13	0.48
14:2S:10:ARG:HG2	14:2S:91:PRO:HA	1.95	0.48
21:2Z:6:LYS:NZ	21:2Z:43:GLU:OE2	2.30	0.48
32:2a:909:A:H2'	32:2a:910:C:O4'	2.14	0.48
32:2a:1190:G:H5'	34:2c:176:HIS:HE1	1.78	0.48
33:2b:218:ALA:O	33:2b:222:ILE:HG23	2.13	0.48
34:2c:78:GLY:HA3	34:2c:83:ARG:H	1.77	0.48
34:2c:151:VAL:HA	34:2c:199:LYS:O	2.13	0.48
35:2d:61:LYS:NZ	35:2d:72:GLU:OE1	2.37	0.48
44:2m:80:ARG:HH22	50:2s:69:HIS:CE1	2.29	0.48
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.48	0.48
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:100:ARG:HH22	35:1d:118:ARG:HH21	1.62	0.48
1:2A:27:G:O2'	1:2A:28:A:OP2	2.28	0.48
1:2A:2134:A:H2'	1:2A:2134:A:N3	2.27	0.48
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.48	0.48
32:2a:620:C:C2	35:2d:135:LEU:HG	2.49	0.48
32:2a:1132:C:H2'	32:2a:1133:G:C8	2.48	0.48
33:2b:42:ILE:HG21	33:2b:202:PRO:O	2.14	0.48
35:2d:59:ARG:HH11	35:2d:59:ARG:HA	1.78	0.48
36:2e:102:ALA:HB2	36:2e:120:THR:HG21	1.96	0.48
2:1B:66:A:H61	2:1B:108:U:H2'	1.79	0.48
32:1a:625:G:H4'	47:1p:16:HIS:CD2	2.48	0.48
32:1a:1221:G:OP1	32:1a:1320:C:N4	2.40	0.48
1:2A:1359:A:H2	1:2A:1372:U:O4	1.97	0.48
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.48	0.48
1:2A:2028:U:O4	61:2A:3830:HOH:O	2.20	0.48
32:2a:114:U:O2'	32:2a:115:G:H5'	2.14	0.48
1:1A:952:G:OP1	12:1Q:16:ARG:NH2	2.46	0.48
30:18:15:LYS:HB3	30:18:23:VAL:HG12	1.94	0.48
32:1a:408:A:H2'	32:1a:409:G:O4'	2.14	0.48
32:1a:749:C:H2'	32:1a:750:G:H8	1.78	0.48
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.95	0.48
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.49	0.48
47:1p:3:LYS:HG3	47:1p:24:ALA:HB2	1.96	0.48
1:2A:2103:C:H2'	1:2A:2104:G:C8	2.48	0.48
32:2a:977:A:O2'	32:2a:981:U:N3	2.45	0.48
44:2m:92:HIS:HA	44:2m:110:ARG:HH21	1.79	0.48
51:2t:98:PRO:O	51:2t:99:LEU:HB2	2.13	0.48
1:1A:484:C:OP1	20:1Y:51:VAL:HG22	2.13	0.48
1:1A:747:U:O2	1:1A:2014:A:H1'	2.14	0.48
32:1a:382:A:H2'	32:1a:383:A:C8	2.48	0.48
32:1a:944:G:OP1	61:1a:1910:HOH:O	2.20	0.48
32:1a:976:G:OP2	32:1a:1358:U:O2'	2.24	0.48
32:1a:1003:G:C4	32:1a:1004:A:H2	2.32	0.48
32:1a:1157:A:H4'	32:1a:1158:C:O5'	2.14	0.48
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.31	0.48
1:2A:2438:U:O2'	1:2A:2440:C:OP1	2.29	0.48
5:2F:24:LEU:HD13	5:2F:114:VAL:HG23	1.94	0.48
5:2F:196:LEU:O	5:2F:200:GLU:N	2.42	0.48
32:2a:109:A:C6	32:2a:326:G:C6	3.02	0.48
39:2h:21:LYS:O	39:2h:65:TYR:OH	2.21	0.48
54:2y:14:A:H3'	54:2y:15:G:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2y:18:G:N2	54:2y:55:PSU:C4	2.74	0.48
1:1A:388:G:O2'	1:1A:389:G:N7	2.45	0.48
1:1A:2156:G:OP2	1:1A:2156:G:H8	1.95	0.48
5:1F:64:ILE:HG21	5:1F:78:ILE:HG23	1.96	0.48
6:1G:45:GLU:H	6:1G:45:GLU:CD	2.21	0.48
41:1j:38:ILE:HG13	41:1j:71:LEU:HB3	1.94	0.48
1:2A:2135:A:OP1	1:2A:2160:G:H1'	2.13	0.48
1:2A:2299:G:H2'	1:2A:2300:G:H8	1.79	0.48
2:2B:105:A:H5'	2:2B:106:G:OP2	2.14	0.48
32:2a:377:G:OP1	47:2p:3:LYS:HE2	2.14	0.48
32:2a:1031:G:H2'	32:2a:1032:G:C8	2.49	0.48
32:2a:1273:G:H3'	32:2a:1274:G:C8	2.49	0.48
33:2b:16:HIS:HB2	33:2b:204:ASN:HD22	1.79	0.48
35:2d:33:MET:HB2	60:2d:302:SF4:S2	2.54	0.48
35:2d:111:ALA:HB1	35:2d:116:GLN:HE21	1.79	0.48
39:2h:51:VAL:HG11	39:2h:60:ARG:HH12	1.79	0.48
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.48	0.48
54:1y:48:C:C2	54:1y:59:U:H1'	2.48	0.48
4:2E:48:GLN:HE21	4:2E:78:LEU:HD22	1.79	0.48
32:2a:925:G:H1'	32:2a:1502:A:C4	2.49	0.48
32:2a:1060:C:H2'	32:2a:1061:G:H8	1.78	0.48
32:2a:1264:C:C4	32:2a:1272:G:O6	2.67	0.48
44:2m:15:VAL:O	44:2m:19:LEU:HG	2.14	0.48
1:1A:1858:G:N2	1:1A:1883:G:H2'	2.29	0.47
2:1B:24:G:N7	2:1B:56:G:H2'	2.29	0.47
8:1I:123:LEU:HA	8:1I:144:VAL:HG23	1.97	0.47
26:14:57:GLU:HA	26:14:58:ARG:HA	1.48	0.47
32:1a:373:A:H2'	32:1a:374:A:H8	1.78	0.47
32:1a:783:C:OP1	32:1a:1515:C:O2'	2.28	0.47
32:1a:1004:A:C5'	32:1a:1024:G:H22	2.27	0.47
48:1q:56:VAL:HB	48:1q:78:GLU:HB3	1.96	0.47
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.14	0.47
1:2A:2334:G:H5'	14:2S:9:ARG:HG2	1.96	0.47
15:2T:51:ARG:HG3	15:2T:98:LYS:HD3	1.95	0.47
21:2Z:54:HIS:HB3	21:2Z:101:PRO:HD3	1.95	0.47
32:2a:392:G:H2'	32:2a:393:A:H8	1.79	0.47
32:2a:501:C:H2'	32:2a:502:G:C8	2.48	0.47
55:2x:15:G:H2'	55:2x:59:A:N1	2.29	0.47
1:1A:1430:C:H2'	1:1A:1431:U:C6	2.49	0.47
1:1A:1851:U:H2'	1:1A:1852:C:O4'	2.15	0.47
13:1R:28:LEU:HD23	13:1R:48:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:110:C:O2'	47:1p:25:ARG:O	2.30	0.47
32:1a:375:U:OP1	47:1p:69:THR:OG1	2.24	0.47
32:1a:1202:G:O4'	45:1n:29:ARG:NH1	2.46	0.47
40:1i:51:ARG:HG2	40:1i:56:LEU:HD21	1.96	0.47
44:1m:23:TYR:CE2	44:1m:71:ARG:HG3	2.49	0.47
48:1q:53:LEU:HB3	48:1q:82:MET:HE1	1.96	0.47
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.49	0.47
1:2A:1685:C:H42	1:2A:1703:G:H1	1.60	0.47
14:2S:30:ARG:HB2	14:2S:35:ILE:HD12	1.96	0.47
32:2a:986:A:H2'	32:2a:987:G:O4'	2.14	0.47
32:2a:1279:A:H5"	41:2j:7:LYS:NZ	2.29	0.47
35:2d:122:ARG:HA	35:2d:122:ARG:HD2	1.73	0.47
44:2m:10:PRO:HG2	44:2m:21:TYR:CD1	2.49	0.47
1:1A:272(G):C:H42	1:1A:363(C):G:H1	1.62	0.47
1:1A:2389:G:H5"	1:1A:2390:U:O4'	2.14	0.47
2:1B:1:U:H2'	2:1B:2:C:C6	2.49	0.47
11:1P:59:LEU:HD11	30:18:10:ALA:HA	1.96	0.47
40:1i:51:ARG:HA	40:1i:56:LEU:HD11	1.96	0.47
44:1m:122:LYS:HA	44:1m:122:LYS:HD2	1.71	0.47
1:2A:1790:C:H5"	1:2A:1791:A:OP1	2.13	0.47
21:2Z:53:ILE:HA	21:2Z:71:VAL:HG23	1.96	0.47
32:2a:671:G:H2'	32:2a:672:U:O4'	2.14	0.47
39:2h:20:TYR:HA	39:2h:65:TYR:CE1	2.49	0.47
54:2y:51:U:H3	54:2y:63:G:H1	1.62	0.47
1:1A:2331:G:N7	61:1A:4185:HOH:O	2.36	0.47
1:1A:2693:A:H2'	1:1A:2694:G:C8	2.49	0.47
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.78	0.47
32:1a:92:C:H2'	32:1a:93:G:H8	1.79	0.47
32:1a:276:G:O3'	48:1q:68:ARG:NH1	2.47	0.47
32:1a:985:C:H2'	32:1a:986:A:H8	1.80	0.47
1:2A:1193:G:OP1	11:2P:14:LYS:NZ	2.22	0.47
1:2A:2533:A:OP1	1:2A:2665:A:O2'	2.30	0.47
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.50	0.47
4:2E:143:ASN:HD22	4:2E:147:PRO:HD3	1.79	0.47
15:2T:127:ALA:C	15:2T:129:ARG:N	2.71	0.47
17:2V:24:LYS:HE2	17:2V:24:LYS:HB3	1.72	0.47
32:2a:1352:C:H2'	32:2a:1353:G:C8	2.49	0.47
40:2i:5:TYR:CD1	40:2i:18:PHE:HE1	2.32	0.47
40:2i:17:VAL:HG11	40:2i:81:ILE:HA	1.95	0.47
43:2l:117:ARG:HB3	43:2l:122:THR:HB	1.95	0.47
1:1A:1607:C:H4'	1:1A:1608:A:O5'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:38:GLN:O	11:1P:39:LYS:HB3	2.14	0.47
12:1Q:85:LYS:HG2	22:10:7:LEU:HB3	1.96	0.47
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.50	0.47
32:1a:222:U:H2'	32:1a:223:U:C6	2.49	0.47
32:1a:865:A:H2	32:1a:918:A:H4'	1.79	0.47
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.50	0.47
54:1y:8:4SU:O2'	54:1y:21:A:N1	2.41	0.47
1:2A:579:G:H2'	1:2A:580:C:C6	2.50	0.47
1:2A:921:G:O6	61:2A:3836:HOH:O	2.20	0.47
1:2A:922:U:H2'	1:2A:923:C:C6	2.49	0.47
1:2A:2314:C:H5'	6:2G:38:VAL:HG21	1.95	0.47
4:2E:170:LEU:HB3	4:2E:184:VAL:HG22	1.95	0.47
6:2G:98:ARG:H	6:2G:98:ARG:HG2	1.36	0.47
14:2S:5:THR:OG1	14:2S:8:GLU:HG3	2.14	0.47
21:2Z:69:THR:HG22	21:2Z:90:VAL:HG22	1.96	0.47
32:2a:401:C:P	35:2d:73:ARG:HH21	2.36	0.47
32:2a:1060:C:HO2'	41:2j:56:HIS:HD1	1.61	0.47
33:2b:178:ARG:NH1	39:2h:74:PRO:HG3	2.30	0.47
35:2d:8:VAL:HG22	35:2d:21:LEU:HD13	1.95	0.47
38:2g:102:ARG:O	38:2g:106:GLN:HG3	2.14	0.47
40:2i:18:PHE:HD2	40:2i:62:TYR:HD2	1.62	0.47
1:1A:271(K):U:H1'	8:1I:50:ARG:HD2	1.96	0.47
1:1A:1937:A:H1'	1:1A:1939:5MU:H72	1.97	0.47
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.96	0.47
32:1a:1172:C:H2'	32:1a:1173:G:H8	1.80	0.47
37:1f:35:ALA:HA	37:1f:67:MET:HB3	1.97	0.47
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.50	0.47
1:2A:2006:C:O2'	1:2A:2823:A:N3	2.47	0.47
5:2F:31:HIS:HB2	11:2P:9:ASN:OD1	2.15	0.47
6:2G:123:ASN:C	6:2G:125:PHE:H	2.22	0.47
32:2a:148:G:H2'	32:2a:149:A:C8	2.48	0.47
32:2a:737:A:H2'	32:2a:738:C:C6	2.49	0.47
46:2o:87:ILE:O	46:2o:88:ARG:HB3	2.14	0.47
55:2x:18:G:O2'	55:2x:19:G:H5'	2.14	0.47
1:1A:536:A:H2'	1:1A:537:C:C6	2.50	0.47
1:1A:2865:U:OP2	15:1T:119:LYS:NZ	2.47	0.47
2:1B:91:C:H5'	12:1Q:18:LYS:HA	1.96	0.47
3:1D:19:ALA:HB3	3:1D:21:PHE:CE1	2.50	0.47
5:1F:103:LYS:HA	5:1F:106:ARG:HD3	1.96	0.47
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.30	0.47
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:963:G:H5'	61:1a:2019:HOH:O	2.13	0.47
32:1a:973:G:H3'	32:1a:974:A:H5"	1.97	0.47
32:1a:985:C:H2'	32:1a:986:A:C8	2.50	0.47
32:1a:1007:C:H2'	32:1a:1008:C:C6	2.49	0.47
32:1a:1039:C:H2'	32:1a:1040:U:C6	2.49	0.47
32:1a:1144:G:N2	32:1a:1146:A:H62	2.13	0.47
37:1f:100:ASN:HB2	49:1r:28:GLU:HA	1.97	0.47
40:1i:8:GLY:HA3	40:1i:76:ALA:O	2.14	0.47
44:1m:91:ARG:HB2	44:1m:98:VAL:HG12	1.96	0.47
46:1o:18:PHE:CZ	46:1o:21:ASP:HB2	2.49	0.47
46:1o:24:SER:O	46:1o:28:GLN:HG3	2.15	0.47
51:1t:60:GLU:HG3	51:1t:81:LYS:HD2	1.95	0.47
54:1w:9:A:O2'	54:1w:10:G:N7	2.46	0.47
1:2A:287:C:H2'	1:2A:288:C:H6	1.80	0.47
1:2A:570:G:H2'	1:2A:2030:A:C5	2.48	0.47
1:2A:643:A:N1	1:2A:2369:A:O2'	2.46	0.47
1:2A:657:U:H2'	1:2A:658:C:C6	2.49	0.47
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.15	0.47
1:2A:1652:A:OP1	13:2R:8:ARG:NH1	2.46	0.47
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.50	0.47
3:2D:132:PRO:HD3	3:2D:190:TYR:CZ	2.49	0.47
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.32	0.47
21:2Z:70:LEU:HD12	21:2Z:70:LEU:HA	1.77	0.47
21:2Z:75:ASN:O	21:2Z:84:GLU:HG3	2.14	0.47
24:22:35:LEU:HD12	24:22:53:LEU:HD12	1.96	0.47
26:24:34:GLU:HB3	44:2m:57:ARG:HH21	1.79	0.47
32:2a:692:U:O2'	32:2a:694:A:N7	2.35	0.47
32:2a:972:C:O2'	41:2j:55:LYS:O	2.31	0.47
32:2a:984:C:H2'	32:2a:985:C:H6	1.79	0.47
32:2a:1371:G:O3'	40:2i:69:GLY:HA3	2.15	0.47
35:2d:104:VAL:HG21	35:2d:140:VAL:HG21	1.97	0.47
36:2e:78:HIS:CD2	36:2e:142:LEU:HD23	2.49	0.47
36:2e:91:LEU:HB3	36:2e:118:ILE:HD11	1.97	0.47
54:2y:18:G:H1'	54:2y:60:U:H5	1.79	0.47
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.50	0.47
1:1A:1364:G:P	23:11:3:LYS:HG3	2.54	0.47
1:1A:2461:C:H2'	1:1A:2462:U:C6	2.50	0.47
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	1.96	0.47
6:1G:44:GLY:O	6:1G:47:LYS:HE3	2.15	0.47
8:1I:93:THR:H	8:1I:96:ASP:HB2	1.80	0.47
9:1N:35:ARG:HD3	9:1N:37:LYS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:270:A:H2'	32:1a:271:C:C6	2.49	0.47
40:1i:77:ILE:O	40:1i:81:ILE:HG22	2.15	0.47
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.47	0.47
1:2A:1539:G:H2'	1:2A:1540:U:O4'	2.15	0.47
1:2A:2592:G:OP1	61:2A:3835:HOH:O	2.20	0.47
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	1.97	0.47
21:2Z:171:ILE:H	21:2Z:171:ILE:HG13	1.49	0.47
32:2a:189(K):U:H2'	32:2a:189(L):G:C8	2.50	0.47
32:2a:448:A:P	32:2a:485:G:H22	2.38	0.47
36:2e:145:LYS:O	36:2e:149:GLU:HG2	2.15	0.47
38:2g:151:TYR:OH	42:2k:54:ARG:HD3	2.15	0.47
1:1A:1359:A:H2	1:1A:1372:U:O4	1.98	0.47
1:1A:2022:U:OP1	61:1A:4129:HOH:O	2.21	0.47
9:1N:42:TRP:CH2	9:1N:44:PRO:HB3	2.49	0.47
6:2G:126:ASP:HB2	6:2G:130:ASN:O	2.15	0.47
21:2Z:72:ARG:NH1	21:2Z:97:GLU:O	2.46	0.47
32:2a:663:A:O3'	49:2r:64:ARG:NH2	2.46	0.47
32:2a:946:A:H2'	32:2a:947:G:C8	2.50	0.47
1:1A:247:G:H4'	1:1A:386:G:C5	2.50	0.47
5:1F:164:ARG:O	5:1F:168:ARG:HB3	2.14	0.47
21:1Z:126:VAL:HG12	21:1Z:128:VAL:HB	1.97	0.47
26:14:24:THR:OG1	26:14:25:TYR:N	2.48	0.47
32:1a:193:C:H2'	32:1a:194:C:C6	2.50	0.47
33:1b:100:GLY:N	33:1b:176:GLU:OE2	2.43	0.47
35:1d:178:VAL:HG12	35:1d:179:GLU:H	1.80	0.47
49:1r:59:SER:OG	49:1r:60:ALA:N	2.48	0.47
1:2A:848:G:H2'	1:2A:849:A:C8	2.50	0.47
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.32	0.47
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.51	0.47
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.29	0.47
33:2b:219:VAL:HA	33:2b:222:ILE:HG12	1.96	0.47
36:2e:95:ALA:O	36:2e:97:GLY:N	2.44	0.47
1:1A:876:C:H2'	1:1A:877:U:O4'	2.15	0.46
1:1A:2537:U:H2'	1:1A:2538:C:C6	2.50	0.46
32:1a:1500:A:OP2	61:1a:1909:HOH:O	2.20	0.46
33:1b:78:GLN:NE2	33:1b:94:ASN:O	2.40	0.46
51:1t:42:GLN:NE2	51:1t:46:GLU:OE2	2.44	0.46
54:1y:36:A:H2'	54:1y:37:MIA:O4'	2.15	0.46
1:2A:1446:C:H42	1:2A:1465:G:H1	1.62	0.46
14:1S:5:THR:OG1	14:1S:8:GLU:HG3	2.15	0.46
32:1a:1039:C:H2'	32:1a:1040:U:H6	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.80	0.46
33:1b:124:SER:HA	33:1b:125:PRO:HA	1.68	0.46
32:2a:1065:U:H5"	32:2a:1190:G:H22	1.80	0.46
36:2e:42:GLY:HA2	36:2e:65:ASN:O	2.15	0.46
38:2g:105:VAL:O	38:2g:109:ASN:ND2	2.42	0.46
1:1A:118:A:C8	1:1A:119:A:C8	3.03	0.46
1:1A:1022:G:N7	9:1N:66:LYS:HE2	2.30	0.46
1:1A:1876:A:H2'	1:1A:1877:A:C8	2.51	0.46
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.50	0.46
1:1A:2405:G:O2'	1:1A:2406:U:OP1	2.22	0.46
5:1F:9:ILE:HD12	5:1F:123:LEU:HD23	1.97	0.46
6:1G:5:VAL:HG22	6:1G:8:LYS:H	1.80	0.46
26:14:18:CYS:SG	26:14:20:ASN:HB2	2.55	0.46
32:1a:116:A:H61	32:1a:313:A:H1'	1.80	0.46
32:1a:1005:A:H5"	32:1a:1006:C:C5	2.51	0.46
33:1b:82:ARG:HH11	33:1b:92:TYR:HH	1.57	0.46
1:2A:479:A:N3	1:2A:481:G:H5"	2.30	0.46
1:2A:686:G:N2	1:2A:788:A:H61	2.13	0.46
1:2A:1186:G:C2	1:2A:1187:G:H1'	2.49	0.46
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.15	0.46
6:2G:39:ILE:HG23	6:2G:157:ILE:HD13	1.97	0.46
6:2G:125:PHE:HB3	6:2G:166:ASP:OD2	2.14	0.46
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.15	0.46
21:2Z:144:LEU:O	21:2Z:145:GLU:HB2	2.14	0.46
1:1A:1239:G:H2'	1:1A:1240:U:O4'	2.16	0.46
1:1A:2233:U:H2'	1:1A:2234:G:C8	2.50	0.46
2:1B:48:A:P	14:1S:30:ARG:HH12	2.39	0.46
32:1a:748:C:H4'	32:1a:749:C:O5'	2.16	0.46
33:1b:48:MET:HA	33:1b:51:LEU:HB2	1.97	0.46
1:2A:631:A:H2'	1:2A:632:A:O4'	2.15	0.46
1:2A:1509(B):A:H2'	1:2A:1510:G:C8	2.50	0.46
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.50	0.46
1:2A:2127:G:H1	1:2A:2161:C:N4	2.14	0.46
1:2A:2611:U:H6	1:2A:2611:U:H5'	1.81	0.46
5:2F:116:ASP:OD1	5:2F:119:ARG:NH2	2.49	0.46
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.49	0.46
32:2a:1190:G:H5'	34:2c:176:HIS:CE1	2.51	0.46
32:2a:1226:C:H4'	50:2s:80:TYR:CZ	2.50	0.46
36:2e:36:ASP:C	36:2e:38:GLN:H	2.20	0.46
1:1A:55:G:O2'	1:1A:127:A:N1	2.45	0.46
1:1A:667:U:O2	30:18:2:PRO:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.15	0.46
1:1A:2134:A:N3	1:1A:2159:G:H1'	2.31	0.46
1:1A:2794:C:N4	1:1A:2802:G:H22	2.13	0.46
32:1a:96:U:H2'	32:1a:97:G:C8	2.50	0.46
32:1a:1358:U:OP1	45:1n:35:ARG:HG3	2.16	0.46
33:1b:16:HIS:HB2	33:1b:204:ASN:CB	2.46	0.46
33:1b:55:PHE:HA	33:1b:58:ILE:HG12	1.96	0.46
35:1d:88:VAL:O	35:1d:92:VAL:HG23	2.16	0.46
35:1d:178:VAL:C	35:1d:180:GLY:H	2.24	0.46
40:1i:42:ARG:NH2	40:1i:75:ASP:OD2	2.49	0.46
1:2A:154(A):C:H42	1:2A:171:G:H1	1.62	0.46
1:2A:184:C:H2'	1:2A:185:U:H6	1.78	0.46
1:2A:927:G:H2'	1:2A:928:G:O4'	2.14	0.46
1:2A:2105:C:H2'	1:2A:2106:G:H8	1.79	0.46
1:2A:2110:G:H3'	1:2A:2111:C:C5'	2.45	0.46
18:2W:12:ILE:HD13	18:2W:17:VAL:HG13	1.96	0.46
20:2Y:6:HIS:CD2	20:2Y:7:VAL:HG23	2.51	0.46
32:2a:64:G:H4'	32:2a:65:U:H3'	1.98	0.46
32:2a:428:G:OP2	35:2d:10:ARG:NH1	2.48	0.46
32:2a:918:A:H2'	32:2a:919:A:C8	2.50	0.46
32:2a:983:A:N1	32:2a:1222:G:N2	2.63	0.46
32:2a:1070:U:H2'	32:2a:1071:C:H6	1.81	0.46
32:2a:1126:U:H3	41:2j:40:LEU:HD11	1.80	0.46
33:2b:92:TYR:CE2	33:2b:151:GLY:HA3	2.51	0.46
54:2y:67:C:H2'	54:2y:68:C:C6	2.51	0.46
1:1A:671:C:N4	61:1A:4296:HOH:O	2.48	0.46
1:1A:1815:A:OP2	3:1D:54:ARG:NH2	2.47	0.46
5:1F:123:LEU:HD13	5:1F:192:LEU:HD13	1.98	0.46
6:1G:59:GLU:CD	6:1G:153:ARG:HH21	2.23	0.46
7:1H:90:LYS:HE3	7:1H:159:GLU:HG2	1.98	0.46
21:1Z:45:ASP:CG	21:1Z:49:ARG:HE	2.24	0.46
26:14:54:GLY:N	26:14:55:ARG:HA	2.28	0.46
32:1a:328:C:H4'	32:1a:329:A:H5'	1.98	0.46
1:2A:2336:A:H61	22:20:43:THR:CG2	2.28	0.46
3:2D:125:ILE:HB	37:2f:81:ILE:HD11	1.98	0.46
12:2Q:110:THR:HB	12:2Q:113:GLN:H	1.81	0.46
32:2a:107:G:H2'	32:2a:108:G:O4'	2.15	0.46
32:2a:580:U:H2'	32:2a:581:G:O4'	2.15	0.46
32:2a:779:C:H2'	32:2a:780:A:O4'	2.16	0.46
32:2a:1014:A:H2'	32:2a:1015:A:C8	2.50	0.46
32:2a:1316:G:N2	32:2a:1319:A:H5"	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.80	0.46
40:2i:55:ALA:HA	40:2i:58:HIS:HD2	1.81	0.46
43:2l:7:ILE:O	43:2l:11:VAL:HG13	2.15	0.46
1:1A:1094:U:H1'	1:1A:1097:U:C4	2.51	0.46
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.51	0.46
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.51	0.46
1:1A:2791:C:H2'	1:1A:2792:G:H8	1.80	0.46
17:1V:1:MET:HE3	17:1V:43:GLU:HB2	1.96	0.46
32:1a:731:G:H5'	32:1a:766:A:H4'	1.97	0.46
33:1b:12:GLU:O	33:1b:15:VAL:HG22	2.15	0.46
35:1d:142:PRO:HA	35:1d:185:PHE:HD2	1.80	0.46
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.32	0.46
1:2A:272(B):G:H2'	1:2A:272(C):G:C8	2.50	0.46
1:2A:800:A:H8	1:2A:800:A:OP1	1.99	0.46
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.15	0.46
1:2A:2503:2MA:H8	58:2A:3772:WC9:O	2.15	0.46
1:2A:2811:G:N2	1:2A:2891:G:H1'	2.31	0.46
5:2F:12:LEU:HD12	5:2F:124:LEU:HD21	1.97	0.46
8:2I:130:TYR:CE2	8:2I:132:PRO:HB3	2.50	0.46
14:2S:48:LEU:HD23	14:2S:48:LEU:HA	1.78	0.46
16:2U:76:TYR:CE2	16:2U:80:ILE:HG13	2.51	0.46
26:24:13:ARG:HG2	26:24:23:GLU:HA	1.98	0.46
32:2a:660:G:H1	32:2a:745:C:H42	1.64	0.46
39:2h:9:MET:HG3	39:2h:26:VAL:HG11	1.97	0.46
1:1A:593:G:H4'	30:18:4:MET:HE2	1.96	0.46
1:1A:1796:U:H2'	1:1A:1797:C:H6	1.81	0.46
32:1a:1240:U:OP2	38:1g:116:ALA:N	2.49	0.46
32:1a:1260:C:O5'	32:1a:1284:C:H4'	2.16	0.46
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.51	0.46
33:1b:105:PHE:C	33:1b:107:THR:H	2.23	0.46
1:2A:760:G:H2'	1:2A:761:A:O4'	2.15	0.46
1:2A:897:C:H5'	54:2w:56:C:OP1	2.15	0.46
1:2A:1221(A):C:C2	1:2A:1229:G:C2	3.03	0.46
1:2A:2518:A:OP2	61:2A:3837:HOH:O	2.21	0.46
14:2S:35:ILE:HG12	14:2S:101:LEU:HD12	1.98	0.46
23:21:56:GLN:HA	23:21:56:GLN:HE21	1.81	0.46
32:2a:337:C:H2'	32:2a:338:A:C8	2.51	0.46
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.24	0.46
32:2a:1518:MA6:H93	32:2a:1519:MA6:C9	2.46	0.46
43:2l:84:LEU:HB2	43:2l:105:TYR:CE2	2.50	0.46
44:2m:23:TYR:CE2	44:2m:71:ARG:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:34:LEU:HD13	44:2m:41:PRO:HB3	1.96	0.46
48:2q:50:LYS:HD2	48:2q:51:TYR:CZ	2.50	0.46
1:1A:1278:A:OP1	13:1R:36:THR:HG23	2.16	0.46
1:1A:2469:A:O3'	12:1Q:56:ARG:NH1	2.49	0.46
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.30	0.46
32:1a:392:G:H2'	32:1a:393:A:H8	1.81	0.46
44:1m:108:ARG:HD3	44:1m:108:ARG:HA	1.66	0.46
1:2A:436:C:H2'	1:2A:437:G:C8	2.51	0.46
1:2A:639:U:H2'	1:2A:640:C:C6	2.51	0.46
1:2A:1037:G:H1	1:2A:1118:C:H42	1.64	0.46
5:2F:20:LEU:HD13	5:2F:125:LEU:HD13	1.96	0.46
5:2F:116:ASP:O	5:2F:120:GLU:HG2	2.16	0.46
32:2a:192:U:O2'	51:2t:60:GLU:OE1	2.27	0.46
32:2a:266:G:H2'	32:2a:266:G:N3	2.31	0.46
32:2a:405:U:O4	35:2d:2:GLY:N	2.48	0.46
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.81	0.46
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.51	0.46
33:2b:185:ILE:HG22	33:2b:199:TYR:HD2	1.80	0.46
34:2c:152:ILE:HG13	34:2c:199:LYS:HB2	1.97	0.46
35:2d:63:LYS:HD2	35:2d:198:VAL:HG12	1.98	0.46
40:2i:5:TYR:HD1	40:2i:18:PHE:CE1	2.34	0.46
40:2i:9:ARG:HA	40:2i:13:ALA:O	2.16	0.46
1:1A:1041:C:N4	1:1A:1114:G:H1	2.12	0.46
1:1A:1062:G:P	1:1A:1070:A:H1'	2.56	0.46
33:1b:24:TRP:H	33:1b:24:TRP:HD1	1.62	0.46
44:1m:23:TYR:HB3	44:1m:67:GLU:HA	1.98	0.46
54:1y:28:G:H1	54:1y:42:C:H42	1.63	0.46
14:2S:36:TYR:CD2	14:2S:36:TYR:N	2.84	0.46
32:2a:434:U:H2'	32:2a:435:C:C6	2.51	0.46
35:2d:140:VAL:HG11	35:2d:146:ILE:HD11	1.98	0.46
50:2s:49:ILE:HD13	50:2s:71:LEU:HD11	1.97	0.46
1:1A:721:C:H2'	1:1A:722:A:C8	2.51	0.45
1:1A:893:C:H2'	1:1A:894:C:C6	2.51	0.45
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.16	0.45
7:1H:17:VAL:HG11	7:1H:50:VAL:HG21	1.98	0.45
32:1a:421:U:O4	34:1c:127:ARG:NH2	2.46	0.45
44:1m:20:THR:C	44:1m:22:ILE:H	2.24	0.45
51:1t:22:ARG:O	51:1t:26:ASN:ND2	2.49	0.45
1:2A:1341:U:OP2	1:2A:1394:U:O2'	2.22	0.45
1:2A:1359:A:C2	1:2A:1372:U:O4	2.69	0.45
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2129:C:N4	1:2A:2159:G:H1	2.15	0.45
4:2E:48:GLN:NE2	4:2E:78:LEU:HD22	2.31	0.45
14:2S:85:VAL:HG22	14:2S:86:ALA:H	1.81	0.45
26:24:46:GLN:CD	26:24:48:ARG:HD3	2.41	0.45
32:2a:999:C:N4	32:2a:1042:G:H1	2.13	0.45
32:2a:1068:G:H8	32:2a:1068:G:OP2	1.99	0.45
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.51	0.45
42:2k:21:ILE:HB	42:2k:84:VAL:HG12	1.98	0.45
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.82	0.45
32:1a:935:A:O2'	32:1a:1383:C:N3	2.48	0.45
38:1g:74:GLU:HG2	38:1g:91:VAL:HG22	1.98	0.45
47:1p:22:THR:HA	47:1p:33:ILE:HD12	1.99	0.45
54:1y:67:C:H2'	54:1y:68:C:C6	2.51	0.45
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.51	0.45
1:2A:2123:G:H2'	1:2A:2124:G:C8	2.50	0.45
1:2A:2758:A:C4	7:2H:67:LEU:HD21	2.51	0.45
1:2A:2805:G:H2'	1:2A:2807:G:H8	1.78	0.45
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.40	0.45
11:2P:121:LYS:HB3	11:2P:121:LYS:HE2	1.77	0.45
32:2a:222:U:H2'	32:2a:223:U:C6	2.51	0.45
32:2a:328:C:H4'	32:2a:329:A:H5'	1.98	0.45
32:2a:1224:G:H1	32:2a:1363:C:H42	1.64	0.45
32:2a:1263:C:H3'	32:2a:1263:C:H6	1.80	0.45
32:2a:1299:A:H2'	32:2a:1299:A:N3	2.31	0.45
32:2a:1343:G:H2'	32:2a:1344:C:C6	2.51	0.45
34:2c:131:ARG:HH21	34:2c:135:LYS:HE3	1.80	0.45
39:2h:51:VAL:HG12	39:2h:52:ASP:H	1.81	0.45
1:1A:1721:G:H1'	1:1A:1741:A:H61	1.82	0.45
1:1A:1991:U:H2'	1:1A:1992:G:H5"	1.98	0.45
32:1a:160:A:H1'	32:1a:344:A:C5	2.52	0.45
32:1a:532:A:N6	32:1a:1206:G:O2'	2.50	0.45
32:1a:1333:A:H2'	32:1a:1334:G:O4'	2.17	0.45
38:1g:79:ARG:HG3	38:1g:80:VAL:N	2.31	0.45
55:1x:23:C:H2'	55:1x:24:U:C6	2.51	0.45
1:2A:468:G:N7	29:27:39:ARG:NH2	2.53	0.45
6:2G:49:ASP:N	6:2G:49:ASP:OD1	2.49	0.45
11:2P:37:GLY:O	11:2P:40:SER:OG	2.33	0.45
16:2U:50:ARG:HH22	17:2V:72:VAL:HG22	1.80	0.45
26:24:12:ALA:HB3	26:24:26:SER:HB3	1.98	0.45
30:28:63:PRO:HG2	30:28:64:TYR:CE2	2.51	0.45
32:2a:979:C:O2	45:2n:19:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1004:A:C8	32:2a:1005:A:H4'	2.51	0.45
33:2b:52:GLU:HG2	33:2b:56:ARG:HH12	1.81	0.45
33:2b:60:ASP:O	33:2b:64:ARG:HG2	2.16	0.45
34:2c:179:ARG:NH1	34:2c:206:GLU:OE1	2.49	0.45
37:2f:76:ALA:O	37:2f:80:ARG:HG3	2.16	0.45
38:2g:79:ARG:NH2	38:2g:80:VAL:HA	2.31	0.45
43:2l:6:THR:HG23	43:2l:9:GLN:OE1	2.16	0.45
46:2o:87:ILE:HG22	46:2o:88:ARG:N	2.31	0.45
1:1A:492:A:H2'	1:1A:493:G:O4'	2.16	0.45
1:1A:1448:G:O2'	1:1A:1528(A):A:N1	2.45	0.45
1:1A:2102:U:H3	1:1A:2187:G:H1	1.64	0.45
1:1A:2748:A:H5'	7:1H:4:ILE:HD12	1.98	0.45
22:10:10:THR:HG22	22:10:12:ASN:H	1.82	0.45
32:1a:719:C:H1'	49:1r:49:LYS:HB3	1.98	0.45
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.50	0.45
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.41	0.45
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.52	0.45
1:2A:2171:A:H1'	1:2A:2172:U:C6	2.51	0.45
13:2R:36:THR:HG22	13:2R:37:THR:H	1.80	0.45
1:1A:2108:C:H2'	1:1A:2109:U:H6	1.81	0.45
5:1F:125:LEU:HD23	5:1F:194:MET:HB2	1.98	0.45
12:1Q:137:TYR:HB3	21:1Z:76:LEU:HD21	1.99	0.45
32:1a:175:C:H2'	32:1a:176:C:C6	2.51	0.45
35:1d:61:LYS:HD2	35:1d:207:TYR:OH	2.16	0.45
39:1h:114:THR:OG1	39:1h:117:GLY:O	2.34	0.45
1:2A:272(B):G:H2'	1:2A:272(C):G:H8	1.82	0.45
1:2A:2408:U:H2'	1:2A:2409:G:C8	2.51	0.45
6:2G:37:VAL:HG21	6:2G:103:LEU:HD11	1.98	0.45
32:2a:45:U:H2'	32:2a:46:G:C8	2.52	0.45
32:2a:1151:A:O2'	32:2a:1152:A:H8	1.98	0.45
33:2b:43:ASP:OD2	33:2b:46:LYS:N	2.46	0.45
36:2e:80:ILE:HG13	39:2h:104:ARG:NH2	2.32	0.45
44:2m:29:ARG:HB3	44:2m:64:TRP:CZ3	2.51	0.45
44:2m:33:ALA:HB1	44:2m:59:TYR:HE2	1.82	0.45
49:2r:56:THR:OG1	49:2r:63:GLN:NE2	2.48	0.45
55:2x:40:C:H2'	55:2x:41:C:C6	2.51	0.45
1:1A:2074:U:H2'	1:1A:2075:U:C6	2.52	0.45
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.51	0.45
8:1I:70:GLU:O	8:1I:74:ASN:HB2	2.16	0.45
12:1Q:10:ARG:HH12	12:1Q:90:VAL:H	1.63	0.45
18:1W:71:VAL:HA	18:1W:107:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:409:G:OP2	35:1d:22:LYS:HD2	2.17	0.45
32:1a:721:G:H4'	32:1a:722:A:O4'	2.16	0.45
32:1a:966:M2G:HM12	55:1x:34:C:H5'	1.98	0.45
32:1a:1318:A:H5"	50:1s:3:ARG:NH1	2.32	0.45
33:1b:58:ILE:HG13	33:1b:221:LEU:HD12	1.98	0.45
44:1m:3:ARG:HG3	44:1m:4:ILE:H	1.81	0.45
46:1o:10:LYS:HE3	46:1o:10:LYS:HB2	1.83	0.45
48:1q:53:LEU:HD23	48:1q:82:MET:HE1	1.98	0.45
1:2A:593:G:H4'	30:28:4:MET:HE2	1.98	0.45
1:2A:881:G:H3'	1:2A:882:G:H8	1.81	0.45
1:2A:1697:G:OP2	1:2A:1698:A:O2'	2.28	0.45
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.81	0.45
7:2H:127:GLU:C	7:2H:129:THR:H	2.24	0.45
7:2H:156:ALA:O	7:2H:172:LYS:HG2	2.16	0.45
18:2W:14:PRO:O	18:2W:18:ARG:HG3	2.17	0.45
32:2a:1122:U:N3	32:2a:1123:A:N7	2.65	0.45
32:2a:1150:U:H4'	41:2j:41:PRO:HG3	1.97	0.45
33:2b:58:ILE:HG23	33:2b:61:LEU:HD23	1.99	0.45
36:2e:105:VAL:HB	36:2e:106:PRO:HD3	1.99	0.45
54:2w:18:G:H4'	54:2w:60:U:C5	2.52	0.45
1:1A:228:A:H8	1:1A:229:A:H5'	1.81	0.45
1:1A:518:G:H2'	1:1A:519:U:C6	2.52	0.45
1:1A:919:G:N2	1:1A:2269:A:OP2	2.50	0.45
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.99	0.45
21:1Z:126:VAL:HG11	21:1Z:161:VAL:HB	1.98	0.45
24:12:41:ILE:HG13	24:12:43:GLN:HG3	1.99	0.45
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.97	0.45
32:1a:767:A:H2'	32:1a:768:A:O4'	2.17	0.45
33:1b:82:ARG:NH1	33:1b:92:TYR:HH	2.14	0.45
33:1b:188:ALA:HB1	33:1b:192:SER:OG	2.15	0.45
39:1h:73:ASP:OD1	39:1h:75:ARG:NE	2.49	0.45
44:1m:3:ARG:HD2	44:1m:9:ILE:H	1.82	0.45
1:2A:71:A:N7	19:2X:31:HIS:HE1	2.15	0.45
1:2A:674:G:O2'	5:2F:74:ARG:HD3	2.16	0.45
1:2A:2156:G:H2'	1:2A:2157:G:C4	2.51	0.45
9:2N:69:GLN:O	9:2N:71:ILE:HG13	2.17	0.45
14:2S:3:ARG:NH2	14:2S:4:LEU:O	2.50	0.45
32:2a:343:U:H2'	32:2a:345:C:C5	2.52	0.45
32:2a:973:G:H3'	32:2a:974:A:H5"	1.99	0.45
32:2a:1221:G:O3'	50:2s:77:THR:OG1	2.32	0.45
32:2a:1396:A:OP2	61:2a:1914:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:113:ALA:HB2	34:2c:202:ILE:HG13	1.98	0.45
36:2e:20:GLN:HE21	36:2e:20:GLN:HB2	1.61	0.45
41:2j:9:ARG:O	41:2j:16:LEU:HD21	2.17	0.45
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.42	0.45
2:1B:48:A:H4'	14:1S:95:HIS:HD2	1.82	0.45
18:1W:25:ARG:NH2	18:1W:74:ALA:O	2.39	0.45
32:1a:56:U:H2'	32:1a:57:G:C8	2.52	0.45
32:1a:381:C:H2'	32:1a:382:A:O4'	2.17	0.45
36:1e:105:VAL:HB	36:1e:106:PRO:HD3	1.99	0.45
2:2B:75:G:N2	21:2Z:87:ASP:OD1	2.50	0.45
3:2D:253:GLN:HG3	61:2D:411:HOH:O	2.15	0.45
6:2G:68:PRO:HB3	6:2G:92:VAL:HB	1.98	0.45
32:2a:179:A:H2'	32:2a:180:U:C6	2.52	0.45
32:2a:1279:A:O2'	32:2a:1281:U:OP2	2.32	0.45
40:2i:8:GLY:O	40:2i:15:ALA:N	2.41	0.45
41:2j:12:ASP:O	41:2j:15:THR:OG1	2.34	0.45
1:1A:218:A:C2	1:1A:235:U:H4'	2.52	0.45
1:1A:226:G:N2	1:1A:228:A:H62	2.15	0.45
3:1D:145:VAL:HG12	3:1D:146:GLU:O	2.17	0.45
32:1a:667:G:H4'	46:1o:51:HIS:ND1	2.32	0.45
32:1a:695:A:OP2	42:1k:53:SER:N	2.50	0.45
32:1a:1060:C:C5	34:1c:2:GLY:HA3	2.52	0.45
1:2A:422:A:OP2	61:2A:3838:HOH:O	2.21	0.45
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.52	0.45
1:2A:2320:A:H1'	1:2A:2321:G:C2	2.52	0.45
2:2B:24:G:N7	2:2B:56:G:H2'	2.32	0.45
12:2Q:65:PHE:HB2	12:2Q:105:GLU:HB2	1.97	0.45
22:20:53:MET:HG3	22:20:59:LEU:HD23	1.99	0.45
32:2a:9:G:H2'	32:2a:10:A:C8	2.50	0.45
32:2a:597:G:OP2	61:2a:1909:HOH:O	2.21	0.45
38:2g:101:LEU:O	38:2g:105:VAL:HG23	2.17	0.45
40:2i:85:LEU:HB3	40:2i:92:TYR:CD2	2.50	0.45
5:1F:7:TYR:CD2	5:1F:24:LEU:HB2	2.51	0.45
8:1I:81:VAL:HG21	8:1I:88:ILE:HD13	1.99	0.45
18:1W:4:LYS:HD2	18:1W:6:ILE:HD11	1.99	0.45
32:1a:1179:A:O3'	40:1i:103:THR:HB	2.16	0.45
13:2R:118:GLU:CD	13:2R:118:GLU:H	2.24	0.45
32:2a:336:C:H2'	32:2a:337:C:C6	2.52	0.45
32:2a:735:C:H2'	32:2a:736:C:H6	1.82	0.45
32:2a:1318:A:H5"	50:2s:3:ARG:NH2	2.31	0.45
33:2b:114:ARG:HA	33:2b:117:GLU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:158:ILE:H	35:2d:158:ILE:HG13	1.63	0.45
54:2w:21:A:HO2'	54:2w:22:G:P	2.40	0.45
1:1A:1939:5MU:OP1	1:1A:2604:U:O2'	2.31	0.44
1:1A:1971:A:OP2	3:1D:242:ARG:NH2	2.50	0.44
6:1G:66:GLN:HG3	26:14:1:MET:HE1	1.99	0.44
28:16:38:LYS:HE3	28:16:38:LYS:HB3	1.80	0.44
39:1h:21:LYS:O	39:1h:65:TYR:OH	2.27	0.44
1:2A:271(G):C:H2'	1:2A:271(H):G:C8	2.52	0.44
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.51	0.44
1:2A:2206:G:H5"	1:2A:2207:G:C8	2.52	0.44
1:2A:2340:G:H2'	1:2A:2341:G:H8	1.82	0.44
32:2a:1026:G:O6	32:2a:1036:G:N2	2.51	0.44
32:2a:1515:C:H2'	32:2a:1516:G:C8	2.52	0.44
34:2c:131:ARG:NH2	34:2c:135:LYS:HE3	2.32	0.44
35:2d:22:LYS:HB2	35:2d:26:CYS:SG	2.57	0.44
38:2g:69:VAL:HG22	38:2g:135:VAL:HG22	1.99	0.44
43:2l:53:ARG:HB3	43:2l:69:TYR:HE1	1.81	0.44
1:1A:1038:C:H42	1:1A:1117:G:H1	1.65	0.44
1:1A:1557:C:H5"	1:1A:1558:A:OP2	2.17	0.44
1:1A:1594:G:H2'	1:1A:1595:G:O4'	2.17	0.44
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.53	0.44
37:1f:76:ALA:O	37:1f:80:ARG:HG3	2.18	0.44
55:1x:8:4SU:O2	55:1x:21:A:H2	2.00	0.44
1:2A:581:C:H2'	1:2A:582:G:C8	2.52	0.44
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.33	0.44
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.17	0.44
33:2b:76:GLN:HB2	33:2b:208:ILE:HD11	1.98	0.44
41:2j:89:ASP:O	41:2j:91:PRO:HD3	2.18	0.44
1:1A:272(J):C:H2'	1:1A:274:G:C8	2.52	0.44
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.16	0.44
1:1A:896:A:H4'	1:1A:897:C:OP1	2.17	0.44
1:1A:1512:U:H2'	1:1A:1513:C:C6	2.52	0.44
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.32	0.44
1:1A:2121:G:H2'	1:1A:2122:U:C6	2.52	0.44
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.99	0.44
32:1a:562:C:O2	43:1l:16:GLU:N	2.51	0.44
32:1a:892:A:O2'	32:1a:1415:G:H4'	2.17	0.44
32:1a:1239:A:H62	32:1a:1299:A:H62	1.64	0.44
33:1b:178:ARG:NH1	33:1b:196:LEU:O	2.50	0.44
39:1h:10:LEU:HG	39:1h:83:ILE:HD11	1.98	0.44
1:2A:588:U:H2'	1:2A:589:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.35	0.44
1:2A:2872:G:O2'	1:2A:2873:A:H5'	2.17	0.44
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.50	0.44
32:2a:862:C:H1'	32:2a:874:G:H5"	1.99	0.44
32:2a:953:G:H5'	32:2a:965:A:N6	2.26	0.44
32:2a:999:C:C4	32:2a:1000:U:C4	3.04	0.44
32:2a:1268:A:H2'	32:2a:1269:A:C8	2.52	0.44
1:1A:1076:C:H4'	1:1A:1077:A:OP1	2.17	0.44
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.52	0.44
12:1Q:20:ALA:HB2	21:1Z:79:ARG:HG3	1.98	0.44
32:1a:1370:G:C2	32:1a:1371:G:C8	3.05	0.44
32:1a:1429:C:H2'	32:1a:1430:C:H6	1.83	0.44
33:1b:102:LEU:HB3	33:1b:180:LEU:HD12	1.98	0.44
1:2A:236:C:H2'	1:2A:237:C:H6	1.83	0.44
1:2A:375:C:H2'	1:2A:376:C:C6	2.52	0.44
1:2A:600:G:O3'	5:2F:108:LYS:HE3	2.18	0.44
1:2A:1803:A:HO2'	3:2D:259:THR:HG21	1.81	0.44
1:2A:2138:C:H2'	1:2A:2139:C:O4'	2.16	0.44
1:2A:2788:C:N4	1:2A:2789:C:H41	2.16	0.44
1:2A:2846:G:H2'	1:2A:2847:U:O4'	2.17	0.44
6:2G:31:VAL:HG22	6:2G:32:PRO:HD2	2.00	0.44
8:2I:54:GLN:HA	8:2I:57:ARG:HG2	2.00	0.44
32:2a:7:G:H5'	32:2a:298:A:O4'	2.17	0.44
32:2a:1073:U:H2'	32:2a:1074:G:H8	1.82	0.44
32:2a:1104:G:O3'	33:2b:111:ARG:NH2	2.46	0.44
33:2b:91:PRO:HG3	33:2b:154:LEU:HB2	2.00	0.44
1:1A:2188:C:H2'	1:1A:2189:U:O4'	2.17	0.44
1:1A:2320:A:H2'	1:1A:2320:A:N3	2.33	0.44
7:1H:9:ILE:HD12	7:1H:50:VAL:HG12	2.00	0.44
26:14:59:PHE:C	26:14:61:ARG:H	2.26	0.44
32:1a:560:U:HO2'	32:1a:561:U:P	2.38	0.44
34:1c:81:GLY:O	34:1c:85:ARG:HB2	2.17	0.44
36:1e:10:MET:H	36:1e:10:MET:HG2	1.58	0.44
1:2A:236:C:H2'	1:2A:237:C:C6	2.52	0.44
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.17	0.44
1:2A:903:C:H2'	1:2A:904:C:C6	2.52	0.44
1:2A:981:A:N1	1:2A:2027:G:O2'	2.45	0.44
1:2A:2406:U:C2	11:2P:72:PRO:HG2	2.52	0.44
7:2H:3:ARG:HE	7:2H:54:ARG:NH1	2.12	0.44
9:2N:123:TYR:OH	9:2N:130:HIS:NE2	2.37	0.44
32:2a:392:G:H2'	32:2a:393:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:685:G:C2	32:2a:686:U:C4	3.06	0.44
32:2a:1250:A:H4'	40:2i:68:GLY:N	2.32	0.44
33:2b:9:GLU:O	33:2b:11:LEU:N	2.50	0.44
43:2l:8:ASN:O	43:2l:12:ARG:HG3	2.18	0.44
54:2y:58:A:O2'	54:2y:60:U:OP2	2.28	0.44
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.52	0.44
1:1A:996:A:H4'	16:1U:91:ASP:OD2	2.18	0.44
1:1A:2139:C:H2'	1:1A:2140:C:O4'	2.17	0.44
1:1A:2611:U:H5'	1:1A:2611:U:H6	1.83	0.44
22:10:43:THR:OG1	22:10:46:LYS:HG2	2.18	0.44
32:1a:692:U:O2'	32:1a:694:A:N7	2.47	0.44
32:1a:974:A:H8	32:1a:974:A:OP1	1.99	0.44
32:1a:1101:A:H4'	32:1a:1102:A:O5'	2.17	0.44
33:1b:163:PHE:HA	33:1b:185:ILE:HG12	2.00	0.44
47:1p:60:LEU:HD12	47:1p:60:LEU:HA	1.69	0.44
50:1s:63:THR:OG1	50:1s:65:ASN:OD1	2.27	0.44
1:2A:141:A:H8	1:2A:1408:C:O2'	2.00	0.44
1:2A:586:A:N1	1:2A:809:G:O2'	2.37	0.44
1:2A:1027:A:C6	1:2A:1126:A:C4	3.05	0.44
1:2A:1607:C:H5"	1:2A:1608:A:H5'	2.00	0.44
1:2A:2121:G:H1	1:2A:2177:C:H42	1.66	0.44
5:2F:33:LEU:HB3	11:2P:6:LEU:HD21	1.99	0.44
25:23:52:HIS:CD2	25:23:53:LEU:HG	2.53	0.44
32:2a:1388:C:H2'	32:2a:1389:C:C6	2.52	0.44
35:2d:193:ASP:OD1	35:2d:193:ASP:N	2.50	0.44
1:1A:862:G:H2'	1:1A:863:A:O4'	2.18	0.44
1:1A:1048:A:N1	1:1A:1112:G:O2'	2.40	0.44
1:1A:2144:U:H3	1:1A:2147:G:H22	1.66	0.44
4:1E:176:ILE:HB	4:1E:181:LEU:HB2	1.99	0.44
32:1a:148:G:H2'	32:1a:149:A:C8	2.53	0.44
32:1a:148:G:H2'	32:1a:149:A:H8	1.83	0.44
32:1a:392:G:H2'	32:1a:393:A:C8	2.52	0.44
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.18	0.44
1:2A:2478:A:OP2	31:29:2:LYS:NZ	2.33	0.44
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.17	0.44
3:2D:159:ALA:HB1	3:2D:198:ASN:O	2.18	0.44
7:2H:46:GLU:HB2	7:2H:49:VAL:HG12	1.99	0.44
12:2Q:12:GLN:HE21	12:2Q:72:LYS:HG3	1.83	0.44
25:23:40:THR:HG22	25:23:42:ALA:H	1.82	0.44
32:2a:108:G:C6	51:2t:15:ARG:HG2	2.52	0.44
32:2a:841:U:H6	32:2a:841:U:P	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:65:LYS:HG3	44:2m:69:GLU:OE1	2.17	0.44
1:1A:558:G:OP1	9:1N:111:PRO:HD2	2.18	0.44
1:1A:637:A:H4'	1:1A:638:G:O5'	2.18	0.44
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.53	0.44
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.18	0.44
7:1H:88:LEU:HD23	7:1H:130:ARG:HG2	1.99	0.44
32:1a:161:A:H2'	32:1a:162:A:C8	2.53	0.44
32:1a:600:C:H2'	32:1a:601:C:C6	2.53	0.44
32:1a:1273:G:H3'	32:1a:1274:G:H8	1.83	0.44
32:1a:1304:G:OP1	52:1u:2:GLY:N	2.51	0.44
35:1d:43:HIS:CE1	35:1d:46:LYS:HZ2	2.36	0.44
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	1.98	0.44
38:1g:78:ARG:HD3	38:1g:79:ARG:H	1.83	0.44
45:1n:14:PRO:HG2	45:1n:16:PHE:O	2.18	0.44
1:2A:747:U:O2	1:2A:2014:A:H1'	2.17	0.44
1:2A:1364:G:C8	23:21:3:LYS:HD2	2.52	0.44
1:2A:2390:U:P	30:28:35:GLN:HE22	2.40	0.44
1:2A:2590:A:O3'	3:2D:239:ARG:NH2	2.51	0.44
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.42	0.44
14:2S:84:GLN:H	14:2S:111:GLU:HB2	1.82	0.44
20:2Y:7:VAL:CG1	20:2Y:27:VAL:HG21	2.48	0.44
26:24:1:MET:HE2	26:24:6:HIS:CD2	2.53	0.44
30:28:23:VAL:HG22	30:28:47:LYS:HB3	1.99	0.44
32:2a:447:G:O6	32:2a:485:G:O2'	2.19	0.44
32:2a:1006:C:C4	32:2a:1007:C:C4	3.06	0.44
32:2a:1027:C:C2	32:2a:1034:G:N2	2.82	0.44
54:2y:61:C:H2'	54:2y:62:C:C6	2.53	0.44
1:1A:242:G:C8	30:18:5:LYS:HG2	2.53	0.44
1:1A:1021:A:H3'	1:1A:1021:A:N3	2.33	0.44
11:1P:45:LEU:HD12	11:1P:45:LEU:HA	1.78	0.44
17:1V:55:ALA:CA	17:1V:101:GLY:HA2	2.40	0.44
32:1a:184:G:H2'	32:1a:185:A:C8	2.52	0.44
32:1a:580:U:H2'	32:1a:581:G:O4'	2.18	0.44
32:1a:955:U:O2'	50:1s:83:HIS:HD2	2.00	0.44
41:1j:49:VAL:HG21	45:1n:41:ARG:O	2.18	0.44
1:2A:322:A:OP1	5:2F:168:ARG:HD2	2.17	0.44
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.61	0.44
21:2Z:138:GLU:H	21:2Z:156:LYS:CE	2.31	0.44
22:20:43:THR:HG23	22:20:43:THR:O	2.18	0.44
32:2a:67:C:H2'	32:2a:68:G:H8	1.82	0.44
32:2a:508:C:OP1	35:2d:209:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:583:A:H2'	32:2a:584:G:O4'	2.18	0.44
32:2a:1125:U:OP1	41:2j:35:SER:OG	2.20	0.44
32:2a:1272:G:H5'	32:2a:1273:G:OP2	2.18	0.44
34:2c:162:GLN:NE2	53:2v:24:A:O2'	2.51	0.44
36:2e:110:LEU:HD21	36:2e:139:LEU:HD21	2.00	0.44
39:2h:6:ILE:O	39:2h:10:LEU:HD13	2.18	0.44
54:2y:51:U:H2'	54:2y:52:G:H8	1.82	0.44
1:1A:271(M):G:O2'	1:1A:271(N):U:H5"	2.18	0.43
1:1A:284:U:H2'	1:1A:285:C:C6	2.53	0.43
1:1A:1007:C:OP1	9:1N:37:LYS:HE2	2.17	0.43
1:1A:1371:G:H2'	1:1A:1372:U:H5	1.83	0.43
1:1A:1740:G:H2'	1:1A:1741:A:C8	2.53	0.43
19:1X:92:LEU:O	19:1X:94:GLY:N	2.50	0.43
21:1Z:1:MET:HA	21:1Z:2:GLU:HA	1.70	0.43
32:1a:130:A:O2'	32:1a:131:C:O5'	2.36	0.43
32:1a:881:G:P	43:1l:12:ARG:HH22	2.41	0.43
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.53	0.43
1:2A:2359:C:H2'	1:2A:2360:A:O4'	2.18	0.43
1:2A:2572:A:C8	4:2E:144:ARG:HD3	2.52	0.43
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.53	0.43
5:2F:165:ARG:HG2	5:2F:168:ARG:HH21	1.82	0.43
38:2g:97:GLN:O	38:2g:101:LEU:HG	2.18	0.43
1:1A:1803:A:H4'	3:1D:259:THR:HG23	2.00	0.43
1:1A:2779:U:H5'	1:1A:2781:A:O4'	2.18	0.43
7:1H:56:SER:OG	7:1H:58:GLU:HG2	2.18	0.43
32:1a:343:U:O2'	32:1a:346:G:O6	2.31	0.43
32:1a:890:G:O2'	32:1a:906:G:O6	2.34	0.43
32:1a:922:G:C6	32:1a:923:A:C6	3.06	0.43
32:1a:1112:C:H1'	34:1c:179:ARG:NH1	2.33	0.43
32:1a:1140:C:H2'	32:1a:1141:C:C6	2.53	0.43
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	2.01	0.43
1:2A:1924:C:H4'	55:2x:13:C:O2'	2.18	0.43
1:2A:2305:A:H2'	1:2A:2306:C:O4'	2.19	0.43
1:2A:2319:G:H22	14:2S:3:ARG:HD2	1.83	0.43
6:2G:25:TYR:CD2	6:2G:31:VAL:HG23	2.53	0.43
6:2G:45:GLU:H	6:2G:45:GLU:HG2	1.40	0.43
37:2f:30:LEU:HD23	37:2f:75:LEU:HD11	1.98	0.43
37:2f:61:LEU:HB3	37:2f:63:TYR:CE2	2.53	0.43
45:2n:15:LYS:HB3	45:2n:15:LYS:HE2	1.82	0.43
54:2w:11:C:N4	54:2w:24:G:H1	2.13	0.43
1:1A:910:A:N1	1:1A:2277:G:H1'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.53	0.43
2:1B:92:C:H5"	21:1Z:79:ARG:NH1	2.33	0.43
5:1F:136:THR:HA	5:1F:166:ALA:O	2.18	0.43
11:1P:63:PRO:HG2	30:18:25:MET:HB2	2.00	0.43
32:1a:299:G:C6	32:1a:300:A:C6	3.07	0.43
35:1d:108:LEU:HD23	35:1d:174:LEU:HD13	2.00	0.43
36:1e:41:VAL:O	36:1e:66:MET:HA	2.18	0.43
48:1q:24:GLU:HA	48:1q:39:SER:HA	2.00	0.43
1:2A:801:G:O6	5:2F:53:THR:OG1	2.35	0.43
1:2A:994:C:O2'	1:2A:996:A:OP1	2.34	0.43
1:2A:1112:G:H2'	1:2A:1113:U:O4'	2.19	0.43
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.33	0.43
1:2A:2166:G:H3'	1:2A:2167:U:H5"	2.00	0.43
10:2O:34:THR:OG1	10:2O:35:VAL:N	2.52	0.43
21:2Z:5:LEU:HD11	21:2Z:44:PHE:HA	1.99	0.43
21:2Z:23:LYS:HB3	21:2Z:38:TYR:CD1	2.53	0.43
32:2a:1072:G:H2'	32:2a:1073:U:C6	2.54	0.43
39:2h:41:ARG:NH2	39:2h:123:GLU:OE2	2.51	0.43
1:1A:918:A:H5"	2:1B:98:G:O2'	2.18	0.43
1:1A:2612:C:OP2	27:15:2:ALA:N	2.51	0.43
1:1A:2615:U:H2'	1:1A:2616:C:C6	2.53	0.43
3:1D:242:ARG:N	3:1D:242:ARG:HD3	2.33	0.43
16:1U:81:HIS:CE1	16:1U:85:LYS:HE2	2.54	0.43
30:18:4:MET:HE3	30:18:63:PRO:HG3	2.01	0.43
32:1a:1002:G:C2	32:1a:1004:A:H1'	2.53	0.43
41:1j:47:PHE:HB2	41:1j:63:PHE:HB2	2.00	0.43
47:1p:67:THR:H	47:1p:70:ALA:HB3	1.84	0.43
54:1y:6:G:O6	54:1y:7:A:N6	2.51	0.43
1:2A:1153:C:H2'	1:2A:1154:G:O4'	2.18	0.43
1:2A:1423:G:OP1	1:2A:1492:G:O2'	2.36	0.43
1:2A:1805:U:O2	3:2D:50:THR:HB	2.18	0.43
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.52	0.43
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.33	0.43
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.54	0.43
2:2B:24:G:H4'	2:2B:25:A:C8	2.53	0.43
4:2E:54:GLN:NE2	4:2E:76:ARG:HG2	2.33	0.43
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.53	0.43
12:2Q:110:THR:HG22	12:2Q:112:GLU:H	1.84	0.43
32:2a:523:A:H61	43:2l:92:0TD:CG	2.30	0.43
32:2a:537:G:H5"	43:2l:113:ARG:NH1	2.33	0.43
32:2a:1002:G:H1	32:2a:1038:C:N4	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1004:A:N3	32:2a:1038:C:C2	2.87	0.43
32:2a:1023:G:H3'	32:2a:1024:G:H8	1.83	0.43
32:2a:1065:U:H5"	32:2a:1190:G:N2	2.33	0.43
32:2a:1198:G:H2'	32:2a:1199:U:C6	2.54	0.43
33:2b:215:LEU:HD23	33:2b:215:LEU:HA	1.81	0.43
34:2c:52:LEU:HD12	34:2c:53:ALA:H	1.83	0.43
40:2i:28:VAL:HA	40:2i:63:ILE:O	2.17	0.43
54:2w:19:G:H1	54:2w:56:C:N4	2.16	0.43
1:1A:1080:C:H5'	1:1A:1081:U:OP2	2.19	0.43
4:1E:120:TRP:CE3	4:1E:155:LYS:HD3	2.53	0.43
12:1Q:12:GLN:NE2	12:1Q:72:LYS:HG3	2.33	0.43
32:1a:22:G:H4'	32:1a:885:G:C8	2.54	0.43
32:1a:562:C:H1'	43:1l:15:ARG:HB3	2.01	0.43
32:1a:737:A:H2'	32:1a:738:C:C6	2.54	0.43
32:1a:875:C:O2'	39:1h:14:ARG:HD2	2.18	0.43
33:1b:158:LEU:HD23	33:1b:158:LEU:HA	1.91	0.43
1:2A:383:U:H2'	1:2A:385:C:H5	1.83	0.43
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.17	0.43
1:2A:2114:A:H1'	1:2A:2168:G:H1'	2.01	0.43
7:2H:33:LEU:HD21	7:2H:136:ILE:HG13	1.99	0.43
32:2a:1321:C:O2'	50:2s:77:THR:HG21	2.18	0.43
32:2a:1356:G:H2'	32:2a:1357:A:C8	2.54	0.43
33:2b:47:THR:O	33:2b:51:LEU:N	2.51	0.43
34:2c:42:LEU:O	34:2c:43:LEU:HD22	2.19	0.43
38:2g:99:LEU:HD22	38:2g:103:TRP:CZ2	2.53	0.43
1:1A:9:U:OP1	9:1N:115:ARG:NH2	2.52	0.43
1:1A:652(E):G:H1	1:1A:652(T):C:H42	1.67	0.43
1:1A:1999:C:H4'	1:1A:2723:C:O2	2.19	0.43
7:1H:127:GLU:OE2	7:1H:130:ARG:NE	2.37	0.43
19:1X:1:MET:HE1	24:12:26:ARG:HH21	1.83	0.43
21:1Z:105:VAL:N	21:1Z:139:VAL:O	2.46	0.43
32:1a:107:G:H2'	32:1a:108:G:O4'	2.19	0.43
1:2A:55:G:O2'	1:2A:127:A:N1	2.48	0.43
1:2A:307:G:H21	1:2A:330:A:N6	2.16	0.43
2:2B:11:C:H3'	2:2B:12:C:H6	1.84	0.43
3:2D:242:ARG:HD3	3:2D:242:ARG:N	2.34	0.43
4:2E:30:PRO:HB3	4:2E:92:THR:HG22	2.00	0.43
5:2F:11:VAL:HG21	5:2F:20:LEU:HD12	2.00	0.43
5:2F:157:VAL:HG11	5:2F:181:LEU:HD13	2.00	0.43
6:2G:43:LEU:C	6:2G:45:GLU:H	2.27	0.43
32:2a:1053:G:H4'	32:2a:1054:C:H3'	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.54	0.43
35:2d:158:ILE:O	35:2d:162:LEU:HD12	2.19	0.43
39:2h:96:GLY:H	39:2h:99:GLU:CD	2.25	0.43
1:1A:947:G:H2'	1:1A:948:G:C8	2.53	0.43
1:1A:1001:A:H2'	1:1A:1002:G:O4'	2.19	0.43
1:1A:2771:C:H2'	1:1A:2772:C:C6	2.54	0.43
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.53	0.43
21:1Z:124:ILE:HG23	21:1Z:126:VAL:HG23	2.00	0.43
35:1d:11:LEU:HD13	35:1d:66:ARG:HG2	2.01	0.43
35:1d:172:PRO:C	35:1d:174:LEU:H	2.27	0.43
39:1h:121:ASP:OD1	39:1h:121:ASP:N	2.50	0.43
40:1i:8:GLY:O	40:1i:15:ALA:N	2.51	0.43
1:2A:108:U:H2'	1:2A:109:G:C8	2.54	0.43
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.54	0.43
1:2A:855:G:H2'	1:2A:856:C:C6	2.54	0.43
1:2A:863:A:H2'	1:2A:864:G:C8	2.54	0.43
1:2A:1824:G:N3	3:2D:254:THR:OG1	2.50	0.43
1:2A:2150:U:C2'	1:2A:2151:G:H5'	2.49	0.43
15:2T:15:VAL:HG13	15:2T:79:HIS:CE1	2.53	0.43
32:2a:1054:C:C5	54:2w:34:G:H1'	2.53	0.43
32:2a:1106:G:H4'	34:2c:171:GLY:O	2.18	0.43
36:2e:60:TYR:O	36:2e:64:ARG:HG3	2.19	0.43
42:2k:81:ASP:OD1	42:2k:106:LYS:HB2	2.19	0.43
1:1A:1448:G:H4'	1:1A:1542:A:OP1	2.18	0.43
1:1A:2128:C:N3	1:1A:2160:G:N2	2.64	0.43
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.52	0.43
1:1A:2203:U:O4'	3:1D:151:LYS:HE2	2.19	0.43
1:1A:2206:G:H5"	1:1A:2207:G:C5	2.53	0.43
9:1N:4:TYR:HB2	16:1U:101:ARG:NH1	2.34	0.43
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.36	0.43
32:1a:262:A:C6	32:1a:263:A:C6	3.06	0.43
44:1m:37:THR:O	44:1m:55:ARG:NH1	2.47	0.43
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.53	0.43
54:1y:66:U:C4	54:1y:67:C:C4	3.07	0.43
1:2A:796:C:H2'	1:2A:797:C:C6	2.53	0.43
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.53	0.43
14:2S:87:PHE:CE1	14:2S:102:ALA:HB2	2.54	0.43
21:2Z:146:ILE:HA	21:2Z:174:VAL:O	2.19	0.43
32:2a:587:G:N2	32:2a:754:C:OP2	2.47	0.43
35:2d:50:ARG:NH1	36:2e:10:MET:HE3	2.34	0.43
42:2k:16:SER:OG	42:2k:106:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:2l:88:GLY:O	43:2l:99:HIS:HD2	2.01	0.43
46:2o:74:ASP:HB3	46:2o:77:ARG:HB2	2.01	0.43
47:2p:41:PRO:O	47:2p:43:LYS:HE2	2.19	0.43
54:2y:59:U:H3'	54:2y:60:U:O2	2.18	0.43
1:1A:271(E):U:H2'	1:1A:271(F):C:C6	2.54	0.43
1:1A:839:U:H2'	1:1A:840:C:C6	2.54	0.43
1:1A:2108:C:H2'	1:1A:2109:U:C6	2.54	0.43
1:1A:2573:C:H3'	61:1A:4188:HOH:O	2.18	0.43
3:1D:37:LEU:HD13	3:1D:87:ASN:ND2	2.33	0.43
32:1a:266:G:H2'	32:1a:266:G:N3	2.34	0.43
32:1a:1292:U:H5'	40:1i:38:GLN:OE1	2.19	0.43
32:1a:1380:U:C4	38:1g:3:ARG:HG2	2.54	0.43
1:2A:287:C:H2'	1:2A:288:C:C6	2.53	0.43
1:2A:492:A:H2'	1:2A:493:G:O4'	2.19	0.43
1:2A:910:A:N1	1:2A:2277:G:H1'	2.34	0.43
1:2A:1038:C:H42	1:2A:1117:G:H1	1.64	0.43
1:2A:1607:C:N4	1:2A:1622:G:OP2	2.47	0.43
1:2A:1823:G:OP1	3:2D:54:ARG:NH1	2.51	0.43
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.19	0.43
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.19	0.43
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.54	0.43
20:2Y:68:HIS:ND1	20:2Y:70:SER:HB3	2.34	0.43
32:2a:89:C:H2'	32:2a:90:U:O4'	2.19	0.43
32:2a:768:A:N3	32:2a:1512:U:O2'	2.48	0.43
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.83	0.43
33:2b:16:HIS:CB	33:2b:204:ASN:HB3	2.39	0.43
40:2i:5:TYR:HD1	40:2i:18:PHE:HE1	1.67	0.43
40:2i:94:ALA:C	40:2i:96:LEU:H	2.27	0.43
40:2i:99:LEU:HB3	40:2i:101:PHE:CE2	2.54	0.43
50:2s:28:LYS:HB3	50:2s:29:ARG:CB	2.49	0.43
53:2v:23:A:H4'	53:2v:24:A:H5'	2.01	0.43
54:2y:8:4SU:H1'	54:2y:48:C:H1'	2.00	0.43
1:1A:185:U:H4'	1:1A:218:A:H4'	2.01	0.43
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.52	0.43
1:1A:1359:A:H2'	1:1A:1360:A:H5'	2.01	0.43
1:1A:2168:G:O6	1:1A:2171:A:H5"	2.19	0.43
1:1A:2544:G:N7	61:1A:4187:HOH:O	2.36	0.43
1:1A:2727:G:O2'	10:1O:70:LYS:NZ	2.51	0.43
1:1A:2820:A:OP2	13:1R:2:ARG:NH2	2.51	0.43
2:1B:75:G:H22	21:1Z:73:GLN:NE2	2.16	0.43
6:1G:28:VAL:O	6:1G:31:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1U:58:ARG:HA	16:1U:61:TRP:CE3	2.54	0.43
32:1a:8:A:C6	35:1d:209:ARG:HB2	2.54	0.43
32:1a:1146:A:H2'	32:1a:1147:C:O4'	2.18	0.43
32:1a:1530:G:H4'	32:1a:1530:G:OP1	2.18	0.43
33:1b:162:ILE:O	33:1b:185:ILE:HG12	2.19	0.43
39:1h:124:ALA:O	39:1h:128:GLY:N	2.51	0.43
1:2A:30:G:H2'	1:2A:31:C:H6	1.83	0.43
1:2A:196:A:N3	1:2A:196:A:H2'	2.34	0.43
1:2A:242:G:C8	30:28:5:LYS:HG2	2.53	0.43
1:2A:323:G:O2'	1:2A:1205:U:N3	2.41	0.43
1:2A:1260:G:C6	1:2A:1261:C:C4	3.07	0.43
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.84	0.43
32:2a:473:G:H2'	32:2a:474:G:H8	1.84	0.43
32:2a:1176:A:H2'	32:2a:1177:G:O4'	2.18	0.43
32:2a:1403:C:C2	32:2a:1404:5MC:HM52	2.54	0.43
33:2b:12:GLU:O	33:2b:15:VAL:HG22	2.19	0.43
33:2b:167:PRO:HD3	33:2b:187:LEU:O	2.19	0.43
50:2s:28:LYS:HA	50:2s:28:LYS:HD3	1.80	0.43
51:2t:60:GLU:HG3	51:2t:81:LYS:HD2	2.01	0.43
1:1A:2097:C:H2'	1:1A:2098:U:O4'	2.19	0.42
3:1D:206:LEU:HD22	3:1D:211:ARG:HG2	2.01	0.42
13:1R:70:LEU:O	13:1R:72:ASP:N	2.51	0.42
32:1a:1346:A:N1	32:1a:1374:A:H5"	2.34	0.42
39:1h:114:THR:HG22	39:1h:130:GLY:O	2.18	0.42
47:1p:20:VAL:HG21	47:1p:32:TYR:CD2	2.53	0.42
51:1t:53:LEU:HA	51:1t:56:MET:HB3	2.01	0.42
1:2A:141:A:C8	1:2A:1408:C:O2'	2.72	0.42
1:2A:1754:C:H5	15:2T:96:ARG:NH2	2.17	0.42
1:2A:1913:A:H4'	1:2A:1914:C:O5'	2.18	0.42
2:2B:74:U:H3'	2:2B:75:G:H5"	2.00	0.42
30:28:63:PRO:HG2	30:28:64:TYR:CD2	2.54	0.42
32:2a:841:U:C4	32:2a:848:C:H1'	2.54	0.42
32:2a:1122:U:C2	32:2a:1123:A:C8	3.06	0.42
32:2a:1241:G:H2'	32:2a:1242:C:C6	2.54	0.42
32:2a:1251:A:H2'	32:2a:1252:A:C8	2.54	0.42
32:2a:1318:A:H1'	50:2s:37:ARG:HE	1.84	0.42
32:2a:1401:G:C2	32:2a:1402:4OC:H1'	2.54	0.42
38:2g:111:ARG:HB3	38:2g:113:GLU:OE1	2.18	0.42
1:1A:897:C:H5'	54:1w:56:C:OP1	2.19	0.42
1:1A:1354:A:H2'	1:1A:1355:G:O4'	2.19	0.42
1:1A:1665:A:H2'	1:1A:1666:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.33	0.42
1:1A:2203:U:H4'	3:1D:151:LYS:HG2	2.01	0.42
7:1H:105:LEU:HD12	7:1H:151:ILE:HD12	2.01	0.42
12:1Q:1:MET:HE3	12:1Q:1:MET:HB2	1.93	0.42
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.34	0.42
31:19:13:LYS:HD3	31:19:28:GLU:OE1	2.19	0.42
32:1a:838:G:H1	32:1a:848:C:H42	1.67	0.42
35:1d:155:LEU:HB3	35:1d:158:ILE:CD1	2.49	0.42
40:1i:20:ARG:O	40:1i:60:ASP:N	2.30	0.42
41:1j:57:LYS:HE2	41:1j:60:ARG:NH2	2.35	0.42
1:2A:883:G:N1	1:2A:894:C:O2	2.53	0.42
1:2A:1003:G:N2	1:2A:1153:C:C2	2.87	0.42
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.55	0.42
5:2F:158:THR:O	5:2F:164:ARG:HD3	2.19	0.42
6:2G:36:LYS:HE2	6:2G:95:ARG:HH12	1.83	0.42
32:2a:1010:G:H2'	32:2a:1011:G:C8	2.54	0.42
32:2a:1013:G:N2	32:2a:1016:A:OP2	2.52	0.42
36:2e:100:VAL:O	36:2e:107:ARG:NH2	2.45	0.42
48:2q:12:SER:HB3	48:2q:20:THR:HB	2.00	0.42
48:2q:27:PHE:CE1	48:2q:36:ILE:HD11	2.55	0.42
1:1A:576:U:H2'	1:1A:577:G:C8	2.54	0.42
1:1A:588:U:H2'	1:1A:589:C:C6	2.54	0.42
1:1A:1094:U:H2'	1:1A:1095:A:C8	2.55	0.42
1:1A:2693:A:H2'	1:1A:2694:G:H8	1.82	0.42
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.19	0.42
22:10:43:THR:O	22:10:43:THR:HG23	2.18	0.42
32:1a:1273:G:C2	32:1a:1274:G:H1'	2.54	0.42
39:1h:95:VAL:HB	39:1h:99:GLU:HB2	2.01	0.42
40:1i:3:GLN:NE2	40:1i:20:ARG:HH21	2.16	0.42
40:1i:28:VAL:HG22	40:1i:63:ILE:HB	2.00	0.42
51:1t:47:GLY:N	51:1t:48:LYS:HB2	2.34	0.42
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.18	0.42
1:2A:1427:A:H4'	1:2A:1428:C:O5'	2.18	0.42
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.54	0.42
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.34	0.42
5:2F:20:LEU:HD23	5:2F:21:ALA:H	1.85	0.42
6:2G:105:LYS:NZ	6:2G:143:GLU:OE2	2.42	0.42
32:2a:1251:A:N1	32:2a:1354:C:O2'	2.38	0.42
35:2d:172:PRO:HB2	35:2d:187:ARG:HH21	1.85	0.42
40:2i:24:GLY:HA2	40:2i:59:PHE:O	2.18	0.42
55:2x:50:U:H2'	55:2x:51:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2y:44:G:C6	54:2y:45:U:C2	3.08	0.42
1:1A:279:C:H42	1:1A:361:G:H1	1.67	0.42
8:1I:72:LEU:HD21	8:1I:107:VAL:HG11	2.01	0.42
8:1I:77:LEU:HD23	8:1I:77:LEU:HA	1.77	0.42
11:1P:126:VAL:HG12	11:1P:148:LEU:HD13	2.01	0.42
12:1Q:111:GLU:O	12:1Q:115:MET:HG2	2.20	0.42
17:1V:24:LYS:HE2	17:1V:24:LYS:HB3	1.81	0.42
26:14:59:PHE:HD2	50:1s:64:GLU:HB3	1.84	0.42
32:1a:828:A:H2'	32:1a:829:G:O4'	2.19	0.42
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.42	0.42
1:2A:2118:U:OP1	1:2A:2148:G:H4'	2.19	0.42
1:2A:2277:G:OP2	22:20:10:THR:HG21	2.20	0.42
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.54	0.42
1:2A:2439:A:H5'	1:2A:2439:A:C8	2.55	0.42
9:2N:24:GLY:O	9:2N:28:THR:HG23	2.18	0.42
20:2Y:83:THR:OG1	20:2Y:84:ARG:N	2.51	0.42
32:2a:814:A:N7	32:2a:816:A:C4	2.88	0.42
32:2a:942:G:C2	32:2a:1342:C:C2	3.08	0.42
44:2m:20:THR:C	44:2m:22:ILE:H	2.27	0.42
1:1A:1119:C:N4	61:1A:4335:HOH:O	2.52	0.42
1:1A:2271:G:OP1	22:10:18:ALA:HB1	2.19	0.42
3:1D:152:GLY:O	3:1D:154:LYS:HD3	2.20	0.42
32:1a:165:C:H2'	32:1a:166:G:C8	2.50	0.42
32:1a:176:C:H2'	32:1a:177:C:C6	2.54	0.42
32:1a:523:A:N1	43:1l:92:0TD:H6	2.35	0.42
32:1a:996:A:N1	32:1a:1045:C:O2'	2.43	0.42
32:1a:1241:G:H2'	32:1a:1242:C:C6	2.55	0.42
33:1b:231:GLU:HB3	33:1b:232:PRO:HD3	2.01	0.42
40:1i:4:TYR:CD1	40:1i:88:TYR:HA	2.54	0.42
40:1i:49:PRO:HD3	40:1i:78:LYS:HG3	2.02	0.42
51:1t:56:MET:HE3	51:1t:85:MET:HG2	2.01	0.42
54:1y:34:G:H3'	54:1y:35:A:H8	1.83	0.42
1:2A:72:U:OP2	24:22:29:LYS:NZ	2.48	0.42
1:2A:1630:G:H2'	1:2A:1631:C:C6	2.54	0.42
1:2A:1851:U:H2'	1:2A:1852:C:O4'	2.20	0.42
2:2B:20:C:H42	2:2B:63:G:H1	1.67	0.42
21:2Z:102:LEU:HD21	21:2Z:124:ILE:HG13	2.00	0.42
21:2Z:121:HIS:N	21:2Z:171:ILE:O	2.53	0.42
25:23:16:PRO:HB2	25:23:18:ASP:OD1	2.20	0.42
32:2a:519:C:H2'	32:2a:520:A:O4'	2.19	0.42
32:2a:857:C:H2'	32:2a:858:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1265:G:C4	32:2a:1271:G:N2	2.88	0.42
1:1A:414:C:H2'	1:1A:415:A:C8	2.54	0.42
1:1A:484:C:H2'	1:1A:485:C:C6	2.55	0.42
1:1A:848:G:H2'	1:1A:849:A:C8	2.54	0.42
1:1A:2029:G:H2'	1:1A:2031:A:OP1	2.19	0.42
15:1T:127:ALA:C	15:1T:129:ARG:N	2.77	0.42
21:1Z:125:LEU:HG	21:1Z:164:ALA:HB3	2.01	0.42
32:1a:540:G:H2'	32:1a:541:G:O4'	2.19	0.42
32:1a:685:G:O2'	32:1a:686:U:H5'	2.20	0.42
32:1a:690:G:C6	32:1a:691:G:C6	3.08	0.42
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	2.02	0.42
33:1b:155:LEU:HD12	33:1b:155:LEU:HA	1.78	0.42
33:1b:178:ARG:NH2	39:1h:74:PRO:HB3	2.35	0.42
54:1w:18:G:H4'	54:1w:60:U:C5	2.54	0.42
54:1w:51:U:H2'	54:1w:52:G:H8	1.85	0.42
1:2A:171:G:H2'	1:2A:172:C:C6	2.54	0.42
1:2A:658:C:H2'	1:2A:659:C:C6	2.54	0.42
1:2A:868:U:C4	1:2A:869:G:N7	2.87	0.42
1:2A:1843:C:H5'	3:2D:253:GLN:OE1	2.20	0.42
1:2A:2136:C:N4	1:2A:2155:G:N1	2.64	0.42
1:2A:2355:C:H4'	22:20:24:LYS:HG3	2.01	0.42
5:2F:102:PRO:HB2	5:2F:105:VAL:HG23	2.00	0.42
11:2P:59:LEU:HD11	30:28:10:ALA:HA	2.02	0.42
15:2T:65:LYS:HE3	15:2T:67:SER:HB2	2.01	0.42
26:24:58:ARG:HB3	50:2s:67:VAL:HG13	2.00	0.42
32:2a:163:C:H2'	32:2a:164:U:O4'	2.20	0.42
32:2a:542:G:P	35:2d:10:ARG:HH22	2.42	0.42
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.54	0.42
32:2a:1135:U:H2'	32:2a:1137:C:N3	2.34	0.42
32:2a:1434:A:H2'	32:2a:1435:G:O4'	2.20	0.42
38:2g:79:ARG:HG3	38:2g:80:VAL:H	1.84	0.42
52:2u:5:ASP:O	52:2u:11:GLY:HA3	2.19	0.42
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.20	0.42
1:1A:2685:G:H5'	10:1O:68:GLU:OE2	2.19	0.42
7:1H:24:VAL:HG22	7:1H:35:VAL:HB	2.02	0.42
24:12:53:LEU:HD23	24:12:53:LEU:HA	1.78	0.42
32:1a:461:A:O2'	32:1a:470:C:H5'	2.19	0.42
32:1a:1151:A:O2'	32:1a:1152:A:H8	2.03	0.42
47:1p:75:ARG:C	47:1p:77:ALA:H	2.28	0.42
49:1r:84:LYS:HE2	49:1r:84:LYS:HB2	1.89	0.42
50:1s:40:ILE:HB	50:1s:67:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:172:C:H2'	1:2A:173:G:H8	1.85	0.42
1:2A:902:C:H2'	1:2A:903:C:C6	2.55	0.42
1:2A:1037:G:H2'	1:2A:1038:C:O4'	2.19	0.42
1:2A:1815:A:OP2	3:2D:54:ARG:NH2	2.52	0.42
1:2A:2134:A:H2	1:2A:2159:G:H1'	1.85	0.42
15:2T:16:ARG:HB3	15:2T:18:ASP:OD1	2.20	0.42
30:28:34:TRP:CG	30:28:35:GLN:N	2.88	0.42
32:2a:302:G:N3	32:2a:556:C:H4'	2.35	0.42
32:2a:384:G:H2'	32:2a:385:C:C6	2.55	0.42
32:2a:983:A:H3'	32:2a:983:A:N3	2.35	0.42
32:2a:1103:C:H2'	32:2a:1104:G:O4'	2.20	0.42
34:2c:121:ALA:HB2	34:2c:198:VAL:HG21	2.01	0.42
39:2h:106:GLY:O	39:2h:122:ARG:NH2	2.52	0.42
44:2m:27:LYS:HE2	44:2m:27:LYS:HB2	1.89	0.42
1:1A:1429:G:H2'	1:1A:1430:C:H6	1.81	0.42
1:1A:1790:C:H5"	1:1A:1791:A:OP1	2.20	0.42
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.54	0.42
11:1P:125:VAL:HG13	11:1P:138:LEU:HD21	2.02	0.42
32:1a:142:G:H2'	32:1a:143:A:H8	1.84	0.42
32:1a:1028:C:H2'	32:1a:1029:C:O4'	2.20	0.42
32:1a:1140:C:H2'	32:1a:1141:C:H6	1.85	0.42
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.55	0.42
35:1d:141:ARG:HG3	35:1d:144:ASP:OD1	2.19	0.42
1:2A:1665:A:H2'	1:2A:1666:G:O4'	2.19	0.42
1:2A:1782:C:H1'	1:2A:2609:U:H5"	2.02	0.42
1:2A:1999:C:H4'	1:2A:2723:C:O2	2.19	0.42
1:2A:2689:U:P	1:2A:2719:G:H22	2.43	0.42
4:2E:56:PRO:C	4:2E:58:ARG:H	2.28	0.42
6:2G:41:GLN:HB3	6:2G:43:LEU:HD22	2.02	0.42
7:2H:98:LEU:HD11	7:2H:124:GLU:HA	2.02	0.42
10:2O:105:GLU:OE1	10:2O:105:GLU:N	2.44	0.42
21:2Z:19:ARG:HG3	21:2Z:25:PRO:HD3	2.01	0.42
21:2Z:102:LEU:HD23	21:2Z:137:ILE:HB	2.02	0.42
32:2a:573:A:N3	32:2a:883:C:O2'	2.50	0.42
33:2b:33:TYR:HB3	33:2b:41:ILE:HD11	2.02	0.42
44:2m:89:GLY:O	44:2m:93:ARG:HG2	2.20	0.42
46:2o:62:GLN:O	46:2o:66:LEU:HG	2.20	0.42
48:2q:45:HIS:NE2	48:2q:47:PRO:HG3	2.35	0.42
1:1A:119:A:H4'	1:1A:120:U:OP1	2.20	0.42
1:1A:444:C:H4'	5:1F:49:ALA:HB2	2.01	0.42
1:1A:1639:U:O2'	1:1A:2699:C:H4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1916:A:H2'	1:1A:1917:PSU:O4'	2.20	0.42
1:1A:2376:A:H2'	1:1A:2377:A:O4'	2.20	0.42
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.20	0.42
27:15:16:ARG:O	27:15:20:ARG:HG3	2.20	0.42
32:1a:294:U:OP1	32:1a:610:G:O2'	2.30	0.42
32:1a:353:A:H5'	32:1a:353:A:H8	1.84	0.42
32:1a:1291:G:O2'	40:1i:38:GLN:OE1	2.31	0.42
32:1a:1325:C:OP1	52:1u:15:ARG:NH1	2.51	0.42
1:2A:93:G:H2'	1:2A:94:C:C6	2.54	0.42
1:2A:191:A:H2'	1:2A:192:C:C6	2.55	0.42
1:2A:521:G:H2'	1:2A:522:G:H8	1.85	0.42
1:2A:645:C:H5"	1:2A:646:A:OP2	2.20	0.42
1:2A:2059:A:O2'	5:2F:69:HIS:HD2	2.03	0.42
1:2A:2564:A:OP1	1:2A:2648:C:H4'	2.19	0.42
1:2A:2749:A:H1'	7:2H:63:SER:HB3	2.02	0.42
2:2B:13:A:O2'	2:2B:14:U:H3'	2.20	0.42
3:2D:25:THR:HG21	3:2D:113:VAL:HG21	2.02	0.42
12:2Q:1:MET:HG2	12:2Q:44:ALA:HB1	2.00	0.42
32:2a:8:A:H5'	36:2e:101:ILE:HG22	2.02	0.42
32:2a:148:G:H2'	32:2a:149:A:H8	1.85	0.42
32:2a:401:C:O2'	32:2a:621:A:N3	2.45	0.42
33:2b:92:TYR:CZ	33:2b:151:GLY:HA3	2.54	0.42
33:2b:207:ALA:O	33:2b:211:ILE:HG13	2.20	0.42
35:2d:76:ARG:NE	35:2d:80:GLU:OE2	2.37	0.42
37:2f:46:ARG:HH22	49:2r:37:VAL:HG11	1.84	0.42
38:2g:92:SER:O	38:2g:96:GLN:HG3	2.20	0.42
41:2j:32:ALA:HA	41:2j:33:GLN:HA	1.88	0.42
50:2s:80:TYR:C	50:2s:82:GLY:H	2.27	0.42
54:2y:2:C:H42	54:2y:71:G:H1	1.67	0.42
1:1A:196:A:H2'	1:1A:196:A:N3	2.35	0.42
1:1A:1477:A:C2	1:1A:1515:G:C2	3.08	0.42
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.84	0.42
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	2.02	0.42
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.34	0.42
5:1F:132:VAL:HA	5:1F:138:GLU:HB3	2.02	0.42
14:1S:105:ALA:HB1	14:1S:110:LEU:HD12	2.02	0.42
21:1Z:31:ARG:NE	21:1Z:94:GLU:OE2	2.53	0.42
32:1a:430:A:OP2	35:1d:8:VAL:HG12	2.20	0.42
32:1a:1095:U:P	32:1a:1108:G:H1	2.43	0.42
42:1k:30:VAL:HG11	42:1k:65:ALA:HA	2.02	0.42
51:1t:100:ILE:HB	51:1t:101:GLY:H	1.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:455:C:N3	1:2A:472:A:H2'	2.35	0.42
1:2A:478:A:N1	1:2A:500:G:H4'	2.35	0.42
1:2A:855:G:C5	1:2A:856:C:C4	3.08	0.42
1:2A:2031:A:N3	1:2A:2455:G:O2'	2.47	0.42
1:2A:2165:G:H2'	1:2A:2166:G:O4'	2.20	0.42
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.20	0.42
7:2H:80:SER:OG	7:2H:81:GLU:N	2.51	0.42
9:2N:71:ILE:HG21	9:2N:84:LYS:HB3	2.01	0.42
32:2a:943:U:H1'	40:2i:124:GLN:HE22	1.85	0.42
32:2a:1068:G:N2	32:2a:1191:A:N3	2.66	0.42
32:2a:1070:U:H2'	32:2a:1071:C:C6	2.55	0.42
34:2c:6:HIS:ND1	45:2n:49:HIS:HB3	2.35	0.42
34:2c:131:ARG:NH2	36:2e:50:GLU:HG3	2.35	0.42
34:2c:184:TYR:HD1	34:2c:201:TYR:CE1	2.38	0.42
1:1A:962:G:C2'	1:1A:963:U:H5'	2.50	0.41
7:1H:101:ARG:NH2	7:1H:122:THR:HA	2.35	0.41
32:1a:250:A:H4'	32:1a:251:G:O5'	2.20	0.41
32:1a:974:A:OP2	45:1n:29:ARG:NH2	2.42	0.41
32:1a:1316:G:N2	32:1a:1318:A:H3'	2.34	0.41
52:1u:5:ASP:O	52:1u:11:GLY:HA3	2.20	0.41
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.20	0.41
1:2A:1359:A:H2'	1:2A:1360:A:H5'	2.02	0.41
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.19	0.41
1:2A:1598:C:H2'	1:2A:1599:C:H6	1.84	0.41
1:2A:1813:G:H1'	3:2D:50:THR:OG1	2.20	0.41
1:2A:2191:G:H2'	1:2A:2192:G:O4'	2.20	0.41
1:2A:2238:G:H2'	1:2A:2238:G:N3	2.35	0.41
1:2A:2556:C:H2'	1:2A:2557:G:O4'	2.20	0.41
1:2A:2690:C:OP1	13:2R:17:ARG:NH2	2.52	0.41
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.30	0.41
9:2N:15:LEU:HD23	9:2N:137:LYS:HG3	2.02	0.41
21:2Z:54:HIS:HE2	21:2Z:123:ASP:HB3	1.85	0.41
32:2a:1278:U:H5'	32:2a:1279:A:C5'	2.44	0.41
32:2a:1329:A:H5'	44:2m:29:ARG:NE	2.35	0.41
34:2c:101:LEU:HD22	34:2c:102:ASN:H	1.84	0.41
40:2i:16:ARG:HB2	40:2i:64:THR:CG2	2.45	0.41
41:2j:47:PHE:HB2	41:2j:63:PHE:HB2	2.02	0.41
42:2k:41:THR:HG21	42:2k:71:LYS:HB2	2.01	0.41
50:2s:28:LYS:HB3	50:2s:29:ARG:CA	2.50	0.41
54:2y:11:C:N4	54:2y:24:G:H1	2.15	0.41
1:1A:1035:U:H2'	1:1A:1036:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1173:G:N1	1:1A:1176:G:OP2	2.49	0.41
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.20	0.41
1:1A:1750:G:O2'	1:1A:2860:A:N1	2.50	0.41
1:1A:2168:G:N1	1:1A:2171:A:C8	2.88	0.41
9:1N:120:LEU:HG	9:1N:122:VAL:HG23	2.02	0.41
11:1P:39:LYS:HG3	11:1P:45:LEU:HD22	2.01	0.41
16:1U:104:GLN:NE2	16:1U:105:VAL:HG23	2.35	0.41
32:1a:160:A:H2'	32:1a:161:A:O4'	2.20	0.41
32:1a:256:U:H2'	32:1a:257:G:O4'	2.21	0.41
32:1a:679:C:H2'	32:1a:680:C:C6	2.55	0.41
32:1a:691:G:H2'	32:1a:692:U:C6	2.55	0.41
32:1a:975:A:O2'	45:1n:32:SER:OG	2.26	0.41
32:1a:1054:C:C5	54:1w:34:G:H1'	2.55	0.41
36:1e:78:HIS:CE1	36:1e:143:ARG:H	2.38	0.41
1:2A:271(S):G:C6	1:2A:271(T):C:C4	3.08	0.41
1:2A:852:G:H2'	1:2A:853:G:C8	2.50	0.41
1:2A:1669:A:H5"	1:2A:2550:G:OP1	2.20	0.41
1:2A:2156:G:H2'	1:2A:2157:G:C5	2.55	0.41
1:2A:2203:U:H2'	1:2A:2205:C:C6	2.55	0.41
6:2G:67:LYS:HD3	26:24:5:ILE:HD12	2.02	0.41
21:2Z:7:ALA:HB3	21:2Z:61:LEU:HD12	2.02	0.41
21:2Z:99:TYR:CE1	21:2Z:125:LEU:HB2	2.55	0.41
32:2a:131:C:H2'	32:2a:132:C:C6	2.55	0.41
32:2a:137:C:H2'	32:2a:138:G:H8	1.84	0.41
32:2a:458:C:H2'	32:2a:460:G:O4'	2.20	0.41
32:2a:921:U:O2	36:2e:19:MET:HB2	2.19	0.41
32:2a:1280:A:O2'	32:2a:1281:U:H5'	2.20	0.41
41:2j:5:ARG:O	41:2j:98:ILE:HA	2.20	0.41
42:2k:45:GLY:O	42:2k:50:TYR:HB2	2.21	0.41
47:2p:43:LYS:HG2	47:2p:48:TRP:CD1	2.55	0.41
55:2x:58:A:H4'	55:2x:59:A:OP1	2.20	0.41
1:1A:740:U:OP2	61:1A:4132:HOH:O	2.22	0.41
1:1A:900:A:H2'	1:1A:901:A:O4'	2.20	0.41
1:1A:904:C:O2'	21:1Z:169:GLU:OE2	2.26	0.41
1:1A:1588:C:H2'	1:1A:1589:C:C6	2.56	0.41
1:1A:2483:C:N3	12:1Q:124:LYS:NZ	2.64	0.41
7:1H:55:PRO:HG2	7:1H:61:HIS:CE1	2.55	0.41
32:1a:200:G:H1	32:1a:217:C:N4	2.16	0.41
32:1a:1027:C:C4	32:1a:1034:G:N1	2.89	0.41
32:1a:1456:G:N1	51:1t:51:GLU:OE2	2.52	0.41
33:1b:108:ILE:O	33:1b:111:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:22:LYS:HB2	35:1d:26:CYS:SG	2.61	0.41
39:1h:49:GLU:HG2	39:1h:62:TYR:HE2	1.85	0.41
44:1m:89:GLY:O	44:1m:93:ARG:HG3	2.20	0.41
1:2A:68:G:H2'	1:2A:69:C:O4'	2.19	0.41
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.86	0.41
1:2A:1999:C:H5"	1:2A:2723:C:O2'	2.20	0.41
1:2A:2723:C:OP2	4:2E:109:LYS:NZ	2.53	0.41
2:2B:7:G:H2'	2:2B:8:U:O4'	2.20	0.41
5:2F:161:GLU:O	5:2F:165:ARG:HG3	2.20	0.41
9:2N:1:MET:HE1	16:2U:94:ASN:ND2	2.35	0.41
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.53	0.41
21:2Z:45:ASP:CG	21:2Z:49:ARG:HE	2.28	0.41
32:2a:751:U:H4'	46:2o:24:SER:HA	2.03	0.41
32:2a:1003:G:N2	32:2a:1025:U:O4	2.53	0.41
32:2a:1225:A:OP1	44:2m:103:THR:OG1	2.33	0.41
32:2a:1264:C:N4	32:2a:1265:G:O6	2.53	0.41
32:2a:1366:C:H2'	32:2a:1367:C:C6	2.55	0.41
37:2f:61:LEU:HB3	37:2f:63:TYR:HE2	1.85	0.41
37:2f:86:ARG:O	37:2f:87:ARG:HG2	2.19	0.41
37:2f:100:ASN:HD21	49:2r:23:LYS:HE3	1.85	0.41
45:2n:9:LYS:HG3	45:2n:12:ARG:NH1	2.36	0.41
45:2n:53:LEU:HD23	45:2n:53:LEU:HA	1.77	0.41
1:1A:114:U:O2'	19:1X:33:LYS:NZ	2.53	0.41
1:1A:286:C:H2'	1:1A:287:C:C6	2.56	0.41
1:1A:647:G:H2'	1:1A:648:G:O4'	2.20	0.41
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.56	0.41
1:1A:1889:A:H2'	1:1A:1890:A:C8	2.55	0.41
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.56	0.41
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.55	0.41
26:14:16:CYS:HB3	26:14:20:ASN:HB3	2.02	0.41
32:1a:1272:G:H2'	32:1a:1273:G:O4'	2.21	0.41
38:1g:8:GLU:OE2	38:1g:8:GLU:N	2.46	0.41
44:1m:3:ARG:HG3	44:1m:4:ILE:N	2.36	0.41
48:1q:78:GLU:HG2	48:1q:79:SER:H	1.85	0.41
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.55	0.41
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.55	0.41
4:2E:96:PHE:O	4:2E:175:VAL:HG21	2.20	0.41
10:2O:7:TYR:HE2	10:2O:20:MET:HE3	1.85	0.41
23:21:67:ILE:N	23:21:68:PRO:HD2	2.36	0.41
32:2a:1242:C:H42	32:2a:1295:G:H1	1.67	0.41
32:2a:1310:G:H5'	44:2m:77:ASN:ND2	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1511:G:H2'	32:2a:1512:U:O4'	2.20	0.41
33:2b:88:ALA:HB2	33:2b:219:VAL:CG2	2.51	0.41
34:2c:6:HIS:CG	45:2n:49:HIS:HB3	2.55	0.41
42:2k:48:ILE:HD11	42:2k:64:ALA:HA	2.03	0.41
1:1A:744:G:OP1	4:1E:132:HIS:ND1	2.52	0.41
1:1A:760:G:H2'	1:1A:761:A:O4'	2.20	0.41
1:1A:2181:G:HO2'	1:1A:2182:G:P	2.43	0.41
1:1A:2183:C:HO2'	1:1A:2184:G:P	2.43	0.41
3:1D:246:PRO:O	3:1D:254:THR:HG22	2.20	0.41
5:1F:111:ALA:HB2	5:1F:206:ILE:HG21	2.02	0.41
10:1O:120:GLU:HG2	10:1O:122:LEU:HG	2.03	0.41
16:1U:47:TYR:HA	16:1U:50:ARG:NH2	2.35	0.41
21:1Z:52:SER:O	21:1Z:52:SER:OG	2.36	0.41
27:15:40:LYS:NZ	27:15:44:THR:O	2.50	0.41
32:1a:399:G:H2'	32:1a:400:C:C6	2.55	0.41
32:1a:438:G:H4'	35:1d:123:HIS:ND1	2.35	0.41
32:1a:756:C:H2'	32:1a:757:U:O4'	2.21	0.41
32:1a:909:A:H2'	32:1a:910:C:O4'	2.19	0.41
32:1a:1458:G:OP1	51:1t:35:THR:OG1	2.35	0.41
33:1b:24:TRP:CZ3	33:1b:26:PRO:HA	2.56	0.41
35:1d:158:ILE:O	35:1d:162:LEU:N	2.40	0.41
50:1s:52:TYR:HA	50:1s:56:GLN:O	2.20	0.41
54:1w:8:4SU:O5'	54:1w:8:4SU:H6	2.20	0.41
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.54	0.41
1:2A:811:U:H2'	11:2P:21:ARG:HA	2.03	0.41
1:2A:1198:U:H2'	1:2A:1199:U:C6	2.56	0.41
1:2A:1364:G:N7	23:21:3:LYS:HD2	2.36	0.41
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.55	0.41
1:2A:2396:G:OP1	23:21:25:LYS:NZ	2.41	0.41
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.55	0.41
9:2N:102:ALA:O	9:2N:106:MET:HG3	2.21	0.41
32:2a:372:C:O2	61:2a:1915:HOH:O	2.21	0.41
32:2a:991:U:C5	32:2a:1212:U:H1'	2.55	0.41
32:2a:1003:G:C6	32:2a:1004:A:C6	3.08	0.41
32:2a:1051:C:H2'	32:2a:1052:U:H6	1.84	0.41
39:2h:4:ASP:HB3	39:2h:7:ALA:HB3	2.01	0.41
1:1A:817:C:H4'	1:1A:932:G:C5	2.55	0.41
1:1A:1174:A:H1'	1:1A:1175:U:O5'	2.21	0.41
1:1A:1289:C:H2'	1:1A:1290:C:C6	2.56	0.41
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.21	0.41
4:1E:28:ALA:HB3	4:1E:93:VAL:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:53:LEU:HD11	6:1G:87:PRO:HB2	2.03	0.41
7:1H:3:ARG:HG3	7:1H:4:ILE:N	2.35	0.41
11:1P:121:LYS:O	11:1P:123:LEU:N	2.54	0.41
26:14:63:TYR:N	26:14:64:GLY:HA2	2.34	0.41
32:1a:176:C:H2'	32:1a:177:C:H6	1.85	0.41
32:1a:620:C:H2'	32:1a:621:A:O4'	2.20	0.41
32:1a:1466:C:H2'	32:1a:1467:G:O4'	2.21	0.41
42:1k:33:THR:HA	42:1k:39:PRO:HA	2.02	0.41
47:1p:50:LYS:HA	47:1p:50:LYS:HD2	1.79	0.41
51:1t:74:LYS:H	51:1t:74:LYS:HE2	1.86	0.41
1:2A:438:G:H2'	1:2A:440:G:C8	2.56	0.41
1:2A:2498:C:OP2	61:2A:3818:HOH:O	2.21	0.41
1:2A:2819:G:H2'	1:2A:2821:A:N7	2.35	0.41
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.53	0.41
28:26:40:CYS:O	28:26:44:ARG:N	2.50	0.41
32:2a:7:G:O2'	36:2e:120:THR:O	2.39	0.41
32:2a:203:U:H2'	32:2a:203:U:OP2	2.19	0.41
32:2a:1097:C:H1'	32:2a:1170:A:H1'	2.03	0.41
36:2e:31:LEU:HD23	36:2e:31:LEU:HA	1.85	0.41
40:2i:99:LEU:HB3	40:2i:101:PHE:HE2	1.84	0.41
1:1A:784:A:C8	1:1A:792:G:C5	3.08	0.41
1:1A:1039:G:H1	1:1A:1116:C:H42	1.68	0.41
1:1A:1063:G:H2'	1:1A:1064:C:C5	2.55	0.41
1:1A:1394:U:H2'	1:1A:1395:A:O4'	2.21	0.41
1:1A:2151:G:C6	1:1A:2152:G:C6	3.09	0.41
3:1D:83:GLU:OE1	3:1D:104:TYR:OH	2.33	0.41
6:1G:7:LEU:HD23	6:1G:7:LEU:HA	1.93	0.41
32:1a:66:G:O4'	32:1a:173:U:C4	2.74	0.41
32:1a:431:A:H2'	32:1a:432:A:O4'	2.20	0.41
32:1a:1286:A:H2'	32:1a:1287:A:H4'	2.01	0.41
34:1c:66:VAL:HG11	34:1c:91:LEU:HD21	2.02	0.41
40:1i:108:VAL:HG12	40:1i:109:VAL:H	1.86	0.41
41:1j:13:HIS:HB3	41:1j:68:HIS:CE1	2.55	0.41
1:2A:652(T):C:H2'	1:2A:652(U):G:C8	2.55	0.41
1:2A:881:G:H3'	1:2A:882:G:C8	2.56	0.41
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.49	0.41
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.21	0.41
21:2Z:151:HIS:HD2	21:2Z:168:GLU:C	2.29	0.41
32:2a:19:C:H5"	36:2e:86:ALA:HB1	2.03	0.41
32:2a:1237:C:HO2'	32:2a:1300:G:H1	1.66	0.41
32:2a:1320:C:N3	50:2s:36:ARG:NH2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1379:G:O6	38:2g:2:ALA:HB3	2.21	0.41
32:2a:1438:G:H2'	32:2a:1439:C:C6	2.55	0.41
36:2e:41:VAL:O	36:2e:66:MET:HA	2.20	0.41
36:2e:84:PHE:O	36:2e:86:ALA:N	2.50	0.41
1:1A:764:A:O4'	3:1D:213:ARG:HG3	2.21	0.41
1:1A:922:U:H2'	1:1A:923:C:C6	2.56	0.41
1:1A:1427:A:H4'	1:1A:1428:C:O4'	2.21	0.41
1:1A:2160:G:C6	1:1A:2161:C:N4	2.89	0.41
1:1A:2690:C:N4	1:1A:2713:A:H1'	2.35	0.41
2:1B:33:G:H5'	6:1G:2:PRO:HD3	2.02	0.41
5:1F:72:ARG:HE	5:1F:72:ARG:HB3	1.69	0.41
9:1N:61:ARG:HD3	9:1N:61:ARG:HA	1.96	0.41
21:1Z:153:SER:HA	21:1Z:167:PRO:HB3	2.02	0.41
24:12:3:LEU:HD23	24:12:3:LEU:HA	1.84	0.41
32:1a:837:G:H1	32:1a:849:C:H42	1.69	0.41
32:1a:933:G:OP2	38:1g:3:ARG:HB2	2.20	0.41
32:1a:1026:G:N7	32:1a:1035:A:H2	2.18	0.41
32:1a:1216:G:H5"	45:1n:5:ALA:HB2	2.02	0.41
32:1a:1429:C:H2'	32:1a:1430:C:C6	2.55	0.41
33:1b:125:PRO:O	33:1b:127:ILE:N	2.54	0.41
1:2A:340:A:H2'	1:2A:341:G:O4'	2.19	0.41
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.55	0.41
1:2A:2131:G:N7	1:2A:2133:G:C2	2.89	0.41
1:2A:2137:C:N4	1:2A:2154:G:H1	2.18	0.41
1:2A:2864:G:OP1	15:2T:119:LYS:HE3	2.21	0.41
4:2E:120:TRP:CE3	4:2E:155:LYS:HD3	2.55	0.41
6:2G:7:LEU:HD13	6:2G:104:GLU:HA	2.02	0.41
6:2G:33:ARG:O	6:2G:161:THR:HG23	2.21	0.41
6:2G:38:VAL:HG12	6:2G:93:THR:HA	2.02	0.41
28:26:11:LEU:HD23	28:26:11:LEU:HA	1.88	0.41
32:2a:376:G:H5"	47:2p:5:ARG:HD2	2.03	0.41
32:2a:620:C:H2'	32:2a:621:A:O4'	2.21	0.41
32:2a:836:G:C6	32:2a:851:G:C6	3.09	0.41
32:2a:1182:G:H4'	32:2a:1183:A:H5"	2.02	0.41
32:2a:1279:A:H5"	41:2j:7:LYS:HZ3	1.86	0.41
36:2e:100:VAL:HB	36:2e:107:ARG:NH1	2.35	0.41
1:1A:226:G:H21	1:1A:228:A:H62	1.67	0.41
1:1A:362:U:H6	1:1A:362:U:H2'	1.71	0.41
1:1A:784:A:C5	3:1D:229:VAL:HG21	2.56	0.41
1:1A:819:A:C4	1:1A:1189:A:C2	3.08	0.41
1:1A:947:G:H2'	1:1A:948:G:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1108:U:H2'	1:1A:1109:C:O4'	2.21	0.41
1:1A:1113:U:H2'	1:1A:1114:G:H8	1.86	0.41
1:1A:1495:A:C6	1:1A:1496:A:C6	3.09	0.41
1:1A:1799:G:O2'	3:1D:181:GLU:OE2	2.32	0.41
1:1A:2080:G:OP1	23:11:35:THR:HG21	2.21	0.41
1:1A:2104:G:H2'	1:1A:2105:C:C6	2.56	0.41
1:1A:2273:A:H2'	1:1A:2274:A:C8	2.56	0.41
1:1A:2790:A:H3'	1:1A:2790:A:N3	2.35	0.41
4:1E:64:LYS:HE3	4:1E:64:LYS:HB2	1.97	0.41
6:1G:148:MET:H	6:1G:148:MET:HG3	1.60	0.41
8:1I:114:LEU:HD13	8:1I:130:TYR:HD1	1.86	0.41
11:1P:63:PRO:HD3	30:18:27:THR:HG22	2.01	0.41
21:1Z:70:LEU:HD11	21:1Z:98:MET:HE3	2.03	0.41
28:16:12:GLU:OE1	28:16:52:VAL:HG11	2.20	0.41
32:1a:627:G:O2'	32:1a:628:G:H5'	2.21	0.41
32:1a:662:G:H2'	32:1a:663:A:C8	2.56	0.41
32:1a:1402:4OC:O5'	32:1a:1402:4OC:H6	2.21	0.41
32:1a:1456:G:O6	51:1t:54:LYS:NZ	2.39	0.41
35:1d:7:PRO:HB2	35:1d:10:ARG:HG2	2.03	0.41
36:1e:90:VAL:O	36:1e:120:THR:HA	2.20	0.41
54:1w:71:G:H2'	54:1w:71:G:N3	2.36	0.41
54:1y:13:C:H2'	54:1y:14:A:H5"	2.02	0.41
1:2A:483:A:O2'	20:2Y:49:VAL:O	2.28	0.41
1:2A:900:A:H3'	1:2A:901:A:H8	1.86	0.41
1:2A:1013:C:H2'	1:2A:1014:U:H6	1.86	0.41
1:2A:1473:G:C6	1:2A:1474:C:C4	3.09	0.41
1:2A:1771:C:OP1	61:2A:3840:HOH:O	2.22	0.41
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.56	0.41
1:2A:2330:G:O2'	22:20:41:ARG:O	2.35	0.41
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.85	0.41
1:2A:2512:C:H2'	1:2A:2513:G:O4'	2.19	0.41
5:2F:108:LYS:HB2	5:2F:108:LYS:HE2	1.88	0.41
19:2X:88:LYS:NZ	19:2X:90:GLU:OE1	2.30	0.41
32:2a:4:U:O4	39:2h:105:ARG:HD3	2.21	0.41
32:2a:1134:G:H1	32:2a:1140:C:N4	2.17	0.41
32:2a:1225:A:H2'	32:2a:1226:C:C5	2.56	0.41
32:2a:1316:G:N2	32:2a:1318:A:H3'	2.34	0.41
33:2b:54:THR:HG23	33:2b:199:TYR:HB3	2.03	0.41
34:2c:195:VAL:O	34:2c:196:LEU:HD23	2.20	0.41
35:2d:60:GLU:HG3	35:2d:202:LEU:HD12	2.02	0.41
38:2g:69:VAL:HG11	38:2g:134:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:44:VAL:HG11	41:2j:46:ARG:HE	1.86	0.41
42:2k:34:ASP:OD2	42:2k:38:ASN:HB2	2.21	0.41
52:2u:6:ARG:C	52:2u:8:THR:H	2.28	0.41
1:1A:534:U:H2'	1:1A:535:C:C6	2.56	0.41
1:1A:1028:A:H61	1:1A:1125:G:H2'	1.85	0.41
8:1I:117:GLU:H	8:1I:117:GLU:HG2	1.68	0.41
28:16:35:GLU:OE1	28:16:50:ARG:NH2	2.54	0.41
32:1a:243:A:C2	32:1a:246:A:C8	3.09	0.41
32:1a:724:G:C2	32:1a:725:G:C8	3.10	0.41
32:1a:814:A:H2'	32:1a:816:A:H5"	2.03	0.41
32:1a:1152:A:OP1	41:1j:68:HIS:ND1	2.54	0.41
34:1c:73:PRO:O	34:1c:77:ILE:HG12	2.21	0.41
1:2A:271(M):G:H4'	1:2A:271(N):U:OP1	2.21	0.41
1:2A:705:A:C2	1:2A:727:A:H1'	2.56	0.41
1:2A:748:G:C8	18:2W:89:ALA:HB1	2.55	0.41
1:2A:776:G:H4'	1:2A:777:A:O5'	2.21	0.41
1:2A:1300:U:H4'	1:2A:1301:A:H5'	2.03	0.41
1:2A:2334:G:O6	22:20:74:ARG:NH1	2.26	0.41
1:2A:2540:C:H2'	1:2A:2541:A:O4'	2.21	0.41
1:2A:2785:C:O2'	4:2E:66:HIS:ND1	2.51	0.41
2:2B:33:G:C6	2:2B:34:U:C4	3.09	0.41
5:2F:33:LEU:HD22	5:2F:112:MET:HE3	2.03	0.41
7:2H:154:PRO:HB3	7:2H:163:TYR:CZ	2.56	0.41
11:2P:6:LEU:HD23	11:2P:6:LEU:HA	1.95	0.41
12:2Q:75:THR:HG21	12:2Q:87:LYS:NZ	2.36	0.41
14:2S:4:LEU:HD23	14:2S:4:LEU:HA	1.91	0.41
14:2S:77:ALA:HB1	14:2S:82:ILE:HB	2.02	0.41
20:2Y:7:VAL:HG21	20:2Y:72:VAL:HG12	2.03	0.41
32:2a:70:G:H2'	32:2a:71:C:C6	2.57	0.41
32:2a:444:C:H2'	32:2a:445:G:H8	1.86	0.41
32:2a:671:G:H5'	37:2f:77:ARG:HH22	1.86	0.41
32:2a:1265:G:C2	32:2a:1271:G:C2	3.09	0.41
34:2c:182:ILE:HG22	34:2c:203:PHE:HA	2.02	0.41
39:2h:51:VAL:HG21	39:2h:60:ARG:HB2	2.03	0.41
42:2k:38:ASN:HA	42:2k:39:PRO:HD3	1.98	0.41
47:2p:72:ARG:HG2	47:2p:73:LEU:HD23	2.02	0.41
1:1A:583:G:OP2	16:1U:10:ARG:HD2	2.20	0.40
1:1A:1430:C:H2'	1:1A:1431:U:H6	1.86	0.40
5:1F:28:ILE:HD13	5:1F:116:ASP:HB2	2.03	0.40
6:1G:60:LEU:HD12	6:1G:60:LEU:HA	1.95	0.40
6:1G:124:SER:HB2	6:1G:131:TYR:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:97:ARG:NE	7:1H:104:GLU:OE1	2.38	0.40
8:1I:109:ILE:HG23	8:1I:130:TYR:CE1	2.56	0.40
23:11:44:PRO:HB2	23:11:46:LEU:HD13	2.03	0.40
30:18:52:LYS:N	30:18:53:PRO:HD2	2.37	0.40
32:1a:942:G:C2	32:1a:1342:C:C2	3.09	0.40
35:1d:60:GLU:HG3	35:1d:202:LEU:HD12	2.02	0.40
54:1w:5:G:H1	54:1w:68:C:H42	1.68	0.40
1:2A:323:G:H1'	1:2A:1205:U:O2	2.20	0.40
1:2A:764:A:O4'	3:2D:213:ARG:HG3	2.21	0.40
1:2A:956:G:H2'	1:2A:957:A:H2'	2.03	0.40
1:2A:2104:G:C2	1:2A:2186:G:C2	3.09	0.40
1:2A:2335:A:C8	1:2A:2337:G:C5	3.09	0.40
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.52	0.40
11:2P:57:THR:O	11:2P:61:ARG:HG3	2.21	0.40
13:2R:1:MET:HE3	13:2R:1:MET:HB2	1.97	0.40
13:2R:9:LYS:O	13:2R:17:ARG:HD3	2.21	0.40
14:2S:3:ARG:NH1	14:2S:4:LEU:H	2.19	0.40
18:2W:11:ARG:NH1	18:2W:99:ARG:O	2.50	0.40
19:2X:44:GLU:HG2	19:2X:49:VAL:O	2.22	0.40
26:24:10:VAL:HG22	26:24:11:PRO:HD2	2.03	0.40
32:2a:8:A:N6	35:2d:205:GLU:O	2.50	0.40
32:2a:1206:G:C6	32:2a:1207:2MG:C5	3.09	0.40
32:2a:1273:G:C6	32:2a:1274:G:C4	3.09	0.40
34:2c:7:PRO:HG2	34:2c:184:TYR:HB2	2.03	0.40
36:2e:136:MET:HE3	36:2e:139:LEU:HD12	2.02	0.40
38:2g:113:GLU:HG3	38:2g:118:VAL:HG23	2.02	0.40
41:2j:51:ARG:O	45:2n:45:ARG:NH1	2.54	0.40
54:2y:58:A:H4'	54:2y:59:U:OP1	2.21	0.40
1:1A:27:G:C2	1:1A:512:G:N3	2.89	0.40
1:1A:64:A:O3'	19:1X:71:GLY:HA3	2.22	0.40
1:1A:548:A:H1'	1:1A:549:G:OP1	2.20	0.40
1:1A:700:G:H2'	1:1A:701:G:O4'	2.21	0.40
1:1A:1769:G:O2'	1:1A:1958:C:OP1	2.34	0.40
1:1A:2130:U:H6	1:1A:2130:U:O5'	2.04	0.40
6:1G:108:ASN:HB3	26:14:22:ILE:HD13	2.03	0.40
13:1R:70:LEU:C	13:1R:72:ASP:H	2.29	0.40
32:1a:4:U:O4	39:1h:105:ARG:HD3	2.22	0.40
32:1a:189:G:C6	32:1a:189(L):G:N1	2.89	0.40
32:1a:277:C:P	48:1q:68:ARG:HH12	2.44	0.40
32:1a:715:A:H2'	32:1a:716:A:C8	2.56	0.40
32:1a:800:G:O6	61:1a:1912:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1126:U:O2	32:1a:1280:A:H2'	2.22	0.40
33:1b:28:PHE:O	33:1b:32:ILE:HG13	2.21	0.40
35:1d:184:LYS:HE2	35:1d:184:LYS:HB3	1.88	0.40
39:1h:51:VAL:HG21	39:1h:60:ARG:HH11	1.86	0.40
39:1h:110:ALA:HB3	39:1h:121:ASP:HB3	2.03	0.40
50:1s:22:LEU:HD12	50:1s:31:ILE:HD11	2.02	0.40
1:2A:1161:C:H2'	1:2A:1162:G:C8	2.57	0.40
1:2A:1759:A:H1'	1:2A:2711:A:C2	2.56	0.40
1:2A:2134:A:C2	1:2A:2159:G:H1'	2.56	0.40
1:2A:2232:U:P	23:21:40:ARG:HH12	2.44	0.40
2:2B:29:A:H2'	2:2B:30:C:C6	2.57	0.40
10:2O:4:PRO:O	10:2O:5:GLN:HB2	2.21	0.40
32:2a:555:C:H2'	32:2a:556:C:C6	2.56	0.40
32:2a:1006:C:N3	32:2a:1023:G:N2	2.63	0.40
32:2a:1032:G:H2'	32:2a:1033:G:C8	2.56	0.40
32:2a:1201:A:H4'	32:2a:1202:G:O5'	2.21	0.40
38:2g:71:PRO:HG3	38:2g:103:TRP:CH2	2.56	0.40
41:2j:33:GLN:HG2	41:2j:34:VAL:H	1.86	0.40
41:2j:50:ILE:HD11	41:2j:57:LYS:HD2	2.02	0.40
54:2y:62:C:H2'	54:2y:63:G:H8	1.86	0.40
1:1A:278:A:O2'	1:1A:279:C:OP1	2.33	0.40
1:1A:1156:A:OP1	16:1U:55:ARG:NH1	2.54	0.40
1:1A:1568:G:H5'	3:1D:60:ARG:HA	2.03	0.40
1:1A:1800:C:OP1	3:1D:260:ARG:NH2	2.54	0.40
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.62	0.40
14:1S:48:LEU:HD12	14:1S:48:LEU:HA	1.92	0.40
14:1S:65:VAL:O	14:1S:69:VAL:HG12	2.21	0.40
16:1U:29:SER:O	16:1U:30:LYS:HD3	2.22	0.40
32:1a:555:C:H2'	32:1a:556:C:C6	2.56	0.40
32:1a:938:A:C6	32:1a:939:G:C5	3.10	0.40
32:1a:1529:G:H4'	32:1a:1530:G:OP2	2.21	0.40
34:1c:120:VAL:O	34:1c:124:ILE:HG13	2.22	0.40
35:1d:103:ASN:O	35:1d:107:ARG:HG2	2.21	0.40
36:1e:66:MET:HE3	36:1e:66:MET:HB3	1.96	0.40
38:1g:78:ARG:HE	38:1g:79:ARG:HG2	1.87	0.40
40:1i:24:GLY:HA2	40:1i:59:PHE:O	2.20	0.40
1:2A:42:G:H2'	1:2A:43:A:O4'	2.22	0.40
1:2A:468:G:H5"	5:2F:60:SER:HB2	2.02	0.40
1:2A:495:G:N3	18:2W:61:ASN:ND2	2.63	0.40
1:2A:571:A:N6	1:2A:2499:C:O3'	2.54	0.40
1:2A:1160:G:C6	1:2A:1161:C:C4	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1321:A:H2'	1:2A:1322:A:O4'	2.21	0.40
1:2A:2145:C:O2'	1:2A:2147:G:N7	2.52	0.40
1:2A:2198:A:OP1	8:2I:33:ARG:NH2	2.54	0.40
6:2G:36:LYS:HG2	6:2G:160:VAL:HB	2.04	0.40
11:2P:102:ARG:C	11:2P:104:GLY:H	2.29	0.40
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	2.02	0.40
32:2a:1401:G:H2'	32:2a:1402:4OC:O4'	2.22	0.40
32:2a:1427:U:H2'	32:2a:1428:A:H8	1.87	0.40
35:2d:173:TRP:CE2	35:2d:189:PRO:HB3	2.57	0.40
38:2g:68:ASN:HD22	38:2g:128:ALA:HA	1.86	0.40
49:2r:43:PHE:C	49:2r:51:LEU:HD12	2.46	0.40
1:1A:1023:U:OP2	61:1A:4131:HOH:O	2.21	0.40
1:1A:1062:G:C8	1:1A:1088:A:H2'	2.57	0.40
1:1A:2171:A:O2'	1:1A:2172:U:H5"	2.21	0.40
1:1A:2576:G:H1'	61:1A:4649:HOH:O	2.20	0.40
1:1A:2785:C:OP1	4:1E:41:LYS:HE3	2.21	0.40
6:1G:108:ASN:HD22	26:14:22:ILE:HD13	1.86	0.40
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.21	0.40
32:1a:271:C:H2'	32:1a:272:C:H6	1.86	0.40
32:1a:575:G:O2'	32:1a:821:G:H5'	2.22	0.40
32:1a:621:A:H2'	32:1a:622:A:C8	2.56	0.40
32:1a:1002:G:C5	32:1a:1003:G:H1'	2.56	0.40
54:1y:11:C:H2'	54:1y:12:U:C6	2.55	0.40
1:2A:288:C:H2'	1:2A:289:A:H8	1.85	0.40
1:2A:531:C:H4'	1:2A:532:A:H5"	2.03	0.40
1:2A:862:G:H2'	1:2A:863:A:O4'	2.21	0.40
1:2A:1181:C:H2'	1:2A:1182:A:C8	2.56	0.40
1:2A:2647:U:H2'	1:2A:2648:C:C6	2.57	0.40
13:2R:36:THR:HG22	13:2R:37:THR:N	2.36	0.40
32:2a:44:G:H2'	32:2a:45:U:O4'	2.22	0.40
32:2a:512:U:H2'	32:2a:513:C:C6	2.55	0.40
32:2a:735:C:H2'	32:2a:736:C:C6	2.56	0.40
32:2a:993:G:N3	32:2a:993:G:H2'	2.35	0.40
32:2a:1227:A:C8	50:2s:83:HIS:HB3	2.57	0.40
34:2c:138:VAL:HG11	34:2c:169:ALA:HA	2.03	0.40
44:2m:13:LYS:HA	44:2m:44:ARG:HH11	1.86	0.40
50:2s:36:ARG:HD2	50:2s:52:TYR:O	2.22	0.40
51:2t:72:LEU:HA	51:2t:72:LEU:HD12	1.89	0.40
54:2w:14:A:H61	54:2w:21:A:H2	1.70	0.40
1:1A:244:A:C2	1:1A:255:A:C4	3.10	0.40
1:1A:466:A:N3	1:1A:683:C:H1'	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:700:G:O2'	1:1A:1632:A:N3	2.43	0.40
1:1A:723:G:H2'	1:1A:724:U:O4'	2.22	0.40
1:1A:897:C:H4'	54:1w:55:PSU:O3'	2.22	0.40
1:1A:1084:A:H2'	1:1A:1085:A:O4'	2.22	0.40
1:1A:1153:C:H2'	1:1A:1154:G:O4'	2.22	0.40
1:1A:2052:G:H4'	4:1E:143:ASN:O	2.21	0.40
1:1A:2250:G:O2'	1:1A:2496:C:OP1	2.34	0.40
1:1A:2712:U:O2'	1:1A:2713:A:H5'	2.22	0.40
1:1A:2846:G:H2'	1:1A:2847:U:O4'	2.22	0.40
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.56	0.40
6:1G:15:VAL:HG21	6:1G:176:LEU:HD23	2.04	0.40
6:1G:47:LYS:O	6:1G:86:MET:HE2	2.21	0.40
25:13:7:LYS:HE3	25:13:32:GLN:HE21	1.87	0.40
31:19:7:VAL:HG12	31:19:34:GLN:HB3	2.04	0.40
32:1a:266:G:H5"	32:1a:268:C:H41	1.86	0.40
32:1a:524:G:H2'	32:1a:525:C:C6	2.56	0.40
32:1a:619:U:C2	35:1d:135:LEU:HD22	2.57	0.40
35:1d:83:SER:HA	35:1d:89:THR:HG21	2.04	0.40
35:1d:138:TYR:HE2	35:1d:140:VAL:HA	1.86	0.40
37:1f:89:MET:SD	49:1r:76:LEU:HD22	2.62	0.40
38:1g:97:GLN:O	38:1g:101:LEU:HG	2.22	0.40
42:1k:15:ALA:HA	42:1k:76:GLY:O	2.22	0.40
1:2A:108:U:H2'	1:2A:109:G:H8	1.87	0.40
1:2A:276:A:H5"	1:2A:277:C:H5'	2.03	0.40
1:2A:1651:G:H2'	1:2A:1652:A:O4'	2.20	0.40
1:2A:1799:G:O2'	3:2D:181:GLU:OE2	2.36	0.40
1:2A:2137:C:H42	1:2A:2154:G:H1	1.70	0.40
1:2A:2340:G:H2'	1:2A:2341:G:C8	2.56	0.40
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.54	0.40
7:2H:89:ILE:O	7:2H:129:THR:HG22	2.22	0.40
10:2O:7:TYR:CZ	10:2O:44:LYS:HG3	2.56	0.40
12:2Q:7:MET:HE2	12:2Q:7:MET:HB3	1.87	0.40
32:2a:607:A:H2'	32:2a:608:A:O4'	2.21	0.40
32:2a:978:A:O2'	32:2a:1322:C:N3	2.42	0.40
32:2a:1108:G:H5'	34:2c:176:HIS:CD2	2.56	0.40
32:2a:1247:U:H1'	32:2a:1291:G:N2	2.36	0.40
34:2c:42:LEU:HA	34:2c:45:LYS:NZ	2.37	0.40
37:2f:97:PHE:HD2	49:2r:31:LEU:HD11	1.85	0.40
38:2g:22:LEU:HG	38:2g:62:PHE:HE2	1.86	0.40
51:2t:89:ARG:O	51:2t:93:GLU:HG2	2.22	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%)	263 (96%)	10 (4%)	0	100 100
3	2D	273/276 (99%)	263 (96%)	10 (4%)	0	100 100
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	24 48
4	2E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24 48
5	1F	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	24 48
5	2F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	24 48
6	1G	179/182 (98%)	165 (92%)	14 (8%)	0	100 100
6	2G	179/182 (98%)	154 (86%)	21 (12%)	4 (2%)	5 14
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	21 44
7	2H	172/180 (96%)	156 (91%)	14 (8%)	2 (1%)	10 27
8	1I	144/148 (97%)	129 (90%)	15 (10%)	0	100 100
8	2I	144/148 (97%)	125 (87%)	18 (12%)	1 (1%)	18 41
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100 100
9	2N	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	18 41
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100 100
10	2O	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	16 37
11	1P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	9 23
11	2P	147/150 (98%)	130 (88%)	13 (9%)	4 (3%)	4 10
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100 100
12	2Q	139/141 (99%)	131 (94%)	8 (6%)	0	100 100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100 100
13	2R	116/118 (98%)	111 (96%)	4 (3%)	1 (1%)	14 35
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100 100
14	2S	108/112 (96%)	97 (90%)	8 (7%)	3 (3%)	4 9
15	1T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	16 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100 100
16	1U	114/118 (97%)	114 (100%)	0	0	100 100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100 100
17	1V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	6 16
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12 32
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
18	2W	110/113 (97%)	110 (100%)	0	0	100 100
19	1X	93/96 (97%)	89 (96%)	2 (2%)	2 (2%)	5 14
19	2X	93/96 (97%)	90 (97%)	3 (3%)	0	100 100
20	1Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	12 32
20	2Y	105/110 (96%)	95 (90%)	10 (10%)	0	100 100
21	1Z	148/206 (72%)	137 (93%)	10 (7%)	1 (1%)	18 41
21	2Z	156/206 (76%)	125 (80%)	28 (18%)	3 (2%)	6 17
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100 100
22	20	81/85 (95%)	76 (94%)	5 (6%)	0	100 100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11 29
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11 29
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100 100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
26	14	67/71 (94%)	50 (75%)	13 (19%)	4 (6%)	1 2
26	24	67/71 (94%)	52 (78%)	13 (19%)	2 (3%)	3 8
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100 100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
29	17	46/49 (94%)	46 (100%)	0	0	100 100
29	27	46/49 (94%)	46 (100%)	0	0	100 100
30	18	62/65 (95%)	62 (100%)	0	0	100 100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
33	1b	229/256 (90%)	198 (86%)	24 (10%)	7 (3%)	3 8
33	2b	229/256 (90%)	192 (84%)	29 (13%)	8 (4%)	3 6
34	1c	204/239 (85%)	190 (93%)	14 (7%)	0	100 100
34	2c	204/239 (85%)	169 (83%)	33 (16%)	2 (1%)	12 32
35	1d	206/209 (99%)	195 (95%)	11 (5%)	0	100 100
35	2d	206/209 (99%)	190 (92%)	16 (8%)	0	100 100
36	1e	146/162 (90%)	138 (94%)	7 (5%)	1 (1%)	18 41
36	2e	146/162 (90%)	129 (88%)	13 (9%)	4 (3%)	4 10
37	1f	98/101 (97%)	92 (94%)	5 (5%)	1 (1%)	12 32
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100 100
38	1g	153/156 (98%)	147 (96%)	5 (3%)	1 (1%)	18 41
38	2g	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	9 25
39	1h	135/138 (98%)	127 (94%)	8 (6%)	0	100 100
39	2h	135/138 (98%)	124 (92%)	11 (8%)	0	100 100
40	1i	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	16 37
40	2i	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	16 37
41	1j	95/105 (90%)	79 (83%)	15 (16%)	1 (1%)	11 29
41	2j	94/105 (90%)	78 (83%)	14 (15%)	2 (2%)	5 15
42	1k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	6 18
42	2k	112/129 (87%)	103 (92%)	8 (7%)	1 (1%)	14 35
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100 100
43	2l	119/132 (90%)	110 (92%)	9 (8%)	0	100 100
44	1m	121/126 (96%)	109 (90%)	11 (9%)	1 (1%)	16 37
44	2m	120/126 (95%)	103 (86%)	15 (12%)	2 (2%)	7 19
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100 100
45	2n	58/61 (95%)	51 (88%)	7 (12%)	0	100 100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100 100
46	2o	86/89 (97%)	84 (98%)	1 (1%)	1 (1%)	10 27
47	1p	80/88 (91%)	74 (92%)	6 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
47	2p	80/88 (91%)	77 (96%)	3 (4%)	0	100 100
48	1q	97/105 (92%)	91 (94%)	6 (6%)	0	100 100
48	2q	97/105 (92%)	93 (96%)	4 (4%)	0	100 100
49	1r	66/88 (75%)	63 (96%)	3 (4%)	0	100 100
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100 100
50	1s	81/93 (87%)	74 (91%)	6 (7%)	1 (1%)	10 27
50	2s	81/93 (87%)	70 (86%)	9 (11%)	2 (2%)	4 11
51	1t	94/106 (89%)	85 (90%)	6 (6%)	3 (3%)	3 7
51	2t	94/106 (89%)	83 (88%)	9 (10%)	2 (2%)	5 15
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
52	2u	21/27 (78%)	19 (90%)	1 (5%)	1 (5%)	2 3
All	All	11370/12128 (94%)	10547 (93%)	733 (6%)	90 (1%)	16 37

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
17	1V	79	VAL
21	1Z	53	ILE
33	1b	17	PHE
33	1b	126	GLU
40	1i	54	ASP
41	1j	79	ARG
44	1m	67	GLU
5	2F	130	ALA
6	2G	84	LYS
8	2I	10	GLU
11	2P	36	LYS
21	2Z	144	LEU
33	2b	8	LYS
33	2b	17	PHE
38	2g	80	VAL
44	2m	67	GLU
7	1H	126	PRO
20	1Y	54	LYS
23	11	3	LYS
26	14	49	PHE
26	14	62	ARG

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Mol	Chain	Res	Type
26	14	68	ARG
36	1e	85	GLY
42	1k	49	GLY
6	2G	42	GLY
7	2H	47	GLU
7	2H	126	PRO
10	2O	5	GLN
17	2V	79	VAL
21	2Z	145	GLU
26	24	45	GLY
33	2b	74	LYS
41	2j	75	ILE
41	2j	79	ARG
42	2k	49	GLY
50	2s	9	VAL
4	1E	52	LEU
11	1P	38	GLN
19	1X	93	GLU
33	1b	38	GLY
51	1t	47	GLY
51	1t	100	ILE
6	2G	51	ARG
11	2P	29	LYS
11	2P	38	GLN
14	2S	84	GLN
23	21	3	LYS
33	2b	20	GLU
33	2b	125	PRO
34	2c	179	ARG
36	2e	37	ARG
36	2e	85	GLY
36	2e	97	GLY
40	2i	121	ARG
51	2t	47	GLY
17	1V	43	GLU
26	14	45	GLY
33	1b	124	SER
4	2E	52	LEU
9	2N	2	LYS
14	2S	20	ARG
14	2S	96	GLY
26	24	49	PHE

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Mol	Chain	Res	Type
33	2b	10	LEU
33	2b	121	LEU
33	2b	123	ALA
44	2m	58	GLU
51	2t	95	ALA
15	1T	37	GLY
33	1b	37	ASN
33	1b	231	GLU
38	1g	54	THR
6	2G	124	SER
46	2o	88	ARG
52	2u	7	ARG
11	1P	45	LEU
19	1X	2	LYS
37	1f	40	VAL
42	1k	105	VAL
50	1s	27	GLU
51	1t	102	GLY
11	2P	45	LEU
34	2c	95	THR
21	2Z	171	ILE
36	2e	69	VAL
38	2g	55	GLY
50	2s	76	PRO
33	1b	125	PRO
13	2R	58	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1D	215/218 (99%)	206 (96%)	9 (4%)	26 55
3	2D	215/218 (99%)	206 (96%)	9 (4%)	26 55
4	1E	164/166 (99%)	156 (95%)	8 (5%)	22 49
4	2E	164/166 (99%)	153 (93%)	11 (7%)	15 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	1F	160/166 (96%)	147 (92%)	13 (8%)	11 27
5	2F	159/166 (96%)	150 (94%)	9 (6%)	18 43
6	1G	143/156 (92%)	130 (91%)	13 (9%)	9 22
6	2G	143/156 (92%)	119 (83%)	24 (17%)	2 6
7	1H	144/148 (97%)	137 (95%)	7 (5%)	22 49
7	2H	144/148 (97%)	129 (90%)	15 (10%)	7 17
8	1I	113/124 (91%)	96 (85%)	17 (15%)	3 7
8	2I	105/124 (85%)	93 (89%)	12 (11%)	5 14
9	1N	118/119 (99%)	111 (94%)	7 (6%)	18 42
9	2N	118/119 (99%)	111 (94%)	7 (6%)	18 42
10	1O	100/100 (100%)	100 (100%)	0	100 100
10	2O	100/100 (100%)	98 (98%)	2 (2%)	48 76
11	1P	115/116 (99%)	107 (93%)	8 (7%)	14 34
11	2P	115/116 (99%)	109 (95%)	6 (5%)	21 47
12	1Q	111/111 (100%)	106 (96%)	5 (4%)	24 52
12	2Q	111/111 (100%)	109 (98%)	2 (2%)	51 78
13	1R	101/101 (100%)	97 (96%)	4 (4%)	28 56
13	2R	101/101 (100%)	98 (97%)	3 (3%)	36 66
14	1S	86/88 (98%)	77 (90%)	9 (10%)	6 17
14	2S	85/88 (97%)	78 (92%)	7 (8%)	10 27
15	1T	115/127 (91%)	109 (95%)	6 (5%)	21 47
15	2T	113/127 (89%)	110 (97%)	3 (3%)	39 69
16	1U	93/94 (99%)	86 (92%)	7 (8%)	12 31
16	2U	93/94 (99%)	89 (96%)	4 (4%)	26 54
17	1V	80/82 (98%)	74 (92%)	6 (8%)	12 31
17	2V	80/82 (98%)	73 (91%)	7 (9%)	9 23
18	1W	90/92 (98%)	85 (94%)	5 (6%)	19 44
18	2W	90/92 (98%)	83 (92%)	7 (8%)	11 29
19	1X	77/78 (99%)	75 (97%)	2 (3%)	40 70
19	2X	77/78 (99%)	76 (99%)	1 (1%)	61 83
20	1Y	85/91 (93%)	78 (92%)	7 (8%)	10 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	2Y	85/91 (93%)	74 (87%)	11 (13%)	4 10
21	1Z	135/179 (75%)	121 (90%)	14 (10%)	7 17
21	2Z	137/179 (76%)	124 (90%)	13 (10%)	8 20
22	10	65/67 (97%)	63 (97%)	2 (3%)	35 65
22	20	65/67 (97%)	61 (94%)	4 (6%)	16 39
23	11	80/83 (96%)	79 (99%)	1 (1%)	61 83
23	21	80/83 (96%)	77 (96%)	3 (4%)	29 58
24	12	65/67 (97%)	63 (97%)	2 (3%)	35 65
24	22	65/67 (97%)	61 (94%)	4 (6%)	16 39
25	13	51/52 (98%)	47 (92%)	4 (8%)	11 29
25	23	50/52 (96%)	46 (92%)	4 (8%)	11 28
26	14	59/63 (94%)	51 (86%)	8 (14%)	3 9
26	24	53/63 (84%)	45 (85%)	8 (15%)	3 7
27	15	50/52 (96%)	47 (94%)	3 (6%)	17 41
27	25	50/52 (96%)	48 (96%)	2 (4%)	28 56
28	16	51/52 (98%)	47 (92%)	4 (8%)	11 29
28	26	50/52 (96%)	48 (96%)	2 (4%)	28 56
29	17	41/42 (98%)	35 (85%)	6 (15%)	3 8
29	27	41/42 (98%)	37 (90%)	4 (10%)	7 19
30	18	54/55 (98%)	52 (96%)	2 (4%)	30 59
30	28	54/55 (98%)	52 (96%)	2 (4%)	30 59
31	19	34/34 (100%)	34 (100%)	0	100 100
31	29	34/34 (100%)	33 (97%)	1 (3%)	37 67
33	1b	192/220 (87%)	175 (91%)	17 (9%)	9 23
33	2b	187/220 (85%)	156 (83%)	31 (17%)	2 6
34	1c	142/188 (76%)	133 (94%)	9 (6%)	16 39
34	2c	140/188 (74%)	126 (90%)	14 (10%)	7 19
35	1d	169/181 (93%)	149 (88%)	20 (12%)	5 13
35	2d	173/181 (96%)	158 (91%)	15 (9%)	9 24
36	1e	113/123 (92%)	104 (92%)	9 (8%)	11 28
36	2e	114/123 (93%)	101 (89%)	13 (11%)	5 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
37	1f	84/90 (93%)	78 (93%)	6 (7%)	13 33
37	2f	85/90 (94%)	78 (92%)	7 (8%)	10 27
38	1g	119/127 (94%)	107 (90%)	12 (10%)	7 18
38	2g	120/127 (94%)	112 (93%)	8 (7%)	15 36
39	1h	114/119 (96%)	106 (93%)	8 (7%)	14 34
39	2h	114/119 (96%)	104 (91%)	10 (9%)	9 23
40	1i	90/99 (91%)	81 (90%)	9 (10%)	7 19
40	2i	89/99 (90%)	82 (92%)	7 (8%)	11 28
41	1j	66/92 (72%)	61 (92%)	5 (8%)	12 30
41	2j	69/92 (75%)	61 (88%)	8 (12%)	5 13
42	1k	82/99 (83%)	74 (90%)	8 (10%)	7 19
42	2k	83/99 (84%)	80 (96%)	3 (4%)	31 60
43	1l	96/108 (89%)	91 (95%)	5 (5%)	21 47
43	2l	96/108 (89%)	89 (93%)	7 (7%)	13 32
44	1m	93/101 (92%)	86 (92%)	7 (8%)	12 31
44	2m	92/101 (91%)	82 (89%)	10 (11%)	6 16
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5 12
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7 18
46	1o	78/80 (98%)	74 (95%)	4 (5%)	21 48
46	2o	78/80 (98%)	75 (96%)	3 (4%)	29 58
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5 13
47	2p	68/74 (92%)	62 (91%)	6 (9%)	9 23
48	1q	94/97 (97%)	89 (95%)	5 (5%)	20 46
48	2q	94/97 (97%)	89 (95%)	5 (5%)	20 46
49	1r	59/77 (77%)	55 (93%)	4 (7%)	14 35
49	2r	59/77 (77%)	52 (88%)	7 (12%)	5 13
50	1s	69/80 (86%)	67 (97%)	2 (3%)	37 67
50	2s	67/80 (84%)	57 (85%)	10 (15%)	3 8
51	1t	70/82 (85%)	67 (96%)	3 (4%)	26 54
51	2t	70/82 (85%)	66 (94%)	4 (6%)	18 43
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19 44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19 44
All	All	9303/10064 (92%)	8615 (93%)	688 (7%)	13 32

All (688) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	38	LYS
3	1D	39	LYS
3	1D	99	ASP
3	1D	106	ILE
3	1D	142	VAL
3	1D	173	VAL
3	1D	229	VAL
3	1D	273	ARG
4	1E	9	VAL
4	1E	21	VAL
4	1E	33	VAL
4	1E	59	VAL
4	1E	93	VAL
4	1E	116	VAL
4	1E	184	VAL
4	1E	195	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	72	ARG
5	1F	74	ARG
5	1F	95	ARG
5	1F	132	VAL
5	1F	140	LEU
5	1F	144	LYS
5	1F	145	GLU
5	1F	162	LEU
5	1F	168	ARG
5	1F	183	VAL
5	1F	192	LEU
6	1G	3	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	21	ARG
6	1G	22	ARG
6	1G	28	VAL

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Mol	Chain	Res	Type
6	1G	31	VAL
6	1G	43	LEU
6	1G	82	LEU
6	1G	133	LEU
6	1G	140	ILE
6	1G	148	MET
6	1G	161	THR
7	1H	47	GLU
7	1H	50	VAL
7	1H	95	ARG
7	1H	116	GLU
7	1H	119	GLU
7	1H	124	GLU
7	1H	149	ARG
8	1I	9	LEU
8	1I	10	GLU
8	1I	12	LEU
8	1I	20	ASP
8	1I	42	SER
8	1I	47	LEU
8	1I	74	ASN
8	1I	75	LEU
8	1I	77	LEU
8	1I	85	GLU
8	1I	87	LYS
8	1I	92	VAL
8	1I	101	LEU
8	1I	109	ILE
8	1I	123	LEU
8	1I	129	THR
8	1I	142	VAL
9	1N	1	MET
9	1N	9	VAL
9	1N	48	MET
9	1N	62	VAL
9	1N	83	LYS
9	1N	88	GLU
9	1N	138	LEU
11	1P	45	LEU
11	1P	94	GLU
11	1P	95	VAL
11	1P	125	VAL

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Mol	Chain	Res	Type
11	1P	126	VAL
11	1P	132	LYS
11	1P	133	SER
11	1P	148	LEU
12	1Q	8	LYS
12	1Q	56	ARG
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	118	LEU
13	1R	36	THR
13	1R	73	VAL
13	1R	91	GLN
13	1R	114	VAL
14	1S	14	VAL
14	1S	25	ARG
14	1S	36	TYR
14	1S	46	VAL
14	1S	48	LEU
14	1S	68	GLN
14	1S	69	VAL
14	1S	73	LEU
14	1S	85	VAL
15	1T	28	VAL
15	1T	34	VAL
15	1T	67	SER
15	1T	96	ARG
15	1T	108	ARG
15	1T	128	GLU
16	1U	17	ILE
16	1U	31	SER
16	1U	74	LEU
16	1U	77	SER
16	1U	78	THR
16	1U	84	LYS
16	1U	95	LEU
17	1V	28	GLU
17	1V	32	THR
17	1V	56	SER
17	1V	61	VAL
17	1V	73	SER
17	1V	79	VAL
18	1W	4	LYS

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Mol	Chain	Res	Type
18	1W	11	ARG
18	1W	17	VAL
18	1W	92	ARG
18	1W	96	ILE
19	1X	38	GLU
19	1X	88	LYS
20	1Y	1	MET
20	1Y	7	VAL
20	1Y	43	ASN
20	1Y	64	GLU
20	1Y	72	VAL
20	1Y	85	VAL
20	1Y	99	CYS
21	1Z	33	LEU
21	1Z	53	ILE
21	1Z	70	LEU
21	1Z	72	ARG
21	1Z	102	LEU
21	1Z	138	GLU
21	1Z	139	VAL
21	1Z	140	ASP
21	1Z	146	ILE
21	1Z	153	SER
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	161	VAL
21	1Z	171	ILE
22	10	7	LEU
22	10	49	LYS
23	11	46	LEU
24	12	1	MET
24	12	65	ASN
25	13	54	VAL
25	13	55	ARG
25	13	56	VAL
25	13	60	GLU
26	14	21	VAL
26	14	27	THR
26	14	49	PHE
26	14	50	VAL
26	14	52	THR
26	14	53	GLU

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Mol	Chain	Res	Type
26	14	63	TYR
26	14	69	LYS
27	15	6	VAL
27	15	26	THR
27	15	40	LYS
28	16	5	VAL
28	16	44	ARG
28	16	47	THR
28	16	48	VAL
29	17	1	MET
29	17	24	THR
29	17	29	LYS
29	17	32	LYS
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	29	LYS
33	1b	7	VAL
33	1b	10	LEU
33	1b	12	GLU
33	1b	35	GLU
33	1b	54	THR
33	1b	80	ILE
33	1b	83	MET
33	1b	93	VAL
33	1b	112	VAL
33	1b	122	PHE
33	1b	126	GLU
33	1b	138	LEU
33	1b	170	GLU
33	1b	185	ILE
33	1b	208	ILE
33	1b	215	LEU
33	1b	236	TYR
34	1c	3	ASN
34	1c	43	LEU
34	1c	49	SER
34	1c	70	VAL
34	1c	77	ILE
34	1c	89	GLU
34	1c	190	ARG
34	1c	195	VAL

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Mol	Chain	Res	Type
34	1c	198	VAL
35	1d	5	ILE
35	1d	18	LYS
35	1d	19	LEU
35	1d	59	ARG
35	1d	70	ILE
35	1d	76	ARG
35	1d	83	SER
35	1d	91	SER
35	1d	100	ARG
35	1d	119	GLN
35	1d	127	THR
35	1d	135	LEU
35	1d	144	ASP
35	1d	157	LEU
35	1d	158	ILE
35	1d	177	ASP
35	1d	178	VAL
35	1d	181	MET
35	1d	190	ASP
35	1d	194	LEU
36	1e	10	MET
36	1e	16	THR
36	1e	18	ARG
36	1e	31	LEU
36	1e	41	VAL
36	1e	56	GLN
36	1e	82	VAL
36	1e	98	THR
36	1e	131	ILE
37	1f	19	LEU
37	1f	45	LEU
37	1f	55	ASP
37	1f	65	VAL
37	1f	75	LEU
37	1f	92	LYS
38	1g	12	LEU
38	1g	16	LEU
38	1g	23	VAL
38	1g	50	ILE
38	1g	59	LEU
38	1g	61	VAL

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Mol	Chain	Res	Type
38	1g	78	ARG
38	1g	79	ARG
38	1g	94	ARG
38	1g	98	SER
38	1g	104	LEU
38	1g	113	GLU
39	1h	29	SER
39	1h	37	ARG
39	1h	39	LEU
39	1h	51	VAL
39	1h	52	ASP
39	1h	54	ASP
39	1h	122	ARG
39	1h	133	LEU
40	1i	17	VAL
40	1i	23	ASN
40	1i	42	ARG
40	1i	53	VAL
40	1i	64	THR
40	1i	96	LEU
40	1i	97	LYS
40	1i	103	THR
40	1i	108	VAL
41	1j	5	ARG
41	1j	8	LEU
41	1j	34	VAL
41	1j	46	ARG
41	1j	96	ILE
42	1k	14	VAL
42	1k	30	VAL
42	1k	48	ILE
42	1k	87	THR
42	1k	104	GLN
42	1k	109	VAL
42	1k	114	VAL
42	1k	116	HIS
43	1l	11	VAL
43	1l	18	VAL
43	1l	46	LYS
43	1l	83	VAL
43	1l	123	LYS
44	1m	4	ILE

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Mol	Chain	Res	Type
44	1m	15	VAL
44	1m	19	LEU
44	1m	43	THR
44	1m	49	THR
44	1m	70	LEU
44	1m	109	THR
45	1n	12	ARG
45	1n	13	THR
45	1n	18	VAL
45	1n	22	THR
45	1n	32	SER
45	1n	33	VAL
46	1o	24	SER
46	1o	27	VAL
46	1o	39	LEU
46	1o	76	GLU
47	1p	20	VAL
47	1p	21	VAL
47	1p	27	LYS
47	1p	45	THR
47	1p	60	LEU
47	1p	62	VAL
47	1p	67	THR
47	1p	72	ARG
48	1q	19	VAL
48	1q	26	GLN
48	1q	53	LEU
48	1q	70	ARG
48	1q	97	SER
49	1r	31	LEU
49	1r	46	GLU
49	1r	54	ARG
49	1r	76	LEU
50	1s	12	ASP
50	1s	19	VAL
51	1t	10	LEU
51	1t	24	LEU
51	1t	84	LEU
52	1u	15	ARG
3	2D	3	VAL
3	2D	18	VAL
3	2D	22	SER

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Mol	Chain	Res	Type
3	2D	106	ILE
3	2D	142	VAL
3	2D	171	ASP
3	2D	229	VAL
3	2D	259	THR
3	2D	260	ARG
4	2E	7	VAL
4	2E	9	VAL
4	2E	14	ILE
4	2E	21	VAL
4	2E	33	VAL
4	2E	90	THR
4	2E	116	VAL
4	2E	134	ILE
4	2E	175	VAL
4	2E	184	VAL
4	2E	195	LEU
5	2F	12	LEU
5	2F	20	LEU
5	2F	33	LEU
5	2F	53	THR
5	2F	70	THR
5	2F	74	ARG
5	2F	157	VAL
5	2F	192	LEU
5	2F	197	ASP
6	2G	5	VAL
6	2G	16	ARG
6	2G	18	GLU
6	2G	21	ARG
6	2G	31	VAL
6	2G	43	LEU
6	2G	45	GLU
6	2G	49	ASP
6	2G	53	LEU
6	2G	58	GLN
6	2G	60	LEU
6	2G	70	VAL
6	2G	79	ASN
6	2G	91	ARG
6	2G	98	ARG
6	2G	130	ASN

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Mol	Chain	Res	Type
6	2G	140	ILE
6	2G	148	MET
6	2G	150	ASP
6	2G	152	LEU
6	2G	159	VAL
6	2G	162	THR
6	2G	164	GLU
6	2G	170	ARG
7	2H	17	VAL
7	2H	45	VAL
7	2H	47	GLU
7	2H	49	VAL
7	2H	50	VAL
7	2H	57	ASP
7	2H	68	THR
7	2H	70	THR
7	2H	84	SER
7	2H	119	GLU
7	2H	124	GLU
7	2H	127	GLU
7	2H	129	THR
7	2H	133	VAL
7	2H	141	VAL
8	2I	15	VAL
8	2I	31	LEU
8	2I	38	LEU
8	2I	40	THR
8	2I	51	ILE
8	2I	58	LEU
8	2I	77	LEU
8	2I	117	GLU
8	2I	122	GLU
8	2I	127	VAL
8	2I	139	GLN
8	2I	142	VAL
9	2N	1	MET
9	2N	5	VAL
9	2N	9	VAL
9	2N	48	MET
9	2N	62	VAL
9	2N	83	LYS
9	2N	138	LEU

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Mol	Chain	Res	Type
10	2O	28	SER
10	2O	52	VAL
11	2P	45	LEU
11	2P	65	ARG
11	2P	70	GLN
11	2P	95	VAL
11	2P	96	THR
11	2P	135	LEU
12	2Q	56	ARG
12	2Q	98	LYS
13	2R	102	GLU
13	2R	114	VAL
13	2R	118	GLU
14	2S	35	ILE
14	2S	36	TYR
14	2S	38	GLN
14	2S	52	SER
14	2S	58	LEU
14	2S	63	THR
14	2S	110	LEU
15	2T	28	VAL
15	2T	72	VAL
15	2T	96	ARG
16	2U	5	LYS
16	2U	31	SER
16	2U	74	LEU
16	2U	100	VAL
17	2V	7	THR
17	2V	28	GLU
17	2V	32	THR
17	2V	45	THR
17	2V	56	SER
17	2V	61	VAL
17	2V	79	VAL
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	21	VAL
18	2W	60	ASN
18	2W	67	ASP
18	2W	78	GLU
19	2X	52	VAL

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Mol	Chain	Res	Type
20	2Y	1	MET
20	2Y	3	VAL
20	2Y	49	VAL
20	2Y	63	LYS
20	2Y	67	LEU
20	2Y	72	VAL
20	2Y	83	THR
20	2Y	85	VAL
20	2Y	91	GLU
20	2Y	97	ARG
20	2Y	106	LEU
21	2Z	14	LYS
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	71	VAL
21	2Z	74	VAL
21	2Z	84	GLU
21	2Z	121	HIS
21	2Z	148	ASP
21	2Z	150	LEU
21	2Z	154	ASP
21	2Z	161	VAL
21	2Z	171	ILE
21	2Z	174	VAL
22	20	10	THR
22	20	30	VAL
22	20	63	VAL
22	20	74	ARG
23	21	35	THR
23	21	56	GLN
23	21	81	LYS
24	22	12	GLU
24	22	45	SER
24	22	53	LEU
24	22	66	GLU
25	23	31	LEU
25	23	37	LEU
25	23	54	VAL
25	23	59	VAL
26	24	3	GLU
26	24	5	ILE
26	24	10	VAL

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Mol	Chain	Res	Type
26	24	31	ILE
26	24	34	GLU
26	24	50	VAL
26	24	59	PHE
26	24	63	TYR
27	25	6	VAL
27	25	58	LEU
28	26	9	LEU
28	26	19	ARG
29	27	1	MET
29	27	24	THR
29	27	43	THR
29	27	46	VAL
30	28	14	VAL
30	28	46	ARG
31	29	6	SER
33	2b	7	VAL
33	2b	8	LYS
33	2b	9	GLU
33	2b	11	LEU
33	2b	23	ARG
33	2b	37	ASN
33	2b	39	ILE
33	2b	41	ILE
33	2b	47	THR
33	2b	48	MET
33	2b	61	LEU
33	2b	67	THR
33	2b	71	VAL
33	2b	76	GLN
33	2b	80	ILE
33	2b	94	ASN
33	2b	107	THR
33	2b	112	VAL
33	2b	115	LEU
33	2b	127	ILE
33	2b	158	LEU
33	2b	164	VAL
33	2b	179	LYS
33	2b	185	ILE
33	2b	187	LEU
33	2b	189	ASP

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Mol	Chain	Res	Type
33	2b	197	VAL
33	2b	204	ASN
33	2b	224	GLN
33	2b	229	VAL
33	2b	236	TYR
34	2c	14	ILE
34	2c	15	THR
34	2c	34	LEU
34	2c	43	LEU
34	2c	44	GLU
34	2c	91	LEU
34	2c	140	ARG
34	2c	143	GLU
34	2c	152	ILE
34	2c	165	THR
34	2c	182	ILE
34	2c	190	ARG
34	2c	192	THR
34	2c	202	ILE
35	2d	8	VAL
35	2d	28	SER
35	2d	31	CYS
35	2d	53	ASP
35	2d	59	ARG
35	2d	76	ARG
35	2d	78	LEU
35	2d	83	SER
35	2d	118	ARG
35	2d	127	THR
35	2d	135	LEU
35	2d	158	ILE
35	2d	162	LEU
35	2d	178	VAL
35	2d	193	ASP
36	2e	13	ILE
36	2e	20	GLN
36	2e	31	LEU
36	2e	41	VAL
36	2e	51	VAL
36	2e	55	VAL
36	2e	57	LYS
36	2e	75	THR

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Mol	Chain	Res	Type
36	2e	111	GLU
36	2e	120	THR
36	2e	136	MET
36	2e	144	THR
36	2e	151	LEU
37	2f	21	LEU
37	2f	37	VAL
37	2f	63	TYR
37	2f	70	ASP
37	2f	81	ILE
37	2f	92	LYS
37	2f	93	SER
38	2g	15	ASP
38	2g	24	THR
38	2g	49	ILE
38	2g	52	GLU
38	2g	78	ARG
38	2g	79	ARG
38	2g	98	SER
38	2g	135	VAL
39	2h	23	SER
39	2h	26	VAL
39	2h	29	SER
39	2h	51	VAL
39	2h	61	VAL
39	2h	99	GLU
39	2h	103	VAL
39	2h	112	LEU
39	2h	133	LEU
39	2h	137	VAL
40	2i	54	ASP
40	2i	75	ASP
40	2i	89	ASN
40	2i	93	ARG
40	2i	99	LEU
40	2i	103	THR
40	2i	128	ARG
41	2j	8	LEU
41	2j	9	ARG
41	2j	29	ARG
41	2j	34	VAL
41	2j	67	THR

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Mol	Chain	Res	Type
41	2j	96	ILE
41	2j	98	ILE
41	2j	100	THR
42	2k	14	VAL
42	2k	24	SER
42	2k	82	VAL
43	2l	11	VAL
43	2l	18	VAL
43	2l	40	VAL
43	2l	62	SER
43	2l	83	VAL
43	2l	86	ARG
43	2l	116	SER
44	2m	4	ILE
44	2m	22	ILE
44	2m	32	GLU
44	2m	39	ILE
44	2m	45	VAL
44	2m	47	ASP
44	2m	53	VAL
44	2m	62	ASN
44	2m	81	LEU
44	2m	121	LYS
45	2n	3	ARG
45	2n	12	ARG
45	2n	18	VAL
45	2n	33	VAL
45	2n	35	ARG
46	2o	27	VAL
46	2o	39	LEU
46	2o	76	GLU
47	2p	2	VAL
47	2p	20	VAL
47	2p	45	THR
47	2p	67	THR
47	2p	69	THR
47	2p	74	LEU
48	2q	5	VAL
48	2q	9	VAL
48	2q	53	LEU
48	2q	63	ARG
48	2q	99	SER

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Mol	Chain	Res	Type
49	2r	31	LEU
49	2r	35	ARG
49	2r	37	VAL
49	2r	54	ARG
49	2r	76	LEU
49	2r	82	THR
49	2r	84	LYS
50	2s	12	ASP
50	2s	27	GLU
50	2s	31	ILE
50	2s	37	ARG
50	2s	45	VAL
50	2s	47	HIS
50	2s	48	THR
50	2s	56	GLN
50	2s	65	ASN
50	2s	67	VAL
51	2t	46	GLU
51	2t	72	LEU
51	2t	90	GLN
51	2t	100	ILE
52	2u	7	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	116	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
6	1G	108	ASN
8	1I	133	HIS
9	1N	56	ASN
9	1N	94	HIS
10	1O	89	ASN
12	1Q	12	GLN
12	1Q	141	GLN
13	1R	71	GLN
14	1S	68	GLN
14	1S	95	HIS
15	1T	58	ASN

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Mol	Chain	Res	Type
16	1U	81	HIS
16	1U	94	ASN
18	1W	111	HIS
19	1X	31	HIS
19	1X	82	GLN
20	1Y	43	ASN
21	1Z	73	GLN
21	1Z	75	ASN
21	1Z	132	ASN
23	11	56	GLN
24	12	38	GLN
24	12	43	GLN
25	13	32	GLN
26	14	46	GLN
26	14	60	GLN
34	1c	6	HIS
34	1c	69	HIS
34	1c	98	ASN
34	1c	110	ASN
34	1c	118	GLN
34	1c	162	GLN
35	1d	42	GLN
35	1d	116	GLN
36	1e	78	HIS
37	1f	73	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	110	GLN
40	1i	23	ASN
40	1i	31	GLN
40	1i	124	GLN
41	1j	56	HIS
41	1j	69	ASN
43	1l	80	HIS
43	1l	99	HIS
44	1m	77	ASN
44	1m	92	HIS
46	1o	13	GLN
47	1p	14	ASN
48	1q	26	GLN
49	1r	36	ASN
49	1r	63	GLN

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Mol	Chain	Res	Type
50	1s	23	ASN
50	1s	47	HIS
50	1s	83	HIS
3	2D	87	ASN
4	2E	48	GLN
5	2F	69	HIS
5	2F	133	ASN
6	2G	130	ASN
7	2H	74	ASN
8	2I	133	HIS
10	2O	5	GLN
11	2P	70	GLN
12	2Q	123	HIS
13	2R	71	GLN
14	2S	38	GLN
15	2T	58	ASN
16	2U	81	HIS
16	2U	94	ASN
18	2W	60	ASN
19	2X	31	HIS
20	2Y	43	ASN
21	2Z	73	GLN
21	2Z	151	HIS
23	21	56	GLN
24	22	38	GLN
26	24	20	ASN
28	26	20	ASN
33	2b	94	ASN
33	2b	135	GLN
34	2c	31	HIS
34	2c	98	ASN
34	2c	123	GLN
34	2c	139	GLN
34	2c	162	GLN
34	2c	170	GLN
35	2d	42	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

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Mol	Chain	Res	Type
35	2d	160	GLN
36	2e	72	GLN
36	2e	73	ASN
37	2f	13	ASN
37	2f	73	ASN
37	2f	100	ASN
38	2g	28	ASN
38	2g	68	ASN
40	2i	3	GLN
40	2i	58	HIS
40	2i	73	GLN
41	2j	13	HIS
41	2j	33	GLN
41	2j	69	ASN
42	2k	38	ASN
42	2k	117	ASN
43	2l	99	HIS
44	2m	12	ASN
44	2m	77	ASN
46	2o	13	GLN
48	2q	26	GLN
49	2r	63	GLN
50	2s	47	HIS
50	2s	57	HIS
50	2s	65	ASN
50	2s	69	HIS
51	2t	45	GLN
51	2t	75	ASN
51	2t	90	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	402 (14%)	26 (0%)
1	2A	2791/2915 (95%)	426 (15%)	25 (0%)
2	1B	119/121 (98%)	8 (6%)	0
2	2B	118/121 (97%)	24 (20%)	0
32	1a	1497/1521 (98%)	222 (14%)	0
32	2a	1501/1521 (98%)	278 (18%)	0
53	1v	12/24 (50%)	0	0
53	2v	12/24 (50%)	1 (8%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	1w	70/76 (92%)	21 (30%)	0
54	1y	72/76 (94%)	28 (38%)	0
54	2w	67/76 (88%)	15 (22%)	0
54	2y	70/76 (92%)	24 (34%)	0
55	1x	74/77 (96%)	8 (10%)	0
55	2x	74/77 (96%)	8 (10%)	0
All	All	9341/9620 (97%)	1465 (15%)	51 (0%)

All (1465) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	78	A
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	272(A)	U

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Mol	Chain	Res	Type
1	1A	272(B)	G
1	1A	272(I)	U
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	363(C)	G
1	1A	370	G
1	1A	380	U
1	1A	386	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	456	C
1	1A	457	A
1	1A	481	G
1	1A	494	G
1	1A	504	U
1	1A	505	A
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	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

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Mol	Chain	Res	Type
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(D)	C
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	764	A
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
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	890	A
1	1A	894	C
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	910	A
1	1A	932	G
1	1A	938	G
1	1A	945	A

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Mol	Chain	Res	Type
1	1A	946	G
1	1A	959	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1038	C
1	1A	1041	C
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1064	C
1	1A	1068	G
1	1A	1069	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1078	U
1	1A	1079	C
1	1A	1081	U
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1094	U
1	1A	1096	A
1	1A	1097	U
1	1A	1101	U
1	1A	1111	A

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Mol	Chain	Res	Type
1	1A	1112	G
1	1A	1116	C
1	1A	1128	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1170	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1308	A
1	1A	1321	A
1	1A	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1370	C
1	1A	1384	A
1	1A	1385	G
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	1437	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G

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Mol	Chain	Res	Type
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1540	U
1	1A	1541	G
1	1A	1543	C
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1648	C
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1745(A)	C
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1829	A

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Mol	Chain	Res	Type
1	1A	1839	G
1	1A	1847	A
1	1A	1861	G
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2034	U
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2099	U
1	1A	2108	C
1	1A	2110	G
1	1A	2113	U
1	1A	2114	A
1	1A	2116	G
1	1A	2121	G
1	1A	2122	U

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Mol	Chain	Res	Type
1	1A	2127	G
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2140	C
1	1A	2141	G
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2149	G
1	1A	2150	U
1	1A	2151	G
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2164	C
1	1A	2165	G
1	1A	2166	G
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A

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Mol	Chain	Res	Type
1	1A	2269	A
1	1A	2278	A
1	1A	2280	G
1	1A	2283	C
1	1A	2286	A
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2312	U
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2347	C
1	1A	2350	C
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2407	G
1	1A	2422	A
1	1A	2423	U
1	1A	2424	C
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2476	A
1	1A	2477	C
1	1A	2478	A
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2520	C
1	1A	2529	G
1	1A	2535	G
1	1A	2549	G
1	1A	2554	U
1	1A	2555	U
1	1A	2566	A

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Mol	Chain	Res	Type
1	1A	2567	G
1	1A	2573	C
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2689	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2758	A
1	1A	2764	A
1	1A	2765	A
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2802	G
1	1A	2805	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2839	G
1	1A	2872	G
1	1A	2879	C
1	1A	2880	C
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	13	A
2	1B	25	A
2	1B	52	A
2	1B	56	G
2	1B	73	A
2	1B	106	G

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Mol	Chain	Res	Type
2	1B	110	G
32	1a	5	U
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	51	A
32	1a	61	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	115	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	147	G
32	1a	162	A
32	1a	163	C
32	1a	174	C
32	1a	180	U
32	1a	182	U
32	1a	189	G
32	1a	195	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	220	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	342	C

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Mol	Chain	Res	Type
32	1a	345	C
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	388	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	482	A
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	531	U
32	1a	532	A
32	1a	533	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G

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Mol	Chain	Res	Type
32	1a	596	C
32	1a	630	G
32	1a	631	G
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	723	U
32	1a	724	G
32	1a	731	G
32	1a	734	G
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	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	885	G
32	1a	902	G
32	1a	913	A
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G

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Mol	Chain	Res	Type
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
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	1039	C
32	1a	1044	A
32	1a	1046	A
32	1a	1053	G
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1124	G
32	1a	1125	U
32	1a	1131	G
32	1a	1132	C
32	1a	1134	G
32	1a	1135	U
32	1a	1137	C
32	1a	1138	G

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Mol	Chain	Res	Type
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1160	G
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1213	A
32	1a	1222	G
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	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	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
32	1a	1381	U
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1446	U

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Mol	Chain	Res	Type
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1469	G
32	1a	1487	G
32	1a	1492	A
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1519	MA6
32	1a	1529	G
32	1a	1530	G
54	1w	2	C
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	50	U
54	1w	61	C
54	1w	63	G
54	1w	68	C
54	1w	69	G
54	1w	73	A
54	1w	74	C
55	1x	6	G
55	1x	9	G
55	1x	13	C
55	1x	19	G
55	1x	20	U
55	1x	47	U
55	1x	61	C
55	1x	63	G

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Mol	Chain	Res	Type
54	1y	5	G
54	1y	6	G
54	1y	7	A
54	1y	8	4SU
54	1y	11	C
54	1y	13	C
54	1y	14	A
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	23	A
54	1y	26	A
54	1y	34	G
54	1y	35	A
54	1y	44	G
54	1y	45	U
54	1y	46	G7M
54	1y	47	U
54	1y	48	C
54	1y	49	C
54	1y	56	C
54	1y	57	G
54	1y	58	A
54	1y	59	U
54	1y	64	A
54	1y	65	G
54	1y	70	G
54	1y	71	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A

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Mol	Chain	Res	Type
1	2A	120	U
1	2A	125	G
1	2A	141	A
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	266	G
1	2A	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	311	A
1	2A	317	G
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	363	G
1	2A	363(B)	G
1	2A	380	U
1	2A	386	G
1	2A	396	G
1	2A	405	U

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Mol	Chain	Res	Type
1	2A	411	G
1	2A	412	A
1	2A	435	C
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	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
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	653	A
1	2A	669	G

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Mol	Chain	Res	Type
1	2A	686	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	832	G
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	874	G
1	2A	875	G
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	892	G
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	941	A
1	2A	945	A

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Mol	Chain	Res	Type
1	2A	946	G
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1020	A
1	2A	1022	G
1	2A	1025	G
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1042	G
1	2A	1043	C
1	2A	1114	G
1	2A	1117	G
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1170	G
1	2A	1171	G
1	2A	1206	G
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1236	G
1	2A	1247	A
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1284	A

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Mol	Chain	Res	Type
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1314	C
1	2A	1321	A
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	1395	A
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	1435	G
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1478	G
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G

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Mol	Chain	Res	Type
1	2A	1543	C
1	2A	1545	A
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1583	A
1	2A	1584	C
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	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
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G

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Mol	Chain	Res	Type
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	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	2032	G
1	2A	2033	A
1	2A	2036	C
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2099	U
1	2A	2108	C
1	2A	2111	C
1	2A	2112	G
1	2A	2114	A
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G

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Mol	Chain	Res	Type
1	2A	2126	A
1	2A	2127	G
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	2146	C
1	2A	2150	U
1	2A	2151	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
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	2174	C
1	2A	2176	A
1	2A	2178	C
1	2A	2182	G
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C

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Mol	Chain	Res	Type
1	2A	2287	A
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2406	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2440	C
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2465	C
1	2A	2468	G
1	2A	2469	A
1	2A	2476	A
1	2A	2490	G
1	2A	2502	G
1	2A	2505	G
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C

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Mol	Chain	Res	Type
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2669	G
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2752	C
1	2A	2758	A
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	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	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	13	A
2	2B	17	C
2	2B	32	C
2	2B	34	U
2	2B	41	U
2	2B	42	C

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Mol	Chain	Res	Type
2	2B	53	A
2	2B	56	G
2	2B	69	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	88	C
2	2B	94	C
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	111	G
2	2B	116	G
2	2B	119	G
2	2B	120	A
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	65	U
32	2a	66	G
32	2a	73	G
32	2a	89	C
32	2a	101	A
32	2a	105	G
32	2a	115	G
32	2a	116	A
32	2a	117	G
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	142	G
32	2a	144	G
32	2a	146	G
32	2a	156	G
32	2a	159	G
32	2a	163	C

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Mol	Chain	Res	Type
32	2a	182	U
32	2a	189(A)	C
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	231	G
32	2a	247	G
32	2a	251	G
32	2a	266	G
32	2a	267	C
32	2a	281	G
32	2a	289	G
32	2a	301	G
32	2a	306	G
32	2a	318	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	339	C
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	424	G
32	2a	429	U
32	2a	438	G

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Mol	Chain	Res	Type
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	457	C
32	2a	470	C
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	517	G
32	2a	518	C
32	2a	521	G
32	2a	527	G7M
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	576	G
32	2a	596	C
32	2a	607	A
32	2a	630	G
32	2a	653	A
32	2a	657	G
32	2a	665	A
32	2a	666	G
32	2a	687	A
32	2a	688	G
32	2a	693	G
32	2a	695	A
32	2a	723	U
32	2a	731	G
32	2a	749	C
32	2a	755	G

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Mol	Chain	Res	Type
32	2a	760	G
32	2a	774	G
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	870	U
32	2a	873	A
32	2a	874	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	942	G
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	963	G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	984	C
32	2a	991	U
32	2a	992	U
32	2a	993	G
32	2a	995	C

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Mol	Chain	Res	Type
32	2a	996	A
32	2a	997	U
32	2a	998	G
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	1021	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1035	A
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1044	A
32	2a	1050	G
32	2a	1051	C
32	2a	1053	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1086	U
32	2a	1091	U
32	2a	1092	A
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A

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Mol	Chain	Res	Type
32	2a	1108	G
32	2a	1109	C
32	2a	1113	C
32	2a	1117	G
32	2a	1122	U
32	2a	1125	U
32	2a	1126	U
32	2a	1129	C
32	2a	1130	A
32	2a	1132	C
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	1146	A
32	2a	1152	A
32	2a	1155	G
32	2a	1157	A
32	2a	1159	U
32	2a	1172	C
32	2a	1182	G
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1204	A
32	2a	1211	U
32	2a	1213	A
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1262	C
32	2a	1264	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G

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Mol	Chain	Res	Type
32	2a	1275	A
32	2a	1276	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1299	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1323	G
32	2a	1338	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1358	U
32	2a	1363	C
32	2a	1368	G
32	2a	1370	G
32	2a	1378	C
32	2a	1381	U
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1508	G
32	2a	1517	G
32	2a	1519	MA6
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U

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Mol	Chain	Res	Type
53	2v	14	A
54	2w	4	C
54	2w	5	G
54	2w	6	G
54	2w	11	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	27	G
54	2w	46	G7M
54	2w	47	U
54	2w	48	C
54	2w	63	G
54	2w	70	G
54	2w	71	G
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	16	C
55	2x	19	G
55	2x	21	A
55	2x	47	U
55	2x	48	C
55	2x	52	G
54	2y	7	A
54	2y	14	A
54	2y	15	G
54	2y	19	G
54	2y	23	A
54	2y	27	G
54	2y	28	G
54	2y	35	A
54	2y	41	C
54	2y	44	G
54	2y	45	U
54	2y	46	G7M
54	2y	48	C
54	2y	49	C
54	2y	50	U
54	2y	51	U
54	2y	53	G
54	2y	55	PSU

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Mol	Chain	Res	Type
54	2y	56	C
54	2y	58	A
54	2y	60	U
54	2y	65	G
54	2y	69	G
54	2y	70	G

All (51) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	199	A
1	1A	266	G
1	1A	278	A
1	1A	548	A
1	1A	685	A
1	1A	746	A
1	1A	764	A
1	1A	827	U
1	1A	974	G
1	1A	1047	G
1	1A	1067	A
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1176	G
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	2422	A
1	1A	2430	A
1	1A	2439	A
1	2A	196	A
1	2A	228	A
1	2A	249	C
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C

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Mol	Chain	Res	Type
1	2A	310	A
1	2A	528	A
1	2A	752	A
1	2A	774	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1608	A
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2406	U
1	2A	2439	A
1	2A	2689	U

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

86 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	$\#\|Z\| > 2$
1	OMG	1A	2251	55,56,1	23,26,27	1.21	3 (13%)	32,38,41	2.02	6 (18%)
32	5MC	1a	1404	32	19,22,23	1.57	3 (15%)	26,32,35	1.18	3 (11%)
1	PSU	2A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	1.93	3 (14%)
32	5MC	2a	967	32	19,22,23	1.63	3 (15%)	26,32,35	1.13	2 (7%)
43	0TD	1l	92	43	8,9,10	4.47	1 (12%)	6,11,13	4.99	2 (33%)
1	5MC	1A	1962	1	19,22,23	1.77	3 (15%)	26,32,35	1.22	3 (11%)
54	MIA	1w	37	54	28,31,32	2.32	6 (21%)	38,44,47	2.75	12 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	PSU	2w	55	54	18,21,22	1.41	2 (11%)	21,30,33	1.99	3 (14%)
54	PSU	1y	39	54	18,21,22	1.39	2 (11%)	21,30,33	1.87	3 (14%)
1	OMU	1A	2552	56,1	19,22,23	1.22	3 (15%)	25,31,34	1.80	5 (20%)
54	PSU	2w	39	54	18,21,22	1.40	2 (11%)	21,30,33	1.69	3 (14%)
1	5MU	1A	1939	56,1	19,22,23	1.43	4 (21%)	27,32,35	2.22	6 (22%)
54	MIA	1y	37	54	21,24,32	1.66	4 (19%)	30,35,47	1.98	7 (23%)
32	MA6	1a	1518	32	23,26,27	0.42	0	33,38,41	2.06	9 (27%)
55	5MC	2x	32	55	19,22,23	1.66	3 (15%)	26,32,35	1.19	3 (11%)
54	PSU	1w	32	56,54	18,21,22	1.33	2 (11%)	21,30,33	1.94	3 (14%)
54	5MU	2y	54	54	19,22,23	1.45	4 (21%)	27,32,35	2.01	6 (22%)
54	5MU	1w	54	54	19,22,23	1.37	5 (26%)	27,32,35	2.02	6 (22%)
1	OMG	2A	2251	55,56,1	23,26,27	1.20	3 (13%)	32,38,41	2.08	7 (21%)
32	4OC	2a	1402	32	20,23,24	0.74	0	25,32,35	0.97	1 (4%)
1	2MA	2A	2503	56,1	22,25,26	1.53	5 (22%)	32,37,40	2.32	8 (25%)
43	0TD	2l	92	43	8,9,10	4.63	1 (12%)	6,11,13	2.01	3 (50%)
32	4OC	1a	1402	32	20,23,24	0.77	0	25,32,35	1.04	3 (12%)
32	M2G	2a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.85	5 (15%)
54	PSU	2y	55	54	18,21,22	1.36	2 (11%)	21,30,33	2.15	5 (23%)
1	PSU	2A	1911	1	18,21,22	1.35	2 (11%)	21,30,33	2.01	3 (14%)
54	G7M	1w	46	54	23,26,27	1.56	3 (13%)	34,39,42	1.64	4 (11%)
54	PSU	1w	39	54	18,21,22	1.35	2 (11%)	21,30,33	1.90	4 (19%)
1	5MC	2A	1942	1	19,22,23	1.60	3 (15%)	26,32,35	1.13	2 (7%)
32	PSU	1a	516	32	18,21,22	1.36	3 (16%)	21,30,33	2.07	5 (23%)
54	PSU	2y	32	54	18,21,22	1.35	2 (11%)	21,30,33	1.94	3 (14%)
32	UR3	1a	1498	32	19,22,23	0.98	1 (5%)	26,32,35	1.84	4 (15%)
32	5MC	1a	1407	32	19,22,23	1.63	3 (15%)	26,32,35	1.10	3 (11%)
54	4SU	2w	8	54	18,21,22	1.76	5 (27%)	25,30,33	1.94	4 (16%)
1	5MU	1A	1915	1	19,22,23	1.44	5 (26%)	27,32,35	2.19	8 (29%)
32	5MC	1a	967	32	19,22,23	1.55	3 (15%)	26,32,35	1.09	2 (7%)
32	G7M	2a	527	56,32	23,26,27	1.46	4 (17%)	34,39,42	1.66	5 (14%)
55	31H	1x	76	55,56	31,34,35	1.19	3 (9%)	35,47,50	1.93	10 (28%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	0.94	1 (4%)
54	MIA	2w	37	54,53	24,27,32	2.20	5 (20%)	32,39,47	2.66	11 (34%)
32	UR3	2a	1498	56,32	19,22,23	1.02	2 (10%)	26,32,35	1.72	3 (11%)
1	PSU	1A	2605	56,1	18,21,22	1.42	4 (22%)	21,30,33	2.00	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	2MA	1A	2503	56,1	22,25,26	1.48	4 (18%)	32,37,40	2.38	9 (28%)
55	4SU	1x	8	55	18,21,22	2.23	6 (33%)	25,30,33	1.68	6 (24%)
54	5MU	2w	54	54	19,22,23	1.37	4 (21%)	27,32,35	1.93	7 (25%)
55	PSU	2x	55	55	18,21,22	1.34	2 (11%)	21,30,33	2.03	4 (19%)
54	4SU	1w	8	54	18,21,22	1.81	5 (27%)	25,30,33	2.00	5 (20%)
32	MA6	2a	1518	32	23,26,27	0.42	0	33,38,41	2.00	9 (27%)
32	5MC	1a	1400	32	19,22,23	1.62	3 (15%)	26,32,35	1.20	3 (11%)
55	4SU	2x	8	55	18,21,22	2.15	6 (33%)	25,30,33	1.29	6 (24%)
54	PSU	1y	55	54	18,21,22	1.38	2 (11%)	21,30,33	2.00	5 (23%)
54	4SU	1y	8	54	18,21,22	1.84	5 (27%)	25,30,33	1.84	4 (16%)
54	G7M	1y	46	54	23,26,27	1.53	4 (17%)	34,39,42	1.71	5 (14%)
54	G7M	2w	46	54	23,26,27	1.46	4 (17%)	34,39,42	1.69	5 (14%)
1	5MC	1A	1942	56,1	19,22,23	1.53	3 (15%)	26,32,35	1.12	2 (7%)
32	5MC	2a	1404	32	19,22,23	1.69	3 (15%)	26,32,35	1.17	3 (11%)
54	PSU	2y	39	54	18,21,22	1.41	2 (11%)	21,30,33	1.66	4 (19%)
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.05	9 (27%)
1	5MC	2A	1962	56,1	19,22,23	1.59	3 (15%)	26,32,35	1.16	2 (7%)
54	PSU	2w	32	54	18,21,22	1.34	2 (11%)	21,30,33	1.96	3 (14%)
54	G7M	2y	46	54	23,26,27	1.59	3 (13%)	34,39,42	1.79	4 (11%)
55	5MU	2x	54	55	19,22,23	1.40	5 (26%)	27,32,35	2.11	6 (22%)
32	2MG	2a	1207	32	23,26,27	1.23	2 (8%)	33,38,41	2.26	7 (21%)
32	5MC	2a	1400	32	19,22,23	1.63	3 (15%)	26,32,35	1.25	3 (11%)
54	MIA	2y	37	54	21,24,32	1.65	4 (19%)	30,35,47	2.01	7 (23%)
32	G7M	1a	527	56,32	23,26,27	1.53	3 (13%)	34,39,42	1.71	5 (14%)
32	M2G	1a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.82	6 (18%)
54	PSU	1w	55	54	18,21,22	1.38	2 (11%)	21,30,33	2.00	3 (14%)
1	OMU	2A	2552	56,1	19,22,23	1.23	2 (10%)	25,31,34	1.76	5 (20%)
55	5MU	1x	54	55,56	19,22,23	1.43	6 (31%)	27,32,35	2.04	6 (22%)
54	5MU	1y	54	54	19,22,23	1.41	5 (26%)	27,32,35	1.85	7 (25%)
55	31H	2x	76	55,56,57	31,34,35	1.20	3 (9%)	35,47,50	1.92	9 (25%)
55	PSU	1x	55	55	18,21,22	1.33	2 (11%)	21,30,33	2.06	4 (19%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	2.02	5 (23%)
1	PSU	2A	2605	1	18,21,22	1.32	2 (11%)	21,30,33	2.10	4 (19%)
55	5MC	1x	32	55	19,22,23	1.66	3 (15%)	26,32,35	1.23	2 (7%)
32	5MC	2a	1407	56,32	19,22,23	1.48	3 (15%)	26,32,35	1.22	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5MU	2A	1939	56,1	19,22,23	1.44	6 (31%)	27,32,35	2.38	6 (22%)
32	MA6	2a	1519	32	23,26,27	0.40	0	33,38,41	2.06	9 (27%)
1	PSU	1A	1917	1	18,21,22	1.41	2 (11%)	21,30,33	2.03	3 (14%)
54	4SU	2y	8	54	18,21,22	1.79	5 (27%)	25,30,33	2.06	5 (20%)
1	5MU	2A	1915	56,1	19,22,23	1.44	5 (26%)	27,32,35	2.15	6 (22%)
1	OMC	2A	1920	1	19,22,23	0.78	0	25,31,34	0.85	0
1	PSU	1A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	1.98	3 (14%)
54	PSU	1y	32	54	18,21,22	1.34	2 (11%)	21,30,33	1.96	4 (19%)
32	2MG	1a	1207	32	23,26,27	1.21	2 (8%)	33,38,41	2.23	8 (24%)

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
1	OMG	1A	2251	55,56,1	-	0/9/27/28	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	2/15/33/34	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	56,1	-	0/9/27/28	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	56,1	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/7/25/34	0/3/3/3
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	56,54	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	1/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,56,1	-	0/9/27/28	0/3/3/3
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
1	2MA	2A	2503	56,1	-	2/7/25/26	0/3/3/3
43	0TD	2l	92	43	-	2/7/12/14	-
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	2y	55	54	-	3/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	56,32	-	3/7/25/26	0/3/3/3
55	31H	1x	76	55,56	-	4/22/40/41	0/3/3/3
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
54	MIA	2w	37	54,53	-	4/11/29/34	0/3/3/3
32	UR3	2a	1498	56,32	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	56,1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	56,1	-	1/7/25/26	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	3/7/25/26	0/2/2/2
54	G7M	1y	46	54	-	2/7/25/26	0/3/3/3
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
1	5MC	1A	1942	56,1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
1	5MC	2A	1962	56,1	-	2/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	G7M	2y	46	54	-	1/7/25/26	0/3/3/3
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	2/9/27/28	0/3/3/3
32	5MC	2a	1400	32	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	MIA	2y	37	54	-	0/7/25/34	0/3/3/3
32	G7M	1a	527	56,32	-	3/7/25/26	0/3/3/3
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	56,1	-	0/9/27/28	0/2/2/2
55	5MU	1x	54	55,56	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	0/7/25/26	0/2/2/2
55	31H	2x	76	55,56,57	-	4/22/40/41	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	56,32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	56,1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	56,1	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3

All (253) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.80	1.69	1.82
43	1l	92	0TD	CB-SB	-12.14	1.70	1.82
54	2w	37	MIA	C2-S10	-7.41	1.69	1.75
54	1w	37	MIA	C13-C14	6.97	1.53	1.32
1	1A	1962	5MC	C5-C4	6.64	1.49	1.44
54	1w	37	MIA	C2-S10	-6.39	1.70	1.75
32	1a	1407	5MC	C5-C4	6.02	1.48	1.44
55	1x	32	5MC	C5-C4	5.96	1.48	1.44
32	2a	967	5MC	C5-C4	5.95	1.48	1.44
55	2x	32	5MC	C5-C4	5.92	1.48	1.44
32	2a	1404	5MC	C5-C4	5.90	1.48	1.44
32	2a	1400	5MC	C5-C4	5.82	1.48	1.44
32	1a	1400	5MC	C5-C4	5.79	1.48	1.44
1	2A	1962	5MC	C5-C4	5.71	1.48	1.44
1	2A	1942	5MC	C5-C4	5.62	1.48	1.44
55	1x	8	4SU	C4-N3	-5.54	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	8	4SU	C4-N3	-5.44	1.32	1.37
32	1a	967	5MC	C5-C4	5.43	1.48	1.44
32	1a	1404	5MC	C5-C4	5.40	1.48	1.44
1	1A	1942	5MC	C5-C4	5.37	1.48	1.44
54	1y	37	MIA	C5-C4	5.30	1.48	1.39
54	2y	37	MIA	C5-C4	5.27	1.48	1.39
54	2w	37	MIA	C5-C4	5.16	1.48	1.39
54	1w	37	MIA	C5-C4	5.05	1.48	1.39
32	2a	1407	5MC	C5-C4	4.94	1.47	1.44
54	1w	8	4SU	C4-S4	-4.77	1.60	1.68
32	1a	527	G7M	C5-N7	-4.76	1.33	1.39
54	1w	46	G7M	C5-N7	-4.76	1.33	1.39
54	2y	46	G7M	C5-N7	-4.73	1.33	1.39
54	2y	8	4SU	C4-S4	-4.67	1.60	1.68
54	1y	8	4SU	C4-S4	-4.65	1.60	1.68
54	2w	8	4SU	C4-S4	-4.63	1.60	1.68
54	1y	46	G7M	C5-N7	-4.46	1.34	1.39
1	2A	2503	2MA	C5-C4	4.45	1.47	1.39
55	2x	8	4SU	C4-S4	-4.35	1.61	1.68
55	1x	8	4SU	C4-S4	-4.29	1.61	1.68
54	2w	46	G7M	C5-N7	-4.27	1.34	1.39
1	1A	2503	2MA	C5-C4	4.24	1.46	1.39
32	2a	527	G7M	C5-N7	-4.19	1.34	1.39
55	1x	76	31H	C5-N7	-4.11	1.31	1.39
54	1w	55	PSU	C6-C5	4.00	1.39	1.35
55	2x	76	31H	C5-N7	-3.99	1.31	1.39
54	2w	55	PSU	C6-C5	3.96	1.39	1.35
54	1y	39	PSU	C6-C5	3.87	1.39	1.35
54	1y	55	PSU	C6-C5	3.86	1.39	1.35
54	2w	39	PSU	C6-C5	3.79	1.39	1.35
54	2y	39	PSU	C6-C5	3.79	1.39	1.35
54	2y	32	PSU	C6-C5	3.78	1.39	1.35
55	1x	8	4SU	C2-N3	-3.78	1.31	1.38
1	1A	1917	PSU	C6-C5	3.75	1.39	1.35
54	1y	32	PSU	C6-C5	3.69	1.39	1.35
54	1y	8	4SU	C4-N3	-3.69	1.33	1.37
1	2A	1917	PSU	C6-C5	3.62	1.39	1.35
32	2a	516	PSU	C6-C5	3.61	1.39	1.35
54	2y	46	G7M	C5-C4	3.59	1.47	1.38
54	2w	32	PSU	C6-C5	3.57	1.39	1.35
55	2x	55	PSU	C6-C5	3.56	1.39	1.35
54	1y	46	G7M	C5-C4	3.49	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	32	PSU	C6-C5	3.49	1.39	1.35
1	1A	1911	PSU	C6-C5	3.44	1.39	1.35
54	1w	39	PSU	C6-C5	3.43	1.39	1.35
54	1w	46	G7M	C5-C4	3.42	1.46	1.38
1	2A	2605	PSU	C6-C5	3.41	1.39	1.35
55	1x	8	4SU	C5-C4	-3.40	1.38	1.42
32	1a	527	G7M	C5-C4	3.39	1.46	1.38
32	2a	1404	5MC	C6-C5	3.34	1.40	1.34
55	1x	55	PSU	C6-C5	3.32	1.39	1.35
54	2w	46	G7M	C5-C4	3.32	1.46	1.38
55	2x	8	4SU	C2-N3	-3.30	1.32	1.38
54	2w	8	4SU	C4-N3	-3.30	1.34	1.37
1	2A	1911	PSU	C6-C5	3.30	1.38	1.35
32	2a	527	G7M	C5-C4	3.30	1.46	1.38
54	2y	8	4SU	C4-N3	-3.28	1.34	1.37
32	2a	966	M2G	C5-C4	3.25	1.47	1.38
1	1A	1939	5MU	C4-N3	-3.23	1.32	1.38
32	1a	516	PSU	C6-C5	3.21	1.38	1.35
55	2x	8	4SU	C5-C4	-3.20	1.38	1.42
32	2a	1207	2MG	C5-C4	3.18	1.47	1.38
1	2A	2251	OMG	C5-C4	3.09	1.47	1.38
54	1w	8	4SU	C4-N3	-3.05	1.34	1.37
55	1x	76	31H	C5-C4	-3.04	1.33	1.39
54	2w	37	MIA	C5-C6	3.03	1.49	1.41
32	1a	966	M2G	C2-N2	3.03	1.40	1.35
55	2x	76	31H	C5-C4	-3.02	1.33	1.39
1	2A	1942	5MC	C6-C5	3.00	1.39	1.34
1	1A	2605	PSU	C4-N3	-2.99	1.33	1.38
32	1a	1207	2MG	C5-C4	2.97	1.46	1.38
32	1a	966	M2G	C5-C4	2.97	1.46	1.38
54	2y	55	PSU	C6-C5	2.96	1.38	1.35
55	1x	54	5MU	C6-C5	2.95	1.39	1.34
1	1A	2251	OMG	C5-C4	2.95	1.46	1.38
54	2y	54	5MU	C6-C5	2.95	1.39	1.34
54	2y	37	MIA	C5-C6	2.94	1.49	1.41
55	2x	32	5MC	C6-C5	2.93	1.39	1.34
54	1y	37	MIA	C5-C6	2.92	1.49	1.41
54	1w	37	MIA	C5-C6	2.90	1.48	1.41
32	1a	967	5MC	C6-C5	2.90	1.39	1.34
1	1A	1939	5MU	C6-C5	2.87	1.39	1.34
1	2A	1915	5MU	C6-C5	2.87	1.39	1.34
55	1x	32	5MC	C6-C5	2.85	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	54	5MU	C2-N1	2.83	1.42	1.38
54	2y	39	PSU	C4-N3	-2.81	1.33	1.38
1	2A	2552	OMU	C4-N3	-2.79	1.33	1.38
54	2w	54	5MU	C6-C5	2.77	1.39	1.34
1	2A	1939	5MU	C4-N3	-2.77	1.33	1.38
54	1y	54	5MU	C6-C5	2.77	1.39	1.34
54	1w	8	4SU	C5-C4	-2.76	1.39	1.42
32	1a	1404	5MC	C6-C5	2.76	1.39	1.34
1	1A	2552	OMU	C4-N3	-2.75	1.33	1.38
54	2y	55	PSU	C4-N3	-2.74	1.33	1.38
55	1x	54	5MU	C4-N3	-2.74	1.33	1.38
1	2A	1939	5MU	C6-C5	2.73	1.39	1.34
54	2w	39	PSU	C4-N3	-2.70	1.33	1.38
1	1A	1915	5MU	C2-N1	2.70	1.42	1.38
1	1A	2503	2MA	C5-C6	2.70	1.48	1.41
32	1a	1400	5MC	C6-C5	2.70	1.39	1.34
55	2x	54	5MU	C6-C5	2.68	1.39	1.34
1	1A	1911	PSU	C4-N3	-2.68	1.33	1.38
32	1a	1407	5MC	C6-C5	2.67	1.39	1.34
1	1A	2251	OMG	C6-N1	-2.66	1.33	1.38
1	1A	1942	5MC	C6-C5	2.66	1.39	1.34
32	2a	1407	5MC	C6-C5	2.65	1.38	1.34
54	1w	39	PSU	C4-N3	-2.64	1.33	1.38
1	1A	1915	5MU	C6-C5	2.64	1.38	1.34
32	2a	1400	5MC	C6-C5	2.62	1.38	1.34
32	1a	516	PSU	C4-N3	-2.61	1.34	1.38
1	1A	1915	5MU	C4-N3	-2.60	1.34	1.38
54	1w	54	5MU	C6-C5	2.59	1.38	1.34
1	2A	1911	PSU	C4-N3	-2.59	1.34	1.38
1	2A	1915	5MU	C2-N1	2.58	1.42	1.38
1	2A	1962	5MC	C6-C5	2.56	1.38	1.34
32	2a	967	5MC	C6-C5	2.56	1.38	1.34
1	2A	1915	5MU	C4-N3	-2.56	1.34	1.38
1	1A	2503	2MA	C5-N7	-2.55	1.34	1.39
55	2x	54	5MU	C4-N3	-2.55	1.34	1.38
54	1y	54	5MU	C4-N3	-2.55	1.34	1.38
1	1A	2605	PSU	C2-N1	-2.54	1.33	1.36
32	1a	1207	2MG	C6-N1	-2.54	1.34	1.38
1	2A	1915	5MU	C4-C5	2.53	1.48	1.44
1	1A	2503	2MA	C8-N7	2.53	1.36	1.31
54	1y	39	PSU	C4-N3	-2.52	1.34	1.38
54	1w	54	5MU	C4-N3	-2.52	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C5-N7	-2.52	1.34	1.39
1	1A	1915	5MU	C4-C5	2.51	1.48	1.44
54	2y	54	5MU	C4-C5	2.50	1.48	1.44
32	2a	966	M2G	C2-N2	2.50	1.39	1.35
55	2x	55	PSU	C4-N3	-2.50	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.49	1.33	1.38
55	1x	55	PSU	C4-N3	-2.49	1.34	1.38
55	1x	76	31H	C5-C6	-2.49	1.34	1.41
1	2A	2503	2MA	C5-N7	-2.49	1.34	1.39
1	2A	2552	OMU	C2-N3	-2.49	1.33	1.38
54	1y	32	PSU	C4-N3	-2.49	1.34	1.38
55	1x	8	4SU	O2-C2	2.48	1.27	1.23
54	1y	37	MIA	C8-N7	2.47	1.36	1.31
32	1a	966	M2G	C6-N1	-2.47	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.46	1.33	1.38
54	2y	54	5MU	C4-N3	-2.45	1.34	1.38
1	1A	1962	5MC	C6-C5	2.45	1.38	1.34
54	2y	46	G7M	C6-N1	-2.45	1.34	1.38
54	1y	8	4SU	C5-C4	-2.45	1.39	1.42
1	1A	1939	5MU	C6-N1	-2.45	1.33	1.38
54	2w	55	PSU	C4-N3	-2.44	1.34	1.38
1	1A	1917	PSU	C4-N3	-2.43	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.42	1.33	1.38
55	2x	76	31H	C5-C6	-2.42	1.34	1.41
54	1w	46	G7M	C6-N1	-2.42	1.34	1.38
54	2y	8	4SU	C5-C4	-2.42	1.39	1.42
1	1A	1939	5MU	C2-N3	-2.41	1.33	1.38
54	2w	8	4SU	C5-C4	-2.41	1.39	1.42
54	2w	54	5MU	C4-N3	-2.40	1.34	1.38
54	1w	54	5MU	C4-C5	2.39	1.48	1.44
54	2y	32	PSU	C4-N3	-2.39	1.34	1.38
32	2a	966	M2G	C6-N1	-2.39	1.34	1.38
1	2A	2605	PSU	C4-N3	-2.39	1.34	1.38
54	2w	54	5MU	C4-C5	2.39	1.48	1.44
55	2x	54	5MU	C4-C5	2.38	1.48	1.44
32	2a	527	G7M	C6-N1	-2.38	1.34	1.38
54	1y	54	5MU	C2-N1	2.38	1.42	1.38
1	1A	2552	OMU	C2-N3	-2.38	1.33	1.38
55	2x	54	5MU	C2-N1	2.38	1.42	1.38
54	2y	8	4SU	C2-N1	2.38	1.42	1.38
1	2A	2251	OMG	C6-N1	-2.37	1.34	1.38
54	2y	37	MIA	C8-N7	2.37	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	516	PSU	C4-N3	-2.36	1.34	1.38
1	1A	2605	PSU	C6-C5	2.35	1.37	1.35
54	1w	32	PSU	C4-N3	-2.35	1.34	1.38
54	2w	32	PSU	C4-N3	-2.35	1.34	1.38
54	1w	55	PSU	C4-N3	-2.34	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.34	1.34	1.38
54	1w	8	4SU	C2-N1	2.34	1.42	1.38
1	2A	1917	PSU	C4-N3	-2.34	1.34	1.38
54	1y	55	PSU	C4-N3	-2.33	1.34	1.38
55	1x	54	5MU	C2-N1	2.32	1.42	1.38
1	2A	1939	5MU	C4-C5	2.32	1.48	1.44
32	2a	1207	2MG	C6-N1	-2.32	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.32	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.31	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.30	1.34	1.38
54	1y	54	5MU	C4-C5	2.30	1.48	1.44
55	1x	54	5MU	C4-C5	2.29	1.48	1.44
54	1y	46	G7M	C6-N1	-2.29	1.34	1.38
55	1x	32	5MC	C6-N1	-2.27	1.34	1.38
54	1w	37	MIA	C8-N7	2.27	1.36	1.31
54	1y	8	4SU	C2-N1	2.27	1.42	1.38
1	1A	2552	OMU	C5-C4	-2.27	1.38	1.43
1	2A	2251	OMG	C5-N7	-2.25	1.34	1.39
1	2A	2503	2MA	C5-C6	2.24	1.47	1.41
1	1A	1942	5MC	C6-N1	-2.24	1.34	1.38
32	2a	1498	UR3	C2-N1	2.23	1.41	1.38
54	1w	54	5MU	C2-N1	2.23	1.42	1.38
54	2y	8	4SU	C2-N3	-2.22	1.34	1.38
54	2w	8	4SU	C2-N3	-2.22	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.21	1.34	1.38
1	1A	2605	PSU	C2-N3	-2.20	1.33	1.37
54	2w	37	MIA	C5-N7	-2.19	1.35	1.39
55	2x	32	5MC	C6-N1	-2.17	1.34	1.38
54	1y	8	4SU	C2-N3	-2.16	1.34	1.38
55	2x	54	5MU	C6-N1	-2.16	1.34	1.38
1	2A	2503	2MA	C8-N7	2.15	1.35	1.31
1	2A	1942	5MC	C6-N1	-2.15	1.34	1.38
54	2w	37	MIA	C8-N7	2.15	1.35	1.31
1	1A	1915	5MU	C6-N1	-2.15	1.34	1.38
32	2a	967	5MC	C6-N1	-2.15	1.34	1.38
54	2w	54	5MU	C2-N1	2.14	1.41	1.38
32	1a	966	M2G	C5-N7	-2.14	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1939	5MU	C2-N1	2.14	1.41	1.38
1	2A	2503	2MA	C4-N9	-2.14	1.33	1.37
54	2y	37	MIA	C5-N7	-2.13	1.35	1.39
32	1a	516	PSU	C2-N3	-2.13	1.34	1.37
55	2x	8	4SU	O2-C2	2.11	1.26	1.23
1	1A	2251	OMG	C5-N7	-2.11	1.34	1.39
55	1x	54	5MU	C2-N3	-2.10	1.34	1.38
32	1a	1498	UR3	C2-N1	2.10	1.41	1.38
32	2a	1404	5MC	C6-N1	-2.09	1.34	1.38
32	1a	527	G7M	C6-N1	-2.09	1.34	1.38
32	1a	967	5MC	C6-N1	-2.07	1.34	1.38
55	1x	8	4SU	C6-C5	2.06	1.39	1.35
1	2A	1915	5MU	C6-N1	-2.05	1.34	1.38
54	1y	37	MIA	C5-N7	-2.05	1.35	1.39
32	1a	1407	5MC	C6-N1	-2.05	1.34	1.38
32	2a	527	G7M	C5-C6	2.04	1.48	1.43
32	2a	966	M2G	C5-N7	-2.04	1.35	1.39
54	2w	8	4SU	C2-N1	2.03	1.41	1.38
54	1y	46	G7M	C5-C6	2.03	1.48	1.43
54	1y	54	5MU	C2-N3	-2.03	1.34	1.38
32	2a	1498	UR3	C6-C5	2.02	1.39	1.35
54	2w	46	G7M	C6-N1	-2.02	1.35	1.38
54	2w	46	G7M	C5-C6	2.02	1.48	1.43
54	1w	8	4SU	C2-N3	-2.01	1.34	1.38
55	2x	8	4SU	C6-C5	2.01	1.39	1.35
55	1x	54	5MU	C6-N1	-2.00	1.34	1.38
54	1w	54	5MU	C6-N1	-2.00	1.34	1.38

All (414) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	-11.56	81.59	102.36
54	2w	37	MIA	C5-C4-N3	-8.96	117.74	127.18
54	1w	37	MIA	C12-C13-C14	-8.86	111.11	127.01
1	1A	2503	2MA	C5-C4-N3	-8.56	118.16	127.18
54	1w	37	MIA	C5-C4-N3	-8.27	118.47	127.18
1	2A	2503	2MA	C5-C4-N3	-7.73	119.04	127.18
32	1a	1498	UR3	C4-N3-C2	-7.25	118.75	124.58
54	2w	37	MIA	N3-C4-N9	7.25	136.19	126.99
32	1a	1207	2MG	C2-N3-C4	7.01	120.77	112.00
32	2a	1207	2MG	C2-N3-C4	6.97	120.72	112.00
32	2a	1498	UR3	C4-N3-C2	-6.77	119.13	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	37	MIA	N3-C4-N9	6.58	135.34	126.99
1	2A	2503	2MA	N3-C4-N9	6.55	135.30	126.99
1	2A	2605	PSU	N1-C2-N3	6.46	121.98	115.17
1	2A	2251	OMG	C5-C4-N3	-6.44	118.14	128.39
32	1a	516	PSU	N1-C2-N3	6.43	121.95	115.17
54	1y	55	PSU	N1-C2-N3	6.37	121.89	115.17
54	2y	55	PSU	N1-C2-N3	6.35	121.86	115.17
55	2x	55	PSU	N1-C2-N3	6.34	121.85	115.17
1	2A	1911	PSU	N1-C2-N3	6.33	121.84	115.17
55	1x	55	PSU	N1-C2-N3	6.23	121.74	115.17
1	1A	2605	PSU	N1-C2-N3	6.23	121.74	115.17
1	1A	1917	PSU	N1-C2-N3	6.23	121.74	115.17
32	2a	516	PSU	N1-C2-N3	6.21	121.72	115.17
54	2w	55	PSU	N1-C2-N3	6.21	121.72	115.17
1	1A	1911	PSU	N1-C2-N3	6.20	121.71	115.17
1	1A	2503	2MA	N3-C4-N9	6.17	134.82	126.99
54	1w	55	PSU	N1-C2-N3	6.15	121.65	115.17
32	2a	966	M2G	C5-C4-N3	-6.08	118.72	128.39
54	2w	32	PSU	N1-C2-N3	6.07	121.57	115.17
54	2y	46	G7M	N9-C4-N3	6.05	138.06	125.95
1	2A	1939	5MU	C4-N3-C2	-5.99	119.49	127.34
54	1w	32	PSU	N1-C2-N3	5.99	121.48	115.17
1	2A	1917	PSU	N1-C2-N3	5.97	121.47	115.17
1	1A	2251	OMG	C5-C4-N3	-5.96	118.90	128.39
54	2y	32	PSU	N1-C2-N3	5.94	121.43	115.17
54	2y	37	MIA	C5-C4-N3	-5.94	118.54	126.72
54	2y	8	4SU	C4-N3-C2	-5.93	121.63	127.31
54	1y	37	MIA	C5-C4-N3	-5.93	118.56	126.72
54	1y	39	PSU	N1-C2-N3	5.92	121.42	115.17
54	1y	32	PSU	N1-C2-N3	5.88	121.37	115.17
54	1w	39	PSU	N1-C2-N3	5.87	121.36	115.17
32	1a	966	M2G	C5-C4-N3	-5.79	119.18	128.39
32	1a	1207	2MG	C5-C4-N3	-5.74	119.26	128.39
55	2x	76	31H	N1-C2-N3	-5.71	119.93	128.58
32	2a	1207	2MG	C5-C4-N3	-5.70	119.32	128.39
1	1A	1939	5MU	C5-C4-N3	5.69	120.27	115.32
55	1x	76	31H	N1-C2-N3	-5.66	120.02	128.58
54	2w	8	4SU	C4-N3-C2	-5.60	121.95	127.31
54	1y	46	G7M	N9-C4-N3	5.55	137.06	125.95
1	2A	1939	5MU	C5-C4-N3	5.49	120.09	115.32
54	1w	8	4SU	C4-N3-C2	-5.43	122.11	127.31
54	1w	46	G7M	N9-C4-N3	5.37	136.70	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1y	46	G7M	C5-C4-N3	-5.34	118.05	128.15
54	2y	46	G7M	C5-C4-N3	-5.32	118.09	128.15
1	1A	1915	5MU	C4-N3-C2	-5.32	120.36	127.34
54	1y	8	4SU	C4-N3-C2	-5.31	122.22	127.31
54	2w	39	PSU	N1-C2-N3	5.29	120.75	115.17
1	2A	1915	5MU	C4-N3-C2	-5.28	120.42	127.34
1	1A	1939	5MU	C4-N3-C2	-5.27	120.42	127.34
1	1A	1915	5MU	N3-C2-N1	5.27	121.75	114.89
32	2a	527	G7M	C5-C4-N3	-5.27	118.20	128.15
32	2a	527	G7M	N9-C4-N3	5.25	136.44	125.95
54	1w	8	4SU	C5-C4-N3	5.24	119.63	114.75
32	1a	527	G7M	N9-C4-N3	5.23	136.41	125.95
1	2A	1939	5MU	N3-C2-N1	5.22	121.69	114.89
54	2y	39	PSU	N1-C2-N3	5.20	120.66	115.17
1	1A	2251	OMG	C2-N3-C4	5.19	121.24	112.30
55	1x	54	5MU	N3-C2-N1	5.19	121.65	114.89
54	2w	46	G7M	N9-C4-N3	5.19	136.33	125.95
55	2x	54	5MU	N3-C2-N1	5.19	121.64	114.89
32	1a	527	G7M	C5-C4-N3	-5.17	118.38	128.15
54	2y	8	4SU	C5-C4-N3	5.13	119.53	114.75
54	2w	37	MIA	C11-S10-C2	-5.13	98.40	102.25
1	2A	1915	5MU	N3-C2-N1	5.12	121.56	114.89
55	2x	54	5MU	C4-N3-C2	-5.12	120.63	127.34
54	2w	46	G7M	C5-C4-N3	-5.04	118.63	128.15
54	2w	8	4SU	C5-C4-N3	5.00	119.40	114.75
1	2A	2251	OMG	N9-C4-N3	4.95	135.84	125.95
1	2A	2251	OMG	C2-N3-C4	4.93	120.78	112.30
54	1w	54	5MU	N3-C2-N1	4.91	121.28	114.89
55	1x	54	5MU	C4-N3-C2	-4.89	120.93	127.34
54	1y	46	G7M	C2-N3-C4	4.88	120.70	112.30
54	1w	54	5MU	C4-N3-C2	-4.87	120.96	127.34
54	2y	37	MIA	N3-C4-N9	4.86	135.43	127.17
55	2x	76	31H	C5-C4-N3	-4.84	120.05	126.72
32	2a	1518	MA6	N1-C2-N3	-4.82	121.28	128.58
54	1w	46	G7M	C5-C4-N3	-4.82	119.05	128.15
54	1y	8	4SU	C5-C4-N3	4.77	119.19	114.75
54	2y	54	5MU	N3-C2-N1	4.77	121.10	114.89
54	2y	54	5MU	C4-N3-C2	-4.74	121.13	127.34
32	1a	1518	MA6	N1-C2-N3	-4.73	121.42	128.58
1	2A	1915	5MU	C5-C4-N3	4.72	119.43	115.32
32	2a	1519	MA6	N1-C2-N3	-4.72	121.44	128.58
54	1y	37	MIA	N3-C4-N9	4.71	135.18	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2552	OMU	C4-N3-C2	-4.71	120.76	126.61
54	2y	55	PSU	C4-N3-C2	-4.69	119.92	126.37
32	2a	527	G7M	C2-N3-C4	4.68	120.35	112.30
1	1A	2251	OMG	N9-C4-N3	4.66	135.27	125.95
54	2y	46	G7M	C2-N3-C4	4.65	120.32	112.30
32	1a	1519	MA6	N1-C2-N3	-4.65	121.54	128.58
1	2A	1939	5MU	O4-C4-C5	-4.65	119.60	124.92
54	2w	46	G7M	C2-N3-C4	4.64	120.29	112.30
55	1x	76	31H	C5-C4-N3	-4.63	120.33	126.72
32	1a	527	G7M	C2-N3-C4	4.63	120.28	112.30
1	2A	2552	OMU	C4-N3-C2	-4.59	120.92	126.61
1	1A	1939	5MU	O4-C4-C5	-4.57	119.69	124.92
1	1A	1915	5MU	C5-C4-N3	4.56	119.29	115.32
32	1a	1519	MA6	C5-C4-N3	-4.56	120.43	126.72
54	2w	54	5MU	N3-C2-N1	4.52	120.77	114.89
32	2a	1518	MA6	C5-C4-N3	-4.51	120.50	126.72
1	1A	1939	5MU	C5-C6-N1	-4.51	118.41	123.31
32	1a	966	M2G	N9-C4-N3	4.47	134.90	125.95
1	2A	1939	5MU	C5-C6-N1	-4.44	118.49	123.31
54	2w	54	5MU	C4-N3-C2	-4.44	121.52	127.34
1	2A	2605	PSU	C4-N3-C2	-4.41	120.29	126.37
1	1A	1939	5MU	N3-C2-N1	4.38	120.59	114.89
32	2a	966	M2G	C2-N3-C4	4.33	120.52	112.51
32	1a	966	M2G	C2-N3-C4	4.33	120.52	112.51
55	1x	55	PSU	C4-N3-C2	-4.32	120.42	126.37
1	2A	2552	OMU	N3-C2-N1	4.32	120.51	114.89
32	1a	516	PSU	C4-N3-C2	-4.31	120.44	126.37
32	2a	1519	MA6	C5-C4-N3	-4.29	120.80	126.72
32	2a	966	M2G	N9-C4-N3	4.27	134.50	125.95
54	2y	54	5MU	C5-C4-N3	4.26	119.02	115.32
55	2x	55	PSU	C4-N3-C2	-4.25	120.52	126.37
54	1w	54	5MU	C5-C4-N3	4.23	119.00	115.32
55	2x	54	5MU	C5-C4-N3	4.23	119.00	115.32
54	1w	46	G7M	C2-N3-C4	4.21	119.56	112.30
54	1y	54	5MU	N3-C2-N1	4.16	120.31	114.89
32	1a	1518	MA6	C5-N7-C8	4.14	109.96	103.45
1	1A	2552	OMU	N3-C2-N1	4.14	120.28	114.89
1	2A	1911	PSU	C4-N3-C2	-4.13	120.68	126.37
55	1x	8	4SU	C6-C5-C4	-4.12	116.38	119.95
1	2A	1915	5MU	O4-C4-C5	-4.11	120.21	124.92
1	1A	2503	2MA	C4-C5-N7	-4.09	105.91	110.58
54	2y	8	4SU	N3-C2-N1	4.09	120.21	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	54	5MU	O4-C4-C5	-4.09	120.24	124.92
32	1a	1518	MA6	C4-C5-N7	-4.08	105.92	110.58
32	2a	516	PSU	C4-N3-C2	-4.07	120.76	126.37
54	1y	54	5MU	C4-N3-C2	-4.06	122.02	127.34
55	1x	32	5MC	C5-C6-N1	-4.06	118.91	123.31
55	1x	54	5MU	C5-C4-N3	4.05	118.84	115.32
32	1a	1518	MA6	C2-N1-C6	4.04	121.71	111.83
54	1y	32	PSU	C4-N3-C2	-4.02	120.84	126.37
32	1a	1518	MA6	C5-C4-N3	-4.02	121.18	126.72
54	1w	37	MIA	C15-C14-C13	-4.01	110.63	122.66
32	2a	1207	2MG	C6-C5-N7	4.00	137.57	130.29
32	1a	1207	2MG	C6-C5-N7	3.99	137.56	130.29
32	2a	1518	MA6	C2-N1-C6	3.99	121.58	111.83
32	2a	1519	MA6	C5-N7-C8	3.97	109.69	103.45
1	1A	1911	PSU	C4-N3-C2	-3.96	120.92	126.37
54	2w	32	PSU	C4-N3-C2	-3.94	120.94	126.37
54	2y	54	5MU	O4-C4-C5	-3.93	120.43	124.92
1	1A	2552	OMU	C5-C4-N3	3.92	120.28	114.80
32	2a	1519	MA6	C4-C5-N7	-3.91	106.11	110.58
32	2a	1519	MA6	C2-N1-C6	3.90	121.36	111.83
54	2y	32	PSU	C4-N3-C2	-3.90	121.00	126.37
1	1A	1962	5MC	C5-C6-N1	-3.90	119.08	123.31
54	1w	54	5MU	O4-C4-C5	-3.89	120.46	124.92
54	2w	54	5MU	C5-C4-N3	3.89	118.70	115.32
55	1x	54	5MU	O4-C4-C5	-3.86	120.50	124.92
1	1A	1917	PSU	C4-N3-C2	-3.84	121.08	126.37
54	1y	54	5MU	C5-C4-N3	3.83	118.65	115.32
32	1a	1519	MA6	C2-N1-C6	3.81	121.15	111.83
32	1a	1519	MA6	C4-C5-N7	-3.81	106.22	110.58
54	1w	55	PSU	C4-N3-C2	-3.81	121.12	126.37
32	1a	1519	MA6	C5-N7-C8	3.81	109.43	103.45
54	2w	55	PSU	C4-N3-C2	-3.80	121.14	126.37
32	1a	1207	2MG	N9-C4-N3	3.80	133.54	125.95
54	1y	55	PSU	C4-N3-C2	-3.78	121.17	126.37
54	2w	8	4SU	N3-C2-N1	3.78	119.81	114.89
54	1w	39	PSU	C4-N3-C2	-3.77	121.17	126.37
54	1w	32	PSU	C4-N3-C2	-3.77	121.18	126.37
54	2y	55	PSU	O2-C2-N1	-3.77	118.91	122.79
1	1A	1915	5MU	O4-C4-C5	-3.76	120.62	124.92
1	1A	2605	PSU	O2-C2-N1	-3.76	118.91	122.79
54	1y	54	5MU	O4-C4-C5	-3.74	120.64	124.92
54	1w	8	4SU	C5-C4-S4	-3.74	120.03	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2w	54	5MU	O4-C4-C5	-3.74	120.64	124.92
1	1A	2605	PSU	C4-N3-C2	-3.74	121.22	126.37
1	1A	1917	PSU	O2-C2-N1	-3.73	118.94	122.79
32	1a	1518	MA6	N9-C8-N7	-3.73	108.65	113.94
54	1y	8	4SU	N3-C2-N1	3.71	119.72	114.89
1	2A	1962	5MC	C5-C6-N1	-3.70	119.29	123.31
1	2A	1917	PSU	C4-N3-C2	-3.70	121.27	126.37
54	1y	39	PSU	C4-N3-C2	-3.68	121.31	126.37
1	2A	1917	PSU	O2-C2-N1	-3.67	119.00	122.79
32	1a	1404	5MC	C5-C6-N1	-3.66	119.34	123.31
54	1w	32	PSU	O2-C2-N1	-3.64	119.04	122.79
55	1x	8	4SU	O2-C2-N1	3.63	127.52	122.80
54	2y	37	MIA	C2-N3-C4	3.61	120.64	111.83
54	1y	37	MIA	C2-N3-C4	3.59	120.61	111.83
32	2a	1404	5MC	C5-C6-N1	-3.59	119.42	123.31
32	2a	1519	MA6	N9-C8-N7	-3.57	108.87	113.94
32	2a	1518	MA6	C5-N7-C8	3.57	109.06	103.45
1	2A	2552	OMU	C5-C4-N3	3.56	119.78	114.80
32	2a	1518	MA6	C4-C5-N7	-3.56	106.52	110.58
54	2w	32	PSU	O2-C2-N1	-3.55	119.13	122.79
32	2a	1207	2MG	N1-C2-N2	3.53	120.16	116.56
54	1w	37	MIA	C16-C14-C13	-3.52	112.08	122.66
32	2a	516	PSU	O2-C2-N1	-3.52	119.16	122.79
55	1x	54	5MU	C5-C6-N1	-3.52	119.49	123.31
54	2w	55	PSU	O2-C2-N1	-3.51	119.17	122.79
54	1y	55	PSU	O2-C2-N1	-3.50	119.18	122.79
32	1a	1400	5MC	C5-C6-N1	-3.49	119.52	123.31
32	1a	967	5MC	C5-C6-N1	-3.48	119.53	123.31
1	2A	1942	5MC	C5-C6-N1	-3.48	119.53	123.31
54	1w	8	4SU	N3-C2-N1	3.47	119.41	114.89
32	2a	1407	5MC	C5-C6-N1	-3.47	119.55	123.31
32	2a	1207	2MG	N9-C4-N3	3.46	132.88	125.95
54	1y	32	PSU	O2-C2-N1	-3.45	119.23	122.79
1	2A	2503	2MA	C4-N9-C8	3.45	109.36	105.74
1	2A	1915	5MU	C5-C6-N1	-3.44	119.57	123.31
54	2w	37	MIA	C4-C5-N7	-3.43	106.66	110.58
55	2x	76	31H	N9-C8-N7	-3.43	109.07	113.94
54	2y	32	PSU	O2-C2-N1	-3.43	119.25	122.79
55	1x	76	31H	N9-C8-N7	-3.43	109.07	113.94
32	1a	1498	UR3	C5-C4-N3	3.42	119.55	115.04
1	1A	1911	PSU	O2-C2-N1	-3.41	119.27	122.79
54	1y	37	MIA	C4-C5-N7	-3.41	106.68	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	55	PSU	O2-C2-N1	-3.41	119.27	122.79
32	2a	1518	MA6	C2-N3-C4	3.40	120.14	111.83
32	1a	1519	MA6	C2-N3-C4	3.40	120.14	111.83
55	2x	76	31H	C2-N3-C4	3.35	120.01	111.83
54	1w	37	MIA	C2-N3-C4	3.34	121.05	112.29
32	2a	1519	MA6	C2-N3-C4	3.34	119.98	111.83
32	2a	966	M2G	C6-C5-N7	3.33	136.36	130.29
55	2x	32	5MC	C5-C6-N1	-3.33	119.70	123.31
32	1a	1519	MA6	N9-C8-N7	-3.33	109.21	113.94
54	2y	37	MIA	C4-C5-N7	-3.33	106.78	110.58
55	1x	55	PSU	O2-C2-N1	-3.30	119.39	122.79
32	2a	1498	UR3	C5-C4-N3	3.30	119.38	115.04
32	1a	516	PSU	O2-C2-N1	-3.29	119.40	122.79
1	1A	2251	OMG	C6-C5-N7	3.28	136.27	130.29
1	2A	2605	PSU	O2-C2-N1	-3.28	119.40	122.79
55	1x	76	31H	C2-N3-C4	3.28	119.84	111.83
32	2a	967	5MC	C5-C6-N1	-3.28	119.75	123.31
32	1a	1407	5MC	C5-C6-N1	-3.27	119.76	123.31
54	1w	37	MIA	C4-C5-N7	-3.26	106.86	110.58
32	2a	1400	5MC	C5-C6-N1	-3.25	119.78	123.31
1	1A	1942	5MC	C5-C4-N3	-3.25	118.43	121.75
54	2y	37	MIA	N3-C2-N1	-3.24	123.67	128.58
43	2l	92	0TD	OD2-CG-CB	3.23	120.12	113.15
54	1y	37	MIA	N3-C2-N1	-3.22	123.71	128.58
54	2w	37	MIA	C2-N3-C4	3.20	120.68	112.29
54	1w	39	PSU	O2-C2-N1	-3.20	119.48	122.79
1	2A	1911	PSU	O2-C2-N1	-3.20	119.49	122.79
54	2w	8	4SU	C5-C4-S4	-3.20	120.66	124.31
55	2x	54	5MU	C5-C6-N1	-3.20	119.84	123.31
32	2a	1207	2MG	N2-C2-N3	-3.19	116.45	120.51
54	2w	39	PSU	C4-N3-C2	-3.19	121.98	126.37
1	2A	2503	2MA	C4-C5-N7	-3.18	106.94	110.58
32	1a	1518	MA6	C2-N3-C4	3.18	119.61	111.83
32	2a	1207	2MG	C4-C5-N7	-3.15	105.67	110.67
1	1A	1915	5MU	C5-C6-N1	-3.14	119.90	123.31
32	1a	1207	2MG	C4-C5-N7	-3.13	105.72	110.67
55	1x	8	4SU	C4-N3-C2	3.11	130.30	127.31
54	2y	8	4SU	C5-C4-S4	-3.11	120.76	124.31
32	2a	1518	MA6	N9-C8-N7	-3.10	109.54	113.94
55	1x	76	31H	C5-N7-C8	3.06	108.26	103.45
55	2x	55	PSU	O2-C2-N1	-3.06	119.64	122.79
54	2y	54	5MU	C5-C6-N1	-3.04	120.01	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2251	OMG	C6-C5-N7	3.04	135.82	130.29
1	1A	2503	2MA	C5-N7-C8	3.04	108.22	103.45
1	1A	2552	OMU	O4-C4-C5	-3.04	119.93	125.16
54	2y	39	PSU	C4-N3-C2	-3.03	122.19	126.37
1	2A	1939	5MU	O2-C2-N1	-3.03	118.85	122.80
43	1l	92	0TD	OD2-CG-CB	3.03	119.69	113.15
1	2A	2503	2MA	C2-N1-C6	3.02	122.74	118.10
1	2A	2503	2MA	N6-C6-N1	3.02	121.10	117.03
55	2x	76	31H	C5-N7-C8	2.99	108.15	103.45
54	2w	54	5MU	C5-C6-N1	-2.98	120.08	123.31
32	1a	966	M2G	C6-C5-N7	2.98	135.70	130.29
54	1w	54	5MU	C5-C6-N1	-2.95	120.11	123.31
32	2a	1404	5MC	C5-C4-N3	-2.92	118.76	121.75
54	1w	37	MIA	C6-C5-N7	2.92	135.62	132.43
54	1y	54	5MU	C5-C6-N1	-2.85	120.22	123.31
55	1x	32	5MC	C5-C4-N3	-2.85	118.83	121.75
32	1a	1207	2MG	N1-C2-N2	2.84	119.46	116.56
32	2a	1407	5MC	C5-C4-N3	-2.84	118.84	121.75
55	1x	8	4SU	S4-C4-N3	-2.84	117.23	120.20
1	2A	1942	5MC	C5-C4-N3	-2.83	118.85	121.75
32	2a	1518	MA6	N3-C4-N9	2.79	131.91	127.17
32	2a	966	M2G	C4-C5-N7	-2.78	106.26	110.67
1	1A	1942	5MC	C5-C6-N1	-2.76	120.31	123.31
1	1A	2552	OMU	O2-C2-N1	-2.76	119.20	122.80
32	1a	1519	MA6	N3-C4-N9	2.75	131.84	127.17
1	2A	2251	OMG	C4-C5-N7	-2.75	106.32	110.67
32	2a	1400	5MC	O2-C2-N3	-2.74	118.01	122.33
55	2x	8	4SU	C6-C5-C4	-2.73	117.59	119.95
55	2x	32	5MC	C5-C4-N3	-2.70	118.98	121.75
1	2A	1962	5MC	C5-C4-N3	-2.70	118.99	121.75
32	1a	1400	5MC	C5-C4-N3	-2.68	119.01	121.75
54	2w	54	5MU	O2-C2-N1	-2.64	119.36	122.80
1	2A	2552	OMU	O2-C2-N1	-2.64	119.37	122.80
32	1a	1404	5MC	C5-C4-N3	-2.63	119.06	121.75
32	1a	1407	5MC	C5-C4-N3	-2.63	119.06	121.75
55	2x	76	31H	C4'-O4'-C1'	-2.62	103.67	109.47
54	1w	54	5MU	O2-C2-N1	-2.60	119.41	122.80
1	1A	2503	2MA	C6-C5-N7	2.60	137.10	132.09
54	1w	37	MIA	C2-N1-C6	2.60	122.47	117.54
1	2A	2503	2MA	C5-N7-C8	2.59	107.52	103.45
1	1A	1915	5MU	C5M-C5-C4	2.59	121.54	118.78
54	2w	46	G7M	O6-C6-C5	-2.58	122.24	128.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1519	MA6	N3-C4-N9	2.58	131.56	127.17
55	2x	32	5MC	O2-C2-N3	-2.57	118.28	122.33
55	1x	76	31H	CA-N-CN	-2.55	118.90	122.82
32	1a	527	G7M	O6-C6-C5	-2.52	122.38	128.01
1	1A	2503	2MA	C2-N1-C6	2.52	121.97	118.10
54	1w	8	4SU	C1'-N1-C2	2.51	122.10	117.59
1	1A	1939	5MU	O2-C2-N1	-2.51	119.53	122.80
55	2x	76	31H	N3-C4-N9	2.51	131.43	127.17
54	1y	39	PSU	O2-C2-N1	-2.50	120.21	122.79
32	2a	1518	MA6	C4-C5-C6	2.49	118.49	115.91
55	2x	76	31H	C5-C4-N9	2.48	108.52	105.81
55	1x	76	31H	C4'-O4'-C1'	-2.47	104.00	109.47
54	2w	37	MIA	C5-N7-C8	2.46	107.32	103.45
55	2x	8	4SU	C5-C4-N3	2.46	117.04	114.75
55	2x	54	5MU	O2-C2-N1	-2.46	119.60	122.80
54	1y	8	4SU	C5-C4-S4	-2.46	121.50	124.31
54	2y	37	MIA	C5-N7-C8	2.45	107.30	103.45
32	1a	966	M2G	O6-C6-C5	-2.45	120.07	126.53
1	1A	1962	5MC	C5-C4-N3	-2.44	119.25	121.75
32	1a	1519	MA6	C4-C5-C6	2.44	118.43	115.91
1	1A	2503	2MA	C4-N9-C8	2.44	108.30	105.74
1	1A	2251	OMG	C4-C5-N7	-2.43	106.81	110.67
32	1a	1207	2MG	N2-C2-N3	-2.43	117.41	120.51
55	2x	8	4SU	C1'-N1-C2	2.43	121.96	117.59
32	1a	1404	5MC	O2-C2-N3	-2.43	118.50	122.33
55	1x	76	31H	N3-C4-N9	2.42	131.29	127.17
54	1y	37	MIA	C5-N7-C8	2.42	107.25	103.45
1	2A	2503	2MA	N9-C8-N7	-2.42	110.51	113.94
54	2y	37	MIA	C4-N9-C8	2.41	108.27	105.74
1	2A	2552	OMU	O4-C4-C5	-2.41	121.00	125.16
43	2l	92	0TD	CSB-SB-CB	-2.40	98.05	102.36
55	1x	54	5MU	O2-C2-N1	-2.40	119.68	122.80
43	2l	92	0TD	OD1-CG-CB	-2.39	117.43	122.44
55	1x	8	4SU	C1'-N1-C2	2.38	121.87	117.59
1	1A	2503	2MA	N9-C8-N7	-2.38	110.56	113.94
1	1A	2503	2MA	N6-C6-N1	2.38	120.23	117.03
1	1A	2251	OMG	O6-C6-C5	-2.38	120.26	126.53
32	2a	1400	5MC	C5-C4-N3	-2.36	119.33	121.75
54	2w	37	MIA	C12-N6-C6	-2.36	120.66	122.85
55	1x	76	31H	C5-C4-N9	2.35	108.38	105.81
32	2a	967	5MC	C5-C4-N3	-2.34	119.36	121.75
54	1w	46	G7M	O6-C6-C5	-2.34	122.79	128.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	37	MIA	N3-C2-N1	-2.33	122.74	127.00
32	2a	1402	4OC	C6-C5-C4	2.33	119.81	117.00
32	1a	516	PSU	C5-C6-N1	-2.32	118.92	122.14
32	2a	1407	5MC	O2-C2-N3	-2.32	118.67	122.33
55	1x	76	31H	OCN-CN-N	-2.32	119.34	125.32
32	1a	1518	MA6	N3-C4-N9	2.31	131.09	127.17
54	2w	54	5MU	C5M-C5-C4	2.30	121.24	118.78
54	2y	46	G7M	O6-C6-C5	-2.30	122.87	128.01
32	2a	516	PSU	O4'-C1'-C2'	2.30	108.33	105.15
1	1A	1962	5MC	CM5-C5-C6	-2.30	119.74	122.85
54	1w	37	MIA	C5-N7-C8	2.29	107.05	103.45
54	2y	55	PSU	C5-C6-N1	-2.29	118.97	122.14
55	1x	55	PSU	C5-C6-N1	-2.29	118.97	122.14
55	2x	8	4SU	S4-C4-N3	-2.28	117.81	120.20
32	1a	1402	4OC	C6-C5-C4	2.28	119.75	117.00
32	1a	1498	UR3	C3U-N3-C4	2.28	121.03	117.87
32	1a	967	5MC	C5-C4-N3	-2.27	119.42	121.75
32	1a	966	M2G	C4-C5-N7	-2.27	107.08	110.67
32	2a	1498	UR3	C3U-N3-C4	2.25	120.99	117.87
1	1A	1915	5MU	O2-C2-N1	-2.25	119.87	122.80
1	2A	2251	OMG	O6-C6-C5	-2.24	120.61	126.53
54	2w	37	MIA	C4-N9-C8	2.24	108.09	105.74
55	2x	8	4SU	O2-C2-N1	2.24	125.71	122.80
54	1y	37	MIA	C4-N9-C8	2.22	108.07	105.74
1	2A	1915	5MU	O2-C2-N1	-2.22	119.91	122.80
54	1y	46	G7M	O6-C6-C5	-2.22	123.07	128.01
54	2w	37	MIA	C4-C5-C6	2.21	118.62	116.78
1	2A	2251	OMG	C8-N7-C5	2.21	108.19	104.26
55	2x	55	PSU	C5-C6-N1	-2.20	119.08	122.14
54	2y	54	5MU	C1'-N1-C2	2.20	121.54	117.59
1	1A	1915	5MU	C5M-C5-C6	-2.19	119.89	122.85
1	1A	1920	OMC	O2-C2-N3	-2.18	118.90	122.33
1	2A	2605	PSU	C5-C6-N1	-2.18	119.12	122.14
54	2w	37	MIA	C1'-N9-C8	-2.18	122.27	127.09
32	1a	1518	MA6	C4-C5-C6	2.17	118.15	115.91
32	2a	1404	5MC	O2-C2-N3	-2.16	118.92	122.33
54	1y	54	5MU	C1'-N1-C2	2.16	121.47	117.59
54	2y	8	4SU	C1'-N1-C2	2.16	121.47	117.59
54	2y	55	PSU	O4'-C1'-C2'	2.15	108.13	105.15
32	1a	516	PSU	O4'-C1'-C2'	2.14	108.11	105.15
32	1a	527	G7M	C5-C6-N1	2.14	116.26	111.84
54	1w	37	MIA	C4-N9-C8	2.12	107.97	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1207	2MG	C8-N7-C5	2.12	108.03	104.26
55	1x	8	4SU	C5-C4-N3	2.11	116.72	114.75
54	2w	46	G7M	C5-C6-N1	2.11	116.20	111.84
54	2w	37	MIA	C6-C5-N7	2.11	134.73	132.43
32	2a	1519	MA6	C4-C5-C6	2.11	118.09	115.91
54	1y	55	PSU	C5-C6-N1	-2.11	119.22	122.14
55	2x	8	4SU	C6-N1-C2	-2.10	118.44	121.00
32	2a	527	G7M	C5-C6-N1	2.09	116.17	111.84
54	1y	32	PSU	C5-C6-N1	-2.08	119.26	122.14
32	2a	516	PSU	C5-C6-N1	-2.06	119.28	122.14
32	1a	1498	UR3	C1'-N1-C2	2.06	120.42	117.04
1	1A	2605	PSU	C5-C6-N1	-2.06	119.29	122.14
55	2x	76	31H	C4-C5-N7	-2.05	108.23	110.58
54	2y	39	PSU	C5-C6-N1	-2.05	119.29	122.14
54	1w	39	PSU	C5-C6-N1	-2.04	119.31	122.14
32	1a	1400	5MC	O2-C2-N3	-2.04	119.11	122.33
54	2y	39	PSU	O2-C2-N3	-2.03	118.25	121.86
32	1a	1407	5MC	O2-C2-N3	-2.03	119.13	122.33
32	1a	1402	4OC	CM4-N4-C4	-2.03	118.48	122.45
54	1y	55	PSU	O4'-C1'-C2'	2.01	107.94	105.15
32	2a	527	G7M	O6-C6-C5	-2.01	123.52	128.01
32	1a	1402	4OC	O2-C2-N3	-2.01	119.16	122.33
54	1y	54	5MU	C5M-C5-C4	2.01	120.93	118.78
54	1y	46	G7M	C5-C6-N1	2.01	115.99	111.84
54	2w	39	PSU	O2-C2-N3	-2.01	118.30	121.86

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C16
54	1y	46	G7M	C4'-C5'-O5'-P
32	2a	1207	2MG	N1-C2-N2-CM2
32	2a	1207	2MG	N3-C2-N2-CM2
32	2a	1519	MA6	O4'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
54	2w	37	MIA	C5-C6-N6-C12
54	2w	37	MIA	N1-C6-N6-C12
54	2w	37	MIA	N1-C2-S10-C11
54	2w	37	MIA	N3-C2-S10-C11
54	2y	55	PSU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
55	1x	76	31H	C3'-C4'-C5'-O5'
55	2x	76	31H	C3'-C4'-C5'-O5'
54	1y	8	4SU	O4'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
55	2x	76	31H	CB-CG-SD-CE
32	1a	1402	4OC	O4'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
55	2x	76	31H	O4'-C4'-C5'-O5'
54	2y	55	PSU	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
55	1x	76	31H	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C15
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
55	1x	76	31H	C4'-C5'-O5'-P
55	2x	76	31H	C4'-C5'-O5'-P
1	2A	1917	PSU	O4'-C4'-C5'-O5'
1	2A	2503	2MA	C3'-C4'-C5'-O5'
54	1y	46	G7M	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
54	2w	46	G7M	C4'-C5'-O5'-P
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C4'-C5'-O5'-P
54	1w	46	G7M	C4'-C5'-O5'-P
32	1a	1402	4OC	C3'-C4'-C5'-O5'
54	2y	54	5MU	O4'-C4'-C5'-O5'
43	2l	92	0TD	CA-CB-SB-CSB
32	2a	527	G7M	C4'-C5'-O5'-P
55	1x	76	31H	CB-CG-SD-CE
1	2A	1962	5MC	C2'-C1'-N1-C6
32	2a	1400	5MC	C2'-C1'-N1-C6
1	1A	2503	2MA	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
54	2y	55	PSU	C2'-C1'-C5-C6
54	2y	46	G7M	C2'-C1'-N9-C8
54	1y	8	4SU	C4'-C5'-O5'-P
32	2a	1400	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	O4'-C1'-N1-C6
32	1a	527	G7M	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P

There are no ring outliers.

31 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	1l	92	0TD	1	0
54	1y	39	PSU	1	0
1	1A	1939	5MU	2	0
54	1y	37	MIA	1	0
32	1a	1518	MA6	1	0
54	2y	54	5MU	1	0
32	2a	1402	4OC	3	0
1	2A	2503	2MA	1	0
43	2l	92	0TD	1	0
32	1a	1402	4OC	1	0
32	2a	966	M2G	1	0
54	2y	55	PSU	7	0
54	1w	46	G7M	1	0
1	1A	2503	2MA	1	0
55	1x	8	4SU	2	0
55	2x	55	PSU	1	0
54	1w	8	4SU	1	0
32	2a	1518	MA6	2	0
55	2x	8	4SU	1	0
54	1y	55	PSU	1	0
54	1y	8	4SU	2	0
32	2a	1404	5MC	1	0
32	1a	1519	MA6	1	0
32	2a	1207	2MG	1	0
32	1a	966	M2G	2	0
54	1w	55	PSU	1	0
1	2A	2552	OMU	1	0
1	2A	1939	5MU	1	0
32	2a	1519	MA6	2	0
1	1A	1917	PSU	1	0
54	2y	8	4SU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2589 ligands modelled in this entry, 2585 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
60	SF4	2d	302	35	0,12,12	-	-	-		
58	WC9	2A	3772	-	34,37,37	1.31	2 (5%)	31,53,53	1.07	3 (9%)
58	WC9	1A	4061	-	34,37,37	1.30	3 (8%)	31,53,53	1.30	4 (12%)
60	SF4	1d	302	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	2d	302	35	-	-	0/6/5/5
58	WC9	2A	3772	-	-	2/28/71/71	0/3/4/4
58	WC9	1A	4061	-	-	3/28/71/71	0/3/4/4
60	SF4	1d	302	35	-	-	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1A	4061	WC9	CAM-CBF	-4.99	1.39	1.51
58	2A	3772	WC9	CAM-CBF	-4.86	1.39	1.51
58	2A	3772	WC9	OAW-CB	2.94	1.45	1.42
58	1A	4061	WC9	CD2-CAZ	-2.94	1.50	1.53
58	1A	4061	WC9	CBF-CBH	2.09	1.40	1.31

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	1A	4061	WC9	CBC-CBB-CAZ	-3.84	109.23	116.68
58	1A	4061	WC9	CAF-OAA-CAB	-3.49	109.60	114.17
58	2A	3772	WC9	CAF-OAA-CAB	-3.14	110.06	114.17
58	2A	3772	WC9	CBC-CBB-CAZ	-3.07	110.73	116.68
58	1A	4061	WC9	CD2-CAZ-CAY	-2.69	109.76	113.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	1A	4061	WC9	CB-CA-C	2.40	115.17	110.46
58	2A	3772	WC9	CD2-CAZ-CAY	-2.18	110.53	113.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1A	4061	WC9	O-C-CA-CB
58	1A	4061	WC9	NAL-C-CA-CB
58	2A	3772	WC9	O-C-CA-CB
58	2A	3772	WC9	NAL-C-CA-CB
58	1A	4061	WC9	O-C-CA-N

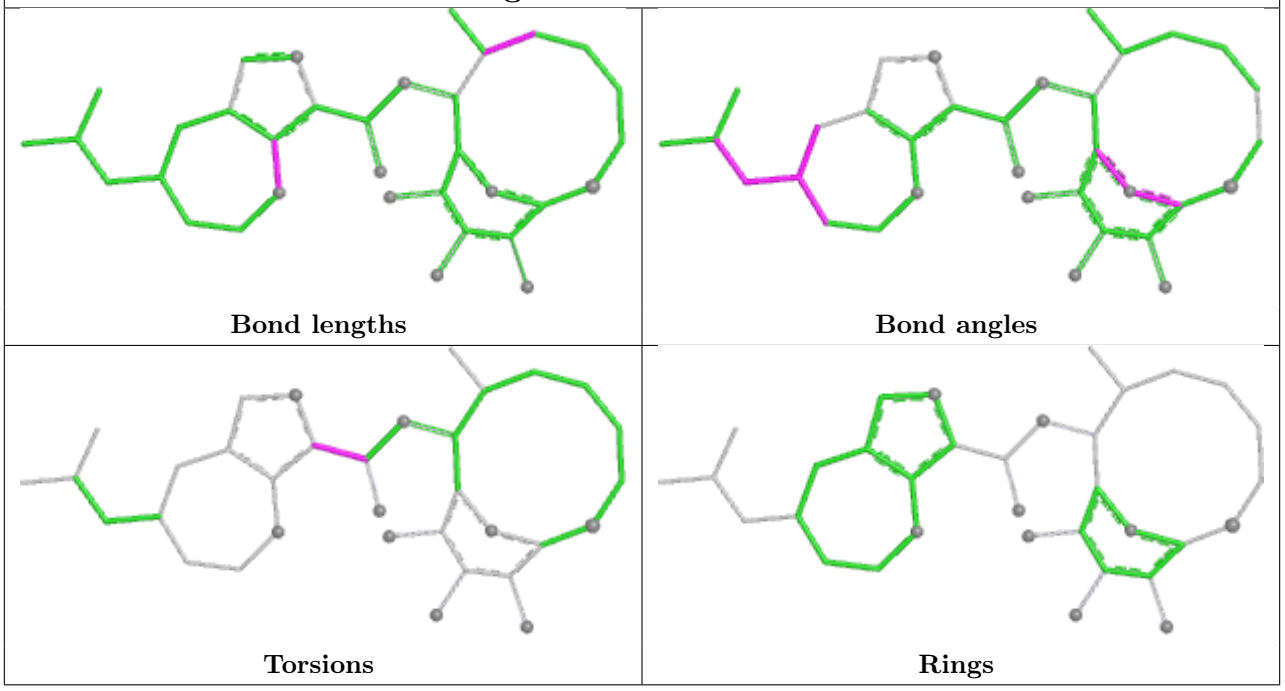
There are no ring outliers.

3 monomers are involved in 3 short contacts:

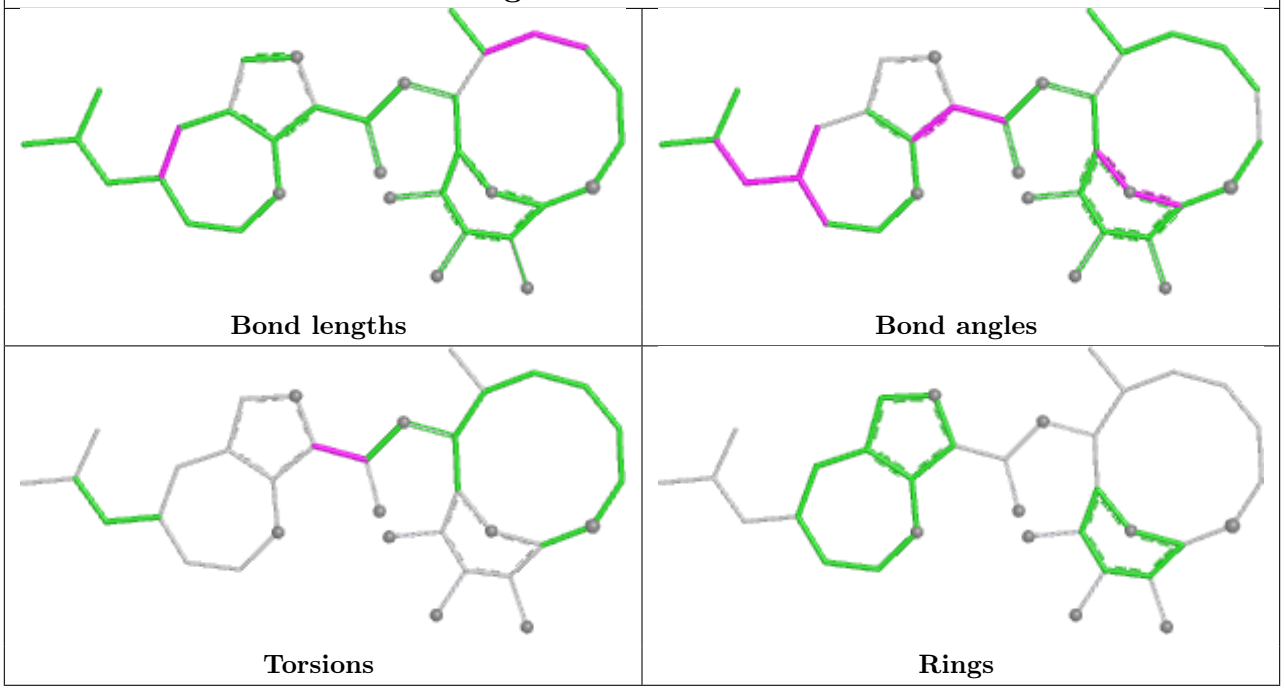
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	2d	302	SF4	1	0
58	2A	3772	WC9	1	0
58	1A	4061	WC9	1	0

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

Ligand WC9 2A 3772



Ligand WC9 1A 4061



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.54	119 (4%) 40 37	25, 41, 102, 117	0
1	2A	2789/2915 (95%)	-0.02	119 (4%) 40 36	36, 62, 101, 117	0
2	1B	120/121 (99%)	-0.35	0 100 100	37, 56, 70, 99	0
2	2B	120/121 (99%)	0.97	4 (3%) 49 45	69, 87, 93, 104	0
3	1D	275/276 (99%)	-0.26	4 (1%) 72 70	27, 40, 56, 86	0
3	2D	275/276 (99%)	0.08	3 (1%) 78 76	34, 53, 66, 88	0
4	1E	204/206 (99%)	-0.30	1 (0%) 87 86	25, 43, 64, 81	0
4	2E	204/206 (99%)	0.22	2 (0%) 79 78	39, 62, 77, 89	0
5	1F	203/210 (96%)	-0.10	1 (0%) 87 86	24, 47, 73, 94	0
5	2F	203/210 (96%)	0.45	2 (0%) 79 78	39, 73, 87, 94	0
6	1G	181/182 (99%)	0.55	11 (6%) 27 24	46, 66, 82, 96	0
6	2G	181/182 (99%)	1.39	40 (22%) 2 2	76, 87, 94, 103	0
7	1H	174/180 (96%)	0.17	2 (1%) 78 76	45, 59, 72, 81	0
7	2H	174/180 (96%)	1.28	30 (17%) 4 3	76, 90, 98, 103	0
8	1I	146/148 (98%)	0.73	7 (4%) 35 32	47, 79, 89, 93	0
8	2I	146/148 (98%)	0.83	7 (4%) 35 32	56, 79, 89, 93	0
9	1N	140/140 (100%)	-0.18	0 100 100	31, 43, 69, 82	0
9	2N	140/140 (100%)	0.51	5 (3%) 46 42	52, 69, 83, 93	0
10	1O	122/122 (100%)	-0.21	0 100 100	35, 45, 63, 67	0
10	2O	122/122 (100%)	0.24	0 100 100	49, 60, 75, 80	0
11	1P	149/150 (99%)	0.00	2 (1%) 75 73	27, 50, 74, 84	0
11	2P	149/150 (99%)	0.54	5 (3%) 48 44	43, 74, 91, 99	0
12	1Q	141/141 (100%)	-0.11	1 (0%) 84 83	33, 47, 63, 84	0
12	2Q	141/141 (100%)	1.00	19 (13%) 7 6	55, 73, 86, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	1R	118/118 (100%)	-0.43	0 100 100	30, 39, 58, 66	0
13	2R	118/118 (100%)	0.11	0 100 100	43, 56, 68, 78	0
14	1S	110/112 (98%)	0.15	2 (1%) 67 65	46, 56, 70, 71	0
14	2S	110/112 (98%)	1.21	14 (12%) 8 7	71, 81, 90, 93	0
15	1T	131/146 (89%)	0.01	4 (3%) 51 48	38, 49, 77, 84	0
15	2T	131/146 (89%)	0.41	4 (3%) 51 48	54, 64, 83, 89	0
16	1U	116/118 (98%)	-0.49	1 (0%) 81 80	27, 35, 49, 70	0
16	2U	116/118 (98%)	0.49	1 (0%) 81 80	50, 66, 83, 89	0
17	1V	101/101 (100%)	-0.36	0 100 100	27, 45, 62, 73	0
17	2V	101/101 (100%)	0.67	1 (0%) 79 78	49, 77, 86, 97	0
18	1W	112/113 (99%)	-0.33	2 (1%) 67 65	26, 37, 56, 94	0
18	2W	112/113 (99%)	0.06	2 (1%) 67 65	44, 53, 74, 92	0
19	1X	95/96 (98%)	-0.14	2 (2%) 63 61	29, 44, 69, 87	0
19	2X	95/96 (98%)	0.56	5 (5%) 32 28	50, 65, 80, 93	0
20	1Y	107/110 (97%)	0.16	2 (1%) 66 63	42, 55, 76, 83	0
20	2Y	107/110 (97%)	1.14	17 (15%) 5 4	65, 78, 90, 100	0
21	1Z	154/206 (74%)	0.71	18 (11%) 9 7	48, 70, 94, 99	0
21	2Z	160/206 (77%)	1.65	40 (25%) 2 1	72, 89, 102, 106	0
22	10	83/85 (97%)	0.28	7 (8%) 17 14	34, 44, 76, 95	0
22	20	83/85 (97%)	1.25	11 (13%) 7 6	53, 71, 87, 96	0
23	11	97/98 (98%)	0.08	1 (1%) 79 78	34, 49, 76, 81	0
23	21	97/98 (98%)	0.39	1 (1%) 79 78	42, 59, 81, 84	0
24	12	70/72 (97%)	0.11	1 (1%) 73 72	41, 54, 66, 79	0
24	22	70/72 (97%)	0.62	0 100 100	64, 76, 86, 88	0
25	13	59/60 (98%)	-0.22	1 (1%) 69 67	31, 43, 66, 82	0
25	23	59/60 (98%)	0.67	4 (6%) 23 20	62, 71, 85, 94	0
26	14	69/71 (97%)	0.89	8 (11%) 9 8	59, 82, 99, 102	0
26	24	69/71 (97%)	1.73	22 (31%) 1 1	86, 94, 103, 104	0
27	15	59/60 (98%)	-0.46	1 (1%) 69 67	24, 37, 60, 66	0
27	25	59/60 (98%)	0.05	1 (1%) 69 67	40, 56, 72, 88	0
28	16	53/54 (98%)	-0.28	0 100 100	39, 47, 62, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.59	1 (1%) 66 63	57, 68, 76, 84	0
29	17	48/49 (97%)	-0.22	2 (4%) 40 37	28, 34, 64, 69	0
29	27	48/49 (97%)	0.07	2 (4%) 40 37	38, 44, 71, 78	0
30	18	64/65 (98%)	-0.37	0 100 100	31, 38, 47, 57	0
30	28	64/65 (98%)	0.47	1 (1%) 70 68	53, 59, 68, 74	0
31	19	37/37 (100%)	-0.29	0 100 100	36, 45, 63, 69	0
31	29	37/37 (100%)	1.05	3 (8%) 18 15	66, 73, 83, 89	0
32	1a	1488/1521 (97%)	0.28	61 (4%) 41 37	40, 71, 101, 118	0
32	2a	1491/1521 (98%)	0.76	166 (11%) 10 8	49, 82, 104, 116	0
33	1b	231/256 (90%)	1.10	32 (13%) 6 5	68, 85, 96, 101	0
33	2b	231/256 (90%)	1.70	72 (31%) 1 1	81, 93, 99, 105	0
34	1c	206/239 (86%)	0.84	12 (5%) 29 25	63, 77, 91, 98	0
34	2c	206/239 (86%)	1.86	90 (43%) 0 0	79, 92, 98, 101	0
35	1d	208/209 (99%)	0.96	15 (7%) 21 18	58, 75, 86, 90	0
35	2d	208/209 (99%)	0.82	10 (4%) 35 32	66, 75, 84, 92	0
36	1e	148/162 (91%)	0.50	2 (1%) 73 72	50, 68, 79, 87	0
36	2e	148/162 (91%)	1.22	20 (13%) 7 6	67, 82, 89, 96	0
37	1f	100/101 (99%)	0.58	3 (3%) 52 49	60, 72, 82, 85	0
37	2f	100/101 (99%)	0.66	3 (3%) 52 49	60, 73, 84, 89	0
38	1g	155/156 (99%)	0.68	9 (5%) 29 25	65, 75, 91, 95	0
38	2g	155/156 (99%)	1.05	17 (10%) 10 9	74, 85, 94, 98	0
39	1h	137/138 (99%)	0.48	2 (1%) 72 70	58, 71, 78, 84	0
39	2h	137/138 (99%)	1.14	12 (8%) 15 13	72, 82, 88, 94	0
40	1i	127/128 (99%)	1.14	19 (14%) 5 4	60, 82, 91, 94	0
40	2i	127/128 (99%)	1.75	43 (33%) 1 1	79, 91, 97, 100	0
41	1j	97/105 (92%)	1.23	14 (14%) 6 5	64, 83, 95, 100	0
41	2j	96/105 (91%)	2.29	55 (57%) 0 0	86, 93, 101, 103	0
42	1k	114/129 (88%)	0.57	4 (3%) 47 43	47, 70, 83, 90	0
42	2k	114/129 (88%)	0.77	8 (7%) 22 19	59, 78, 88, 94	0
43	1l	121/132 (91%)	0.25	5 (4%) 41 37	47, 58, 72, 79	0
43	2l	121/132 (91%)	0.99	12 (9%) 13 10	61, 75, 84, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.75	7 (5%) 29 26	60, 76, 86, 95	0
44	2m	122/126 (96%)	1.85	47 (38%) 1 0	77, 91, 97, 100	0
45	1n	60/61 (98%)	0.87	3 (5%) 34 30	63, 72, 80, 82	0
45	2n	60/61 (98%)	2.74	47 (78%) 0 0	85, 93, 97, 102	0
46	1o	88/89 (98%)	0.66	4 (4%) 38 34	52, 71, 81, 87	0
46	2o	88/89 (98%)	0.83	3 (3%) 48 44	64, 78, 86, 94	0
47	1p	82/88 (93%)	1.40	10 (12%) 8 7	61, 76, 85, 91	0
47	2p	82/88 (93%)	0.91	7 (8%) 16 14	63, 74, 84, 92	0
48	1q	99/105 (94%)	0.61	1 (1%) 79 78	58, 73, 83, 85	0
48	2q	99/105 (94%)	0.68	6 (6%) 27 24	69, 78, 88, 90	0
49	1r	68/88 (77%)	0.41	1 (1%) 72 70	61, 70, 84, 86	0
49	2r	68/88 (77%)	0.68	1 (1%) 72 70	62, 76, 87, 93	0
50	1s	83/93 (89%)	0.68	3 (3%) 46 42	69, 80, 88, 91	0
50	2s	83/93 (89%)	2.11	37 (44%) 0 0	87, 95, 100, 104	0
51	1t	96/106 (90%)	0.90	5 (5%) 33 29	65, 76, 85, 90	0
51	2t	96/106 (90%)	0.85	9 (9%) 14 12	63, 75, 89, 91	0
52	1u	23/27 (85%)	1.15	3 (13%) 7 6	68, 71, 78, 81	0
52	2u	23/27 (85%)	2.46	16 (69%) 0 0	82, 87, 94, 94	0
53	1v	13/24 (54%)	0.42	1 (7%) 19 17	52, 64, 85, 101	0
53	2v	13/24 (54%)	1.61	5 (38%) 1 0	73, 88, 100, 107	0
54	1w	65/76 (85%)	0.97	9 (13%) 6 5	65, 93, 107, 112	0
54	1y	67/76 (88%)	1.03	11 (16%) 4 4	43, 100, 108, 112	0
54	2w	63/76 (82%)	1.37	12 (19%) 3 3	86, 102, 111, 116	0
54	2y	66/76 (86%)	1.35	16 (24%) 2 1	59, 106, 111, 114	0
55	1x	71/77 (92%)	0.29	3 (4%) 40 37	33, 66, 90, 97	0
55	2x	71/77 (92%)	0.66	2 (2%) 55 51	49, 85, 97, 106	0
All	All	20869/21748 (95%)	0.37	1521 (7%) 21 18	24, 68, 97, 118	0

All (1521) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	10	6	GLY	8.5
45	1n	2	ALA	7.9

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Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	7.8
22	10	3	HIS	7.4
45	2n	2	ALA	7.3
44	2m	124	PRO	6.8
44	1m	123	ALA	6.5
23	21	2	SER	6.2
23	11	2	SER	6.1
22	10	7	LEU	6.0
44	1m	124	PRO	5.9
33	2b	165	VAL	5.9
21	2Z	174	VAL	5.7
22	20	2	ALA	5.6
21	1Z	141	VAL	5.6
21	2Z	172	ALA	5.4
21	2Z	173	ALA	5.4
32	2a	1219	U	5.3
32	1a	1503	A	5.1
1	2A	2155	G	5.1
50	2s	2	PRO	5.1
54	1w	74	C	5.0
1	1A	1094	U	5.0
44	2m	102	ARG	5.0
45	2n	18	VAL	5.0
21	2Z	171	ILE	4.9
1	2A	1536	C	4.9
32	1a	1532	U	4.9
22	10	5	LYS	4.9
1	1A	885	C	4.8
38	2g	82	GLY	4.8
1	1A	1078	U	4.8
33	1b	237	ALA	4.8
44	1m	2	ALA	4.7
44	2m	122	LYS	4.7
40	2i	105	ASP	4.7
45	2n	39	LEU	4.7
7	2H	2	SER	4.7
41	2j	93	GLY	4.7
21	2Z	146	ILE	4.7
33	2b	21	ARG	4.7
40	2i	126	SER	4.7
21	1Z	146	ILE	4.6
15	1T	131	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
22	10	2	ALA	4.6
34	2c	2	GLY	4.6
22	20	3	HIS	4.6
40	2i	102	LEU	4.6
45	2n	6	LEU	4.6
1	1A	888	C	4.5
1	2A	2154	G	4.5
32	1a	1034	G	4.5
40	1i	19	LEU	4.5
37	2f	21	LEU	4.5
32	1a	1531	A	4.5
51	1t	103	GLY	4.5
52	2u	2	GLY	4.5
50	2s	9	VAL	4.5
32	1a	1027	C	4.4
32	2a	1038	C	4.4
50	2s	22	LEU	4.4
41	2j	47	PHE	4.4
32	2a	1033	G	4.4
41	2j	65	LEU	4.4
45	2n	3	ARG	4.4
22	20	7	LEU	4.4
44	2m	6	GLY	4.4
32	1a	1035	A	4.4
45	2n	7	ILE	4.4
1	2A	883	G	4.4
1	2A	2147	G	4.4
33	2b	71	VAL	4.4
34	2c	188	LEU	4.3
1	1A	1064	C	4.3
21	2Z	141	VAL	4.3
40	2i	14	VAL	4.3
32	1a	1001(A)	G	4.3
1	2A	896	A	4.3
45	2n	13	THR	4.3
32	1a	1030(A)	G	4.3
32	1a	1036	G	4.3
1	1A	1096	A	4.3
50	2s	11	VAL	4.2
40	2i	11	LYS	4.2
1	2A	2138	C	4.2
54	2w	3	C	4.2

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Mol	Chain	Res	Type	RSRZ
26	14	56	VAL	4.2
1	2A	2111	C	4.2
33	2b	237	ALA	4.1
7	1H	2	SER	4.1
1	2A	2146	C	4.1
32	2a	1030(B)	C	4.1
1	2A	2156	G	4.1
41	2j	10	GLY	4.1
41	2j	42	THR	4.1
1	2A	2136	C	4.1
54	2w	4	C	4.1
21	2Z	149	SER	4.1
1	2A	2113	U	4.1
26	24	51	ASP	4.1
22	10	4	LYS	4.0
21	2Z	150	LEU	4.0
32	1a	1001	A	4.0
32	2a	974	A	4.0
41	2j	41	PRO	4.0
32	2a	1030(A)	G	4.0
34	2c	137	ALA	4.0
45	2n	21	TYR	4.0
50	2s	13	ASP	4.0
22	20	5	LYS	3.9
32	1a	1286	A	3.9
32	2a	965	A	3.9
1	2A	2137	C	3.9
1	1A	2113	U	3.9
21	1Z	150	LEU	3.9
22	20	6	GLY	3.9
32	2a	1149	C	3.9
54	2w	72	C	3.9
54	1w	73	A	3.9
41	2j	63	PHE	3.9
41	2j	58	ASP	3.9
41	2j	91	PRO	3.8
47	1p	82	GLN	3.8
41	2j	38	ILE	3.8
33	2b	161	ALA	3.8
45	2n	30	ALA	3.8
50	1s	9	VAL	3.8
41	2j	55	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
32	2a	1224	G	3.8
1	2A	2145	C	3.8
54	2w	74	C	3.8
31	29	37	GLY	3.8
34	1c	2	GLY	3.8
1	1A	2159	G	3.8
32	2a	1002	G	3.8
44	1m	122	LYS	3.8
54	1w	1	G	3.8
50	2s	4	SER	3.8
34	2c	149	ALA	3.8
34	2c	189	ALA	3.8
35	1d	167	GLY	3.8
20	2Y	54	LYS	3.8
41	2j	37	PRO	3.8
1	1A	1095	A	3.7
54	2w	73	A	3.7
38	2g	2	ALA	3.7
41	2j	88	LEU	3.7
42	2k	49	GLY	3.7
1	2A	882	G	3.7
1	2A	2133	G	3.7
32	2a	1030	C	3.7
14	2S	35	ILE	3.7
32	1a	1025	U	3.7
1	1A	1068	G	3.7
1	1A	1087	G	3.7
1	2A	2149	G	3.7
1	1A	889	C	3.7
12	2Q	104	PHE	3.7
33	2b	163	PHE	3.7
21	1Z	139	VAL	3.7
33	2b	187	LEU	3.6
34	2c	8	ILE	3.6
50	1s	13	ASP	3.6
15	1T	130	ALA	3.6
33	2b	236	TYR	3.6
41	2j	32	ALA	3.6
51	2t	103	GLY	3.6
6	2G	17	PRO	3.6
33	2b	136	VAL	3.6
3	1D	276	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
33	2b	39	ILE	3.6
26	24	65	ASP	3.6
26	24	54	GLY	3.6
1	2A	2125	G	3.6
1	2A	2117	A	3.6
19	1X	95	LEU	3.6
21	2Z	144	LEU	3.6
34	2c	157	ILE	3.6
50	2s	68	GLY	3.6
1	1A	2119	A	3.6
32	2a	983	A	3.6
1	2A	885	C	3.5
1	2A	2115	G	3.5
54	2w	71	G	3.5
45	2n	17	LYS	3.5
41	1j	4	ILE	3.5
38	1g	83	ALA	3.5
50	2s	84	GLY	3.5
40	2i	2	GLU	3.5
1	1A	2110	G	3.5
1	2A	2112	G	3.5
1	2A	2319	G	3.5
32	2a	976	G	3.5
32	2a	1001(A)	G	3.5
1	2A	2118	U	3.5
32	2a	994	A	3.5
45	2n	38	GLY	3.5
33	1b	134	GLU	3.5
21	2Z	125	LEU	3.5
1	1A	886	C	3.5
45	2n	34	TYR	3.5
20	2Y	1	MET	3.5
32	1a	1026	G	3.5
6	1G	182	LYS	3.5
21	2Z	164	ALA	3.5
38	2g	81	GLY	3.5
52	2u	16	GLY	3.5
33	2b	121	LEU	3.5
47	2p	82	GLN	3.5
33	1b	230	VAL	3.5
1	1A	2145	C	3.4
1	1A	2130	U	3.4

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Mol	Chain	Res	Type	RSRZ
54	1w	20	U	3.4
32	1a	1023	G	3.4
32	2a	1034	G	3.4
32	2a	1202	G	3.4
34	2c	194	GLY	3.4
36	2e	21	ALA	3.4
45	2n	10	ALA	3.4
1	2A	2119	A	3.4
26	24	56	VAL	3.4
44	2m	88	ARG	3.4
21	2Z	106	GLY	3.4
1	1A	1081	U	3.4
8	2I	82	ARG	3.4
7	2H	52	VAL	3.4
14	2S	46	VAL	3.4
34	2c	124	ILE	3.4
32	1a	1447	A	3.4
32	2a	1503	A	3.4
21	1Z	168	GLU	3.4
25	23	2	PRO	3.4
33	2b	152	PHE	3.4
35	1d	170	VAL	3.4
6	2G	157	ILE	3.4
32	1a	630	G	3.4
1	2A	2173	A	3.4
52	2u	8	THR	3.4
33	2b	26	PRO	3.4
33	2b	22	LYS	3.3
45	2n	14	PRO	3.3
51	1t	10	LEU	3.3
1	1A	2160	G	3.3
32	1a	1003	G	3.3
45	2n	33	VAL	3.3
41	2j	74	ILE	3.3
32	1a	1257	U	3.3
45	2n	22	THR	3.3
32	2a	1223	C	3.3
34	1c	87	LEU	3.3
45	2n	54	PRO	3.3
8	2I	146	ALA	3.3
26	24	49	PHE	3.3
40	2i	41	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	1A	548	A	3.3
1	1A	1069	A	3.3
54	1y	36	A	3.3
32	1a	1024	G	3.3
32	2a	993	G	3.3
40	1i	2	GLU	3.3
47	1p	81	ARG	3.3
40	2i	67	GLY	3.3
50	2s	24	ALA	3.3
1	1A	2794	C	3.3
1	2A	2139	C	3.3
32	1a	1029	C	3.3
1	2A	2126	A	3.3
32	2a	969	A	3.3
44	2m	104	ARG	3.3
1	1A	2166	G	3.3
1	2A	11	G	3.3
1	2A	1171	G	3.3
32	2a	1032	G	3.3
34	2c	196	LEU	3.3
33	2b	48	MET	3.3
38	2g	85	TYR	3.3
40	2i	125	TYR	3.3
36	1e	85	GLY	3.3
52	2u	11	GLY	3.3
1	1A	1066	U	3.3
26	24	31	ILE	3.3
45	2n	25	VAL	3.3
32	2a	962	C	3.2
21	1Z	1	MET	3.2
21	1Z	104	PHE	3.2
33	2b	122	PHE	3.2
44	2m	60	VAL	3.2
38	2g	84	ASN	3.2
1	1A	1065	U	3.2
1	2A	1113	U	3.2
34	2c	190	ARG	3.2
1	2A	884	C	3.2
22	20	4	LYS	3.2
39	2h	9	MET	3.2
1	1A	887	A	3.2
33	1b	229	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
34	2c	207	VAL	3.2
36	2e	67	VAL	3.2
36	2e	109	ILE	3.2
50	2s	45	VAL	3.2
35	2d	154	ASN	3.2
42	1k	36	ASP	3.2
1	1A	2190	G	3.2
40	2i	9	ARG	3.2
55	2x	47	U	3.2
1	1A	898	C	3.2
32	1a	1030(B)	C	3.2
54	1w	72	C	3.2
40	2i	36	TYR	3.2
6	2G	20	ILE	3.2
38	2g	80	VAL	3.2
1	1A	2117	A	3.2
1	1A	2173	A	3.2
32	2a	977	A	3.2
6	2G	35	GLU	3.2
22	20	68	GLU	3.2
22	20	84	LEU	3.2
39	2h	2	LEU	3.2
1	1A	2141	G	3.2
1	1A	2162	G	3.2
1	2A	2318	G	3.2
32	2a	973	G	3.2
54	2y	33	U	3.2
6	2G	28	VAL	3.2
32	2a	1362	C	3.1
12	2Q	59	ARG	3.1
1	2A	2169	A	3.1
14	2S	32	LEU	3.1
32	2a	1001	A	3.1
46	1o	19	PRO	3.1
34	2c	191	THR	3.1
41	2j	48	THR	3.1
41	2j	31	GLY	3.1
26	24	66	SER	3.1
38	1g	80	VAL	3.1
32	2a	1117	G	3.1
42	2k	25	TYR	3.1
26	24	55	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
40	2i	104	ARG	3.1
40	2i	127	LYS	3.1
52	2u	6	ARG	3.1
32	1a	1030	C	3.1
33	1b	11	LEU	3.1
1	2A	652(B)	A	3.1
32	2a	1225	A	3.1
21	1Z	170	THR	3.1
35	2d	183	GLY	3.1
21	1Z	120	ILE	3.1
38	2g	83	ALA	3.1
48	2q	65	ILE	3.1
33	1b	17	PHE	3.1
39	2h	53	VAL	3.1
38	2g	76	ARG	3.1
42	1k	51	LYS	3.1
43	1l	19	ARG	3.1
45	2n	4	LYS	3.1
51	2t	86	ARG	3.1
6	1G	146	TYR	3.1
43	1l	64	TYR	3.1
40	1i	105	ASP	3.1
44	2m	90	LEU	3.1
1	1A	2112	G	3.1
32	2a	1036	G	3.1
32	2a	1061	G	3.1
45	2n	8	GLU	3.1
50	2s	77	THR	3.1
18	1W	112	GLY	3.1
34	2c	158	GLY	3.1
44	2m	68	GLY	3.1
44	2m	4	ILE	3.1
1	2A	2170	A	3.1
32	2a	1447	A	3.1
53	2v	24	A	3.1
41	2j	49	VAL	3.1
20	2Y	55	TYR	3.1
32	2a	1532	U	3.1
33	2b	140	HIS	3.1
1	1A	2151	G	3.1
3	2D	38	LYS	3.1
41	2j	14	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	1A	1075	C	3.1
1	1A	1076	C	3.1
32	1a	163	C	3.1
32	2a	995	C	3.1
34	2c	68	VAL	3.1
32	2a	1531	A	3.0
33	2b	44	LEU	3.0
50	2s	71	LEU	3.0
41	2j	62	HIS	3.0
1	2A	2132	U	3.0
20	2Y	94	LYS	3.0
34	2c	182	ILE	3.0
40	2i	115	GLY	3.0
50	2s	79	THR	3.0
1	1A	1093	G	3.0
1	2A	2157	G	3.0
32	2a	630	G	3.0
32	2a	1220	G	3.0
54	1w	71	G	3.0
21	2Z	157	LEU	3.0
1	1A	2164	C	3.0
1	2A	886	C	3.0
19	2X	69	TYR	3.0
32	2a	1037	C	3.0
32	2a	1114	C	3.0
32	2a	1363	C	3.0
33	1b	9	GLU	3.0
1	1A	1077	A	3.0
1	1A	2114	A	3.0
45	2n	9	LYS	3.0
40	1i	15	ALA	3.0
22	20	69	PHE	3.0
33	2b	164	VAL	3.0
38	2g	16	LEU	3.0
41	2j	90	LEU	3.0
33	1b	125	PRO	3.0
33	1b	234	PRO	3.0
50	2s	80	TYR	3.0
44	2m	101	GLN	3.0
45	2n	15	LYS	3.0
1	2A	2128	C	3.0
32	2a	980	C	3.0

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Mol	Chain	Res	Type	RSRZ
1	1A	896	A	3.0
45	2n	31	ARG	3.0
21	2Z	21	ALA	3.0
32	1a	204	U	3.0
34	2c	167	TRP	3.0
26	14	63	TYR	3.0
33	2b	199	TYR	3.0
36	1e	10	MET	3.0
40	2i	66	ARG	3.0
33	1b	18	GLY	3.0
1	1A	2152	G	3.0
1	2A	2148	G	3.0
33	1b	188	ALA	3.0
45	2n	48	ALA	3.0
54	1y	15	G	3.0
1	1A	1057	A	3.0
1	1A	2135	A	3.0
1	2A	2134	A	3.0
34	2c	138	VAL	3.0
34	2c	153	VAL	3.0
32	2a	1257	U	2.9
6	1G	48	GLU	2.9
34	2c	6	HIS	2.9
7	2H	175	LYS	2.9
21	1Z	149	SER	2.9
33	1b	236	TYR	2.9
44	2m	78	ILE	2.9
34	2c	9	GLY	2.9
33	2b	17	PHE	2.9
8	1I	38	LEU	2.9
1	1A	2116	G	2.9
1	2A	2166	G	2.9
32	1a	1002	G	2.9
32	1a	1033	G	2.9
32	2a	1286	A	2.9
55	2x	70	G	2.9
35	1d	173	TRP	2.9
54	2w	45	U	2.9
15	2T	112	ARG	2.9
41	2j	43	ARG	2.9
52	2u	24	ARG	2.9
33	2b	31	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
43	2l	64	TYR	2.9
33	2b	185	ILE	2.9
33	2b	77	ALA	2.9
44	2m	75	ALA	2.9
34	1c	207	VAL	2.9
21	2Z	121	HIS	2.9
43	1l	91	LYS	2.9
44	1m	27	LYS	2.9
45	2n	49	HIS	2.9
47	1p	43	LYS	2.9
32	2a	1030(D)	A	2.9
1	1A	12	U	2.9
1	1A	2165	G	2.9
54	1y	18	G	2.9
26	24	63	TYR	2.9
21	2Z	26	GLY	2.9
26	14	45	GLY	2.9
36	2e	86	ALA	2.9
42	2k	89	ALA	2.9
14	2S	29	PHE	2.9
33	1b	7	VAL	2.9
33	1b	163	PHE	2.9
33	2b	70	PHE	2.9
40	1i	14	VAL	2.9
50	2s	5	LEU	2.9
20	1Y	1	MET	2.9
33	2b	166	ASP	2.9
1	1A	884	C	2.9
12	2Q	15	GLY	2.9
32	2a	1092	A	2.9
32	2a	1115	C	2.9
32	2a	1325	C	2.9
34	2c	201	TYR	2.9
54	1y	20	U	2.9
21	2Z	170	THR	2.9
1	1A	1176	G	2.9
6	2G	53	LEU	2.9
12	2Q	102	VAL	2.9
32	2a	1053	G	2.9
32	2a	1190	G	2.9
32	2a	1222	G	2.9
34	2c	92	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
26	14	59	PHE	2.9
40	1i	59	PHE	2.9
33	1b	19	HIS	2.9
26	24	57	GLU	2.8
50	2s	62	ILE	2.8
50	2s	82	GLY	2.8
4	2E	204	ALA	2.8
8	1I	146	ALA	2.8
6	2G	15	VAL	2.8
32	2a	1004	A	2.8
32	2a	1016	A	2.8
54	2y	36	A	2.8
1	2A	889	C	2.8
1	2A	2164	C	2.8
32	2a	972	C	2.8
32	2a	979	C	2.8
32	2a	1249	C	2.8
50	2s	76	PRO	2.8
1	1A	2131	G	2.8
1	2A	2127	G	2.8
14	1S	3	ARG	2.8
32	1a	346	G	2.8
32	2a	1310	G	2.8
52	2u	14	TRP	2.8
6	2G	76	SER	2.8
21	2Z	166	SER	2.8
45	2n	50	LYS	2.8
8	2I	68	LEU	2.8
34	2c	193	TYR	2.8
50	2s	15	LEU	2.8
50	2s	63	THR	2.8
33	1b	15	VAL	2.8
34	2c	141	VAL	2.8
1	1A	2136	C	2.8
1	2A	2140	C	2.8
32	2a	1116	C	2.8
32	2a	1260	C	2.8
34	2c	5	ILE	2.8
38	2g	156	TRP	2.8
1	1A	2115	G	2.8
1	2A	2165	G	2.8
32	2a	1182	G	2.8

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Mol	Chain	Res	Type	RSRZ
54	2w	44	G	2.8
14	2S	45	GLY	2.8
22	10	8	GLY	2.8
33	2b	221	LEU	2.8
45	2n	55	GLY	2.8
37	1f	55	ASP	2.8
52	2u	5	ASP	2.8
21	2Z	105	VAL	2.8
41	2j	94	VAL	2.8
45	2n	16	PHE	2.8
20	2Y	53	PRO	2.8
34	2c	73	PRO	2.8
39	2h	67	PRO	2.8
52	1u	24	ARG	2.8
1	2A	2167	U	2.8
32	2a	978	A	2.8
33	2b	214	ILE	2.8
1	2A	652(T)	C	2.8
32	2a	1217	C	2.8
45	2n	61	TRP	2.8
20	2Y	90	LEU	2.8
36	2e	74	GLY	2.8
41	2j	36	GLY	2.8
44	2m	119	GLY	2.8
7	2H	45	VAL	2.8
33	2b	7	VAL	2.8
1	1A	1058	G	2.8
1	2A	2153	G	2.8
1	2A	2206	G	2.8
12	2Q	60	ARG	2.8
38	1g	85	TYR	2.8
52	2u	15	ARG	2.8
21	2Z	95	PRO	2.7
34	1c	47	LEU	2.7
47	1p	59	TRP	2.7
32	2a	1035	A	2.7
5	2F	130	ALA	2.7
33	2b	67	THR	2.7
40	1i	13	ALA	2.7
25	23	29	ARG	2.7
43	1l	18	VAL	2.7
52	2u	23	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	2A	1533	G	2.7
32	2a	1058	G	2.7
34	2c	152	ILE	2.7
41	1j	36	GLY	2.7
41	2j	59	SER	2.7
48	2q	99	SER	2.7
1	1A	271(K)	U	2.7
1	1A	2109	U	2.7
1	2A	2144	U	2.7
33	2b	15	VAL	2.7
34	2c	79	ARG	2.7
35	1d	195	ALA	2.7
37	2f	55	ASP	2.7
44	2m	7	VAL	2.7
45	2n	37	PHE	2.7
33	2b	234	PRO	2.7
3	1D	38	LYS	2.7
34	2c	4	LYS	2.7
34	2c	48	TYR	2.7
40	2i	124	GLN	2.7
32	2a	1018	C	2.7
41	1j	74	ILE	2.7
1	2A	652(U)	G	2.7
21	2Z	147	GLY	2.7
40	2i	69	GLY	2.7
54	2y	18	G	2.7
54	2y	57	G	2.7
6	2G	48	GLU	2.7
12	2Q	121	ALA	2.7
20	2Y	45	VAL	2.7
33	2b	34	ALA	2.7
33	2b	55	PHE	2.7
33	2b	184	VAL	2.7
41	2j	72	VAL	2.7
34	2c	62	ASP	2.7
32	1a	90	U	2.7
52	2u	18	TYR	2.7
1	1A	1045	A	2.7
1	1A	1098	A	2.7
1	1A	2790	A	2.7
1	2A	229	A	2.7
1	2A	528	A	2.7

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Mol	Chain	Res	Type	RSRZ
32	1a	344	A	2.7
54	2y	38	A	2.7
41	2j	23	ILE	2.7
1	1A	34	C	2.7
1	1A	2128	C	2.7
1	1A	2146	C	2.7
32	1a	1028	C	2.7
20	2Y	5	MET	2.7
39	1h	2	LEU	2.7
41	2j	28	ARG	2.7
41	2j	78	ASN	2.7
12	2Q	52	VAL	2.7
33	2b	91	PRO	2.7
1	2A	1042	G	2.6
1	2A	2116	G	2.6
32	2a	1065	U	2.6
32	2a	1205	U	2.6
1	1A	1067	A	2.6
1	2A	6	A	2.6
1	2A	2114	A	2.6
7	2H	64	LEU	2.6
32	2a	1324	A	2.6
33	2b	10	LEU	2.6
34	2c	32	LEU	2.6
41	2j	85	LEU	2.6
35	1d	191	ARG	2.6
40	2i	10	ARG	2.6
40	2i	20	ARG	2.6
36	2e	99	GLY	2.6
44	2m	100	GLY	2.6
50	2s	72	GLY	2.6
1	2A	2174	C	2.6
32	2a	1063	C	2.6
45	2n	58	LYS	2.6
54	2w	2	C	2.6
54	2y	56	C	2.6
41	2j	76	ASN	2.6
34	2c	53	ALA	2.6
45	2n	56	VAL	2.6
50	2s	10	PHE	2.6
16	1U	117	GLN	2.6
41	2j	73	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
33	1b	200	ILE	2.6
42	2k	48	ILE	2.6
1	1A	2167	U	2.6
1	2A	881	G	2.6
1	2A	2159	G	2.6
32	2a	953	G	2.6
32	2a	961	U	2.6
32	2a	1003	G	2.6
32	2a	1042	G	2.6
32	2a	1150	U	2.6
54	2w	19	G	2.6
1	1A	2158	A	2.6
32	1a	1030(D)	A	2.6
6	2G	50	ALA	2.6
15	2T	130	ALA	2.6
20	2Y	85	VAL	2.6
21	2Z	136	PHE	2.6
31	29	16	VAL	2.6
33	2b	112	VAL	2.6
41	2j	34	VAL	2.6
33	2b	24	TRP	2.6
34	2c	7	PRO	2.6
41	2j	54	PHE	2.6
47	1p	80	PHE	2.6
51	1t	95	ALA	2.6
1	2A	894	C	2.6
54	1y	56	C	2.6
33	2b	223	ILE	2.6
34	2c	134	ILE	2.6
41	2j	8	LEU	2.6
12	2Q	10	ARG	2.6
18	1W	111	HIS	2.6
38	2g	5	ARG	2.6
1	1A	1082	U	2.6
1	1A	2150	U	2.6
29	27	48	LYS	2.6
32	2a	1040	U	2.6
1	1A	1074	G	2.6
1	1A	2133	G	2.6
1	2A	1114	G	2.6
1	2A	2792	G	2.6
32	1a	1030(C)	G	2.6

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Mol	Chain	Res	Type	RSRZ
6	1G	50	ALA	2.6
6	2G	132	ASN	2.6
8	1I	40	THR	2.6
1	2A	899	A	2.6
32	1a	152	A	2.6
34	2c	57	ILE	2.6
44	2m	22	ILE	2.6
1	2A	888	C	2.6
8	2I	75	LEU	2.6
32	1a	345	C	2.6
32	2a	1027	C	2.6
32	2a	1218	C	2.6
33	2b	196	LEU	2.6
26	14	67	TYR	2.6
21	1Z	2	GLU	2.6
33	2b	12	GLU	2.6
35	1d	179	GLU	2.6
41	2j	61	GLU	2.6
1	1A	1097	U	2.6
1	1A	2172	U	2.6
8	2I	55	ALA	2.6
9	2N	9	VAL	2.6
33	1b	131	PRO	2.6
40	1i	106	ALA	2.6
41	2j	44	VAL	2.6
21	2Z	88	PHE	2.6
44	2m	33	ALA	2.6
44	2m	106	ASN	2.6
51	2t	97	ALA	2.6
33	1b	97	TRP	2.5
1	1A	1089	G	2.5
33	2b	201	ILE	2.5
43	2l	100	ILE	2.5
32	2a	975	A	2.5
33	2b	138	LEU	2.5
41	2j	40	LEU	2.5
43	2l	60	LEU	2.5
53	1v	12	A	2.5
6	1G	83	ARG	2.5
9	2N	83	LYS	2.5
35	1d	169	LYS	2.5
45	1n	3	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
51	2t	8	ARG	2.5
34	2c	90	GLU	2.5
2	2B	6	C	2.5
32	2a	999	C	2.5
21	2Z	71	VAL	2.5
21	2Z	96	VAL	2.5
33	1b	232	PRO	2.5
34	2c	195	VAL	2.5
6	1G	80	PHE	2.5
6	2G	163	ALA	2.5
34	2c	160	ALA	2.5
36	2e	45	PHE	2.5
38	1g	2	ALA	2.5
50	2s	75	ALA	2.5
15	2T	55	ASN	2.5
41	1j	100	THR	2.5
1	2A	2172	U	2.5
50	2s	12	ASP	2.5
6	2G	139	LEU	2.5
20	2Y	106	LEU	2.5
39	2h	30	ARG	2.5
40	2i	19	LEU	2.5
45	2n	12	ARG	2.5
45	2n	47	LEU	2.5
34	2c	31	HIS	2.5
1	1A	1063	G	2.5
1	2A	2131	G	2.5
32	2a	1127	G	2.5
54	2w	70	G	2.5
54	2y	19	G	2.5
55	1x	46	G	2.5
1	1A	2170	A	2.5
1	2A	2320	A	2.5
32	1a	1005	A	2.5
32	2a	1248	A	2.5
32	2a	1357	A	2.5
54	1y	35	A	2.5
54	2y	21	A	2.5
34	2c	171	GLY	2.5
43	1l	63	GLY	2.5
51	1t	102	GLY	2.5
7	2H	15	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
36	2e	115	VAL	2.5
25	23	51	ALA	2.5
41	1j	32	ALA	2.5
41	1j	33	GLN	2.5
1	1A	2129	C	2.5
32	2a	1045	C	2.5
32	2a	1054	C	2.5
32	2a	1192	C	2.5
6	2G	136	ARG	2.5
6	2G	156	ASP	2.5
50	2s	31	ILE	2.5
52	2u	3	LYS	2.5
1	2A	1026	U	2.5
38	1g	4	ARG	2.5
40	1i	20	ARG	2.5
44	2m	48	LEU	2.5
48	2q	98	LEU	2.5
52	1u	9	ARG	2.5
41	2j	68	HIS	2.5
35	1d	150	GLU	2.5
50	2s	61	TYR	2.5
35	2d	23	GLY	2.5
38	1g	82	GLY	2.5
34	2c	174	PRO	2.5
1	1A	890	A	2.5
1	1A	1056	G	2.5
32	2a	1024	G	2.5
32	2a	1253	G	2.5
34	2c	55	VAL	2.5
34	2c	170	GLN	2.5
40	2i	44	VAL	2.5
29	27	45	ALA	2.5
34	2c	24	ALA	2.5
6	2G	19	LEU	2.5
7	2H	170	ARG	2.5
1	1A	2138	C	2.5
1	2A	2163	C	2.5
32	2a	1019	C	2.5
1	2A	271(K)	U	2.5
32	2a	950	U	2.5
54	1y	47	U	2.5
5	1F	14	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
26	24	25	TYR	2.5
12	2Q	109	VAL	2.5
21	1Z	105	VAL	2.5
26	14	50	VAL	2.5
50	2s	41	VAL	2.5
6	2G	57	ALA	2.5
33	2b	123	ALA	2.5
49	2r	43	PHE	2.5
44	1m	121	LYS	2.4
44	2m	121	LYS	2.4
54	2y	58	A	2.4
21	2Z	155	LEU	2.4
33	2b	11	LEU	2.4
34	2c	87	LEU	2.4
45	2n	44	LEU	2.4
48	2q	90	ILE	2.4
1	1A	1071	G	2.4
1	2A	271(M)	G	2.4
32	2a	1047	G	2.4
32	2a	1272	G	2.4
44	2m	64	TRP	2.4
32	2a	1006	C	2.4
32	2a	1320	C	2.4
1	2A	12	U	2.4
19	1X	94	GLY	2.4
32	1a	1000	U	2.4
41	2j	77	PRO	2.4
46	2o	89	GLY	2.4
50	1s	84	GLY	2.4
6	2G	74	LYS	2.4
21	2Z	139	VAL	2.4
34	2c	198	VAL	2.4
33	2b	13	ALA	2.4
44	2m	118	ALA	2.4
26	24	58	ARG	2.4
40	1i	66	ARG	2.4
40	2i	128	ARG	2.4
50	2s	29	ARG	2.4
52	1u	6	ARG	2.4
26	24	9	LEU	2.4
33	1b	127	ILE	2.4
33	2b	145	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
34	2c	33	LEU	2.4
34	2c	52	LEU	2.4
36	2e	118	ILE	2.4
21	1Z	121	HIS	2.4
41	2j	35	SER	2.4
40	2i	91	ASP	2.4
47	1p	48	TRP	2.4
53	2v	13	A	2.4
44	2m	58	GLU	2.4
1	1A	880	G	2.4
1	1A	2156	G	2.4
1	1A	2168	G	2.4
1	1A	2207	G	2.4
1	2A	530	G	2.4
32	1a	1009	G	2.4
32	2a	1048	G	2.4
32	2a	1273	G	2.4
32	2a	1316	G	2.4
54	2y	5	G	2.4
41	2j	86	MET	2.4
51	2t	98	PRO	2.4
1	1A	2140	C	2.4
1	2A	897	C	2.4
2	2B	4	C	2.4
6	2G	159	VAL	2.4
7	2H	35	VAL	2.4
33	2b	92	TYR	2.4
34	2c	29	TYR	2.4
42	1k	14	VAL	2.4
46	2o	27	VAL	2.4
1	1A	1026	U	2.4
1	2A	272(A)	U	2.4
1	2A	614(A)	U	2.4
47	2p	38	TYR	2.4
7	2H	156	ALA	2.4
34	2c	163	ALA	2.4
43	2l	32	PHE	2.4
44	2m	72	ALA	2.4
44	2m	76	ALA	2.4
54	1w	47	U	2.4
33	2b	41	ILE	2.4
34	2c	77	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
40	2i	63	ILE	2.4
44	2m	66	LEU	2.4
44	2m	116	THR	2.4
45	2n	42	ILE	2.4
50	2s	16	LEU	2.4
6	2G	147	ASP	2.4
40	1i	12	GLU	2.4
41	1j	86	MET	2.4
1	1A	1103	A	2.4
1	2A	2158	A	2.4
32	1a	160	A	2.4
32	2a	959	A	2.4
33	1b	22	LYS	2.4
26	14	54	GLY	2.4
34	2c	145	GLY	2.4
34	2c	197	GLY	2.4
35	1d	87	GLY	2.4
47	2p	76	GLN	2.4
26	24	10	VAL	2.4
26	24	50	VAL	2.4
33	1b	165	VAL	2.4
33	2b	230	VAL	2.4
1	1A	2125	G	2.4
12	2Q	49	ALA	2.4
14	2S	7	TYR	2.4
26	24	59	PHE	2.4
32	2a	1009	G	2.4
40	2i	62	TYR	2.4
44	2m	23	TYR	2.4
45	1n	5	ALA	2.4
6	1G	139	LEU	2.4
34	2c	12	LEU	2.4
1	1A	2161	C	2.4
32	1a	92	C	2.4
32	2a	4	U	2.4
40	2i	7	THR	2.4
52	2u	17	THR	2.4
32	2a	970	C	2.4
32	2a	1043	C	2.4
32	2a	1060	C	2.4
32	2a	1359	C	2.4
44	2m	92	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
33	1b	50	GLU	2.4
34	2c	20	SER	2.4
41	1j	30	SER	2.4
7	2H	39	PRO	2.4
21	2Z	167	PRO	2.4
33	2b	202	PRO	2.4
35	1d	180	GLY	2.4
40	1i	68	GLY	2.4
7	2H	17	VAL	2.4
44	2m	53	VAL	2.4
1	1A	229	A	2.4
1	1A	529	A	2.4
1	2A	2135	A	2.4
6	2G	141	PHE	2.4
32	2a	1256	A	2.4
35	2d	21	LEU	2.3
14	2S	40	ILE	2.3
34	2c	202	ILE	2.3
41	2j	75	ILE	2.3
40	2i	27	THR	2.3
1	1A	2132	U	2.3
1	2A	171	G	2.3
1	2A	2802	G	2.3
32	1a	181	G	2.3
32	1a	348	G	2.3
32	1a	1032	G	2.3
32	2a	951	G	2.3
32	2a	971	G	2.3
32	2a	982	U	2.3
32	2a	1057	G	2.3
54	1y	44	G	2.3
1	1A	1052	C	2.3
1	1A	1072	C	2.3
1	1A	1509	C	2.3
1	1A	2139	C	2.3
1	2A	645	C	2.3
8	1I	87	LYS	2.3
32	1a	1137	C	2.3
43	2l	47	LYS	2.3
6	2G	32	PRO	2.3
34	2c	109	PRO	2.3
6	2G	127	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
17	2V	63	GLY	2.3
36	2e	29	GLY	2.3
12	2Q	16	ARG	2.3
36	2e	27	ARG	2.3
46	1o	88	ARG	2.3
47	1p	75	ARG	2.3
6	2G	102	PHE	2.3
26	14	49	PHE	2.3
19	2X	92	LEU	2.3
26	24	32	TYR	2.3
33	2b	33	TYR	2.3
1	1A	1086	A	2.3
34	2c	67	THR	2.3
53	2v	12	A	2.3
38	1g	8	GLU	2.3
21	2Z	87	ASP	2.3
40	1i	91	ASP	2.3
6	2G	29	TRP	2.3
1	2A	2160	G	2.3
32	2a	1021	G	2.3
1	1A	2108	C	2.3
1	2A	898	C	2.3
1	2A	2175	C	2.3
7	2H	3	ARG	2.3
24	12	70	GLN	2.3
32	1a	91	C	2.3
32	2a	1214	C	2.3
51	2t	47	GLY	2.3
7	2H	37	VAL	2.3
7	2H	79	VAL	2.3
8	2I	15	VAL	2.3
34	2c	173	VAL	2.3
20	2Y	65	ALA	2.3
33	2b	218	ALA	2.3
34	2c	187	ALA	2.3
44	2m	18	ALA	2.3
44	2m	81	LEU	2.3
45	2n	53	LEU	2.3
44	2m	84	ILE	2.3
7	2H	61	HIS	2.3
21	2Z	99	TYR	2.3
39	2h	3	THR	2.3

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Mol	Chain	Res	Type	RSRZ
40	1i	4	TYR	2.3
40	1i	103	THR	2.3
44	2m	87	TYR	2.3
47	1p	1	MET	2.3
18	2W	60	ASN	2.3
1	1A	1088	A	2.3
32	2a	1110	A	2.3
32	2a	1183	A	2.3
53	2v	14	A	2.3
21	1Z	166	SER	2.3
7	2H	6	ARG	2.3
11	2P	15	ARG	2.3
26	24	7	PRO	2.3
41	2j	17	ASP	2.3
33	2b	175	ARG	2.3
8	1I	124	GLY	2.3
11	2P	116	GLY	2.3
12	2Q	33	GLY	2.3
1	2A	2150	U	2.3
32	1a	1040	U	2.3
32	2a	1000	U	2.3
21	2Z	33	LEU	2.3
41	2j	71	LEU	2.3
42	2k	103	LEU	2.3
36	2e	94	ALA	2.3
1	1A	883	G	2.3
1	2A	2168	G	2.3
32	1a	1008	C	2.3
32	1a	1021	G	2.3
32	2a	1029	C	2.3
32	2a	1031	G	2.3
32	2a	1050	G	2.3
32	2a	1124	G	2.3
34	2c	135	LYS	2.3
40	2i	5	TYR	2.3
25	13	60	GLU	2.3
33	1b	12	GLU	2.3
50	2s	53	ASN	2.3
21	2Z	103	ARG	2.3
21	2Z	153	SER	2.3
38	1g	115	ARG	2.3
45	2n	29	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	1A	1070	A	2.3
6	2G	129	GLY	2.3
21	2Z	143	GLY	2.3
34	2c	155	GLY	2.3
44	2m	112	GLY	2.3
53	2v	23	A	2.3
6	1G	152	LEU	2.3
26	24	35	VAL	2.3
28	26	11	LEU	2.3
34	2c	130	VAL	2.3
34	2c	175	LEU	2.3
39	2h	61	VAL	2.3
40	2i	86	VAL	2.3
21	2Z	104	PHE	2.3
21	2Z	53	ILE	2.2
29	17	45	ALA	2.2
32	2a	1148	U	2.2
35	2d	164	ALA	2.2
40	2i	45	ALA	2.2
41	1j	38	ILE	2.2
43	2l	37	CYS	2.2
54	1y	33	U	2.2
55	1x	47	U	2.2
21	2Z	151	HIS	2.2
47	2p	16	HIS	2.2
3	1D	275	LYS	2.2
26	24	2	LYS	2.2
29	17	48	LYS	2.2
35	2d	86	LYS	2.2
40	2i	118	LYS	2.2
42	2k	124	LYS	2.2
21	2Z	168	GLU	2.2
25	23	60	GLU	2.2
14	2S	92	TYR	2.2
38	2g	151	TYR	2.2
1	1A	2111	C	2.2
32	1a	1037	C	2.2
55	1x	69	C	2.2
1	1A	2124	G	2.2
1	2A	1112	G	2.2
1	2A	2110	G	2.2
1	2A	2751	G	2.2

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Mol	Chain	Res	Type	RSRZ
54	2w	15	G	2.2
18	2W	92	ARG	2.2
22	20	11	ARG	2.2
34	2c	140	ARG	2.2
38	2g	79	ARG	2.2
41	2j	5	ARG	2.2
41	2j	79	ARG	2.2
52	2u	10	ARG	2.2
6	2G	126	ASP	2.2
43	2l	63	GLY	2.2
33	2b	149	LEU	2.2
34	2c	34	LEU	2.2
39	1h	112	LEU	2.2
44	2m	70	LEU	2.2
1	1A	1046	A	2.2
1	1A	1177	A	2.2
1	2A	2171	A	2.2
6	2G	39	ILE	2.2
7	2H	92	ILE	2.2
22	20	45	PHE	2.2
32	2a	1201	A	2.2
32	2a	1319	A	2.2
33	2b	222	ILE	2.2
34	2c	203	PHE	2.2
34	2c	146	ALA	2.2
41	2j	98	ILE	2.2
43	2l	23	LYS	2.2
48	2q	100	LYS	2.2
7	2H	124	GLU	2.2
32	2a	1126	U	2.2
32	2a	1313	U	2.2
41	1j	87	THR	2.2
6	2G	118	ARG	2.2
14	1S	20	ARG	2.2
38	1g	5	ARG	2.2
38	2g	115	ARG	2.2
45	2n	19	ARG	2.2
1	1A	2174	C	2.2
1	2A	2896	C	2.2
20	2Y	107	ASP	2.2
1	2A	2124	G	2.2
1	2A	2805	G	2.2

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Mol	Chain	Res	Type	RSRZ
7	2H	71	LEU	2.2
14	2S	54	LEU	2.2
19	2X	66	LEU	2.2
32	2a	1184	G	2.2
36	2e	35	GLY	2.2
40	2i	39	GLY	2.2
54	2y	15	G	2.2
36	2e	51	VAL	2.2
40	2i	109	VAL	2.2
50	2s	19	VAL	2.2
21	1Z	136	PHE	2.2
34	2c	176	HIS	2.2
44	2m	5	ALA	2.2
20	2Y	83	THR	2.2
21	1Z	169	GLU	2.2
34	2c	192	THR	2.2
6	2G	128	ARG	2.2
33	2b	137	ARG	2.2
45	2n	57	ARG	2.2
51	2t	83	ARG	2.2
35	2d	20	TYR	2.2
42	1k	25	TYR	2.2
6	2G	122	PRO	2.2
7	2H	10	PRO	2.2
40	2i	90	PRO	2.2
34	1c	107	GLN	2.2
33	2b	215	LEU	2.2
40	1i	126	SER	2.2
7	2H	44	VAL	2.2
39	2h	51	VAL	2.2
41	1j	24	VAL	2.2
43	2l	39	VAL	2.2
50	2s	66	MET	2.2
1	2A	34	C	2.2
1	2A	2804	C	2.2
7	2H	9	ILE	2.2
12	2Q	65	PHE	2.2
32	2a	1322	C	2.2
32	2a	1384	C	2.2
33	1b	201	ILE	2.2
33	2b	162	ILE	2.2
41	2j	96	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
54	2y	48	C	2.2
1	1A	275	G	2.2
1	1A	545	G	2.2
1	2A	880	G	2.2
3	1D	28	GLU	2.2
32	2a	1178	G	2.2
32	2a	1216	G	2.2
32	2a	1356	G	2.2
32	2a	1530	G	2.2
54	1w	15	G	2.2
54	2y	34	G	2.2
54	2y	44	G	2.2
6	2G	161	THR	2.2
40	1i	64	THR	2.2
47	2p	69	THR	2.2
41	2j	9	ARG	2.2
4	1E	56	PRO	2.2
6	2G	12	TYR	2.2
32	1a	143	A	2.2
32	1a	171	A	2.2
33	2b	131	PRO	2.2
34	1c	193	TYR	2.2
38	2g	154	TYR	2.2
40	2i	4	TYR	2.2
40	2i	92	TYR	2.2
41	1j	76	ASN	2.2
43	2l	69	TYR	2.2
54	1y	58	A	2.2
1	2A	895	U	2.2
3	2D	276	LYS	2.2
12	2Q	22	LYS	2.2
14	2S	93	LYS	2.2
32	1a	203	U	2.2
32	2a	1085	U	2.2
47	1p	76	GLN	2.2
4	2E	115	GLY	2.2
16	2U	73	GLY	2.2
34	2c	13	GLY	2.2
36	2e	22	GLY	2.2
38	2g	12	LEU	2.2
31	29	12	ASP	2.2
7	2H	43	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
8	1I	42	SER	2.2
33	1b	136	VAL	2.2
33	2b	197	VAL	2.2
37	1f	88	VAL	2.2
47	2p	2	VAL	2.2
50	2s	60	VAL	2.2
34	2c	60	ALA	2.1
41	2j	27	ALA	2.1
45	2n	59	ALA	2.1
47	2p	48	TRP	2.1
11	1P	149	GLU	2.1
34	1c	90	GLU	2.1
1	2A	2143	C	2.1
15	1T	108	ARG	2.1
32	1a	1038	C	2.1
32	2a	1397	C	2.1
34	2c	15	THR	2.1
52	2u	22	ARG	2.1
1	1A	879	G	2.1
1	1A	1091	G	2.1
1	2A	2207	G	2.1
32	2a	1023	G	2.1
11	2P	68	GLN	2.1
14	2S	61	ASN	2.1
46	1o	69	TYR	2.1
7	2H	41	MET	2.1
33	2b	118	LEU	2.1
39	2h	39	LEU	2.1
44	2m	19	LEU	2.1
1	2A	887	A	2.1
12	2Q	61	GLY	2.1
19	2X	94	GLY	2.1
1	1A	1060	U	2.1
1	2A	362	U	2.1
12	2Q	66	ILE	2.1
27	15	60	VAL	2.1
36	2e	41	VAL	2.1
50	2s	14	HIS	2.1
50	2s	38	SER	2.1
45	2n	20	ALA	2.1
49	1r	24	ALA	2.1
12	1Q	112	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
20	1Y	91	GLU	2.1
33	1b	24	TRP	2.1
41	2j	83	GLU	2.1
50	2s	34	TRP	2.1
15	2T	111	ARG	2.1
33	1b	30	ARG	2.1
35	2d	122	ARG	2.1
41	1j	79	ARG	2.1
33	2b	190	THR	2.1
20	2Y	34	LYS	2.1
40	2i	97	LYS	2.1
45	2n	11	LYS	2.1
1	2A	277	C	2.1
2	2B	5	C	2.1
32	1a	136	C	2.1
32	2a	989	C	2.1
32	2a	1066	C	2.1
32	2a	1189	C	2.1
32	2a	1244	C	2.1
35	2d	160	GLN	2.1
54	1w	2	C	2.1
54	2y	4	C	2.1
33	2b	63	MET	2.1
41	1j	65	LEU	2.1
51	2t	10	LEU	2.1
46	1o	89	GLY	2.1
51	2t	101	GLY	2.1
1	2A	2151	G	2.1
6	1G	49	ASP	2.1
12	2Q	131	ILE	2.1
33	2b	40	HIS	2.1
32	2a	1026	G	2.1
34	2c	120	VAL	2.1
44	2m	98	VAL	2.1
51	1t	100	ILE	2.1
1	1A	899	A	2.1
1	2A	1847	A	2.1
7	2H	102	ALA	2.1
32	1a	149	A	2.1
26	24	30	GLU	2.1
32	2a	997	U	2.1
32	2a	1012	U	2.1

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Mol	Chain	Res	Type	RSRZ
32	2a	1044	A	2.1
32	2a	1062	U	2.1
32	2a	1213	A	2.1
32	2a	1251	A	2.1
34	2c	168	ALA	2.1
44	2m	67	GLU	2.1
54	1y	45	U	2.1
38	2g	32	ARG	2.1
34	1c	15	THR	2.1
42	2k	31	THR	2.1
44	2m	20	THR	2.1
44	1m	120	LYS	2.1
35	1d	189	PRO	2.1
7	2H	7	LEU	2.1
14	2S	80	LEU	2.1
34	2c	178	LEU	2.1
39	2h	63	LEU	2.1
48	1q	98	LEU	2.1
45	2n	40	CYS	2.1
6	2G	131	TYR	2.1
21	2Z	9	TYR	2.1
26	24	67	TYR	2.1
1	2A	2803	C	2.1
7	2H	11	VAL	2.1
20	2Y	44	ILE	2.1
32	1a	1006	C	2.1
32	2a	1007	C	2.1
32	2a	1208	C	2.1
32	2a	1317	C	2.1
33	2b	200	ILE	2.1
34	2c	66	VAL	2.1
40	1i	81	ILE	2.1
40	2i	65	VAL	2.1
36	2e	5	ASP	2.1
39	2h	4	ASP	2.1
45	2n	36	PHE	2.1
7	1H	3	ARG	2.1
19	2X	68	ARG	2.1
43	2l	41	ARG	2.1
44	2m	28	ALA	2.1
1	2A	1169	G	2.1
1	2A	1170	G	2.1

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Mol	Chain	Res	Type	RSRZ
32	2a	631	G	2.1
1	1A	1054	A	2.1
1	2A	878	A	2.1
1	2A	917	A	2.1
32	1a	383	A	2.1
32	2a	532	A	2.1
32	2a	1052	U	2.1
32	2a	1159	U	2.1
50	2s	18	LYS	2.1
52	2u	20	LYS	2.1
40	2i	73	GLN	2.1
6	2G	62	LEU	2.1
6	2G	172	LEU	2.1
7	2H	88	LEU	2.1
8	2I	38	LEU	2.1
21	1Z	102	LEU	2.1
34	2c	204	LEU	2.1
40	2i	79	LEU	2.1
34	2c	3	ASN	2.1
11	1P	44	GLY	2.1
34	2c	74	GLY	2.1
40	2i	117	HIS	2.1
34	1c	182	ILE	2.1
39	2h	48	TYR	2.1
6	2G	160	VAL	2.1
33	2b	93	VAL	2.1
34	2c	116	VAL	2.1
47	1p	21	VAL	2.1
34	1c	179	ARG	2.0
34	2c	17	ASP	2.0
36	2e	28	PHE	2.1
6	1G	136	ARG	2.0
11	2P	79	ARG	2.0
5	2F	21	ALA	2.0
6	1G	46	ALA	2.0
12	2Q	117	ALA	2.0
27	25	59	GLU	2.0
36	2e	24	ARG	2.0
40	1i	10	ARG	2.0
41	2j	60	ARG	2.0
45	2n	41	ARG	2.0
34	2c	129	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	1A	1100	C	2.0
11	2P	76	LYS	2.0
30	28	29	LYS	2.0
32	2a	1112	C	2.0
54	2y	13	C	2.0
33	2b	97	TRP	2.0
34	2c	18	TRP	2.0
44	2m	105	THR	2.0
40	2i	21	PRO	2.0
1	1A	2118	U	2.0
1	2A	2130	U	2.0
6	2G	133	LEU	2.0
12	2Q	113	GLN	2.0
20	2Y	57	GLN	2.0
32	1a	173	U	2.0
32	2a	1056	U	2.0
32	2a	1196	U	2.0
33	1b	10	LEU	2.0
35	1d	120	LEU	2.0
40	2i	99	LEU	2.0
42	2k	13	GLN	2.0
1	1A	892	G	2.0
1	1A	1059	G	2.0
1	2A	1115	G	2.0
2	2B	120	A	2.0
32	1a	78	G	2.0
32	1a	79	G	2.0
32	1a	306	G	2.0
32	1a	1031	G	2.0
32	2a	998	G	2.0
32	2a	1011	G	2.0
32	2a	1093	A	2.0
32	2a	1108	G	2.0
32	2a	1130	A	2.0
32	2a	1193	G	2.0
34	2c	181	ASN	2.0
41	2j	69	ASN	2.0
6	2G	52	ILE	2.0
35	1d	5	ILE	2.0
35	1d	16	GLY	2.0
41	2j	6	ILE	2.0
6	2G	146	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
9	2N	5	VAL	2.0
14	2S	36	TYR	2.0
33	1b	31	TYR	2.0
34	2c	76	VAL	2.0
37	2f	59	TYR	2.0
8	1I	27	ARG	2.0
9	2N	61	ARG	2.0
21	1Z	148	ASP	2.0
33	2b	134	GLU	2.0
34	1c	56	ASP	2.0
34	1c	62	ASP	2.0
48	2q	96	GLU	2.0
9	2N	118	LYS	2.0
34	2c	133	ALA	2.0
45	2n	5	ALA	2.0
33	1b	124	SER	2.0
21	2Z	159	PRO	2.0
46	2o	75	PRO	2.0
1	1A	897	C	2.0
1	1A	1080	C	2.0
1	2A	893	C	2.0
32	2a	1119	C	2.0
32	2a	1242	C	2.0
33	2b	61	LEU	2.0
36	2e	139	LEU	2.0
37	1f	48	LEU	2.0
1	1A	2189	U	2.0
32	2a	1358	U	2.0
7	2H	136	ILE	2.0
20	2Y	38	ILE	2.0
33	2b	211	ILE	2.0
34	2c	78	GLY	2.0
1	1A	1073	A	2.0
1	2A	2176	A	2.0
1	2A	2310	A	2.0
3	2D	262	ARG	2.0
7	2H	51	ARG	2.0
14	2S	3	ARG	2.0
15	1T	111	ARG	2.0
32	2a	964	A	2.0
32	2a	996	A	2.0
32	2a	1041	A	2.0

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Mol	Chain	Res	Type	RSRZ
32	2a	1250	A	2.0
32	2a	1261	A	2.0
35	1d	153	ARG	2.0
35	2d	105	VAL	2.0
43	2l	18	VAL	2.0
44	2m	117	VAL	2.0
44	2m	21	TYR	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
54	PSU	2y	55	20/21	0.54	0.17	106,112,122,123	0
54	G7M	2w	46	24/25	0.57	0.16	92,104,115,130	0
54	4SU	2y	8	20/21	0.62	0.15	103,107,116,123	0
54	G7M	1w	46	24/25	0.62	0.18	81,92,115,135	0
54	G7M	2y	46	24/25	0.68	0.15	100,107,114,133	0
54	G7M	1y	46	24/25	0.68	0.15	96,105,111,121	0
54	5MU	2y	54	21/22	0.71	0.15	101,106,114,134	0
54	PSU	1y	55	20/21	0.71	0.15	96,104,113,126	0
54	MIA	2y	37	22/30	0.73	0.15	92,101,108,121	0
54	4SU	1y	8	20/21	0.75	0.13	96,103,106,113	0
54	5MU	1y	54	21/22	0.76	0.15	92,98,113,125	0
54	PSU	2y	32	20/21	0.76	0.14	89,97,108,112	0
54	PSU	2y	39	20/21	0.78	0.13	93,95,108,119	0
54	MIA	1y	37	22/30	0.79	0.14	89,94,98,103	0
54	PSU	1y	39	20/21	0.82	0.13	90,93,102,104	0
54	4SU	2w	8	20/21	0.82	0.12	98,101,108,119	0
54	MIA	2w	37	25/30	0.83	0.14	81,90,97,108	0
32	2MG	2a	1207	24/25	0.83	0.15	90,96,99,100	0
54	PSU	1w	55	20/21	0.83	0.11	73,88,94,96	0
54	PSU	2w	55	20/21	0.84	0.12	78,99,106,107	0
54	PSU	1y	32	20/21	0.86	0.11	90,93,105,107	0
54	5MU	2w	54	21/22	0.86	0.11	77,88,94,96	0
54	PSU	2w	32	20/21	0.88	0.11	91,96,106,114	0
54	4SU	1w	8	20/21	0.88	0.12	87,90,97,99	0
55	4SU	2x	8	20/21	0.89	0.12	81,88,93,95	0
55	5MU	2x	54	21/22	0.89	0.12	78,89,92,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	PSU	2a	516	20/21	0.89	0.11	80,87,91,91	0
43	0TD	2l	92	10/11	0.90	0.14	71,74,79,88	0
32	M2G	2a	966	25/26	0.91	0.18	67,76,90,98	0
55	PSU	2x	55	20/21	0.91	0.10	81,87,92,95	0
1	5MU	2A	1915	21/22	0.91	0.11	75,79,84,87	0
54	MIA	1w	37	29/30	0.92	0.14	54,64,77,101	0
32	5MC	2a	1404	21/22	0.92	0.11	56,61,70,74	0
55	5MC	2x	32	21/22	0.92	0.13	76,79,86,89	0
54	PSU	2w	39	20/21	0.92	0.08	79,91,95,96	0
32	G7M	2a	527	24/25	0.92	0.14	66,74,83,86	0
55	PSU	1x	55	20/21	0.92	0.11	68,73,85,86	0
55	5MU	1x	54	21/22	0.93	0.10	69,75,81,85	0
32	5MC	2a	967	21/22	0.93	0.14	71,79,91,92	0
54	5MU	1w	54	21/22	0.93	0.09	64,76,83,87	0
32	5MC	2a	1400	21/22	0.93	0.15	71,79,82,83	0
32	4OC	2a	1402	22/23	0.93	0.11	60,69,74,78	0
1	PSU	2A	1917	20/21	0.94	0.09	68,74,79,82	0
54	PSU	1w	32	20/21	0.94	0.11	73,78,87,88	0
43	0TD	1l	92	10/11	0.94	0.10	51,56,58,66	0
1	5MU	1A	1915	21/22	0.94	0.10	53,59,63,68	0
55	31H	2x	76	32/33	0.95	0.09	42,50,61,65	0
32	UR3	2a	1498	21/22	0.95	0.10	58,62,68,73	0
32	MA6	2a	1519	24/25	0.95	0.12	56,68,73,76	0
32	2MG	1a	1207	24/25	0.95	0.09	67,76,78,79	0
55	4SU	1x	8	20/21	0.95	0.09	55,68,73,77	0
55	5MC	1x	32	21/22	0.95	0.13	56,62,68,74	0
54	PSU	1w	39	20/21	0.95	0.08	69,75,83,87	0
1	PSU	2A	1911	20/21	0.95	0.08	65,69,75,79	0
32	MA6	2a	1518	24/25	0.96	0.11	55,69,74,76	0
1	2MA	2A	2503	23/24	0.96	0.10	33,42,46,48	0
1	PSU	1A	1917	20/21	0.96	0.08	48,55,60,63	0
32	MA6	1a	1519	24/25	0.96	0.09	39,46,49,52	0
32	PSU	1a	516	20/21	0.96	0.08	58,64,67,69	0
32	G7M	1a	527	24/25	0.96	0.09	44,52,61,64	0
32	M2G	1a	966	25/26	0.96	0.10	50,57,64,72	0
32	5MC	1a	967	21/22	0.96	0.09	49,57,67,68	0
1	OMC	2A	1920	21/22	0.96	0.09	53,67,71,72	0
1	5MC	2A	1942	21/22	0.96	0.09	50,60,63,66	0
1	OMG	2A	2251	24/25	0.96	0.08	41,45,49,51	0
1	PSU	1A	1911	20/21	0.97	0.07	43,50,53,53	0
1	5MU	1A	1939	21/22	0.97	0.07	27,33,37,39	0
1	5MU	2A	1939	21/22	0.97	0.08	35,40,45,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	5MC	1a	1400	21/22	0.97	0.09	46,54,56,59	0
1	5MC	2A	1962	21/22	0.97	0.07	41,53,59,65	0
32	5MC	1a	1404	21/22	0.97	0.07	37,41,46,47	0
32	5MC	2a	1407	21/22	0.97	0.10	56,60,66,70	0
32	5MC	1a	1407	21/22	0.97	0.07	32,42,46,49	0
32	MA6	1a	1518	24/25	0.97	0.08	36,43,49,51	0
1	5MC	1A	1942	21/22	0.97	0.08	37,42,46,49	0
32	4OC	1a	1402	22/23	0.98	0.07	43,46,51,62	0
1	OMU	1A	2552	21/22	0.98	0.07	28,32,37,42	0
1	OMU	2A	2552	21/22	0.98	0.07	41,47,50,56	0
1	PSU	2A	2605	20/21	0.98	0.06	37,41,47,50	0
1	PSU	1A	2605	20/21	0.98	0.06	27,31,35,38	0
32	UR3	1a	1498	21/22	0.98	0.06	38,44,50,53	0
1	OMC	1A	1920	21/22	0.98	0.07	37,47,51,54	0
1	5MC	1A	1962	21/22	0.98	0.06	33,42,49,56	0
55	31H	1x	76	32/33	0.98	0.07	22,32,39,45	10
1	2MA	1A	2503	23/24	0.99	0.05	24,27,32,33	0
1	OMG	1A	2251	24/25	0.99	0.05	26,30,34,36	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
56	MG	1B	221	1/1	0.37	0.26	84,84,84,84	0
56	MG	1A	4060	1/1	0.43	0.16	129,129,129,129	0
56	MG	1a	1671	1/1	0.47	0.32	80,80,80,80	0
56	MG	2i	202	1/1	0.50	0.36	88,88,88,88	0
56	MG	2A	3313	1/1	0.51	0.39	91,91,91,91	0
56	MG	2a	1758	1/1	0.51	0.38	83,83,83,83	0
56	MG	1B	229	1/1	0.51	0.18	86,86,86,86	0
56	MG	1A	3721	1/1	0.52	0.28	86,86,86,86	0
56	MG	2A	3589	1/1	0.57	0.20	83,83,83,83	0
56	MG	2A	3621	1/1	0.57	0.36	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2q	203	1/1	0.57	0.18	89,89,89,89	0
56	MG	2A	3257	1/1	0.58	0.27	81,81,81,81	0
56	MG	2a	1789	1/1	0.59	0.29	77,77,77,77	0
56	MG	1a	1803	1/1	0.59	0.22	94,94,94,94	0
56	MG	1A	3861	1/1	0.59	0.25	62,62,62,62	0
56	MG	1A	3969	1/1	0.61	0.16	92,92,92,92	0
56	MG	2a	1642	1/1	0.61	0.32	89,89,89,89	0
56	MG	2A	3659	1/1	0.62	0.25	85,85,85,85	0
56	MG	2A	3676	1/1	0.63	0.29	60,60,60,60	0
56	MG	2A	3277	1/1	0.65	0.30	94,94,94,94	0
56	MG	2a	1790	1/1	0.65	0.22	85,85,85,85	0
56	MG	2A	3641	1/1	0.65	0.27	76,76,76,76	0
56	MG	2A	3278	1/1	0.65	0.28	91,91,91,91	0
56	MG	1A	3907	1/1	0.66	0.20	80,80,80,80	0
56	MG	2A	3762	1/1	0.66	0.29	78,78,78,78	0
56	MG	1a	1712	1/1	0.67	0.34	86,86,86,86	0
56	MG	1a	1660	1/1	0.67	0.28	87,87,87,87	0
56	MG	2a	1708	1/1	0.67	0.39	91,91,91,91	0
56	MG	2A	3168	1/1	0.67	0.30	81,81,81,81	0
56	MG	2G	201	1/1	0.68	0.22	81,81,81,81	0
56	MG	2A	3300	1/1	0.68	0.27	74,74,74,74	0
56	MG	1A	3956	1/1	0.68	0.19	76,76,76,76	0
56	MG	2A	3455	1/1	0.68	0.29	71,71,71,71	0
56	MG	2A	3569	1/1	0.69	0.28	68,68,68,68	0
56	MG	1A	3757	1/1	0.69	0.12	83,83,83,83	0
56	MG	2A	3742	1/1	0.69	0.29	81,81,81,81	0
56	MG	2a	1779	1/1	0.69	0.36	77,77,77,77	0
56	MG	1a	1753	1/1	0.69	0.31	81,81,81,81	0
56	MG	2B	214	1/1	0.69	0.36	84,84,84,84	0
56	MG	2F	305	1/1	0.69	0.25	78,78,78,78	0
56	MG	2A	3256	1/1	0.69	0.19	83,83,83,83	0
56	MG	1a	1732	1/1	0.70	0.25	90,90,90,90	0
56	MG	2a	1713	1/1	0.70	0.27	87,87,87,87	0
56	MG	2A	3599	1/1	0.70	0.25	61,61,61,61	0
56	MG	2A	3258	1/1	0.70	0.31	77,77,77,77	0
56	MG	2B	216	1/1	0.70	0.28	74,74,74,74	0
56	MG	2A	3238	1/1	0.70	0.17	66,66,66,66	0
56	MG	2A	3015	1/1	0.70	0.36	85,85,85,85	0
56	MG	2A	3582	1/1	0.70	0.40	81,81,81,81	0
56	MG	1A	4005	1/1	0.71	0.17	67,67,67,67	0
56	MG	2A	3162	1/1	0.71	0.27	87,87,87,87	0
56	MG	2A	3167	1/1	0.71	0.22	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3692	1/1	0.71	0.28	91,91,91,91	0
56	MG	28	102	1/1	0.71	0.39	71,71,71,71	0
56	MG	1A	3472	1/1	0.71	0.15	74,74,74,74	0
56	MG	2A	3276	1/1	0.71	0.40	93,93,93,93	0
56	MG	1A	4034	1/1	0.72	0.21	83,83,83,83	0
56	MG	2A	3080	1/1	0.72	0.26	83,83,83,83	0
56	MG	1A	3955	1/1	0.72	0.22	88,88,88,88	0
56	MG	1a	1793	1/1	0.72	0.21	76,76,76,76	0
56	MG	2A	3424	1/1	0.72	0.30	76,76,76,76	0
56	MG	2a	1698	1/1	0.72	0.31	91,91,91,91	0
56	MG	2j	201	1/1	0.72	0.17	81,81,81,81	0
56	MG	1B	232	1/1	0.72	0.34	89,89,89,89	0
56	MG	1B	215	1/1	0.73	0.25	68,68,68,68	0
56	MG	1A	3490	1/1	0.73	0.28	65,65,65,65	0
56	MG	2A	3022	1/1	0.73	0.29	81,81,81,81	0
56	MG	2A	3193	1/1	0.73	0.26	79,79,79,79	0
56	MG	2A	3235	1/1	0.73	0.39	80,80,80,80	0
56	MG	2i	201	1/1	0.73	0.25	85,85,85,85	0
56	MG	1a	1649	1/1	0.73	0.33	83,83,83,83	0
56	MG	2a	1706	1/1	0.73	0.35	79,79,79,79	0
56	MG	2A	3081	1/1	0.73	0.18	75,75,75,75	0
56	MG	2v	101	1/1	0.73	0.37	87,87,87,87	0
56	MG	1x	107	1/1	0.74	0.24	86,86,86,86	0
56	MG	1A	3277	1/1	0.74	0.18	50,50,50,50	0
56	MG	2B	218	1/1	0.74	0.27	80,80,80,80	0
56	MG	1a	1759	1/1	0.74	0.23	87,87,87,87	0
56	MG	2A	3184	1/1	0.74	0.34	82,82,82,82	0
56	MG	2a	1796	1/1	0.74	0.23	91,91,91,91	0
56	MG	2a	1797	1/1	0.74	0.36	81,81,81,81	0
56	MG	1A	4052	1/1	0.74	0.25	84,84,84,84	0
56	MG	2A	3577	1/1	0.74	0.35	87,87,87,87	0
56	MG	2A	3231	1/1	0.74	0.27	85,85,85,85	0
56	MG	1A	3823	1/1	0.74	0.32	46,46,46,46	0
56	MG	2A	3768	1/1	0.74	0.15	89,89,89,89	0
56	MG	2V	202	1/1	0.75	0.23	72,72,72,72	0
56	MG	1A	3838	1/1	0.75	0.22	62,62,62,62	0
56	MG	2a	1608	1/1	0.75	0.29	77,77,77,77	0
56	MG	1a	1691	1/1	0.75	0.24	80,80,80,80	0
56	MG	2a	1672	1/1	0.75	0.34	78,78,78,78	0
56	MG	2A	3620	1/1	0.75	0.17	94,94,94,94	0
56	MG	1A	3847	1/1	0.75	0.18	43,43,43,43	0
56	MG	2A	3267	1/1	0.75	0.23	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3160	1/1	0.75	0.29	71,71,71,71	0
56	MG	1a	1716	1/1	0.75	0.41	76,76,76,76	0
56	MG	1A	4001	1/1	0.75	0.17	83,83,83,83	0
56	MG	1B	226	1/1	0.75	0.22	71,71,71,71	0
56	MG	1A	3332	1/1	0.75	0.23	65,65,65,65	0
56	MG	2A	3321	1/1	0.75	0.21	80,80,80,80	0
56	MG	2B	203	1/1	0.75	0.33	86,86,86,86	0
56	MG	1A	4026	1/1	0.75	0.23	53,53,53,53	0
56	MG	11	102	1/1	0.75	0.20	56,56,56,56	0
56	MG	1A	3812	1/1	0.75	0.15	69,69,69,69	0
56	MG	2A	3236	1/1	0.75	0.18	91,91,91,91	0
56	MG	1A	3208	1/1	0.75	0.22	76,76,76,76	0
56	MG	2A	3618	1/1	0.76	0.20	71,71,71,71	0
56	MG	2a	1602	1/1	0.76	0.23	88,88,88,88	0
56	MG	1A	3094	1/1	0.76	0.24	69,69,69,69	0
56	MG	2a	1617	1/1	0.76	0.20	79,79,79,79	0
56	MG	2A	3340	1/1	0.76	0.42	73,73,73,73	0
56	MG	1a	1799	1/1	0.76	0.21	75,75,75,75	0
56	MG	2a	1683	1/1	0.76	0.28	88,88,88,88	0
56	MG	1B	222	1/1	0.76	0.20	69,69,69,69	0
56	MG	2a	1701	1/1	0.76	0.26	85,85,85,85	0
56	MG	2A	3462	1/1	0.76	0.21	69,69,69,69	0
56	MG	2A	3501	1/1	0.76	0.17	80,80,80,80	0
56	MG	2A	3725	1/1	0.76	0.20	68,68,68,68	0
56	MG	2A	3511	1/1	0.76	0.28	72,72,72,72	0
56	MG	2a	1772	1/1	0.76	0.30	82,82,82,82	0
56	MG	2A	3552	1/1	0.76	0.21	69,69,69,69	0
56	MG	2A	3240	1/1	0.76	0.26	68,68,68,68	0
56	MG	2A	3242	1/1	0.76	0.26	82,82,82,82	0
56	MG	2a	1794	1/1	0.76	0.25	83,83,83,83	0
56	MG	2A	3290	1/1	0.76	0.31	82,82,82,82	0
56	MG	2A	3587	1/1	0.76	0.14	62,62,62,62	0
56	MG	1A	3781	1/1	0.76	0.30	74,74,74,74	0
56	MG	2B	220	1/1	0.76	0.19	77,77,77,77	0
56	MG	1a	1783	1/1	0.76	0.24	70,70,70,70	0
56	MG	2A	3603	1/1	0.76	0.19	77,77,77,77	0
56	MG	2A	3617	1/1	0.76	0.24	77,77,77,77	0
56	MG	2y	101	1/1	0.76	0.12	99,99,99,99	0
56	MG	2A	3055	1/1	0.77	0.30	78,78,78,78	0
56	MG	2E	301	1/1	0.77	0.28	75,75,75,75	0
56	MG	2a	1724	1/1	0.77	0.37	78,78,78,78	0
56	MG	2a	1737	1/1	0.77	0.11	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3640	1/1	0.77	0.19	74,74,74,74	0
56	MG	2a	1771	1/1	0.77	0.20	73,73,73,73	0
56	MG	1A	4032	1/1	0.77	0.25	82,82,82,82	0
56	MG	1a	1789	1/1	0.77	0.24	80,80,80,80	0
56	MG	2A	3091	1/1	0.77	0.36	85,85,85,85	0
56	MG	2A	3109	1/1	0.77	0.34	78,78,78,78	0
56	MG	1A	3828	1/1	0.77	0.23	81,81,81,81	0
56	MG	1a	1724	1/1	0.77	0.25	69,69,69,69	0
56	MG	1A	3547	1/1	0.77	0.32	56,56,56,56	0
56	MG	2a	1643	1/1	0.77	0.17	79,79,79,79	0
56	MG	2A	3601	1/1	0.77	0.21	82,82,82,82	0
56	MG	1A	3843	1/1	0.77	0.26	76,76,76,76	0
56	MG	1A	3181	1/1	0.77	0.27	63,63,63,63	0
56	MG	2A	3476	1/1	0.77	0.21	56,56,56,56	0
56	MG	1a	1762	1/1	0.77	0.21	82,82,82,82	0
56	MG	1A	3470	1/1	0.78	0.25	79,79,79,79	0
56	MG	1A	3927	1/1	0.78	0.24	82,82,82,82	0
56	MG	1A	3744	1/1	0.78	0.13	28,28,28,28	0
56	MG	2a	1709	1/1	0.78	0.46	73,73,73,73	0
56	MG	2A	3200	1/1	0.78	0.31	79,79,79,79	0
56	MG	2A	3219	1/1	0.78	0.18	77,77,77,77	0
56	MG	2A	3298	1/1	0.78	0.20	75,75,75,75	0
56	MG	2A	3224	1/1	0.78	0.35	76,76,76,76	0
56	MG	15	107	1/1	0.78	0.14	59,59,59,59	0
56	MG	2A	3319	1/1	0.78	0.14	75,75,75,75	0
56	MG	1A	3274	1/1	0.78	0.20	75,75,75,75	0
56	MG	1A	3775	1/1	0.78	0.20	62,62,62,62	0
56	MG	1A	3231	1/1	0.78	0.21	71,71,71,71	0
56	MG	2A	3634	1/1	0.78	0.28	70,70,70,70	0
56	MG	1A	3242	1/1	0.78	0.16	55,55,55,55	0
56	MG	2A	3141	1/1	0.78	0.19	62,62,62,62	0
56	MG	2a	1630	1/1	0.78	0.41	82,82,82,82	0
56	MG	2A	3247	1/1	0.78	0.32	72,72,72,72	0
56	MG	1a	1794	1/1	0.78	0.19	64,64,64,64	0
56	MG	1A	3866	1/1	0.78	0.14	54,54,54,54	0
56	MG	2A	3529	1/1	0.78	0.31	71,71,71,71	0
56	MG	1B	228	1/1	0.78	0.14	80,80,80,80	0
56	MG	2a	1670	1/1	0.79	0.30	83,83,83,83	0
56	MG	2A	3005	1/1	0.79	0.37	69,69,69,69	0
56	MG	1A	3933	1/1	0.79	0.14	70,70,70,70	0
56	MG	2A	3199	1/1	0.79	0.23	67,67,67,67	0
56	MG	1a	1629	1/1	0.79	0.34	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3583	1/1	0.79	0.20	88,88,88,88	0
56	MG	2B	211	1/1	0.79	0.30	84,84,84,84	0
56	MG	1a	1757	1/1	0.79	0.25	78,78,78,78	0
56	MG	1a	1638	1/1	0.79	0.29	67,67,67,67	0
56	MG	1A	3718	1/1	0.79	0.14	33,33,33,33	0
56	MG	1A	3765	1/1	0.79	0.31	69,69,69,69	0
56	MG	2D	306	1/1	0.79	0.28	71,71,71,71	0
56	MG	1A	4045	1/1	0.79	0.30	75,75,75,75	0
56	MG	2A	3122	1/1	0.79	0.20	73,73,73,73	0
56	MG	2A	3407	1/1	0.79	0.27	86,86,86,86	0
56	MG	2A	3135	1/1	0.79	0.32	81,81,81,81	0
56	MG	1a	1688	1/1	0.79	0.32	81,81,81,81	0
56	MG	2A	3155	1/1	0.79	0.49	81,81,81,81	0
56	MG	2a	1607	1/1	0.79	0.33	86,86,86,86	0
56	MG	1A	3619	1/1	0.79	0.23	67,67,67,67	0
56	MG	1A	3683	1/1	0.79	0.21	58,58,58,58	0
56	MG	1A	3782	1/1	0.79	0.20	62,62,62,62	0
56	MG	2a	1641	1/1	0.79	0.21	72,72,72,72	0
56	MG	14	101	1/1	0.79	0.22	83,83,83,83	0
56	MG	2A	3545	1/1	0.79	0.21	76,76,76,76	0
56	MG	2a	1668	1/1	0.79	0.29	71,71,71,71	0
56	MG	1A	3088	1/1	0.80	0.18	71,71,71,71	0
56	MG	1A	3392	1/1	0.80	0.22	65,65,65,65	0
56	MG	2A	3306	1/1	0.80	0.26	73,73,73,73	0
56	MG	2A	3309	1/1	0.80	0.24	82,82,82,82	0
56	MG	2A	3607	1/1	0.80	0.15	71,71,71,71	0
56	MG	2A	3312	1/1	0.80	0.30	72,72,72,72	0
56	MG	1a	1664	1/1	0.80	0.21	63,63,63,63	0
56	MG	2A	3619	1/1	0.80	0.14	89,89,89,89	0
56	MG	2A	3318	1/1	0.80	0.20	77,77,77,77	0
56	MG	1a	1767	1/1	0.80	0.27	73,73,73,73	0
56	MG	2A	3626	1/1	0.80	0.20	75,75,75,75	0
56	MG	2a	1678	1/1	0.80	0.32	84,84,84,84	0
56	MG	1A	3426	1/1	0.80	0.31	81,81,81,81	0
56	MG	2a	1692	1/1	0.80	0.15	80,80,80,80	0
56	MG	2A	3324	1/1	0.80	0.24	64,64,64,64	0
56	MG	1A	4042	1/1	0.80	0.17	75,75,75,75	0
56	MG	2A	3647	1/1	0.80	0.15	61,61,61,61	0
56	MG	2A	3343	1/1	0.80	0.41	65,65,65,65	0
56	MG	2A	3667	1/1	0.80	0.22	60,60,60,60	0
56	MG	1A	3976	1/1	0.80	0.18	71,71,71,71	0
56	MG	2a	1714	1/1	0.80	0.27	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1693	1/1	0.80	0.33	73,73,73,73	0
56	MG	2a	1735	1/1	0.80	0.25	80,80,80,80	0
56	MG	2A	3143	1/1	0.80	0.24	77,77,77,77	0
56	MG	2a	1744	1/1	0.80	0.31	82,82,82,82	0
56	MG	2a	1756	1/1	0.80	0.24	76,76,76,76	0
56	MG	2A	3243	1/1	0.80	0.26	80,80,80,80	0
56	MG	2A	3467	1/1	0.80	0.31	68,68,68,68	0
56	MG	1A	4050	1/1	0.80	0.23	78,78,78,78	0
56	MG	2A	3488	1/1	0.80	0.24	56,56,56,56	0
56	MG	1A	3983	1/1	0.80	0.15	64,64,64,64	0
56	MG	2A	3508	1/1	0.80	0.21	86,86,86,86	0
56	MG	2A	3161	1/1	0.80	0.30	74,74,74,74	0
56	MG	1x	101	1/1	0.80	0.21	80,80,80,80	0
56	MG	2A	3263	1/1	0.80	0.19	70,70,70,70	0
56	MG	2a	1812	1/1	0.80	0.41	85,85,85,85	0
56	MG	1A	3574	1/1	0.80	0.15	65,65,65,65	0
56	MG	1x	108	1/1	0.80	0.36	83,83,83,83	0
56	MG	1A	3252	1/1	0.80	0.17	76,76,76,76	0
56	MG	1a	1750	1/1	0.80	0.34	73,73,73,73	0
56	MG	1A	4020	1/1	0.80	0.15	60,60,60,60	0
56	MG	2A	3297	1/1	0.80	0.34	76,76,76,76	0
56	MG	2A	3170	1/1	0.81	0.17	66,66,66,66	0
56	MG	2A	3635	1/1	0.81	0.15	53,53,53,53	0
56	MG	2A	3472	1/1	0.81	0.18	54,54,54,54	0
56	MG	2a	1657	1/1	0.81	0.19	72,72,72,72	0
56	MG	1x	112	1/1	0.81	0.33	83,83,83,83	0
56	MG	2A	3485	1/1	0.81	0.19	55,55,55,55	0
56	MG	2A	3655	1/1	0.81	0.10	86,86,86,86	0
56	MG	2A	3658	1/1	0.81	0.17	88,88,88,88	0
56	MG	1P	205	1/1	0.81	0.13	65,65,65,65	0
56	MG	2A	3197	1/1	0.81	0.21	68,68,68,68	0
56	MG	2a	1697	1/1	0.81	0.22	82,82,82,82	0
56	MG	1A	3291	1/1	0.81	0.32	66,66,66,66	0
56	MG	2A	3680	1/1	0.81	0.24	86,86,86,86	0
56	MG	1A	3458	1/1	0.81	0.20	57,57,57,57	0
56	MG	1A	3763	1/1	0.81	0.25	78,78,78,78	0
56	MG	2A	3532	1/1	0.81	0.21	74,74,74,74	0
56	MG	2A	3746	1/1	0.81	0.24	78,78,78,78	0
56	MG	1a	1602	1/1	0.81	0.39	79,79,79,79	0
56	MG	2A	3763	1/1	0.81	0.28	72,72,72,72	0
56	MG	2a	1733	1/1	0.81	0.33	80,80,80,80	0
56	MG	1A	3317	1/1	0.81	0.29	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3773	1/1	0.81	0.17	66,66,66,66	0
56	MG	1A	3053	1/1	0.81	0.17	59,59,59,59	0
56	MG	2A	3317	1/1	0.81	0.18	87,87,87,87	0
56	MG	1A	3707	1/1	0.81	0.24	69,69,69,69	0
56	MG	2a	1759	1/1	0.81	0.36	76,76,76,76	0
56	MG	1A	3026	1/1	0.81	0.20	64,64,64,64	0
56	MG	1a	1665	1/1	0.81	0.31	71,71,71,71	0
56	MG	2a	1774	1/1	0.81	0.20	70,70,70,70	0
56	MG	1a	1666	1/1	0.81	0.34	69,69,69,69	0
56	MG	2a	1784	1/1	0.81	0.27	80,80,80,80	0
56	MG	2a	1785	1/1	0.81	0.30	80,80,80,80	0
56	MG	1A	3914	1/1	0.81	0.23	63,63,63,63	0
56	MG	2A	3342	1/1	0.81	0.29	74,74,74,74	0
56	MG	1a	1684	1/1	0.81	0.31	58,58,58,58	0
56	MG	2A	3611	1/1	0.81	0.14	80,80,80,80	0
56	MG	2W	202	1/1	0.81	0.22	80,80,80,80	0
56	MG	2a	1802	1/1	0.81	0.26	76,76,76,76	0
56	MG	2A	3353	1/1	0.81	0.24	67,67,67,67	0
56	MG	2g	201	1/1	0.81	0.24	80,80,80,80	0
56	MG	2A	3390	1/1	0.81	0.23	75,75,75,75	0
56	MG	1A	3540	1/1	0.81	0.15	42,42,42,42	0
56	MG	1A	3819	1/1	0.81	0.12	70,70,70,70	0
56	MG	1A	4039	1/1	0.81	0.14	77,77,77,77	0
56	MG	2a	1629	1/1	0.81	0.39	69,69,69,69	0
56	MG	1D	308	1/1	0.81	0.15	60,60,60,60	0
56	MG	1a	1640	1/1	0.82	0.34	78,78,78,78	0
56	MG	2A	3177	1/1	0.82	0.33	81,81,81,81	0
56	MG	2a	1635	1/1	0.82	0.29	73,73,73,73	0
56	MG	1A	4054	1/1	0.82	0.28	65,65,65,65	0
56	MG	2A	3188	1/1	0.82	0.12	66,66,66,66	0
56	MG	1A	3987	1/1	0.82	0.22	62,62,62,62	0
56	MG	2a	1651	1/1	0.82	0.29	77,77,77,77	0
56	MG	1B	201	1/1	0.82	0.21	68,68,68,68	0
56	MG	2a	1666	1/1	0.82	0.20	83,83,83,83	0
56	MG	2A	3625	1/1	0.82	0.22	79,79,79,79	0
56	MG	1A	3904	1/1	0.82	0.21	76,76,76,76	0
56	MG	1a	1806	1/1	0.82	0.18	64,64,64,64	0
56	MG	2A	3347	1/1	0.82	0.44	71,71,71,71	0
56	MG	1l	201	1/1	0.82	0.21	82,82,82,82	0
56	MG	2A	3362	1/1	0.82	0.23	60,60,60,60	0
56	MG	2A	3385	1/1	0.82	0.18	73,73,73,73	0
56	MG	1A	4003	1/1	0.82	0.23	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3328	1/1	0.82	0.36	67,67,67,67	0
56	MG	2a	1704	1/1	0.82	0.29	80,80,80,80	0
56	MG	1A	4006	1/1	0.82	0.22	50,50,50,50	0
56	MG	1A	3474	1/1	0.82	0.20	59,59,59,59	0
56	MG	1a	1690	1/1	0.82	0.61	77,77,77,77	0
56	MG	1A	4021	1/1	0.82	0.10	60,60,60,60	0
56	MG	2A	3684	1/1	0.82	0.14	62,62,62,62	0
56	MG	1B	231	1/1	0.82	0.24	71,71,71,71	0
56	MG	2A	3709	1/1	0.82	0.26	70,70,70,70	0
56	MG	2A	3029	1/1	0.82	0.12	61,61,61,61	0
56	MG	2A	3038	1/1	0.82	0.39	74,74,74,74	0
56	MG	2a	1742	1/1	0.82	0.14	100,100,100,100	0
56	MG	2a	1743	1/1	0.82	0.30	81,81,81,81	0
56	MG	1a	1700	1/1	0.82	0.15	74,74,74,74	0
56	MG	2A	3070	1/1	0.82	0.21	63,63,63,63	0
56	MG	2A	3507	1/1	0.82	0.19	72,72,72,72	0
56	MG	1a	1701	1/1	0.82	0.32	70,70,70,70	0
56	MG	1a	1704	1/1	0.82	0.36	77,77,77,77	0
56	MG	2A	3527	1/1	0.82	0.30	86,86,86,86	0
56	MG	2a	1773	1/1	0.82	0.27	84,84,84,84	0
56	MG	2B	212	1/1	0.82	0.23	89,89,89,89	0
56	MG	1A	3307	1/1	0.82	0.22	65,65,65,65	0
56	MG	1A	3928	1/1	0.82	0.16	83,83,83,83	0
56	MG	1E	315	1/1	0.82	0.16	71,71,71,71	0
56	MG	1A	4033	1/1	0.82	0.22	80,80,80,80	0
56	MG	2D	305	1/1	0.82	0.40	55,55,55,55	0
56	MG	2A	3279	1/1	0.82	0.18	89,89,89,89	0
56	MG	2A	3573	1/1	0.82	0.17	70,70,70,70	0
56	MG	2A	3285	1/1	0.82	0.36	75,75,75,75	0
56	MG	1A	3534	1/1	0.82	0.20	76,76,76,76	0
56	MG	1A	3355	1/1	0.82	0.17	58,58,58,58	0
56	MG	1A	3375	1/1	0.82	0.22	69,69,69,69	0
56	MG	18	106	1/1	0.82	0.21	78,78,78,78	0
56	MG	1A	3572	1/1	0.82	0.32	73,73,73,73	0
56	MG	1a	1764	1/1	0.82	0.19	80,80,80,80	0
56	MG	1A	3787	1/1	0.82	0.23	76,76,76,76	0
56	MG	1A	3804	1/1	0.82	0.18	68,68,68,68	0
56	MG	2x	103	1/1	0.82	0.39	89,89,89,89	0
56	MG	2a	1620	1/1	0.82	0.35	73,73,73,73	0
56	MG	2y	102	1/1	0.82	0.23	88,88,88,88	0
56	MG	1A	3379	1/1	0.83	0.45	49,49,49,49	0
56	MG	2A	3287	1/1	0.83	0.19	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3205	1/1	0.83	0.21	78,78,78,78	0
56	MG	2A	3294	1/1	0.83	0.22	62,62,62,62	0
56	MG	2A	3212	1/1	0.83	0.24	85,85,85,85	0
56	MG	1F	310	1/1	0.83	0.21	55,55,55,55	0
56	MG	1F	312	1/1	0.83	0.29	67,67,67,67	0
56	MG	1a	1648	1/1	0.83	0.31	76,76,76,76	0
56	MG	2A	3234	1/1	0.83	0.30	83,83,83,83	0
56	MG	1A	3192	1/1	0.83	0.17	58,58,58,58	0
56	MG	1A	3901	1/1	0.83	0.14	38,38,38,38	0
56	MG	2A	3522	1/1	0.83	0.16	74,74,74,74	0
56	MG	1a	1661	1/1	0.83	0.15	68,68,68,68	0
56	MG	1a	1707	1/1	0.83	0.29	63,63,63,63	0
56	MG	12	101	1/1	0.83	0.16	61,61,61,61	0
56	MG	2a	1764	1/1	0.83	0.19	53,53,53,53	0
56	MG	2A	3031	1/1	0.83	0.17	58,58,58,58	0
56	MG	2a	1633	1/1	0.83	0.38	74,74,74,74	0
56	MG	1A	3578	1/1	0.83	0.21	64,64,64,64	0
56	MG	2a	1637	1/1	0.83	0.27	75,75,75,75	0
56	MG	2A	3333	1/1	0.83	0.45	68,68,68,68	0
56	MG	2A	3337	1/1	0.83	0.18	65,65,65,65	0
56	MG	2A	3248	1/1	0.83	0.24	79,79,79,79	0
56	MG	2a	1648	1/1	0.83	0.16	90,90,90,90	0
56	MG	2A	3169	1/1	0.83	0.25	75,75,75,75	0
56	MG	2A	3044	1/1	0.83	0.14	68,68,68,68	0
56	MG	1A	3423	1/1	0.83	0.18	40,40,40,40	0
56	MG	1a	1800	1/1	0.83	0.33	80,80,80,80	0
56	MG	2A	3764	1/1	0.83	0.15	79,79,79,79	0
56	MG	2a	1811	1/1	0.83	0.30	91,91,91,91	0
56	MG	1A	3338	1/1	0.83	0.16	63,63,63,63	0
56	MG	2a	1677	1/1	0.83	0.36	78,78,78,78	0
56	MG	2A	3375	1/1	0.83	0.17	63,63,63,63	0
56	MG	2a	1682	1/1	0.83	0.27	80,80,80,80	0
56	MG	2A	3383	1/1	0.83	0.18	74,74,74,74	0
56	MG	1A	3857	1/1	0.83	0.10	52,52,52,52	0
56	MG	1a	1807	1/1	0.83	0.24	78,78,78,78	0
56	MG	2A	3198	1/1	0.83	0.31	75,75,75,75	0
56	MG	2B	217	1/1	0.83	0.33	79,79,79,79	0
56	MG	2A	3100	1/1	0.83	0.28	90,90,90,90	0
56	MG	2a	1686	1/1	0.84	0.23	79,79,79,79	0
56	MG	1A	3799	1/1	0.84	0.30	71,71,71,71	0
56	MG	2B	213	1/1	0.84	0.34	79,79,79,79	0
56	MG	1A	3263	1/1	0.84	0.20	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3613	1/1	0.84	0.17	75,75,75,75	0
56	MG	1A	3805	1/1	0.84	0.21	64,64,64,64	0
56	MG	2A	3083	1/1	0.84	0.20	55,55,55,55	0
56	MG	1A	3309	1/1	0.84	0.19	65,65,65,65	0
56	MG	1A	3024	1/1	0.84	0.28	69,69,69,69	0
56	MG	1a	1605	1/1	0.84	0.13	67,67,67,67	0
56	MG	1A	3822	1/1	0.84	0.19	72,72,72,72	0
56	MG	2E	303	1/1	0.84	0.13	70,70,70,70	0
56	MG	2a	1725	1/1	0.84	0.36	71,71,71,71	0
56	MG	1a	1632	1/1	0.84	0.19	79,79,79,79	0
56	MG	2A	3497	1/1	0.84	0.25	47,47,47,47	0
56	MG	2A	3311	1/1	0.84	0.17	65,65,65,65	0
56	MG	2A	3140	1/1	0.84	0.21	71,71,71,71	0
56	MG	20	101	1/1	0.84	0.28	62,62,62,62	0
56	MG	1A	3163	1/1	0.84	0.26	73,73,73,73	0
56	MG	2A	3643	1/1	0.84	0.29	77,77,77,77	0
56	MG	1a	1713	1/1	0.84	0.41	80,80,80,80	0
56	MG	2A	3516	1/1	0.84	0.23	78,78,78,78	0
56	MG	2a	1615	1/1	0.84	0.29	80,80,80,80	0
56	MG	2a	1770	1/1	0.84	0.18	88,88,88,88	0
56	MG	1A	3167	1/1	0.84	0.31	47,47,47,47	0
56	MG	2a	1619	1/1	0.84	0.16	78,78,78,78	0
56	MG	1A	3943	1/1	0.84	0.16	47,47,47,47	0
56	MG	2a	1626	1/1	0.84	0.36	72,72,72,72	0
56	MG	2a	1776	1/1	0.84	0.36	82,82,82,82	0
56	MG	1A	3949	1/1	0.84	0.18	37,37,37,37	0
56	MG	2a	1783	1/1	0.84	0.18	77,77,77,77	0
56	MG	2A	3003	1/1	0.84	0.36	72,72,72,72	0
56	MG	2a	1632	1/1	0.84	0.28	71,71,71,71	0
56	MG	1a	1653	1/1	0.84	0.33	78,78,78,78	0
56	MG	1A	3700	1/1	0.84	0.16	53,53,53,53	0
56	MG	2A	3687	1/1	0.84	0.26	87,87,87,87	0
56	MG	1A	3292	1/1	0.84	0.20	76,76,76,76	0
56	MG	2A	3700	1/1	0.84	0.14	54,54,54,54	0
56	MG	1A	3844	1/1	0.84	0.15	30,30,30,30	0
56	MG	2a	1804	1/1	0.84	0.28	71,71,71,71	0
56	MG	2A	3576	1/1	0.84	0.15	76,76,76,76	0
56	MG	2A	3737	1/1	0.84	0.20	74,74,74,74	0
56	MG	2A	3174	1/1	0.84	0.25	70,70,70,70	0
56	MG	1A	3544	1/1	0.84	0.32	71,71,71,71	0
56	MG	2A	3273	1/1	0.84	0.19	68,68,68,68	0
56	MG	1O	205	1/1	0.84	0.13	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3783	1/1	0.84	0.11	46,46,46,46	0
56	MG	1A	3349	1/1	0.84	0.15	72,72,72,72	0
56	MG	2A	3058	1/1	0.84	0.30	73,73,73,73	0
56	MG	2B	204	1/1	0.84	0.19	71,71,71,71	0
56	MG	2A	3283	1/1	0.84	0.23	75,75,75,75	0
56	MG	2A	3307	1/1	0.85	0.28	79,79,79,79	0
56	MG	1A	3378	1/1	0.85	0.31	71,71,71,71	0
56	MG	2a	1631	1/1	0.85	0.36	80,80,80,80	0
56	MG	1a	1771	1/1	0.85	0.16	71,71,71,71	0
56	MG	1B	212	1/1	0.85	0.25	77,77,77,77	0
56	MG	1A	3351	1/1	0.85	0.15	62,62,62,62	0
56	MG	1A	3719	1/1	0.85	0.33	73,73,73,73	0
56	MG	1A	3478	1/1	0.85	0.25	75,75,75,75	0
56	MG	1A	3486	1/1	0.85	0.20	78,78,78,78	0
56	MG	1a	1657	1/1	0.85	0.25	81,81,81,81	0
56	MG	1A	3388	1/1	0.85	0.24	72,72,72,72	0
56	MG	2a	1650	1/1	0.85	0.15	87,87,87,87	0
56	MG	1A	3510	1/1	0.85	0.23	69,69,69,69	0
56	MG	2A	3336	1/1	0.85	0.22	58,58,58,58	0
56	MG	1A	3205	1/1	0.85	0.21	68,68,68,68	0
56	MG	2A	3639	1/1	0.85	0.29	60,60,60,60	0
56	MG	2a	1669	1/1	0.85	0.45	82,82,82,82	0
56	MG	1A	3399	1/1	0.85	0.26	70,70,70,70	0
56	MG	1A	4009	1/1	0.85	0.16	69,69,69,69	0
56	MG	1x	106	1/1	0.85	0.31	71,71,71,71	0
56	MG	1D	312	1/1	0.85	0.33	49,49,49,49	0
56	MG	2A	3654	1/1	0.85	0.24	77,77,77,77	0
56	MG	2A	3350	1/1	0.85	0.34	72,72,72,72	0
56	MG	1a	1679	1/1	0.85	0.30	77,77,77,77	0
56	MG	2A	3354	1/1	0.85	0.15	69,69,69,69	0
56	MG	2A	3357	1/1	0.85	0.26	64,64,64,64	0
56	MG	2A	3360	1/1	0.85	0.26	61,61,61,61	0
56	MG	1a	1680	1/1	0.85	0.09	69,69,69,69	0
56	MG	2A	3222	1/1	0.85	0.33	70,70,70,70	0
56	MG	1E	307	1/1	0.85	0.18	60,60,60,60	0
56	MG	2A	3226	1/1	0.85	0.20	70,70,70,70	0
56	MG	2A	3229	1/1	0.85	0.33	80,80,80,80	0
56	MG	2A	3394	1/1	0.85	0.38	67,67,67,67	0
56	MG	2A	3401	1/1	0.85	0.27	70,70,70,70	0
56	MG	2a	1717	1/1	0.85	0.39	78,78,78,78	0
56	MG	2A	3405	1/1	0.85	0.25	73,73,73,73	0
56	MG	1a	1685	1/1	0.85	0.31	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1729	1/1	0.85	0.42	79,79,79,79	0
56	MG	2A	3419	1/1	0.85	0.26	65,65,65,65	0
56	MG	1E	310	1/1	0.85	0.25	71,71,71,71	0
56	MG	1E	313	1/1	0.85	0.18	55,55,55,55	0
56	MG	1A	3408	1/1	0.85	0.27	76,76,76,76	0
56	MG	1A	3359	1/1	0.85	0.25	64,64,64,64	0
56	MG	1a	1697	1/1	0.85	0.13	66,66,66,66	0
56	MG	1A	3903	1/1	0.85	0.19	73,73,73,73	0
56	MG	2B	205	1/1	0.85	0.22	74,74,74,74	0
56	MG	1G	203	1/1	0.85	0.21	75,75,75,75	0
56	MG	1O	201	1/1	0.85	0.11	68,68,68,68	0
56	MG	1A	3360	1/1	0.85	0.40	67,67,67,67	0
56	MG	2A	3252	1/1	0.85	0.18	70,70,70,70	0
56	MG	2A	3253	1/1	0.85	0.23	74,74,74,74	0
56	MG	2A	3073	1/1	0.85	0.28	73,73,73,73	0
56	MG	1A	3444	1/1	0.85	0.17	65,65,65,65	0
56	MG	2B	219	1/1	0.85	0.36	77,77,77,77	0
56	MG	10	108	1/1	0.85	0.16	72,72,72,72	0
56	MG	2a	1782	1/1	0.85	0.27	84,84,84,84	0
56	MG	1a	1714	1/1	0.85	0.36	76,76,76,76	0
56	MG	1A	3454	1/1	0.85	0.14	63,63,63,63	0
56	MG	1A	3602	1/1	0.85	0.20	58,58,58,58	0
56	MG	2a	1788	1/1	0.85	0.32	71,71,71,71	0
56	MG	2A	3101	1/1	0.85	0.34	70,70,70,70	0
56	MG	2A	3104	1/1	0.85	0.40	79,79,79,79	0
56	MG	1A	3373	1/1	0.85	0.28	35,35,35,35	0
56	MG	2O	201	1/1	0.85	0.19	67,67,67,67	0
56	MG	1a	1741	1/1	0.85	0.32	85,85,85,85	0
56	MG	2a	1798	1/1	0.85	0.26	71,71,71,71	0
56	MG	2a	1799	1/1	0.85	0.20	67,67,67,67	0
56	MG	2A	3127	1/1	0.85	0.33	71,71,71,71	0
56	MG	1A	3469	1/1	0.85	0.12	68,68,68,68	0
56	MG	20	102	1/1	0.85	0.28	75,75,75,75	0
56	MG	1A	3935	1/1	0.85	0.24	81,81,81,81	0
56	MG	19	101	1/1	0.85	0.13	56,56,56,56	0
56	MG	1A	3809	1/1	0.85	0.16	64,64,64,64	0
56	MG	2A	3152	1/1	0.85	0.42	75,75,75,75	0
56	MG	2a	1609	1/1	0.85	0.23	77,77,77,77	0
56	MG	1A	3697	1/1	0.85	0.17	63,63,63,63	0
56	MG	2A	3592	1/1	0.85	0.14	58,58,58,58	0
56	MG	2A	3596	1/1	0.85	0.13	55,55,55,55	0
56	MG	2x	105	1/1	0.85	0.34	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1763	1/1	0.85	0.29	80,80,80,80	0
56	MG	1A	3318	1/1	0.85	0.41	74,74,74,74	0
56	MG	1A	3327	1/1	0.86	0.26	65,65,65,65	0
56	MG	1A	3992	1/1	0.86	0.12	53,53,53,53	0
56	MG	2A	3329	1/1	0.86	0.31	55,55,55,55	0
56	MG	1A	3018	1/1	0.86	0.12	43,43,43,43	0
56	MG	2A	3203	1/1	0.86	0.28	74,74,74,74	0
56	MG	2A	3204	1/1	0.86	0.26	55,55,55,55	0
56	MG	1a	1613	1/1	0.86	0.33	64,64,64,64	0
56	MG	1a	1614	1/1	0.86	0.16	72,72,72,72	0
56	MG	1A	3616	1/1	0.86	0.19	65,65,65,65	0
56	MG	2A	3036	1/1	0.86	0.23	76,76,76,76	0
56	MG	2A	3223	1/1	0.86	0.24	77,77,77,77	0
56	MG	2A	3352	1/1	0.86	0.35	66,66,66,66	0
56	MG	2a	1644	1/1	0.86	0.15	78,78,78,78	0
56	MG	1A	3243	1/1	0.86	0.27	63,63,63,63	0
56	MG	1A	3875	1/1	0.86	0.17	47,47,47,47	0
56	MG	2A	3355	1/1	0.86	0.26	61,61,61,61	0
56	MG	2a	1652	1/1	0.86	0.28	54,54,54,54	0
56	MG	1A	3626	1/1	0.86	0.16	63,63,63,63	0
56	MG	2A	3056	1/1	0.86	0.26	68,68,68,68	0
56	MG	1a	1739	1/1	0.86	0.15	61,61,61,61	0
56	MG	1a	1643	1/1	0.86	0.39	80,80,80,80	0
56	MG	1A	3655	1/1	0.86	0.18	60,60,60,60	0
56	MG	2A	3078	1/1	0.86	0.28	70,70,70,70	0
56	MG	1D	310	1/1	0.86	0.19	68,68,68,68	0
56	MG	1A	3673	1/1	0.86	0.12	30,30,30,30	0
56	MG	1A	3674	1/1	0.86	0.23	68,68,68,68	0
56	MG	2A	3245	1/1	0.86	0.29	72,72,72,72	0
56	MG	2A	3688	1/1	0.86	0.27	73,73,73,73	0
56	MG	2a	1688	1/1	0.86	0.25	76,76,76,76	0
56	MG	1A	3494	1/1	0.86	0.14	69,69,69,69	0
56	MG	2a	1693	1/1	0.86	0.35	80,80,80,80	0
56	MG	2a	1695	1/1	0.86	0.18	76,76,76,76	0
56	MG	2a	1696	1/1	0.86	0.29	75,75,75,75	0
56	MG	2A	3095	1/1	0.86	0.23	77,77,77,77	0
56	MG	2A	3705	1/1	0.86	0.16	83,83,83,83	0
56	MG	1A	3509	1/1	0.86	0.20	72,72,72,72	0
56	MG	2A	3719	1/1	0.86	0.16	57,57,57,57	0
56	MG	2A	3720	1/1	0.86	0.20	46,46,46,46	0
56	MG	2a	1707	1/1	0.86	0.27	67,67,67,67	0
56	MG	2A	3433	1/1	0.86	0.32	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3733	1/1	0.86	0.12	57,57,57,57	0
56	MG	1A	3698	1/1	0.86	0.16	59,59,59,59	0
56	MG	2A	3738	1/1	0.86	0.10	66,66,66,66	0
56	MG	2a	1716	1/1	0.86	0.40	57,57,57,57	0
56	MG	2A	3103	1/1	0.86	0.15	59,59,59,59	0
56	MG	2a	1721	1/1	0.86	0.41	69,69,69,69	0
56	MG	1a	1766	1/1	0.86	0.27	71,71,71,71	0
56	MG	2A	3758	1/1	0.86	0.26	69,69,69,69	0
56	MG	1A	4037	1/1	0.86	0.21	50,50,50,50	0
56	MG	2A	3261	1/1	0.86	0.23	81,81,81,81	0
56	MG	1A	3188	1/1	0.86	0.25	68,68,68,68	0
56	MG	2a	1736	1/1	0.86	0.31	83,83,83,83	0
56	MG	1a	1780	1/1	0.86	0.28	81,81,81,81	0
56	MG	2A	3272	1/1	0.86	0.39	73,73,73,73	0
56	MG	1a	1667	1/1	0.86	0.31	80,80,80,80	0
56	MG	1A	3389	1/1	0.86	0.22	51,51,51,51	0
56	MG	2B	206	1/1	0.86	0.23	82,82,82,82	0
56	MG	2B	210	1/1	0.86	0.13	83,83,83,83	0
56	MG	1a	1674	1/1	0.86	0.22	83,83,83,83	0
56	MG	1a	1677	1/1	0.86	0.19	71,71,71,71	0
56	MG	2a	1765	1/1	0.86	0.29	67,67,67,67	0
56	MG	1A	3365	1/1	0.86	0.30	69,69,69,69	0
56	MG	2A	3518	1/1	0.86	0.21	58,58,58,58	0
56	MG	2A	3519	1/1	0.86	0.28	68,68,68,68	0
56	MG	1A	4048	1/1	0.86	0.16	66,66,66,66	0
56	MG	1a	1802	1/1	0.86	0.16	68,68,68,68	0
56	MG	1A	3945	1/1	0.86	0.16	78,78,78,78	0
56	MG	2A	3288	1/1	0.86	0.32	73,73,73,73	0
56	MG	1a	1804	1/1	0.86	0.26	66,66,66,66	0
56	MG	2A	3291	1/1	0.86	0.37	84,84,84,84	0
56	MG	2A	3553	1/1	0.86	0.27	52,52,52,52	0
56	MG	2E	302	1/1	0.86	0.27	71,71,71,71	0
56	MG	2A	3561	1/1	0.86	0.17	58,58,58,58	0
56	MG	2E	304	1/1	0.86	0.34	76,76,76,76	0
56	MG	1T	202	1/1	0.86	0.14	65,65,65,65	0
56	MG	1A	3541	1/1	0.86	0.12	44,44,44,44	0
56	MG	1A	3397	1/1	0.86	0.24	68,68,68,68	0
56	MG	1r	101	1/1	0.86	0.20	80,80,80,80	0
56	MG	2A	3302	1/1	0.86	0.25	67,67,67,67	0
56	MG	1A	3398	1/1	0.86	0.15	68,68,68,68	0
56	MG	2A	3175	1/1	0.86	0.26	70,70,70,70	0
56	MG	1a	1692	1/1	0.86	0.33	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3178	1/1	0.86	0.46	81,81,81,81	0
56	MG	2a	1603	1/1	0.86	0.21	72,72,72,72	0
56	MG	2a	1606	1/1	0.86	0.40	80,80,80,80	0
56	MG	1A	3840	1/1	0.86	0.16	74,74,74,74	0
56	MG	2A	3185	1/1	0.86	0.14	61,61,61,61	0
56	MG	2A	3600	1/1	0.86	0.28	82,82,82,82	0
56	MG	2q	201	1/1	0.86	0.14	67,67,67,67	0
56	MG	2a	1611	1/1	0.86	0.38	78,78,78,78	0
56	MG	2a	1614	1/1	0.86	0.24	79,79,79,79	0
56	MG	1A	3131	1/1	0.86	0.13	58,58,58,58	0
56	MG	2a	1616	1/1	0.86	0.24	68,68,68,68	0
56	MG	1A	3402	1/1	0.86	0.28	63,63,63,63	0
56	MG	1x	113	1/1	0.86	0.15	70,70,70,70	0
56	MG	1a	1738	1/1	0.87	0.12	64,64,64,64	0
56	MG	1A	4011	1/1	0.87	0.19	58,58,58,58	0
56	MG	2A	3107	1/1	0.87	0.18	58,58,58,58	0
56	MG	2A	3565	1/1	0.87	0.17	41,41,41,41	0
56	MG	1a	1740	1/1	0.87	0.12	70,70,70,70	0
56	MG	2A	3119	1/1	0.87	0.18	76,76,76,76	0
56	MG	2A	3574	1/1	0.87	0.29	74,74,74,74	0
56	MG	1A	3680	1/1	0.87	0.13	31,31,31,31	0
56	MG	2A	3292	1/1	0.87	0.24	87,87,87,87	0
56	MG	1a	1745	1/1	0.87	0.09	74,74,74,74	0
56	MG	1a	1748	1/1	0.87	0.26	63,63,63,63	0
56	MG	2a	1624	1/1	0.87	0.38	73,73,73,73	0
56	MG	13	103	1/1	0.87	0.21	61,61,61,61	0
56	MG	1A	3183	1/1	0.87	0.15	59,59,59,59	0
56	MG	1A	3833	1/1	0.87	0.09	46,46,46,46	0
56	MG	2A	3305	1/1	0.87	0.39	69,69,69,69	0
56	MG	1A	4031	1/1	0.87	0.10	66,66,66,66	0
56	MG	1A	3835	1/1	0.87	0.19	43,43,43,43	0
56	MG	1A	3685	1/1	0.87	0.20	62,62,62,62	0
56	MG	1a	1603	1/1	0.87	0.14	70,70,70,70	0
56	MG	1A	3687	1/1	0.87	0.14	68,68,68,68	0
56	MG	2A	3610	1/1	0.87	0.19	63,63,63,63	0
56	MG	1A	3688	1/1	0.87	0.23	60,60,60,60	0
56	MG	2A	3316	1/1	0.87	0.16	71,71,71,71	0
56	MG	1A	3690	1/1	0.87	0.22	77,77,77,77	0
56	MG	1a	1778	1/1	0.87	0.27	65,65,65,65	0
56	MG	1a	1624	1/1	0.87	0.27	60,60,60,60	0
56	MG	1a	1628	1/1	0.87	0.14	63,63,63,63	0
56	MG	1A	3692	1/1	0.87	0.25	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1664	1/1	0.87	0.23	71,71,71,71	0
56	MG	1a	1790	1/1	0.87	0.33	61,61,61,61	0
56	MG	1a	1631	1/1	0.87	0.38	67,67,67,67	0
56	MG	1A	3346	1/1	0.87	0.26	64,64,64,64	0
56	MG	1a	1635	1/1	0.87	0.26	75,75,75,75	0
56	MG	1A	4047	1/1	0.87	0.15	65,65,65,65	0
56	MG	1A	3083	1/1	0.87	0.23	48,48,48,48	0
56	MG	1A	3497	1/1	0.87	0.32	62,62,62,62	0
56	MG	1A	3706	1/1	0.87	0.12	76,76,76,76	0
56	MG	2A	3645	1/1	0.87	0.24	72,72,72,72	0
56	MG	2A	3348	1/1	0.87	0.20	68,68,68,68	0
56	MG	2A	3651	1/1	0.87	0.22	60,60,60,60	0
56	MG	2a	1691	1/1	0.87	0.21	80,80,80,80	0
56	MG	1A	3507	1/1	0.87	0.18	73,73,73,73	0
56	MG	1A	3713	1/1	0.87	0.18	76,76,76,76	0
56	MG	1A	3001	1/1	0.87	0.13	48,48,48,48	0
56	MG	1l	202	1/1	0.87	0.13	72,72,72,72	0
56	MG	2A	3660	1/1	0.87	0.19	93,93,93,93	0
56	MG	1A	3295	1/1	0.87	0.39	65,65,65,65	0
56	MG	2A	3211	1/1	0.87	0.22	65,65,65,65	0
56	MG	2A	3359	1/1	0.87	0.14	59,59,59,59	0
56	MG	2A	3682	1/1	0.87	0.24	73,73,73,73	0
56	MG	1A	3358	1/1	0.87	0.16	60,60,60,60	0
56	MG	1x	103	1/1	0.87	0.24	72,72,72,72	0
56	MG	2A	3363	1/1	0.87	0.36	72,72,72,72	0
56	MG	2a	1710	1/1	0.87	0.28	66,66,66,66	0
56	MG	2a	1712	1/1	0.87	0.25	64,64,64,64	0
56	MG	2A	3365	1/1	0.87	0.27	72,72,72,72	0
56	MG	2A	3367	1/1	0.87	0.29	75,75,75,75	0
56	MG	1A	3409	1/1	0.87	0.34	80,80,80,80	0
56	MG	2A	3706	1/1	0.87	0.29	77,77,77,77	0
56	MG	2A	3377	1/1	0.87	0.18	63,63,63,63	0
56	MG	2A	3710	1/1	0.87	0.21	74,74,74,74	0
56	MG	2A	3711	1/1	0.87	0.09	52,52,52,52	0
56	MG	1A	3753	1/1	0.87	0.16	45,45,45,45	0
56	MG	1A	3415	1/1	0.87	0.13	69,69,69,69	0
56	MG	1A	3542	1/1	0.87	0.15	66,66,66,66	0
56	MG	1A	3939	1/1	0.87	0.14	45,45,45,45	0
56	MG	2A	3400	1/1	0.87	0.15	66,66,66,66	0
56	MG	2a	1741	1/1	0.87	0.19	85,85,85,85	0
56	MG	1x	114	1/1	0.87	0.22	66,66,66,66	0
56	MG	2A	3403	1/1	0.87	0.26	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3249	1/1	0.87	0.17	70,70,70,70	0
56	MG	2A	3757	1/1	0.87	0.12	71,71,71,71	0
56	MG	1A	3546	1/1	0.87	0.26	61,61,61,61	0
56	MG	2A	3761	1/1	0.87	0.24	78,78,78,78	0
56	MG	2A	3414	1/1	0.87	0.20	65,65,65,65	0
56	MG	1A	3425	1/1	0.87	0.38	81,81,81,81	0
56	MG	2a	1766	1/1	0.87	0.27	81,81,81,81	0
56	MG	2A	3237	1/1	0.87	0.11	74,74,74,74	0
56	MG	1A	3180	1/1	0.87	0.23	46,46,46,46	0
56	MG	2A	3769	1/1	0.87	0.19	72,72,72,72	0
56	MG	2A	3438	1/1	0.87	0.12	60,60,60,60	0
56	MG	1A	3260	1/1	0.87	0.20	71,71,71,71	0
56	MG	1A	3957	1/1	0.87	0.13	54,54,54,54	0
56	MG	1A	3368	1/1	0.87	0.24	59,59,59,59	0
56	MG	2A	3470	1/1	0.87	0.16	69,69,69,69	0
56	MG	1A	3974	1/1	0.87	0.14	70,70,70,70	0
56	MG	2A	3474	1/1	0.87	0.12	50,50,50,50	0
56	MG	1A	3586	1/1	0.87	0.14	65,65,65,65	0
56	MG	2A	3054	1/1	0.87	0.16	73,73,73,73	0
56	MG	1A	3156	1/1	0.87	0.12	44,44,44,44	0
56	MG	2A	3495	1/1	0.87	0.10	39,39,39,39	0
56	MG	1A	3459	1/1	0.87	0.28	65,65,65,65	0
56	MG	1A	3322	1/1	0.87	0.29	64,64,64,64	0
56	MG	1G	204	1/1	0.87	0.10	75,75,75,75	0
56	MG	1A	3326	1/1	0.87	0.36	69,69,69,69	0
56	MG	1A	3266	1/1	0.87	0.27	71,71,71,71	0
56	MG	2a	1801	1/1	0.87	0.23	68,68,68,68	0
56	MG	1A	3813	1/1	0.87	0.17	60,60,60,60	0
56	MG	1R	202	1/1	0.87	0.21	67,67,67,67	0
56	MG	1S	201	1/1	0.87	0.13	58,58,58,58	0
56	MG	2A	3521	1/1	0.87	0.15	43,43,43,43	0
56	MG	2d	301	1/1	0.87	0.09	67,67,67,67	0
56	MG	2A	3086	1/1	0.87	0.20	73,73,73,73	0
56	MG	1A	3272	1/1	0.87	0.16	62,62,62,62	0
56	MG	2A	3528	1/1	0.87	0.23	72,72,72,72	0
56	MG	2P	201	1/1	0.87	0.17	64,64,64,64	0
56	MG	10	104	1/1	0.87	0.15	68,68,68,68	0
56	MG	2A	3531	1/1	0.87	0.24	74,74,74,74	0
56	MG	10	105	1/1	0.87	0.14	63,63,63,63	0
56	MG	2w	101	1/1	0.87	0.19	78,78,78,78	0
56	MG	2A	3541	1/1	0.87	0.17	51,51,51,51	0
56	MG	1A	3218	1/1	0.87	0.23	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3546	1/1	0.87	0.21	57,57,57,57	0
56	MG	2A	3550	1/1	0.87	0.25	67,67,67,67	0
56	MG	1X	104	1/1	0.88	0.15	53,53,53,53	0
56	MG	2A	3399	1/1	0.88	0.27	75,75,75,75	0
56	MG	2a	1634	1/1	0.88	0.40	83,83,83,83	0
56	MG	2A	3105	1/1	0.88	0.23	74,74,74,74	0
56	MG	2A	3106	1/1	0.88	0.52	78,78,78,78	0
56	MG	2a	1639	1/1	0.88	0.15	70,70,70,70	0
56	MG	1A	3244	1/1	0.88	0.21	77,77,77,77	0
56	MG	1A	3617	1/1	0.88	0.10	31,31,31,31	0
56	MG	2A	3116	1/1	0.88	0.10	67,67,67,67	0
56	MG	1a	1682	1/1	0.88	0.28	52,52,52,52	0
56	MG	2A	3417	1/1	0.88	0.41	75,75,75,75	0
56	MG	2A	3121	1/1	0.88	0.22	56,56,56,56	0
56	MG	2A	3422	1/1	0.88	0.22	57,57,57,57	0
56	MG	2A	3662	1/1	0.88	0.23	52,52,52,52	0
56	MG	2A	3269	1/1	0.88	0.21	74,74,74,74	0
56	MG	2A	3426	1/1	0.88	0.46	70,70,70,70	0
56	MG	2A	3428	1/1	0.88	0.24	67,67,67,67	0
56	MG	2a	1667	1/1	0.88	0.17	64,64,64,64	0
56	MG	2A	3432	1/1	0.88	0.28	77,77,77,77	0
56	MG	10	107	1/1	0.88	0.09	62,62,62,62	0
56	MG	2A	3123	1/1	0.88	0.13	83,83,83,83	0
56	MG	1A	3501	1/1	0.88	0.36	72,72,72,72	0
56	MG	2a	1673	1/1	0.88	0.18	61,61,61,61	0
56	MG	1a	1687	1/1	0.88	0.34	72,72,72,72	0
56	MG	2A	3465	1/1	0.88	0.19	56,56,56,56	0
56	MG	2A	3704	1/1	0.88	0.12	89,89,89,89	0
56	MG	1B	210	1/1	0.88	0.15	60,60,60,60	0
56	MG	2a	1684	1/1	0.88	0.37	74,74,74,74	0
56	MG	1a	1689	1/1	0.88	0.24	67,67,67,67	0
56	MG	1A	3977	1/1	0.88	0.15	65,65,65,65	0
56	MG	2A	3284	1/1	0.88	0.31	60,60,60,60	0
56	MG	1b	301	1/1	0.88	0.19	84,84,84,84	0
56	MG	1A	3620	1/1	0.88	0.18	80,80,80,80	0
56	MG	2a	1694	1/1	0.88	0.18	64,64,64,64	0
56	MG	2A	3159	1/1	0.88	0.14	71,71,71,71	0
56	MG	2A	3490	1/1	0.88	0.18	66,66,66,66	0
56	MG	2A	3730	1/1	0.88	0.14	43,43,43,43	0
56	MG	1B	218	1/1	0.88	0.10	50,50,50,50	0
56	MG	2a	1700	1/1	0.88	0.43	78,78,78,78	0
56	MG	1A	3437	1/1	0.88	0.32	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3232	1/1	0.88	0.14	55,55,55,55	0
56	MG	2a	1705	1/1	0.88	0.24	63,63,63,63	0
56	MG	2A	3502	1/1	0.88	0.17	55,55,55,55	0
56	MG	1A	3122	1/1	0.88	0.20	44,44,44,44	0
56	MG	2A	3295	1/1	0.88	0.11	77,77,77,77	0
56	MG	2A	3296	1/1	0.88	0.13	77,77,77,77	0
56	MG	1B	227	1/1	0.88	0.13	48,48,48,48	0
56	MG	1A	3517	1/1	0.88	0.23	44,44,44,44	0
56	MG	1a	1705	1/1	0.88	0.17	59,59,59,59	0
56	MG	1x	109	1/1	0.88	0.23	72,72,72,72	0
56	MG	2A	3304	1/1	0.88	0.36	60,60,60,60	0
56	MG	1A	3678	1/1	0.88	0.20	65,65,65,65	0
56	MG	2a	1718	1/1	0.88	0.41	73,73,73,73	0
56	MG	2a	1719	1/1	0.88	0.44	82,82,82,82	0
56	MG	1A	3895	1/1	0.88	0.15	60,60,60,60	0
56	MG	1A	3518	1/1	0.88	0.22	62,62,62,62	0
56	MG	2A	3181	1/1	0.88	0.21	68,68,68,68	0
56	MG	1a	1623	1/1	0.88	0.17	59,59,59,59	0
56	MG	1A	3456	1/1	0.88	0.11	62,62,62,62	0
56	MG	2A	3007	1/1	0.88	0.21	64,64,64,64	0
56	MG	1a	1718	1/1	0.88	0.32	69,69,69,69	0
56	MG	1A	3103	1/1	0.88	0.10	43,43,43,43	0
56	MG	1A	3788	1/1	0.88	0.14	49,49,49,49	0
56	MG	2B	215	1/1	0.88	0.14	74,74,74,74	0
56	MG	1A	3262	1/1	0.88	0.17	64,64,64,64	0
56	MG	1A	4029	1/1	0.88	0.29	68,68,68,68	0
56	MG	2a	1748	1/1	0.88	0.19	71,71,71,71	0
56	MG	1A	3333	1/1	0.88	0.23	60,60,60,60	0
56	MG	2A	3568	1/1	0.88	0.18	71,71,71,71	0
56	MG	1A	3372	1/1	0.88	0.16	55,55,55,55	0
56	MG	2A	3051	1/1	0.88	0.18	63,63,63,63	0
56	MG	2A	3207	1/1	0.88	0.21	64,64,64,64	0
56	MG	2A	3210	1/1	0.88	0.25	54,54,54,54	0
56	MG	2a	1769	1/1	0.88	0.21	54,54,54,54	0
56	MG	1A	3932	1/1	0.88	0.11	62,62,62,62	0
56	MG	2A	3341	1/1	0.88	0.27	71,71,71,71	0
56	MG	1A	3311	1/1	0.88	0.24	67,67,67,67	0
56	MG	2E	308	1/1	0.88	0.19	81,81,81,81	0
56	MG	1A	3316	1/1	0.88	0.27	70,70,70,70	0
56	MG	2A	3588	1/1	0.88	0.15	53,53,53,53	0
56	MG	1A	3285	1/1	0.88	0.17	61,61,61,61	0
56	MG	1I	201	1/1	0.88	0.15	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2R	202	1/1	0.88	0.13	53,53,53,53	0
56	MG	2A	3595	1/1	0.88	0.19	58,58,58,58	0
56	MG	2A	3072	1/1	0.88	0.15	60,60,60,60	0
56	MG	2A	3598	1/1	0.88	0.24	77,77,77,77	0
56	MG	1a	1656	1/1	0.88	0.25	68,68,68,68	0
56	MG	21	102	1/1	0.88	0.14	65,65,65,65	0
56	MG	2A	3076	1/1	0.88	0.14	63,63,63,63	0
56	MG	2a	1795	1/1	0.88	0.29	83,83,83,83	0
56	MG	1A	3290	1/1	0.88	0.17	52,52,52,52	0
56	MG	2A	3233	1/1	0.88	0.35	84,84,84,84	0
56	MG	2a	1604	1/1	0.88	0.14	85,85,85,85	0
56	MG	1O	204	1/1	0.88	0.13	59,59,59,59	0
56	MG	1A	3488	1/1	0.88	0.14	64,64,64,64	0
56	MG	1A	3424	1/1	0.88	0.12	54,54,54,54	0
56	MG	2A	3361	1/1	0.88	0.28	75,75,75,75	0
56	MG	2A	3084	1/1	0.88	0.14	60,60,60,60	0
56	MG	2a	1612	1/1	0.88	0.25	71,71,71,71	0
56	MG	1A	3587	1/1	0.88	0.16	37,37,37,37	0
56	MG	1A	3598	1/1	0.88	0.10	34,34,34,34	0
56	MG	1A	3382	1/1	0.88	0.17	56,56,56,56	0
56	MG	2A	3098	1/1	0.88	0.15	64,64,64,64	0
56	MG	2A	3376	1/1	0.88	0.23	72,72,72,72	0
56	MG	1T	203	1/1	0.88	0.15	61,61,61,61	0
56	MG	2a	1622	1/1	0.88	0.25	77,77,77,77	0
56	MG	2r	102	1/1	0.88	0.32	81,81,81,81	0
56	MG	2A	3632	1/1	0.88	0.17	45,45,45,45	0
56	MG	1V	202	1/1	0.88	0.25	47,47,47,47	0
56	MG	2a	1627	1/1	0.88	0.27	61,61,61,61	0
56	MG	1a	1675	1/1	0.88	0.27	67,67,67,67	0
56	MG	2x	106	1/1	0.88	0.25	69,69,69,69	0
56	MG	2A	3637	1/1	0.88	0.15	73,73,73,73	0
56	MG	2A	3250	1/1	0.88	0.13	68,68,68,68	0
56	MG	1A	3724	1/1	0.89	0.11	67,67,67,67	0
56	MG	2A	3249	1/1	0.89	0.28	74,74,74,74	0
56	MG	1a	1770	1/1	0.89	0.39	73,73,73,73	0
56	MG	1A	3735	1/1	0.89	0.10	24,24,24,24	0
56	MG	1A	3741	1/1	0.89	0.20	55,55,55,55	0
56	MG	2A	3255	1/1	0.89	0.21	64,64,64,64	0
56	MG	1A	3082	1/1	0.89	0.27	55,55,55,55	0
56	MG	2A	3415	1/1	0.89	0.34	79,79,79,79	0
56	MG	1a	1781	1/1	0.89	0.21	68,68,68,68	0
56	MG	2A	3418	1/1	0.89	0.41	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3671	1/1	0.89	0.09	32,32,32,32	0
56	MG	2A	3421	1/1	0.89	0.51	65,65,65,65	0
56	MG	2a	1649	1/1	0.89	0.28	74,74,74,74	0
56	MG	2A	3657	1/1	0.89	0.13	69,69,69,69	0
56	MG	2A	3260	1/1	0.89	0.23	70,70,70,70	0
56	MG	1N	203	1/1	0.89	0.10	56,56,56,56	0
56	MG	1A	3207	1/1	0.89	0.12	65,65,65,65	0
56	MG	2a	1658	1/1	0.89	0.17	68,68,68,68	0
56	MG	2a	1662	1/1	0.89	0.29	70,70,70,70	0
56	MG	2A	3108	1/1	0.89	0.36	70,70,70,70	0
56	MG	2A	3666	1/1	0.89	0.30	55,55,55,55	0
56	MG	1O	203	1/1	0.89	0.26	69,69,69,69	0
56	MG	2A	3672	1/1	0.89	0.16	74,74,74,74	0
56	MG	1A	3325	1/1	0.89	0.26	62,62,62,62	0
56	MG	2A	3434	1/1	0.89	0.21	76,76,76,76	0
56	MG	2A	3117	1/1	0.89	0.12	82,82,82,82	0
56	MG	2A	3441	1/1	0.89	0.19	77,77,77,77	0
56	MG	2A	3444	1/1	0.89	0.12	32,32,32,32	0
56	MG	2A	3445	1/1	0.89	0.30	65,65,65,65	0
56	MG	2A	3454	1/1	0.89	0.13	55,55,55,55	0
56	MG	2A	3694	1/1	0.89	0.23	69,69,69,69	0
56	MG	2A	3274	1/1	0.89	0.14	60,60,60,60	0
56	MG	2A	3701	1/1	0.89	0.12	78,78,78,78	0
56	MG	1A	3876	1/1	0.89	0.16	49,49,49,49	0
56	MG	2a	1689	1/1	0.89	0.21	70,70,70,70	0
56	MG	1A	3764	1/1	0.89	0.21	64,64,64,64	0
56	MG	1A	3259	1/1	0.89	0.37	74,74,74,74	0
56	MG	1A	3361	1/1	0.89	0.31	63,63,63,63	0
56	MG	1S	202	1/1	0.89	0.19	67,67,67,67	0
56	MG	2A	3129	1/1	0.89	0.18	66,66,66,66	0
56	MG	2A	3713	1/1	0.89	0.13	62,62,62,62	0
56	MG	1a	1805	1/1	0.89	0.21	61,61,61,61	0
56	MG	1A	3682	1/1	0.89	0.18	50,50,50,50	0
56	MG	2A	3724	1/1	0.89	0.16	47,47,47,47	0
56	MG	1A	3776	1/1	0.89	0.07	30,30,30,30	0
56	MG	2A	3728	1/1	0.89	0.14	56,56,56,56	0
56	MG	2A	3489	1/1	0.89	0.17	58,58,58,58	0
56	MG	1a	1808	1/1	0.89	0.23	68,68,68,68	0
56	MG	1A	3909	1/1	0.89	0.14	60,60,60,60	0
56	MG	1W	207	1/1	0.89	0.16	35,35,35,35	0
56	MG	2A	3498	1/1	0.89	0.30	70,70,70,70	0
56	MG	1A	3168	1/1	0.89	0.27	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3756	1/1	0.89	0.16	74,74,74,74	0
56	MG	1m	3002	1/1	0.89	0.28	71,71,71,71	0
56	MG	1p	101	1/1	0.89	0.11	69,69,69,69	0
56	MG	10	103	1/1	0.89	0.22	59,59,59,59	0
56	MG	2A	3163	1/1	0.89	0.31	68,68,68,68	0
56	MG	1A	3684	1/1	0.89	0.13	76,76,76,76	0
56	MG	1A	3045	1/1	0.89	0.11	46,46,46,46	0
56	MG	2a	1720	1/1	0.89	0.35	65,65,65,65	0
56	MG	1A	3786	1/1	0.89	0.12	75,75,75,75	0
56	MG	1A	3057	1/1	0.89	0.11	54,54,54,54	0
56	MG	2A	3771	1/1	0.89	0.30	75,75,75,75	0
56	MG	2a	1727	1/1	0.89	0.27	73,73,73,73	0
56	MG	1A	3059	1/1	0.89	0.14	53,53,53,53	0
56	MG	2a	1732	1/1	0.89	0.37	66,66,66,66	0
56	MG	2A	3525	1/1	0.89	0.21	68,68,68,68	0
56	MG	2A	3526	1/1	0.89	0.11	48,48,48,48	0
56	MG	11	103	1/1	0.89	0.26	67,67,67,67	0
56	MG	1A	3798	1/1	0.89	0.23	63,63,63,63	0
56	MG	1A	3416	1/1	0.89	0.08	69,69,69,69	0
56	MG	1B	211	1/1	0.89	0.23	69,69,69,69	0
56	MG	1A	3944	1/1	0.89	0.12	66,66,66,66	0
56	MG	1A	3800	1/1	0.89	0.11	71,71,71,71	0
56	MG	2A	3186	1/1	0.89	0.30	74,74,74,74	0
56	MG	2a	1749	1/1	0.89	0.33	84,84,84,84	0
56	MG	2A	3006	1/1	0.89	0.19	61,61,61,61	0
56	MG	2A	3547	1/1	0.89	0.22	67,67,67,67	0
56	MG	2A	3192	1/1	0.89	0.12	78,78,78,78	0
56	MG	1A	3802	1/1	0.89	0.13	58,58,58,58	0
56	MG	1a	1601	1/1	0.89	0.15	68,68,68,68	0
56	MG	2A	3327	1/1	0.89	0.29	60,60,60,60	0
56	MG	2A	3019	1/1	0.89	0.14	68,68,68,68	0
56	MG	2A	3566	1/1	0.89	0.13	53,53,53,53	0
56	MG	1A	3310	1/1	0.89	0.15	57,57,57,57	0
56	MG	2A	3334	1/1	0.89	0.36	72,72,72,72	0
56	MG	2A	3571	1/1	0.89	0.23	53,53,53,53	0
56	MG	2A	3027	1/1	0.89	0.16	75,75,75,75	0
56	MG	2F	303	1/1	0.89	0.21	68,68,68,68	0
56	MG	2a	1778	1/1	0.89	0.26	77,77,77,77	0
56	MG	2A	3028	1/1	0.89	0.23	57,57,57,57	0
56	MG	1A	3157	1/1	0.89	0.12	57,57,57,57	0
56	MG	1A	3102	1/1	0.89	0.29	76,76,76,76	0
56	MG	2A	3579	1/1	0.89	0.11	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2R	201	1/1	0.89	0.12	67,67,67,67	0
56	MG	2A	3580	1/1	0.89	0.15	71,71,71,71	0
56	MG	1A	3699	1/1	0.89	0.21	67,67,67,67	0
56	MG	1A	3380	1/1	0.89	0.12	47,47,47,47	0
56	MG	2A	3039	1/1	0.89	0.26	59,59,59,59	0
56	MG	1A	3603	1/1	0.89	0.22	62,62,62,62	0
56	MG	2A	3213	1/1	0.89	0.11	60,60,60,60	0
56	MG	1A	3429	1/1	0.89	0.11	55,55,55,55	0
56	MG	2A	3221	1/1	0.89	0.17	66,66,66,66	0
56	MG	2A	3052	1/1	0.89	0.20	67,67,67,67	0
56	MG	1a	1626	1/1	0.89	0.27	63,63,63,63	0
56	MG	2a	1605	1/1	0.89	0.33	70,70,70,70	0
56	MG	1A	3711	1/1	0.89	0.14	56,56,56,56	0
56	MG	2a	1810	1/1	0.89	0.20	78,78,78,78	0
56	MG	1A	3196	1/1	0.89	0.36	68,68,68,68	0
56	MG	1A	3830	1/1	0.89	0.14	52,52,52,52	0
56	MG	1D	311	1/1	0.89	0.17	53,53,53,53	0
56	MG	1a	1749	1/1	0.89	0.38	82,82,82,82	0
56	MG	1a	1634	1/1	0.89	0.39	78,78,78,78	0
56	MG	1A	3385	1/1	0.89	0.10	50,50,50,50	0
56	MG	1a	1755	1/1	0.89	0.14	67,67,67,67	0
56	MG	2A	3371	1/1	0.89	0.34	79,79,79,79	0
56	MG	1a	1636	1/1	0.89	0.15	56,56,56,56	0
56	MG	1A	4002	1/1	0.89	0.08	22,22,22,22	0
56	MG	2t	201	1/1	0.89	0.24	57,57,57,57	0
56	MG	1A	3447	1/1	0.89	0.24	62,62,62,62	0
56	MG	1A	3353	1/1	0.89	0.11	56,56,56,56	0
56	MG	2x	102	1/1	0.89	0.20	77,77,77,77	0
56	MG	2A	3622	1/1	0.89	0.15	68,68,68,68	0
56	MG	1a	1645	1/1	0.89	0.18	64,64,64,64	0
56	MG	2A	3087	1/1	0.89	0.18	81,81,81,81	0
56	MG	2A	3628	1/1	0.89	0.16	71,71,71,71	0
56	MG	1A	3723	1/1	0.89	0.11	47,47,47,47	0
56	MG	2A	3339	1/1	0.90	0.38	69,69,69,69	0
56	MG	1A	3253	1/1	0.90	0.17	81,81,81,81	0
56	MG	1A	3614	1/1	0.90	0.11	52,52,52,52	0
56	MG	1F	307	1/1	0.90	0.14	60,60,60,60	0
56	MG	1e	201	1/1	0.90	0.16	76,76,76,76	0
56	MG	1e	202	1/1	0.90	0.20	56,56,56,56	0
56	MG	1a	1662	1/1	0.90	0.24	72,72,72,72	0
56	MG	1A	3990	1/1	0.90	0.10	52,52,52,52	0
56	MG	2A	3608	1/1	0.90	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3240	1/1	0.90	0.28	50,50,50,50	0
56	MG	1n	101	1/1	0.90	0.14	59,59,59,59	0
56	MG	1A	3995	1/1	0.90	0.11	39,39,39,39	0
56	MG	2A	3615	1/1	0.90	0.19	64,64,64,64	0
56	MG	1A	3498	1/1	0.90	0.24	48,48,48,48	0
56	MG	1A	3060	1/1	0.90	0.19	59,59,59,59	0
56	MG	1N	202	1/1	0.90	0.15	57,57,57,57	0
56	MG	2a	1636	1/1	0.90	0.23	76,76,76,76	0
56	MG	2A	3194	1/1	0.90	0.25	81,81,81,81	0
56	MG	1A	3505	1/1	0.90	0.33	76,76,76,76	0
56	MG	1A	3624	1/1	0.90	0.09	34,34,34,34	0
56	MG	1A	3352	1/1	0.90	0.11	69,69,69,69	0
56	MG	2A	3364	1/1	0.90	0.30	68,68,68,68	0
56	MG	1A	3746	1/1	0.90	0.14	29,29,29,29	0
56	MG	1A	3639	1/1	0.90	0.10	65,65,65,65	0
56	MG	1A	4015	1/1	0.90	0.13	27,27,27,27	0
56	MG	1Q	203	1/1	0.90	0.14	69,69,69,69	0
56	MG	1a	1686	1/1	0.90	0.32	56,56,56,56	0
56	MG	1A	3651	1/1	0.90	0.13	34,34,34,34	0
56	MG	2a	1653	1/1	0.90	0.21	66,66,66,66	0
56	MG	2a	1656	1/1	0.90	0.25	70,70,70,70	0
56	MG	1R	206	1/1	0.90	0.20	44,44,44,44	0
56	MG	1A	3759	1/1	0.90	0.09	43,43,43,43	0
56	MG	2a	1660	1/1	0.90	0.22	62,62,62,62	0
56	MG	2A	3386	1/1	0.90	0.21	64,64,64,64	0
56	MG	2A	3388	1/1	0.90	0.21	60,60,60,60	0
56	MG	1A	3868	1/1	0.90	0.11	60,60,60,60	0
56	MG	2A	3392	1/1	0.90	0.36	81,81,81,81	0
56	MG	1A	3871	1/1	0.90	0.23	41,41,41,41	0
56	MG	2A	3396	1/1	0.90	0.16	45,45,45,45	0
56	MG	1A	3761	1/1	0.90	0.09	48,48,48,48	0
56	MG	2A	3026	1/1	0.90	0.22	59,59,59,59	0
56	MG	1U	203	1/1	0.90	0.17	60,60,60,60	0
56	MG	1A	3319	1/1	0.90	0.15	64,64,64,64	0
56	MG	2A	3225	1/1	0.90	0.19	64,64,64,64	0
56	MG	2a	1679	1/1	0.90	0.33	72,72,72,72	0
56	MG	2A	3663	1/1	0.90	0.17	75,75,75,75	0
56	MG	1a	1698	1/1	0.90	0.22	60,60,60,60	0
56	MG	1a	1699	1/1	0.90	0.28	71,71,71,71	0
56	MG	2a	1685	1/1	0.90	0.20	73,73,73,73	0
56	MG	2A	3230	1/1	0.90	0.19	68,68,68,68	0
56	MG	2A	3416	1/1	0.90	0.15	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3033	1/1	0.90	0.14	49,49,49,49	0
56	MG	1W	205	1/1	0.90	0.17	47,47,47,47	0
56	MG	1A	3884	1/1	0.90	0.12	30,30,30,30	0
56	MG	1a	1703	1/1	0.90	0.31	68,68,68,68	0
56	MG	1A	3890	1/1	0.90	0.14	70,70,70,70	0
56	MG	2A	3046	1/1	0.90	0.17	73,73,73,73	0
56	MG	2A	3048	1/1	0.90	0.19	66,66,66,66	0
56	MG	2A	3696	1/1	0.90	0.21	65,65,65,65	0
56	MG	1A	3664	1/1	0.90	0.14	32,32,32,32	0
56	MG	2a	1699	1/1	0.90	0.16	69,69,69,69	0
56	MG	2A	3429	1/1	0.90	0.46	77,77,77,77	0
56	MG	1A	3134	1/1	0.90	0.17	53,53,53,53	0
56	MG	1A	3293	1/1	0.90	0.22	58,58,58,58	0
56	MG	1A	4044	1/1	0.90	0.17	65,65,65,65	0
56	MG	1A	3150	1/1	0.90	0.13	44,44,44,44	0
56	MG	1A	3299	1/1	0.90	0.25	56,56,56,56	0
56	MG	1A	3245	1/1	0.90	0.18	52,52,52,52	0
56	MG	1a	1719	1/1	0.90	0.23	63,63,63,63	0
56	MG	2A	3449	1/1	0.90	0.15	60,60,60,60	0
56	MG	2a	1711	1/1	0.90	0.32	72,72,72,72	0
56	MG	2A	3453	1/1	0.90	0.20	74,74,74,74	0
56	MG	2A	3251	1/1	0.90	0.43	66,66,66,66	0
56	MG	1a	1721	1/1	0.90	0.19	60,60,60,60	0
56	MG	1A	3913	1/1	0.90	0.15	70,70,70,70	0
56	MG	2A	3729	1/1	0.90	0.21	75,75,75,75	0
56	MG	2A	3077	1/1	0.90	0.13	60,60,60,60	0
56	MG	1A	3364	1/1	0.90	0.10	55,55,55,55	0
56	MG	2A	3734	1/1	0.90	0.12	47,47,47,47	0
56	MG	1A	3464	1/1	0.90	0.18	53,53,53,53	0
56	MG	2a	1723	1/1	0.90	0.18	65,65,65,65	0
56	MG	1A	3400	1/1	0.90	0.13	55,55,55,55	0
56	MG	18	101	1/1	0.90	0.16	67,67,67,67	0
56	MG	2A	3744	1/1	0.90	0.14	51,51,51,51	0
56	MG	1A	3929	1/1	0.90	0.10	43,43,43,43	0
56	MG	2a	1731	1/1	0.90	0.48	70,70,70,70	0
56	MG	2A	3482	1/1	0.90	0.24	58,58,58,58	0
56	MG	2A	3262	1/1	0.90	0.28	74,74,74,74	0
56	MG	1B	203	1/1	0.90	0.19	59,59,59,59	0
56	MG	1A	3401	1/1	0.90	0.13	59,59,59,59	0
56	MG	1A	3040	1/1	0.90	0.20	64,64,64,64	0
56	MG	2A	3092	1/1	0.90	0.32	73,73,73,73	0
56	MG	1A	3934	1/1	0.90	0.22	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1B	214	1/1	0.90	0.26	66,66,66,66	0
56	MG	2A	3499	1/1	0.90	0.26	75,75,75,75	0
56	MG	1A	3558	1/1	0.90	0.21	51,51,51,51	0
56	MG	2B	201	1/1	0.90	0.23	85,85,85,85	0
56	MG	2B	202	1/1	0.90	0.11	75,75,75,75	0
56	MG	1A	3559	1/1	0.90	0.23	61,61,61,61	0
56	MG	1a	1616	1/1	0.90	0.13	62,62,62,62	0
56	MG	2a	1762	1/1	0.90	0.16	59,59,59,59	0
56	MG	1a	1619	1/1	0.90	0.15	61,61,61,61	0
56	MG	1B	219	1/1	0.90	0.21	59,59,59,59	0
56	MG	1A	3940	1/1	0.90	0.16	37,37,37,37	0
56	MG	1A	3568	1/1	0.90	0.40	68,68,68,68	0
56	MG	2A	3286	1/1	0.90	0.10	73,73,73,73	0
56	MG	1A	3250	1/1	0.90	0.13	54,54,54,54	0
56	MG	1a	1768	1/1	0.90	0.17	52,52,52,52	0
56	MG	2A	3524	1/1	0.90	0.19	70,70,70,70	0
56	MG	2A	3115	1/1	0.90	0.18	65,65,65,65	0
56	MG	1a	1769	1/1	0.90	0.10	65,65,65,65	0
56	MG	2a	1777	1/1	0.90	0.23	75,75,75,75	0
56	MG	1A	3476	1/1	0.90	0.15	62,62,62,62	0
56	MG	1A	3577	1/1	0.90	0.10	59,59,59,59	0
56	MG	1a	1772	1/1	0.90	0.19	55,55,55,55	0
56	MG	2D	301	1/1	0.90	0.20	54,54,54,54	0
56	MG	1A	3950	1/1	0.90	0.12	25,25,25,25	0
56	MG	1B	230	1/1	0.90	0.21	77,77,77,77	0
56	MG	2A	3533	1/1	0.90	0.18	62,62,62,62	0
56	MG	2A	3534	1/1	0.90	0.23	60,60,60,60	0
56	MG	2A	3126	1/1	0.90	0.14	57,57,57,57	0
56	MG	2a	1791	1/1	0.90	0.28	78,78,78,78	0
56	MG	1A	3807	1/1	0.90	0.25	66,66,66,66	0
56	MG	2E	307	1/1	0.90	0.10	38,38,38,38	0
56	MG	1A	3371	1/1	0.90	0.14	61,61,61,61	0
56	MG	2F	302	1/1	0.90	0.09	50,50,50,50	0
56	MG	2A	3131	1/1	0.90	0.23	70,70,70,70	0
56	MG	2A	3134	1/1	0.90	0.14	54,54,54,54	0
56	MG	1a	1785	1/1	0.90	0.17	76,76,76,76	0
56	MG	2A	3136	1/1	0.90	0.29	71,71,71,71	0
56	MG	1a	1637	1/1	0.90	0.26	65,65,65,65	0
56	MG	1B	233	1/1	0.90	0.24	70,70,70,70	0
56	MG	2A	3142	1/1	0.90	0.29	64,64,64,64	0
56	MG	2T	201	1/1	0.90	0.27	74,74,74,74	0
56	MG	1a	1792	1/1	0.90	0.16	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3315	1/1	0.90	0.33	84,84,84,84	0
56	MG	2A	3570	1/1	0.90	0.17	70,70,70,70	0
56	MG	2A	3145	1/1	0.90	0.12	63,63,63,63	0
56	MG	2A	3149	1/1	0.90	0.17	68,68,68,68	0
56	MG	1a	1639	1/1	0.90	0.19	68,68,68,68	0
56	MG	1A	3129	1/1	0.90	0.09	78,78,78,78	0
56	MG	1A	3487	1/1	0.90	0.19	80,80,80,80	0
56	MG	1A	3970	1/1	0.90	0.14	72,72,72,72	0
56	MG	1a	1647	1/1	0.90	0.18	64,64,64,64	0
56	MG	1A	3339	1/1	0.90	0.23	66,66,66,66	0
56	MG	2A	3331	1/1	0.90	0.20	57,57,57,57	0
56	MG	2A	3585	1/1	0.90	0.14	71,71,71,71	0
56	MG	1A	3712	1/1	0.90	0.10	56,56,56,56	0
56	MG	2A	3165	1/1	0.90	0.13	70,70,70,70	0
56	MG	1E	309	1/1	0.90	0.12	64,64,64,64	0
56	MG	1A	3342	1/1	0.90	0.20	57,57,57,57	0
56	MG	2A	3349	1/1	0.91	0.29	63,63,63,63	0
56	MG	1A	3387	1/1	0.91	0.60	81,81,81,81	0
56	MG	2A	3351	1/1	0.91	0.34	64,64,64,64	0
56	MG	2A	3605	1/1	0.91	0.15	73,73,73,73	0
56	MG	1A	3226	1/1	0.91	0.29	71,71,71,71	0
56	MG	1A	3789	1/1	0.91	0.18	63,63,63,63	0
56	MG	2A	3187	1/1	0.91	0.29	69,69,69,69	0
56	MG	1A	3794	1/1	0.91	0.07	38,38,38,38	0
56	MG	2A	3356	1/1	0.91	0.18	54,54,54,54	0
56	MG	2A	3614	1/1	0.91	0.13	62,62,62,62	0
56	MG	2A	3189	1/1	0.91	0.20	80,80,80,80	0
56	MG	2A	3358	1/1	0.91	0.34	65,65,65,65	0
56	MG	1A	3972	1/1	0.91	0.10	69,69,69,69	0
56	MG	1x	111	1/1	0.91	0.27	71,71,71,71	0
56	MG	1N	201	1/1	0.91	0.17	63,63,63,63	0
56	MG	1A	3795	1/1	0.91	0.16	56,56,56,56	0
56	MG	2a	1638	1/1	0.91	0.33	75,75,75,75	0
56	MG	1A	3027	1/1	0.91	0.18	78,78,78,78	0
56	MG	2A	3623	1/1	0.91	0.12	81,81,81,81	0
56	MG	1A	3275	1/1	0.91	0.22	44,44,44,44	0
56	MG	1A	3169	1/1	0.91	0.12	60,60,60,60	0
56	MG	2A	3627	1/1	0.91	0.33	70,70,70,70	0
56	MG	2a	1647	1/1	0.91	0.29	75,75,75,75	0
56	MG	1A	3087	1/1	0.91	0.27	49,49,49,49	0
56	MG	2A	3368	1/1	0.91	0.10	46,46,46,46	0
56	MG	2A	3369	1/1	0.91	0.10	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3803	1/1	0.91	0.16	69,69,69,69	0
56	MG	1O	206	1/1	0.91	0.21	68,68,68,68	0
56	MG	1A	3340	1/1	0.91	0.38	40,40,40,40	0
56	MG	2a	1655	1/1	0.91	0.38	78,78,78,78	0
56	MG	2A	3208	1/1	0.91	0.17	48,48,48,48	0
56	MG	1A	3006	1/1	0.91	0.18	67,67,67,67	0
56	MG	1A	3138	1/1	0.91	0.18	49,49,49,49	0
56	MG	2A	3644	1/1	0.91	0.09	51,51,51,51	0
56	MG	1A	3508	1/1	0.91	0.24	73,73,73,73	0
56	MG	1a	1694	1/1	0.91	0.24	61,61,61,61	0
56	MG	2A	3648	1/1	0.91	0.12	72,72,72,72	0
56	MG	1A	3810	1/1	0.91	0.23	63,63,63,63	0
56	MG	2A	3391	1/1	0.91	0.12	44,44,44,44	0
56	MG	2A	3220	1/1	0.91	0.19	77,77,77,77	0
56	MG	2A	3030	1/1	0.91	0.12	52,52,52,52	0
56	MG	1A	4004	1/1	0.91	0.18	49,49,49,49	0
56	MG	1T	201	1/1	0.91	0.24	51,51,51,51	0
56	MG	2a	1675	1/1	0.91	0.16	73,73,73,73	0
56	MG	2a	1676	1/1	0.91	0.19	63,63,63,63	0
56	MG	1A	3811	1/1	0.91	0.14	59,59,59,59	0
56	MG	1A	3347	1/1	0.91	0.20	62,62,62,62	0
56	MG	1A	3148	1/1	0.91	0.24	39,39,39,39	0
56	MG	2A	3227	1/1	0.91	0.17	62,62,62,62	0
56	MG	2A	3041	1/1	0.91	0.21	63,63,63,63	0
56	MG	2A	3412	1/1	0.91	0.19	51,51,51,51	0
56	MG	1U	204	1/1	0.91	0.17	39,39,39,39	0
56	MG	1U	210	1/1	0.91	0.17	55,55,55,55	0
56	MG	1A	3004	1/1	0.91	0.10	37,37,37,37	0
56	MG	2A	3049	1/1	0.91	0.22	75,75,75,75	0
56	MG	2a	1690	1/1	0.91	0.10	81,81,81,81	0
56	MG	2A	3686	1/1	0.91	0.18	74,74,74,74	0
56	MG	1A	4012	1/1	0.91	0.09	49,49,49,49	0
56	MG	1A	3413	1/1	0.91	0.09	58,58,58,58	0
56	MG	1A	3526	1/1	0.91	0.20	53,53,53,53	0
56	MG	1A	3246	1/1	0.91	0.22	46,46,46,46	0
56	MG	1A	4023	1/1	0.91	0.17	50,50,50,50	0
56	MG	1A	3695	1/1	0.91	0.14	50,50,50,50	0
56	MG	2A	3065	1/1	0.91	0.20	71,71,71,71	0
56	MG	1A	3696	1/1	0.91	0.11	34,34,34,34	0
56	MG	2A	3430	1/1	0.91	0.10	69,69,69,69	0
56	MG	1A	3834	1/1	0.91	0.18	45,45,45,45	0
56	MG	2a	1702	1/1	0.91	0.18	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1731	1/1	0.91	0.23	52,52,52,52	0
56	MG	1A	3298	1/1	0.91	0.17	38,38,38,38	0
56	MG	1A	3247	1/1	0.91	0.09	78,78,78,78	0
56	MG	1A	3303	1/1	0.91	0.20	58,58,58,58	0
56	MG	1A	3248	1/1	0.91	0.10	53,53,53,53	0
56	MG	13	104	1/1	0.91	0.09	50,50,50,50	0
56	MG	1a	1743	1/1	0.91	0.23	57,57,57,57	0
56	MG	1A	3100	1/1	0.91	0.26	74,74,74,74	0
56	MG	1A	3197	1/1	0.91	0.12	48,48,48,48	0
56	MG	1A	3856	1/1	0.91	0.16	74,74,74,74	0
56	MG	2A	3090	1/1	0.91	0.27	68,68,68,68	0
56	MG	2a	1715	1/1	0.91	0.28	73,73,73,73	0
56	MG	1A	3708	1/1	0.91	0.10	67,67,67,67	0
56	MG	1a	1751	1/1	0.91	0.26	57,57,57,57	0
56	MG	1A	3548	1/1	0.91	0.19	73,73,73,73	0
56	MG	2A	3266	1/1	0.91	0.22	70,70,70,70	0
56	MG	1A	3865	1/1	0.91	0.21	66,66,66,66	0
56	MG	1A	3550	1/1	0.91	0.29	71,71,71,71	0
56	MG	1A	3431	1/1	0.91	0.11	69,69,69,69	0
56	MG	2A	3483	1/1	0.91	0.16	46,46,46,46	0
56	MG	1A	3716	1/1	0.91	0.14	36,36,36,36	0
56	MG	2a	1726	1/1	0.91	0.32	70,70,70,70	0
56	MG	1a	1609	1/1	0.91	0.17	65,65,65,65	0
56	MG	2A	3759	1/1	0.91	0.18	66,66,66,66	0
56	MG	1A	4056	1/1	0.91	0.19	48,48,48,48	0
56	MG	1A	3435	1/1	0.91	0.20	62,62,62,62	0
56	MG	1A	3362	1/1	0.91	0.13	63,63,63,63	0
56	MG	1A	3877	1/1	0.91	0.20	66,66,66,66	0
56	MG	1B	207	1/1	0.91	0.13	64,64,64,64	0
56	MG	1A	3570	1/1	0.91	0.17	52,52,52,52	0
56	MG	2A	3500	1/1	0.91	0.11	49,49,49,49	0
56	MG	1A	3046	1/1	0.91	0.17	44,44,44,44	0
56	MG	1a	1627	1/1	0.91	0.26	65,65,65,65	0
56	MG	1a	1774	1/1	0.91	0.22	64,64,64,64	0
56	MG	2a	1745	1/1	0.91	0.17	83,83,83,83	0
56	MG	1A	3162	1/1	0.91	0.20	63,63,63,63	0
56	MG	2A	3289	1/1	0.91	0.23	71,71,71,71	0
56	MG	2a	1751	1/1	0.91	0.21	72,72,72,72	0
56	MG	1a	1779	1/1	0.91	0.12	48,48,48,48	0
56	MG	2a	1757	1/1	0.91	0.16	65,65,65,65	0
56	MG	2B	208	1/1	0.91	0.31	77,77,77,77	0
56	MG	1A	3726	1/1	0.91	0.15	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3453	1/1	0.91	0.14	64,64,64,64	0
56	MG	1A	3256	1/1	0.91	0.10	49,49,49,49	0
56	MG	1a	1784	1/1	0.91	0.24	59,59,59,59	0
56	MG	1A	3064	1/1	0.91	0.19	65,65,65,65	0
56	MG	2a	1768	1/1	0.91	0.28	80,80,80,80	0
56	MG	1a	1788	1/1	0.91	0.12	63,63,63,63	0
56	MG	1A	3457	1/1	0.91	0.11	58,58,58,58	0
56	MG	1A	3216	1/1	0.91	0.21	48,48,48,48	0
56	MG	2A	3137	1/1	0.91	0.33	66,66,66,66	0
56	MG	2A	3303	1/1	0.91	0.22	71,71,71,71	0
56	MG	1a	1791	1/1	0.91	0.17	72,72,72,72	0
56	MG	1A	3320	1/1	0.91	0.35	64,64,64,64	0
56	MG	1A	3924	1/1	0.91	0.20	66,66,66,66	0
56	MG	1A	3261	1/1	0.91	0.14	66,66,66,66	0
56	MG	2D	307	1/1	0.91	0.14	63,63,63,63	0
56	MG	2A	3308	1/1	0.91	0.13	78,78,78,78	0
56	MG	2A	3542	1/1	0.91	0.18	46,46,46,46	0
56	MG	1A	3467	1/1	0.91	0.09	55,55,55,55	0
56	MG	2A	3310	1/1	0.91	0.17	68,68,68,68	0
56	MG	2a	1786	1/1	0.91	0.29	71,71,71,71	0
56	MG	1a	1642	1/1	0.91	0.23	64,64,64,64	0
56	MG	2A	3150	1/1	0.91	0.10	58,58,58,58	0
56	MG	2E	310	1/1	0.91	0.19	62,62,62,62	0
56	MG	1A	3376	1/1	0.91	0.44	53,53,53,53	0
56	MG	2A	3154	1/1	0.91	0.17	53,53,53,53	0
56	MG	1A	3323	1/1	0.91	0.13	45,45,45,45	0
56	MG	2A	3564	1/1	0.91	0.20	64,64,64,64	0
56	MG	1A	3324	1/1	0.91	0.20	67,67,67,67	0
56	MG	1A	3770	1/1	0.91	0.11	22,22,22,22	0
56	MG	1A	3771	1/1	0.91	0.08	45,45,45,45	0
56	MG	1A	3217	1/1	0.91	0.11	62,62,62,62	0
56	MG	1A	3050	1/1	0.91	0.23	44,44,44,44	0
56	MG	2U	201	1/1	0.91	0.20	60,60,60,60	0
56	MG	2a	1809	1/1	0.91	0.20	84,84,84,84	0
56	MG	2A	3164	1/1	0.91	0.21	74,74,74,74	0
56	MG	2A	3328	1/1	0.91	0.25	57,57,57,57	0
56	MG	1A	3384	1/1	0.91	0.13	61,61,61,61	0
56	MG	2A	3330	1/1	0.91	0.24	51,51,51,51	0
56	MG	1a	1659	1/1	0.91	0.18	62,62,62,62	0
56	MG	2A	3578	1/1	0.91	0.14	61,61,61,61	0
56	MG	1E	302	1/1	0.91	0.12	55,55,55,55	0
56	MG	1A	3780	1/1	0.91	0.40	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3335	1/1	0.91	0.23	44,44,44,44	0
56	MG	1A	3634	1/1	0.91	0.19	50,50,50,50	0
56	MG	2A	3172	1/1	0.91	0.19	64,64,64,64	0
56	MG	1a	1663	1/1	0.91	0.09	54,54,54,54	0
56	MG	1A	3638	1/1	0.91	0.07	25,25,25,25	0
56	MG	1A	3223	1/1	0.91	0.18	56,56,56,56	0
56	MG	1A	3954	1/1	0.91	0.13	74,74,74,74	0
56	MG	1A	3646	1/1	0.91	0.08	39,39,39,39	0
56	MG	2x	104	1/1	0.91	0.22	74,74,74,74	0
56	MG	2a	1613	1/1	0.91	0.23	66,66,66,66	0
56	MG	2A	3344	1/1	0.91	0.38	79,79,79,79	0
56	MG	2A	3182	1/1	0.91	0.12	58,58,58,58	0
56	MG	2A	3183	1/1	0.91	0.17	66,66,66,66	0
57	K	2x	101	1/1	0.91	0.21	85,85,85,85	0
56	MG	2a	1623	1/1	0.92	0.34	75,75,75,75	0
56	MG	1A	3640	1/1	0.92	0.11	50,50,50,50	0
56	MG	1a	1606	1/1	0.92	0.30	67,67,67,67	0
56	MG	2A	3395	1/1	0.92	0.14	62,62,62,62	0
56	MG	2a	1628	1/1	0.92	0.32	61,61,61,61	0
56	MG	1A	3255	1/1	0.92	0.12	48,48,48,48	0
56	MG	1A	3146	1/1	0.92	0.11	40,40,40,40	0
56	MG	1a	1758	1/1	0.92	0.16	73,73,73,73	0
56	MG	2A	3244	1/1	0.92	0.41	82,82,82,82	0
56	MG	2A	3402	1/1	0.92	0.19	66,66,66,66	0
56	MG	1A	3919	1/1	0.92	0.08	27,27,27,27	0
56	MG	1a	1760	1/1	0.92	0.23	68,68,68,68	0
56	MG	2A	3406	1/1	0.92	0.08	65,65,65,65	0
56	MG	1A	3921	1/1	0.92	0.10	62,62,62,62	0
56	MG	2A	3411	1/1	0.92	0.16	49,49,49,49	0
56	MG	1A	3922	1/1	0.92	0.19	64,64,64,64	0
56	MG	2a	1640	1/1	0.92	0.09	83,83,83,83	0
56	MG	2A	3094	1/1	0.92	0.25	66,66,66,66	0
56	MG	1A	3436	1/1	0.92	0.20	75,75,75,75	0
56	MG	2A	3096	1/1	0.92	0.15	74,74,74,74	0
56	MG	2A	3097	1/1	0.92	0.15	57,57,57,57	0
56	MG	2a	1646	1/1	0.92	0.10	70,70,70,70	0
56	MG	1A	3656	1/1	0.92	0.12	53,53,53,53	0
56	MG	2A	3650	1/1	0.92	0.19	72,72,72,72	0
56	MG	1A	3125	1/1	0.92	0.28	46,46,46,46	0
56	MG	2A	3420	1/1	0.92	0.25	61,61,61,61	0
56	MG	1A	3172	1/1	0.92	0.07	51,51,51,51	0
56	MG	1A	3445	1/1	0.92	0.13	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3423	1/1	0.92	0.32	69,69,69,69	0
56	MG	1A	3519	1/1	0.92	0.34	59,59,59,59	0
56	MG	1A	3390	1/1	0.92	0.24	73,73,73,73	0
56	MG	1A	3452	1/1	0.92	0.09	68,68,68,68	0
56	MG	1A	3937	1/1	0.92	0.12	55,55,55,55	0
56	MG	1A	3537	1/1	0.92	0.10	48,48,48,48	0
56	MG	1A	3792	1/1	0.92	0.07	29,29,29,29	0
56	MG	2A	3669	1/1	0.92	0.17	64,64,64,64	0
56	MG	2A	3671	1/1	0.92	0.28	66,66,66,66	0
56	MG	1A	3793	1/1	0.92	0.10	37,37,37,37	0
56	MG	1A	3212	1/1	0.92	0.06	57,57,57,57	0
56	MG	2A	3677	1/1	0.92	0.13	70,70,70,70	0
56	MG	1a	1782	1/1	0.92	0.10	50,50,50,50	0
56	MG	2a	1671	1/1	0.92	0.21	65,65,65,65	0
56	MG	2A	3439	1/1	0.92	0.12	38,38,38,38	0
56	MG	2A	3683	1/1	0.92	0.14	60,60,60,60	0
56	MG	1A	3394	1/1	0.92	0.17	54,54,54,54	0
56	MG	2A	3275	1/1	0.92	0.28	63,63,63,63	0
56	MG	1A	3091	1/1	0.92	0.34	64,64,64,64	0
56	MG	1A	3151	1/1	0.92	0.14	43,43,43,43	0
56	MG	2A	3690	1/1	0.92	0.18	76,76,76,76	0
56	MG	2A	3450	1/1	0.92	0.14	53,53,53,53	0
56	MG	1A	3300	1/1	0.92	0.27	59,59,59,59	0
56	MG	2A	3695	1/1	0.92	0.18	87,87,87,87	0
56	MG	2A	3125	1/1	0.92	0.21	61,61,61,61	0
56	MG	2A	3280	1/1	0.92	0.08	68,68,68,68	0
56	MG	2a	1687	1/1	0.92	0.17	57,57,57,57	0
56	MG	1a	1644	1/1	0.92	0.26	66,66,66,66	0
56	MG	1E	303	1/1	0.92	0.20	44,44,44,44	0
56	MG	1A	3104	1/1	0.92	0.25	50,50,50,50	0
56	MG	1A	3461	1/1	0.92	0.10	56,56,56,56	0
56	MG	1A	3694	1/1	0.92	0.16	55,55,55,55	0
56	MG	1a	1650	1/1	0.92	0.16	51,51,51,51	0
56	MG	1a	1798	1/1	0.92	0.28	72,72,72,72	0
56	MG	2A	3479	1/1	0.92	0.16	57,57,57,57	0
56	MG	2A	3716	1/1	0.92	0.17	56,56,56,56	0
56	MG	1A	3967	1/1	0.92	0.11	52,52,52,52	0
56	MG	1A	3549	1/1	0.92	0.10	67,67,67,67	0
56	MG	1A	3463	1/1	0.92	0.18	76,76,76,76	0
56	MG	1A	3334	1/1	0.92	0.12	66,66,66,66	0
56	MG	1A	3267	1/1	0.92	0.28	58,58,58,58	0
56	MG	1A	3468	1/1	0.92	0.20	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3146	1/1	0.92	0.24	67,67,67,67	0
56	MG	1A	3269	1/1	0.92	0.09	51,51,51,51	0
56	MG	1A	3121	1/1	0.92	0.18	54,54,54,54	0
56	MG	2A	3736	1/1	0.92	0.29	78,78,78,78	0
56	MG	1A	3986	1/1	0.92	0.09	61,61,61,61	0
56	MG	1A	3818	1/1	0.92	0.11	70,70,70,70	0
56	MG	1A	3410	1/1	0.92	0.09	58,58,58,58	0
56	MG	2A	3743	1/1	0.92	0.10	65,65,65,65	0
56	MG	2A	3156	1/1	0.92	0.31	65,65,65,65	0
56	MG	1A	3411	1/1	0.92	0.12	65,65,65,65	0
56	MG	2A	3748	1/1	0.92	0.15	54,54,54,54	0
56	MG	2A	3753	1/1	0.92	0.16	60,60,60,60	0
56	MG	2A	3755	1/1	0.92	0.11	68,68,68,68	0
56	MG	1A	3224	1/1	0.92	0.16	64,64,64,64	0
56	MG	1A	3579	1/1	0.92	0.21	56,56,56,56	0
56	MG	2A	3515	1/1	0.92	0.23	55,55,55,55	0
56	MG	1A	3414	1/1	0.92	0.24	57,57,57,57	0
56	MG	1A	3481	1/1	0.92	0.28	51,51,51,51	0
56	MG	1A	3591	1/1	0.92	0.15	55,55,55,55	0
56	MG	1A	3482	1/1	0.92	0.29	46,46,46,46	0
56	MG	1w	102	1/1	0.92	0.13	73,73,73,73	0
56	MG	1Q	204	1/1	0.92	0.11	59,59,59,59	0
56	MG	1a	1683	1/1	0.92	0.28	52,52,52,52	0
56	MG	2A	3770	1/1	0.92	0.21	54,54,54,54	0
56	MG	2a	1730	1/1	0.92	0.27	66,66,66,66	0
56	MG	1A	3720	1/1	0.92	0.15	61,61,61,61	0
56	MG	2A	3171	1/1	0.92	0.18	72,72,72,72	0
56	MG	1A	3601	1/1	0.92	0.13	42,42,42,42	0
56	MG	1A	3841	1/1	0.92	0.07	37,37,37,37	0
56	MG	1A	3484	1/1	0.92	0.22	64,64,64,64	0
56	MG	2A	3326	1/1	0.92	0.21	46,46,46,46	0
56	MG	2a	1740	1/1	0.92	0.17	78,78,78,78	0
56	MG	1A	3344	1/1	0.92	0.13	47,47,47,47	0
56	MG	2B	207	1/1	0.92	0.12	70,70,70,70	0
56	MG	1A	3136	1/1	0.92	0.31	47,47,47,47	0
56	MG	2B	209	1/1	0.92	0.23	70,70,70,70	0
56	MG	2A	3539	1/1	0.92	0.14	34,34,34,34	0
56	MG	2a	1746	1/1	0.92	0.21	59,59,59,59	0
56	MG	1A	3848	1/1	0.92	0.12	56,56,56,56	0
56	MG	1A	3851	1/1	0.92	0.14	33,33,33,33	0
56	MG	2a	1750	1/1	0.92	0.20	69,69,69,69	0
56	MG	1A	3729	1/1	0.92	0.17	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3332	1/1	0.92	0.29	61,61,61,61	0
56	MG	1A	4027	1/1	0.92	0.19	61,61,61,61	0
56	MG	1A	3730	1/1	0.92	0.19	61,61,61,61	0
56	MG	1a	1695	1/1	0.92	0.12	64,64,64,64	0
56	MG	2A	3012	1/1	0.92	0.10	55,55,55,55	0
56	MG	2A	3554	1/1	0.92	0.15	64,64,64,64	0
56	MG	2A	3559	1/1	0.92	0.20	52,52,52,52	0
56	MG	1W	202	1/1	0.92	0.16	51,51,51,51	0
56	MG	2D	304	1/1	0.92	0.47	48,48,48,48	0
56	MG	1A	3615	1/1	0.92	0.10	41,41,41,41	0
56	MG	2A	3190	1/1	0.92	0.08	70,70,70,70	0
56	MG	1A	3739	1/1	0.92	0.09	26,26,26,26	0
56	MG	1A	3740	1/1	0.92	0.12	33,33,33,33	0
56	MG	1X	105	1/1	0.92	0.10	54,54,54,54	0
56	MG	2A	3195	1/1	0.92	0.12	66,66,66,66	0
56	MG	1Z	301	1/1	0.92	0.15	65,65,65,65	0
56	MG	2A	3572	1/1	0.92	0.09	52,52,52,52	0
56	MG	10	102	1/1	0.92	0.09	51,51,51,51	0
56	MG	2E	309	1/1	0.92	0.13	50,50,50,50	0
56	MG	2a	1781	1/1	0.92	0.19	67,67,67,67	0
56	MG	1A	3419	1/1	0.92	0.20	48,48,48,48	0
56	MG	2A	3575	1/1	0.92	0.25	66,66,66,66	0
56	MG	1a	1706	1/1	0.92	0.35	57,57,57,57	0
56	MG	2A	3202	1/1	0.92	0.16	66,66,66,66	0
56	MG	1A	4036	1/1	0.92	0.25	64,64,64,64	0
56	MG	2a	1787	1/1	0.92	0.16	69,69,69,69	0
56	MG	1a	1711	1/1	0.92	0.25	54,54,54,54	0
56	MG	1A	3421	1/1	0.92	0.16	52,52,52,52	0
56	MG	1A	3874	1/1	0.92	0.11	24,24,24,24	0
56	MG	1A	3052	1/1	0.92	0.18	56,56,56,56	0
56	MG	2a	1792	1/1	0.92	0.10	82,82,82,82	0
56	MG	11	101	1/1	0.92	0.28	41,41,41,41	0
56	MG	1a	1717	1/1	0.92	0.14	61,61,61,61	0
56	MG	2V	201	1/1	0.92	0.32	57,57,57,57	0
56	MG	2A	3047	1/1	0.92	0.22	68,68,68,68	0
56	MG	1A	4043	1/1	0.92	0.13	51,51,51,51	0
56	MG	2A	3216	1/1	0.92	0.08	55,55,55,55	0
56	MG	2a	1800	1/1	0.92	0.24	69,69,69,69	0
56	MG	1A	3750	1/1	0.92	0.14	46,46,46,46	0
56	MG	21	101	1/1	0.92	0.34	50,50,50,50	0
56	MG	2a	1803	1/1	0.92	0.27	81,81,81,81	0
56	MG	2A	3050	1/1	0.92	0.22	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1805	1/1	0.92	0.17	81,81,81,81	0
56	MG	2a	1808	1/1	0.92	0.22	64,64,64,64	0
56	MG	25	101	1/1	0.92	0.18	63,63,63,63	0
56	MG	1A	3496	1/1	0.92	0.20	48,48,48,48	0
56	MG	2a	1601	1/1	0.92	0.12	68,68,68,68	0
56	MG	1A	4046	1/1	0.92	0.19	56,56,56,56	0
56	MG	2a	1814	1/1	0.92	0.26	58,58,58,58	0
56	MG	1A	3283	1/1	0.92	0.22	51,51,51,51	0
56	MG	2e	201	1/1	0.92	0.08	87,87,87,87	0
56	MG	1A	3381	1/1	0.92	0.16	51,51,51,51	0
56	MG	1A	3893	1/1	0.92	0.12	42,42,42,42	0
56	MG	16	101	1/1	0.92	0.07	63,63,63,63	0
56	MG	2A	3606	1/1	0.92	0.21	75,75,75,75	0
56	MG	2A	3373	1/1	0.92	0.06	71,71,71,71	0
56	MG	2q	202	1/1	0.92	0.09	81,81,81,81	0
56	MG	2A	3063	1/1	0.92	0.09	58,58,58,58	0
56	MG	2a	1610	1/1	0.92	0.26	75,75,75,75	0
56	MG	2A	3228	1/1	0.92	0.30	78,78,78,78	0
56	MG	1A	3142	1/1	0.92	0.14	61,61,61,61	0
56	MG	18	102	1/1	0.92	0.36	48,48,48,48	0
56	MG	1A	3898	1/1	0.92	0.17	69,69,69,69	0
56	MG	1A	3636	1/1	0.92	0.10	33,33,33,33	0
56	MG	2A	3616	1/1	0.92	0.15	60,60,60,60	0
56	MG	1A	3637	1/1	0.92	0.09	26,26,26,26	0
56	MG	2A	3389	1/1	0.92	0.12	65,65,65,65	0
56	MG	1A	3288	1/1	0.92	0.12	66,66,66,66	0
56	MG	2a	1621	1/1	0.92	0.21	66,66,66,66	0
56	MG	1A	3506	1/1	0.92	0.10	56,56,56,56	0
56	MG	1A	3442	1/1	0.93	0.10	69,69,69,69	0
56	MG	1a	1796	1/1	0.93	0.21	61,61,61,61	0
56	MG	1B	223	1/1	0.93	0.19	71,71,71,71	0
56	MG	2A	3586	1/1	0.93	0.09	38,38,38,38	0
56	MG	1A	3532	1/1	0.93	0.11	42,42,42,42	0
56	MG	1A	3676	1/1	0.93	0.06	27,27,27,27	0
56	MG	2A	3338	1/1	0.93	0.44	66,66,66,66	0
56	MG	1A	3443	1/1	0.93	0.22	70,70,70,70	0
56	MG	1A	3930	1/1	0.93	0.10	65,65,65,65	0
56	MG	1a	1641	1/1	0.93	0.34	73,73,73,73	0
56	MG	1A	3236	1/1	0.93	0.16	56,56,56,56	0
56	MG	1A	3238	1/1	0.93	0.13	42,42,42,42	0
56	MG	1A	3383	1/1	0.93	0.17	54,54,54,54	0
56	MG	1A	3797	1/1	0.93	0.35	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3602	1/1	0.93	0.06	49,49,49,49	0
56	MG	1D	302	1/1	0.93	0.22	39,39,39,39	0
56	MG	1A	3448	1/1	0.93	0.17	55,55,55,55	0
56	MG	1A	3938	1/1	0.93	0.09	26,26,26,26	0
56	MG	1k	201	1/1	0.93	0.18	57,57,57,57	0
56	MG	2A	3180	1/1	0.93	0.22	71,71,71,71	0
56	MG	1A	3055	1/1	0.93	0.28	56,56,56,56	0
56	MG	1A	3545	1/1	0.93	0.12	53,53,53,53	0
56	MG	1a	1654	1/1	0.93	0.09	53,53,53,53	0
56	MG	1A	3002	1/1	0.93	0.12	60,60,60,60	0
56	MG	1A	3143	1/1	0.93	0.20	47,47,47,47	0
56	MG	1E	305	1/1	0.93	0.27	40,40,40,40	0
56	MG	1A	3184	1/1	0.93	0.17	75,75,75,75	0
56	MG	1w	103	1/1	0.93	0.30	79,79,79,79	0
56	MG	1A	3187	1/1	0.93	0.11	47,47,47,47	0
56	MG	1A	3114	1/1	0.93	0.17	54,54,54,54	0
56	MG	2A	3191	1/1	0.93	0.08	50,50,50,50	0
56	MG	1E	311	1/1	0.93	0.10	27,27,27,27	0
56	MG	1A	3951	1/1	0.93	0.18	50,50,50,50	0
56	MG	1A	3953	1/1	0.93	0.13	41,41,41,41	0
56	MG	1F	305	1/1	0.93	0.17	40,40,40,40	0
56	MG	1A	3808	1/1	0.93	0.08	74,74,74,74	0
56	MG	1a	1669	1/1	0.93	0.16	67,67,67,67	0
56	MG	1A	3554	1/1	0.93	0.08	49,49,49,49	0
56	MG	1A	3147	1/1	0.93	0.30	45,45,45,45	0
56	MG	2A	3201	1/1	0.93	0.32	68,68,68,68	0
56	MG	1A	3118	1/1	0.93	0.11	55,55,55,55	0
56	MG	2A	3380	1/1	0.93	0.17	49,49,49,49	0
56	MG	2A	3004	1/1	0.93	0.38	73,73,73,73	0
56	MG	2A	3384	1/1	0.93	0.09	58,58,58,58	0
56	MG	2A	3642	1/1	0.93	0.12	46,46,46,46	0
56	MG	1A	3961	1/1	0.93	0.10	42,42,42,42	0
56	MG	1A	3016	1/1	0.93	0.23	53,53,53,53	0
56	MG	2A	3387	1/1	0.93	0.25	69,69,69,69	0
56	MG	2a	1665	1/1	0.93	0.37	69,69,69,69	0
56	MG	1A	3968	1/1	0.93	0.09	60,60,60,60	0
56	MG	1A	3089	1/1	0.93	0.17	51,51,51,51	0
56	MG	2A	3649	1/1	0.93	0.25	63,63,63,63	0
56	MG	2A	3209	1/1	0.93	0.33	54,54,54,54	0
56	MG	2A	3013	1/1	0.93	0.12	49,49,49,49	0
56	MG	2A	3653	1/1	0.93	0.09	69,69,69,69	0
56	MG	1A	3571	1/1	0.93	0.20	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1N	205	1/1	0.93	0.14	57,57,57,57	0
56	MG	2A	3656	1/1	0.93	0.14	76,76,76,76	0
56	MG	1A	3154	1/1	0.93	0.14	44,44,44,44	0
56	MG	2A	3214	1/1	0.93	0.11	53,53,53,53	0
56	MG	2A	3397	1/1	0.93	0.11	62,62,62,62	0
56	MG	2A	3398	1/1	0.93	0.18	36,36,36,36	0
56	MG	2a	1681	1/1	0.93	0.27	66,66,66,66	0
56	MG	2A	3023	1/1	0.93	0.15	70,70,70,70	0
56	MG	2A	3218	1/1	0.93	0.20	60,60,60,60	0
56	MG	2A	3665	1/1	0.93	0.11	58,58,58,58	0
56	MG	1O	202	1/1	0.93	0.14	56,56,56,56	0
56	MG	1A	3973	1/1	0.93	0.20	63,63,63,63	0
56	MG	1A	3029	1/1	0.93	0.09	50,50,50,50	0
56	MG	2A	3404	1/1	0.93	0.07	53,53,53,53	0
56	MG	1A	3576	1/1	0.93	0.29	66,66,66,66	0
56	MG	2A	3675	1/1	0.93	0.20	49,49,49,49	0
56	MG	1A	3824	1/1	0.93	0.14	48,48,48,48	0
56	MG	1A	3305	1/1	0.93	0.09	61,61,61,61	0
56	MG	2A	3678	1/1	0.93	0.15	69,69,69,69	0
56	MG	1A	3306	1/1	0.93	0.26	55,55,55,55	0
56	MG	2A	3035	1/1	0.93	0.17	38,38,38,38	0
56	MG	1A	3831	1/1	0.93	0.08	48,48,48,48	0
56	MG	1R	201	1/1	0.93	0.18	48,48,48,48	0
56	MG	1A	3407	1/1	0.93	0.17	52,52,52,52	0
56	MG	1R	205	1/1	0.93	0.15	28,28,28,28	0
56	MG	1A	3581	1/1	0.93	0.11	41,41,41,41	0
56	MG	2A	3232	1/1	0.93	0.20	63,63,63,63	0
56	MG	1A	3994	1/1	0.93	0.13	45,45,45,45	0
56	MG	2a	1703	1/1	0.93	0.34	76,76,76,76	0
56	MG	1A	3127	1/1	0.93	0.19	57,57,57,57	0
56	MG	1A	3836	1/1	0.93	0.18	37,37,37,37	0
56	MG	1A	3357	1/1	0.93	0.12	55,55,55,55	0
56	MG	1A	3308	1/1	0.93	0.20	61,61,61,61	0
56	MG	2A	3425	1/1	0.93	0.21	57,57,57,57	0
56	MG	2A	3702	1/1	0.93	0.17	74,74,74,74	0
56	MG	1A	3594	1/1	0.93	0.08	14,14,14,14	0
56	MG	1A	3842	1/1	0.93	0.08	50,50,50,50	0
56	MG	1U	205	1/1	0.93	0.17	47,47,47,47	0
56	MG	2A	3707	1/1	0.93	0.12	77,77,77,77	0
56	MG	1a	1710	1/1	0.93	0.32	79,79,79,79	0
56	MG	2A	3431	1/1	0.93	0.20	61,61,61,61	0
56	MG	1A	3595	1/1	0.93	0.20	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3213	1/1	0.93	0.18	54,54,54,54	0
56	MG	2A	3715	1/1	0.93	0.18	51,51,51,51	0
56	MG	2A	3246	1/1	0.93	0.37	79,79,79,79	0
56	MG	2A	3437	1/1	0.93	0.11	60,60,60,60	0
56	MG	2A	3059	1/1	0.93	0.20	65,65,65,65	0
56	MG	2A	3722	1/1	0.93	0.18	65,65,65,65	0
56	MG	1W	201	1/1	0.93	0.17	58,58,58,58	0
56	MG	2A	3440	1/1	0.93	0.21	65,65,65,65	0
56	MG	2A	3064	1/1	0.93	0.13	71,71,71,71	0
56	MG	2A	3442	1/1	0.93	0.14	39,39,39,39	0
56	MG	2a	1728	1/1	0.93	0.30	75,75,75,75	0
56	MG	1A	3846	1/1	0.93	0.10	31,31,31,31	0
56	MG	1a	1715	1/1	0.93	0.33	79,79,79,79	0
56	MG	1A	3258	1/1	0.93	0.19	56,56,56,56	0
56	MG	1A	4014	1/1	0.93	0.09	55,55,55,55	0
56	MG	2A	3254	1/1	0.93	0.09	59,59,59,59	0
56	MG	2A	3074	1/1	0.93	0.21	57,57,57,57	0
56	MG	1A	3128	1/1	0.93	0.12	45,45,45,45	0
56	MG	2A	3460	1/1	0.93	0.10	43,43,43,43	0
56	MG	2a	1739	1/1	0.93	0.12	75,75,75,75	0
56	MG	1A	4016	1/1	0.93	0.11	69,69,69,69	0
56	MG	2A	3464	1/1	0.93	0.11	73,73,73,73	0
56	MG	1Y	202	1/1	0.93	0.24	56,56,56,56	0
56	MG	2A	3752	1/1	0.93	0.17	62,62,62,62	0
56	MG	2A	3079	1/1	0.93	0.09	57,57,57,57	0
56	MG	1a	1722	1/1	0.93	0.21	65,65,65,65	0
56	MG	1A	3733	1/1	0.93	0.16	54,54,54,54	0
56	MG	1a	1726	1/1	0.93	0.13	41,41,41,41	0
56	MG	2A	3265	1/1	0.93	0.10	64,64,64,64	0
56	MG	1a	1729	1/1	0.93	0.17	67,67,67,67	0
56	MG	1A	3312	1/1	0.93	0.12	46,46,46,46	0
56	MG	2a	1752	1/1	0.93	0.24	68,68,68,68	0
56	MG	2a	1754	1/1	0.93	0.18	70,70,70,70	0
56	MG	2a	1755	1/1	0.93	0.09	84,84,84,84	0
56	MG	1A	3607	1/1	0.93	0.07	37,37,37,37	0
56	MG	2A	3270	1/1	0.93	0.11	64,64,64,64	0
56	MG	2A	3271	1/1	0.93	0.27	73,73,73,73	0
56	MG	2A	3088	1/1	0.93	0.13	56,56,56,56	0
56	MG	1A	3858	1/1	0.93	0.15	42,42,42,42	0
56	MG	2A	3491	1/1	0.93	0.13	44,44,44,44	0
56	MG	2A	3492	1/1	0.93	0.15	58,58,58,58	0
56	MG	1A	3608	1/1	0.93	0.07	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	1767	1/1	0.93	0.13	72,72,72,72	0
56	MG	1A	4028	1/1	0.93	0.25	59,59,59,59	0
56	MG	1A	3313	1/1	0.93	0.27	41,41,41,41	0
56	MG	1a	1742	1/1	0.93	0.18	49,49,49,49	0
56	MG	1A	3035	1/1	0.93	0.07	48,48,48,48	0
56	MG	1a	1744	1/1	0.93	0.23	65,65,65,65	0
56	MG	1A	3164	1/1	0.93	0.10	46,46,46,46	0
56	MG	2A	3282	1/1	0.93	0.20	62,62,62,62	0
56	MG	1A	3869	1/1	0.93	0.11	52,52,52,52	0
56	MG	2A	3510	1/1	0.93	0.12	63,63,63,63	0
56	MG	11	104	1/1	0.93	0.12	50,50,50,50	0
56	MG	2A	3102	1/1	0.93	0.21	52,52,52,52	0
56	MG	1A	3369	1/1	0.93	0.13	55,55,55,55	0
56	MG	1A	3130	1/1	0.93	0.14	61,61,61,61	0
56	MG	1A	3095	1/1	0.93	0.14	60,60,60,60	0
56	MG	1A	3621	1/1	0.93	0.18	31,31,31,31	0
56	MG	1a	1756	1/1	0.93	0.11	59,59,59,59	0
56	MG	15	103	1/1	0.93	0.27	46,46,46,46	0
56	MG	1A	3073	1/1	0.93	0.21	59,59,59,59	0
56	MG	2A	3293	1/1	0.93	0.13	76,76,76,76	0
56	MG	2A	3111	1/1	0.93	0.13	53,53,53,53	0
56	MG	1A	3878	1/1	0.93	0.10	52,52,52,52	0
56	MG	1A	3879	1/1	0.93	0.24	73,73,73,73	0
56	MG	1a	1761	1/1	0.93	0.19	73,73,73,73	0
56	MG	1A	3883	1/1	0.93	0.06	45,45,45,45	0
56	MG	2A	3299	1/1	0.93	0.28	67,67,67,67	0
56	MG	18	105	1/1	0.93	0.20	58,58,58,58	0
56	MG	2A	3536	1/1	0.93	0.13	72,72,72,72	0
56	MG	2A	3538	1/1	0.93	0.13	39,39,39,39	0
56	MG	1A	3428	1/1	0.93	0.15	62,62,62,62	0
56	MG	1a	1765	1/1	0.93	0.20	51,51,51,51	0
56	MG	1A	3888	1/1	0.93	0.09	51,51,51,51	0
56	MG	2A	3544	1/1	0.93	0.10	54,54,54,54	0
56	MG	1A	3504	1/1	0.93	0.18	54,54,54,54	0
56	MG	1A	4049	1/1	0.93	0.16	72,72,72,72	0
56	MG	1A	3891	1/1	0.93	0.17	59,59,59,59	0
56	MG	2a	1806	1/1	0.93	0.22	58,58,58,58	0
56	MG	2A	3548	1/1	0.93	0.08	37,37,37,37	0
56	MG	1A	3228	1/1	0.93	0.17	40,40,40,40	0
56	MG	1A	3894	1/1	0.93	0.11	40,40,40,40	0
56	MG	1a	1608	1/1	0.93	0.33	60,60,60,60	0
56	MG	1A	3268	1/1	0.93	0.11	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3555	1/1	0.93	0.10	41,41,41,41	0
56	MG	2A	3556	1/1	0.93	0.10	58,58,58,58	0
56	MG	1A	4058	1/1	0.93	0.13	57,57,57,57	0
56	MG	2A	3138	1/1	0.93	0.22	43,43,43,43	0
56	MG	2W	201	1/1	0.93	0.09	63,63,63,63	0
56	MG	1A	3433	1/1	0.93	0.15	57,57,57,57	0
56	MG	1A	3900	1/1	0.93	0.08	25,25,25,25	0
56	MG	2l	201	1/1	0.93	0.10	72,72,72,72	0
56	MG	2l	202	1/1	0.93	0.11	81,81,81,81	0
56	MG	2l	203	1/1	0.93	0.15	78,78,78,78	0
56	MG	1A	3434	1/1	0.93	0.25	51,51,51,51	0
56	MG	1A	3774	1/1	0.93	0.11	51,51,51,51	0
56	MG	2A	3144	1/1	0.93	0.20	69,69,69,69	0
56	MG	2A	3320	1/1	0.93	0.16	62,62,62,62	0
56	MG	28	101	1/1	0.93	0.16	67,67,67,67	0
56	MG	1A	3170	1/1	0.93	0.32	49,49,49,49	0
56	MG	1a	1625	1/1	0.93	0.20	66,66,66,66	0
56	MG	2A	3325	1/1	0.93	0.26	48,48,48,48	0
56	MG	1A	3025	1/1	0.93	0.18	40,40,40,40	0
56	MG	1A	3512	1/1	0.93	0.15	41,41,41,41	0
56	MG	1A	3513	1/1	0.93	0.17	62,62,62,62	0
56	MG	1A	3235	1/1	0.93	0.19	39,39,39,39	0
56	MG	1A	3440	1/1	0.93	0.21	57,57,57,57	0
56	MG	1A	3784	1/1	0.93	0.13	54,54,54,54	0
56	MG	1A	3441	1/1	0.93	0.14	61,61,61,61	0
56	MG	1A	3301	1/1	0.94	0.22	58,58,58,58	0
56	MG	1a	1658	1/1	0.94	0.07	61,61,61,61	0
56	MG	2a	1618	1/1	0.94	0.14	80,80,80,80	0
56	MG	2A	3372	1/1	0.94	0.24	52,52,52,52	0
56	MG	1x	110	1/1	0.94	0.09	31,31,31,31	0
56	MG	1A	3925	1/1	0.94	0.27	66,66,66,66	0
56	MG	1A	3926	1/1	0.94	0.24	69,69,69,69	0
56	MG	1A	3777	1/1	0.94	0.10	28,28,28,28	0
56	MG	1A	3779	1/1	0.94	0.10	41,41,41,41	0
56	MG	2A	3001	1/1	0.94	0.33	63,63,63,63	0
56	MG	2A	3206	1/1	0.94	0.11	52,52,52,52	0
56	MG	1A	3622	1/1	0.94	0.08	41,41,41,41	0
56	MG	1A	3190	1/1	0.94	0.14	38,38,38,38	0
56	MG	1A	3030	1/1	0.94	0.27	39,39,39,39	0
56	MG	1A	3631	1/1	0.94	0.10	43,43,43,43	0
56	MG	1A	3195	1/1	0.94	0.35	42,42,42,42	0
56	MG	2A	3624	1/1	0.94	0.12	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3119	1/1	0.94	0.17	47,47,47,47	0
56	MG	1A	3034	1/1	0.94	0.18	41,41,41,41	0
56	MG	1a	1672	1/1	0.94	0.27	68,68,68,68	0
56	MG	2A	3393	1/1	0.94	0.10	54,54,54,54	0
56	MG	2A	3215	1/1	0.94	0.20	56,56,56,56	0
56	MG	2A	3633	1/1	0.94	0.11	59,59,59,59	0
56	MG	1A	3511	1/1	0.94	0.31	45,45,45,45	0
56	MG	2A	3217	1/1	0.94	0.17	60,60,60,60	0
56	MG	2A	3636	1/1	0.94	0.14	65,65,65,65	0
56	MG	1A	3254	1/1	0.94	0.18	41,41,41,41	0
56	MG	1A	3791	1/1	0.94	0.08	55,55,55,55	0
56	MG	2A	3024	1/1	0.94	0.20	52,52,52,52	0
56	MG	1a	1678	1/1	0.94	0.23	69,69,69,69	0
56	MG	1E	314	1/1	0.94	0.18	32,32,32,32	0
56	MG	1A	3941	1/1	0.94	0.14	32,32,32,32	0
56	MG	1E	316	1/1	0.94	0.21	46,46,46,46	0
56	MG	1A	3942	1/1	0.94	0.12	38,38,38,38	0
56	MG	1A	3058	1/1	0.94	0.21	63,63,63,63	0
56	MG	1A	3641	1/1	0.94	0.08	40,40,40,40	0
56	MG	1A	3642	1/1	0.94	0.12	27,27,27,27	0
56	MG	2A	3408	1/1	0.94	0.18	64,64,64,64	0
56	MG	2A	3409	1/1	0.94	0.25	62,62,62,62	0
56	MG	1A	3946	1/1	0.94	0.14	46,46,46,46	0
56	MG	2A	3037	1/1	0.94	0.21	65,65,65,65	0
56	MG	2A	3413	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	3948	1/1	0.94	0.11	63,63,63,63	0
56	MG	1A	3370	1/1	0.94	0.11	59,59,59,59	0
56	MG	1A	3124	1/1	0.94	0.31	42,42,42,42	0
56	MG	2A	3042	1/1	0.94	0.21	56,56,56,56	0
56	MG	1A	3257	1/1	0.94	0.13	49,49,49,49	0
56	MG	2A	3661	1/1	0.94	0.17	60,60,60,60	0
56	MG	1A	3521	1/1	0.94	0.09	55,55,55,55	0
56	MG	1A	3659	1/1	0.94	0.08	50,50,50,50	0
56	MG	2A	3664	1/1	0.94	0.10	38,38,38,38	0
56	MG	1A	3523	1/1	0.94	0.12	30,30,30,30	0
56	MG	2a	1674	1/1	0.94	0.29	68,68,68,68	0
56	MG	2A	3239	1/1	0.94	0.10	50,50,50,50	0
56	MG	1A	3048	1/1	0.94	0.11	34,34,34,34	0
56	MG	1A	3529	1/1	0.94	0.36	44,44,44,44	0
56	MG	1A	3530	1/1	0.94	0.15	53,53,53,53	0
56	MG	1A	3963	1/1	0.94	0.05	37,37,37,37	0
56	MG	2a	1680	1/1	0.94	0.14	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3674	1/1	0.94	0.15	55,55,55,55	0
56	MG	1A	3211	1/1	0.94	0.25	43,43,43,43	0
56	MG	1A	3049	1/1	0.94	0.18	35,35,35,35	0
56	MG	1a	1702	1/1	0.94	0.17	52,52,52,52	0
56	MG	1A	3377	1/1	0.94	0.10	63,63,63,63	0
56	MG	1A	3539	1/1	0.94	0.25	55,55,55,55	0
56	MG	1Q	206	1/1	0.94	0.15	43,43,43,43	0
56	MG	1A	3061	1/1	0.94	0.33	69,69,69,69	0
56	MG	1A	3020	1/1	0.94	0.09	49,49,49,49	0
56	MG	2A	3067	1/1	0.94	0.18	47,47,47,47	0
56	MG	2A	3068	1/1	0.94	0.11	52,52,52,52	0
56	MG	1A	3165	1/1	0.94	0.13	47,47,47,47	0
56	MG	1A	3975	1/1	0.94	0.13	68,68,68,68	0
56	MG	1A	3817	1/1	0.94	0.17	48,48,48,48	0
56	MG	1A	3686	1/1	0.94	0.15	62,62,62,62	0
56	MG	2A	3259	1/1	0.94	0.21	53,53,53,53	0
56	MG	1A	3980	1/1	0.94	0.15	42,42,42,42	0
56	MG	1A	3321	1/1	0.94	0.40	70,70,70,70	0
56	MG	1A	3166	1/1	0.94	0.07	46,46,46,46	0
56	MG	1A	3099	1/1	0.94	0.07	44,44,44,44	0
56	MG	1A	3989	1/1	0.94	0.07	32,32,32,32	0
56	MG	1A	3067	1/1	0.94	0.22	66,66,66,66	0
56	MG	1U	209	1/1	0.94	0.13	66,66,66,66	0
56	MG	1A	3827	1/1	0.94	0.05	49,49,49,49	0
56	MG	2A	3708	1/1	0.94	0.14	53,53,53,53	0
56	MG	1A	3693	1/1	0.94	0.20	54,54,54,54	0
56	MG	2A	3466	1/1	0.94	0.15	53,53,53,53	0
56	MG	1A	3829	1/1	0.94	0.06	29,29,29,29	0
56	MG	2A	3712	1/1	0.94	0.14	56,56,56,56	0
56	MG	2A	3468	1/1	0.94	0.15	60,60,60,60	0
56	MG	2A	3714	1/1	0.94	0.17	59,59,59,59	0
56	MG	1A	3998	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3471	1/1	0.94	0.10	36,36,36,36	0
56	MG	2A	3718	1/1	0.94	0.08	35,35,35,35	0
56	MG	1a	1730	1/1	0.94	0.11	66,66,66,66	0
56	MG	1A	3455	1/1	0.94	0.18	49,49,49,49	0
56	MG	2A	3475	1/1	0.94	0.07	52,52,52,52	0
56	MG	1A	3225	1/1	0.94	0.18	53,53,53,53	0
56	MG	2A	3478	1/1	0.94	0.10	37,37,37,37	0
56	MG	2A	3727	1/1	0.94	0.10	69,69,69,69	0
56	MG	1a	1734	1/1	0.94	0.25	49,49,49,49	0
56	MG	1a	1736	1/1	0.94	0.12	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3832	1/1	0.94	0.14	44,44,44,44	0
56	MG	2A	3732	1/1	0.94	0.07	43,43,43,43	0
56	MG	2A	3484	1/1	0.94	0.14	44,44,44,44	0
56	MG	1A	3271	1/1	0.94	0.22	51,51,51,51	0
56	MG	1Y	201	1/1	0.94	0.25	62,62,62,62	0
56	MG	2A	3281	1/1	0.94	0.09	67,67,67,67	0
56	MG	1A	3551	1/1	0.94	0.22	66,66,66,66	0
56	MG	1A	3552	1/1	0.94	0.22	57,57,57,57	0
56	MG	1A	4007	1/1	0.94	0.05	28,28,28,28	0
56	MG	1A	3553	1/1	0.94	0.10	63,63,63,63	0
56	MG	1A	3132	1/1	0.94	0.09	46,46,46,46	0
56	MG	1A	3839	1/1	0.94	0.13	38,38,38,38	0
56	MG	10	106	1/1	0.94	0.06	53,53,53,53	0
56	MG	1A	3701	1/1	0.94	0.12	63,63,63,63	0
56	MG	1A	3038	1/1	0.94	0.30	48,48,48,48	0
56	MG	10	109	1/1	0.94	0.06	55,55,55,55	0
56	MG	2A	3506	1/1	0.94	0.11	50,50,50,50	0
56	MG	1a	1754	1/1	0.94	0.23	61,61,61,61	0
56	MG	1A	3330	1/1	0.94	0.15	57,57,57,57	0
56	MG	1A	3560	1/1	0.94	0.09	44,44,44,44	0
56	MG	1A	3561	1/1	0.94	0.12	38,38,38,38	0
56	MG	2A	3513	1/1	0.94	0.20	66,66,66,66	0
56	MG	2A	3118	1/1	0.94	0.20	59,59,59,59	0
56	MG	2A	3765	1/1	0.94	0.14	52,52,52,52	0
56	MG	2A	3767	1/1	0.94	0.08	51,51,51,51	0
56	MG	1A	3391	1/1	0.94	0.25	76,76,76,76	0
56	MG	2A	3517	1/1	0.94	0.16	61,61,61,61	0
56	MG	2A	3120	1/1	0.94	0.17	56,56,56,56	0
56	MG	1A	3171	1/1	0.94	0.12	54,54,54,54	0
56	MG	1A	3075	1/1	0.94	0.12	35,35,35,35	0
56	MG	1A	3850	1/1	0.94	0.09	44,44,44,44	0
56	MG	2A	3523	1/1	0.94	0.15	55,55,55,55	0
56	MG	1A	3174	1/1	0.94	0.49	43,43,43,43	0
56	MG	2a	1763	1/1	0.94	0.18	52,52,52,52	0
56	MG	15	102	1/1	0.94	0.20	43,43,43,43	0
56	MG	1A	3854	1/1	0.94	0.06	28,28,28,28	0
56	MG	2A	3128	1/1	0.94	0.17	47,47,47,47	0
56	MG	15	104	1/1	0.94	0.21	59,59,59,59	0
56	MG	1A	3336	1/1	0.94	0.17	44,44,44,44	0
56	MG	2A	3133	1/1	0.94	0.21	46,46,46,46	0
56	MG	1A	3337	1/1	0.94	0.19	47,47,47,47	0
56	MG	1A	3471	1/1	0.94	0.10	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	4035	1/1	0.94	0.19	58,58,58,58	0
56	MG	1A	3176	1/1	0.94	0.08	36,36,36,36	0
56	MG	1A	3286	1/1	0.94	0.17	58,58,58,58	0
56	MG	2a	1775	1/1	0.94	0.22	71,71,71,71	0
56	MG	1A	3287	1/1	0.94	0.20	56,56,56,56	0
56	MG	1A	3582	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	3237	1/1	0.94	0.21	41,41,41,41	0
56	MG	1A	3731	1/1	0.94	0.11	62,62,62,62	0
56	MG	2a	1780	1/1	0.94	0.19	75,75,75,75	0
56	MG	1a	1604	1/1	0.94	0.14	66,66,66,66	0
56	MG	1A	3732	1/1	0.94	0.09	19,19,19,19	0
56	MG	2D	303	1/1	0.94	0.12	38,38,38,38	0
56	MG	1A	3079	1/1	0.94	0.09	66,66,66,66	0
56	MG	1A	3589	1/1	0.94	0.12	47,47,47,47	0
56	MG	1A	3141	1/1	0.94	0.12	59,59,59,59	0
56	MG	1A	3182	1/1	0.94	0.23	53,53,53,53	0
56	MG	2D	308	1/1	0.94	0.13	76,76,76,76	0
56	MG	1a	1786	1/1	0.94	0.12	86,86,86,86	0
56	MG	1a	1787	1/1	0.94	0.23	66,66,66,66	0
56	MG	1A	3106	1/1	0.94	0.08	30,30,30,30	0
56	MG	1A	3881	1/1	0.94	0.07	47,47,47,47	0
56	MG	2E	305	1/1	0.94	0.17	48,48,48,48	0
56	MG	1A	4053	1/1	0.94	0.16	66,66,66,66	0
56	MG	1A	3350	1/1	0.94	0.17	66,66,66,66	0
56	MG	1A	4055	1/1	0.94	0.19	64,64,64,64	0
56	MG	1A	3745	1/1	0.94	0.08	68,68,68,68	0
56	MG	1A	3113	1/1	0.94	0.07	46,46,46,46	0
56	MG	2A	3567	1/1	0.94	0.12	58,58,58,58	0
56	MG	1A	3749	1/1	0.94	0.15	74,74,74,74	0
56	MG	1A	3296	1/1	0.94	0.24	51,51,51,51	0
56	MG	1A	3751	1/1	0.94	0.07	32,32,32,32	0
56	MG	1a	1630	1/1	0.94	0.34	63,63,63,63	0
56	MG	2Q	202	1/1	0.94	0.19	56,56,56,56	0
56	MG	1B	206	1/1	0.94	0.21	53,53,53,53	0
56	MG	2a	1807	1/1	0.94	0.14	68,68,68,68	0
56	MG	1A	3491	1/1	0.94	0.13	51,51,51,51	0
56	MG	1B	208	1/1	0.94	0.29	70,70,70,70	0
56	MG	1A	3605	1/1	0.94	0.07	48,48,48,48	0
56	MG	2A	3346	1/1	0.94	0.20	57,57,57,57	0
56	MG	1A	3493	1/1	0.94	0.21	50,50,50,50	0
56	MG	2a	1813	1/1	0.94	0.21	71,71,71,71	0
56	MG	2A	3176	1/1	0.94	0.10	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3297	1/1	0.94	0.11	38,38,38,38	0
56	MG	2X	102	1/1	0.94	0.14	56,56,56,56	0
56	MG	1A	3611	1/1	0.94	0.13	66,66,66,66	0
56	MG	2A	3581	1/1	0.94	0.15	72,72,72,72	0
56	MG	1A	3417	1/1	0.94	0.20	48,48,48,48	0
56	MG	1B	217	1/1	0.94	0.13	49,49,49,49	0
56	MG	2k	201	1/1	0.94	0.11	67,67,67,67	0
56	MG	1A	3017	1/1	0.94	0.15	69,69,69,69	0
56	MG	1A	3769	1/1	0.94	0.13	28,28,28,28	0
56	MG	1A	3420	1/1	0.94	0.13	46,46,46,46	0
56	MG	1A	3910	1/1	0.94	0.20	67,67,67,67	0
56	MG	1A	3912	1/1	0.94	0.12	55,55,55,55	0
56	MG	1a	1646	1/1	0.94	0.21	57,57,57,57	0
56	MG	2r	101	1/1	0.94	0.22	75,75,75,75	0
56	MG	2A	3593	1/1	0.94	0.13	67,67,67,67	0
56	MG	1B	224	1/1	0.94	0.15	55,55,55,55	0
56	MG	1A	3500	1/1	0.94	0.21	57,57,57,57	0
56	MG	2A	3597	1/1	0.94	0.13	73,73,73,73	0
56	MG	1A	3772	1/1	0.94	0.09	52,52,52,52	0
56	MG	1A	3618	1/1	0.94	0.09	21,21,21,21	0
56	MG	1A	3920	1/1	0.94	0.08	61,61,61,61	0
56	MG	1A	3117	1/1	0.94	0.17	44,44,44,44	0
56	MG	1x	104	1/1	0.94	0.22	75,75,75,75	0
56	MG	2A	3366	1/1	0.94	0.38	57,57,57,57	0
56	MG	1a	1655	1/1	0.94	0.20	60,60,60,60	0
56	MG	1A	3189	1/1	0.94	0.29	47,47,47,47	0
59	ZN	14	102	1/1	0.94	0.11	123,123,123,123	0
59	ZN	24	501	1/1	0.94	0.17	131,131,131,131	0
56	MG	1A	3403	1/1	0.95	0.13	46,46,46,46	0
56	MG	1A	3859	1/1	0.95	0.10	61,61,61,61	0
56	MG	2A	3018	1/1	0.95	0.08	43,43,43,43	0
56	MG	1a	1681	1/1	0.95	0.24	54,54,54,54	0
56	MG	2A	3021	1/1	0.95	0.20	46,46,46,46	0
56	MG	1A	3635	1/1	0.95	0.09	35,35,35,35	0
56	MG	1A	3997	1/1	0.95	0.09	49,49,49,49	0
56	MG	1A	3356	1/1	0.95	0.20	58,58,58,58	0
56	MG	1P	203	1/1	0.95	0.22	35,35,35,35	0
56	MG	1P	204	1/1	0.95	0.54	39,39,39,39	0
56	MG	1A	3999	1/1	0.95	0.14	49,49,49,49	0
56	MG	1A	3028	1/1	0.95	0.17	36,36,36,36	0
56	MG	1A	3126	1/1	0.95	0.35	44,44,44,44	0
56	MG	1Q	205	1/1	0.95	0.12	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3315	1/1	0.95	0.14	47,47,47,47	0
56	MG	1A	3870	1/1	0.95	0.10	46,46,46,46	0
56	MG	1A	3070	1/1	0.95	0.10	39,39,39,39	0
56	MG	2A	3652	1/1	0.95	0.13	44,44,44,44	0
56	MG	1A	3766	1/1	0.95	0.11	55,55,55,55	0
56	MG	1A	3158	1/1	0.95	0.17	40,40,40,40	0
56	MG	1a	1696	1/1	0.95	0.08	65,65,65,65	0
56	MG	2A	3040	1/1	0.95	0.10	65,65,65,65	0
56	MG	1A	3056	1/1	0.95	0.10	29,29,29,29	0
56	MG	1A	3363	1/1	0.95	0.28	48,48,48,48	0
56	MG	2A	3043	1/1	0.95	0.14	36,36,36,36	0
56	MG	2a	1654	1/1	0.95	0.10	60,60,60,60	0
56	MG	1A	3101	1/1	0.95	0.09	51,51,51,51	0
56	MG	2A	3045	1/1	0.95	0.17	67,67,67,67	0
56	MG	2A	3427	1/1	0.95	0.33	65,65,65,65	0
56	MG	1A	3653	1/1	0.95	0.06	30,30,30,30	0
56	MG	2a	1659	1/1	0.95	0.18	57,57,57,57	0
56	MG	1A	3036	1/1	0.95	0.10	37,37,37,37	0
56	MG	2a	1661	1/1	0.95	0.12	58,58,58,58	0
56	MG	1A	3241	1/1	0.95	0.11	58,58,58,58	0
56	MG	2a	1663	1/1	0.95	0.26	82,82,82,82	0
56	MG	1A	4019	1/1	0.95	0.19	64,64,64,64	0
56	MG	1A	3278	1/1	0.95	0.35	43,43,43,43	0
56	MG	1A	3885	1/1	0.95	0.15	44,44,44,44	0
56	MG	1A	4022	1/1	0.95	0.11	43,43,43,43	0
56	MG	2A	3435	1/1	0.95	0.11	45,45,45,45	0
56	MG	2A	3053	1/1	0.95	0.06	48,48,48,48	0
56	MG	1A	3886	1/1	0.95	0.09	51,51,51,51	0
56	MG	1a	1708	1/1	0.95	0.19	52,52,52,52	0
56	MG	1V	203	1/1	0.95	0.35	44,44,44,44	0
56	MG	1A	4025	1/1	0.95	0.16	55,55,55,55	0
56	MG	1A	3008	1/1	0.95	0.12	29,29,29,29	0
56	MG	2A	3061	1/1	0.95	0.12	62,62,62,62	0
56	MG	2A	3062	1/1	0.95	0.15	48,48,48,48	0
56	MG	1A	3666	1/1	0.95	0.07	29,29,29,29	0
56	MG	1A	3667	1/1	0.95	0.11	75,75,75,75	0
56	MG	1A	3198	1/1	0.95	0.14	47,47,47,47	0
56	MG	1A	3556	1/1	0.95	0.07	40,40,40,40	0
56	MG	1X	106	1/1	0.95	0.17	72,72,72,72	0
56	MG	2A	3459	1/1	0.95	0.09	47,47,47,47	0
56	MG	2A	3069	1/1	0.95	0.14	38,38,38,38	0
56	MG	1A	3201	1/1	0.95	0.07	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3896	1/1	0.95	0.07	41,41,41,41	0
56	MG	1a	1720	1/1	0.95	0.21	74,74,74,74	0
56	MG	1A	3897	1/1	0.95	0.13	65,65,65,65	0
56	MG	1Z	302	1/1	0.95	0.24	60,60,60,60	0
56	MG	1A	3202	1/1	0.95	0.07	48,48,48,48	0
56	MG	1A	3489	1/1	0.95	0.16	52,52,52,52	0
56	MG	2A	3268	1/1	0.95	0.08	61,61,61,61	0
56	MG	1A	3080	1/1	0.95	0.13	45,45,45,45	0
56	MG	1A	3681	1/1	0.95	0.08	41,41,41,41	0
56	MG	1A	3563	1/1	0.95	0.24	57,57,57,57	0
56	MG	2A	3082	1/1	0.95	0.08	47,47,47,47	0
56	MG	1A	3906	1/1	0.95	0.09	64,64,64,64	0
56	MG	1a	1733	1/1	0.95	0.15	54,54,54,54	0
56	MG	2A	3085	1/1	0.95	0.10	42,42,42,42	0
56	MG	1A	3564	1/1	0.95	0.08	43,43,43,43	0
56	MG	1A	3427	1/1	0.95	0.08	46,46,46,46	0
56	MG	1a	1737	1/1	0.95	0.17	70,70,70,70	0
56	MG	1A	3569	1/1	0.95	0.29	66,66,66,66	0
56	MG	1A	3492	1/1	0.95	0.25	41,41,41,41	0
56	MG	1A	3133	1/1	0.95	0.13	47,47,47,47	0
56	MG	1A	3105	1/1	0.95	0.16	45,45,45,45	0
56	MG	1A	3915	1/1	0.95	0.16	57,57,57,57	0
56	MG	12	102	1/1	0.95	0.13	50,50,50,50	0
56	MG	2A	3496	1/1	0.95	0.12	56,56,56,56	0
56	MG	13	102	1/1	0.95	0.10	48,48,48,48	0
56	MG	1A	3917	1/1	0.95	0.05	32,32,32,32	0
56	MG	1A	3918	1/1	0.95	0.12	76,76,76,76	0
56	MG	1A	3495	1/1	0.95	0.28	50,50,50,50	0
56	MG	15	101	1/1	0.95	0.37	41,41,41,41	0
56	MG	1A	3691	1/1	0.95	0.10	51,51,51,51	0
56	MG	1A	3135	1/1	0.95	0.19	31,31,31,31	0
56	MG	1A	3039	1/1	0.95	0.30	43,43,43,43	0
56	MG	15	106	1/1	0.95	0.15	48,48,48,48	0
56	MG	2A	3739	1/1	0.95	0.09	65,65,65,65	0
56	MG	1A	4059	1/1	0.95	0.33	58,58,58,58	0
56	MG	1A	3251	1/1	0.95	0.11	42,42,42,42	0
56	MG	2A	3512	1/1	0.95	0.15	55,55,55,55	0
56	MG	17	102	1/1	0.95	0.11	40,40,40,40	0
56	MG	1A	3499	1/1	0.95	0.23	49,49,49,49	0
56	MG	2A	3751	1/1	0.95	0.10	54,54,54,54	0
56	MG	2A	3112	1/1	0.95	0.19	71,71,71,71	0
56	MG	2A	3113	1/1	0.95	0.24	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3754	1/1	0.95	0.16	70,70,70,70	0
56	MG	2A	3114	1/1	0.95	0.25	68,68,68,68	0
56	MG	2A	3301	1/1	0.95	0.15	43,43,43,43	0
56	MG	2A	3520	1/1	0.95	0.11	38,38,38,38	0
56	MG	1A	3335	1/1	0.95	0.17	49,49,49,49	0
56	MG	18	104	1/1	0.95	0.18	57,57,57,57	0
56	MG	2a	1734	1/1	0.95	0.15	71,71,71,71	0
56	MG	2A	3760	1/1	0.95	0.14	64,64,64,64	0
56	MG	1B	204	1/1	0.95	0.25	67,67,67,67	0
56	MG	1A	3806	1/1	0.95	0.06	44,44,44,44	0
56	MG	2a	1738	1/1	0.95	0.08	86,86,86,86	0
56	MG	1A	3110	1/1	0.95	0.14	35,35,35,35	0
56	MG	1A	3583	1/1	0.95	0.09	33,33,33,33	0
56	MG	1A	3502	1/1	0.95	0.08	29,29,29,29	0
56	MG	1A	3931	1/1	0.95	0.12	69,69,69,69	0
56	MG	1A	3051	1/1	0.95	0.09	63,63,63,63	0
56	MG	1B	213	1/1	0.95	0.14	48,48,48,48	0
56	MG	1A	3022	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	3703	1/1	0.95	0.08	60,60,60,60	0
56	MG	2a	1747	1/1	0.95	0.28	67,67,67,67	0
56	MG	1B	216	1/1	0.95	0.08	63,63,63,63	0
56	MG	1a	1612	1/1	0.95	0.14	76,76,76,76	0
56	MG	2A	3537	1/1	0.95	0.12	71,71,71,71	0
56	MG	1a	1775	1/1	0.95	0.15	63,63,63,63	0
56	MG	2A	3132	1/1	0.95	0.26	55,55,55,55	0
56	MG	2A	3540	1/1	0.95	0.10	58,58,58,58	0
56	MG	1a	1776	1/1	0.95	0.20	55,55,55,55	0
56	MG	1A	3062	1/1	0.95	0.24	53,53,53,53	0
56	MG	1A	3936	1/1	0.95	0.09	70,70,70,70	0
56	MG	2A	3322	1/1	0.95	0.19	65,65,65,65	0
56	MG	2A	3323	1/1	0.95	0.17	45,45,45,45	0
56	MG	1A	3814	1/1	0.95	0.14	60,60,60,60	0
56	MG	1A	3386	1/1	0.95	0.19	53,53,53,53	0
56	MG	2A	3549	1/1	0.95	0.09	40,40,40,40	0
56	MG	1a	1620	1/1	0.95	0.06	50,50,50,50	0
56	MG	2A	3139	1/1	0.95	0.08	41,41,41,41	0
56	MG	1a	1621	1/1	0.95	0.28	64,64,64,64	0
56	MG	1a	1622	1/1	0.95	0.22	64,64,64,64	0
56	MG	1A	3219	1/1	0.95	0.14	66,66,66,66	0
56	MG	1A	3709	1/1	0.95	0.08	59,59,59,59	0
56	MG	1A	3710	1/1	0.95	0.13	59,59,59,59	0
56	MG	2A	3560	1/1	0.95	0.15	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1B	225	1/1	0.95	0.12	61,61,61,61	0
56	MG	1A	3596	1/1	0.95	0.13	37,37,37,37	0
56	MG	1A	3597	1/1	0.95	0.14	52,52,52,52	0
56	MG	1A	3825	1/1	0.95	0.08	46,46,46,46	0
56	MG	1A	3826	1/1	0.95	0.13	50,50,50,50	0
56	MG	2A	3153	1/1	0.95	0.12	53,53,53,53	0
56	MG	1A	3341	1/1	0.95	0.17	42,42,42,42	0
56	MG	1A	3599	1/1	0.95	0.06	32,32,32,32	0
56	MG	1A	3717	1/1	0.95	0.08	56,56,56,56	0
56	MG	2A	3157	1/1	0.95	0.13	47,47,47,47	0
56	MG	1a	1797	1/1	0.95	0.22	67,67,67,67	0
56	MG	1A	3600	1/1	0.95	0.09	35,35,35,35	0
56	MG	1B	234	1/1	0.95	0.10	41,41,41,41	0
56	MG	1A	3220	1/1	0.95	0.13	49,49,49,49	0
56	MG	1D	307	1/1	0.95	0.11	50,50,50,50	0
56	MG	1A	3952	1/1	0.95	0.10	24,24,24,24	0
56	MG	2F	304	1/1	0.95	0.16	50,50,50,50	0
56	MG	1A	3446	1/1	0.95	0.24	47,47,47,47	0
56	MG	1A	3302	1/1	0.95	0.10	36,36,36,36	0
56	MG	2N	201	1/1	0.95	0.06	62,62,62,62	0
56	MG	1A	3221	1/1	0.95	0.10	61,61,61,61	0
56	MG	1A	3451	1/1	0.95	0.23	48,48,48,48	0
56	MG	1A	3003	1/1	0.95	0.08	28,28,28,28	0
56	MG	1E	304	1/1	0.95	0.15	41,41,41,41	0
56	MG	1d	301	1/1	0.95	0.43	67,67,67,67	0
56	MG	2A	3173	1/1	0.95	0.15	47,47,47,47	0
56	MG	2T	202	1/1	0.95	0.23	59,59,59,59	0
56	MG	1A	3958	1/1	0.95	0.09	37,37,37,37	0
56	MG	1A	3959	1/1	0.95	0.07	32,32,32,32	0
56	MG	1f	201	1/1	0.95	0.16	53,53,53,53	0
56	MG	1A	3837	1/1	0.95	0.22	42,42,42,42	0
56	MG	2A	3594	1/1	0.95	0.12	71,71,71,71	0
56	MG	2X	101	1/1	0.95	0.09	72,72,72,72	0
56	MG	1A	3609	1/1	0.95	0.06	32,32,32,32	0
56	MG	1A	3348	1/1	0.95	0.13	44,44,44,44	0
56	MG	1m	3001	1/1	0.95	0.09	65,65,65,65	0
56	MG	1E	312	1/1	0.95	0.15	67,67,67,67	0
56	MG	1A	3395	1/1	0.95	0.31	69,69,69,69	0
56	MG	21	103	1/1	0.95	0.12	55,55,55,55	0
56	MG	1A	3522	1/1	0.95	0.15	40,40,40,40	0
56	MG	1A	3090	1/1	0.95	0.22	60,60,60,60	0
56	MG	1A	3065	1/1	0.95	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1F	302	1/1	0.95	0.15	35,35,35,35	0
56	MG	2f	201	1/1	0.95	0.10	52,52,52,52	0
56	MG	2A	3604	1/1	0.95	0.25	63,63,63,63	0
56	MG	1F	303	1/1	0.95	0.10	47,47,47,47	0
56	MG	1x	102	1/1	0.95	0.22	69,69,69,69	0
56	MG	1F	304	1/1	0.95	0.13	49,49,49,49	0
56	MG	1A	3527	1/1	0.95	0.23	48,48,48,48	0
56	MG	2A	3609	1/1	0.95	0.12	65,65,65,65	0
56	MG	1x	105	1/1	0.95	0.20	63,63,63,63	0
56	MG	1A	3845	1/1	0.95	0.10	33,33,33,33	0
56	MG	1F	309	1/1	0.95	0.12	36,36,36,36	0
56	MG	1A	3528	1/1	0.95	0.13	42,42,42,42	0
56	MG	1A	3092	1/1	0.95	0.16	59,59,59,59	0
56	MG	1A	3066	1/1	0.95	0.06	36,36,36,36	0
56	MG	1A	3265	1/1	0.95	0.11	45,45,45,45	0
56	MG	1a	1668	1/1	0.95	0.14	65,65,65,65	0
56	MG	1G	205	1/1	0.95	0.14	69,69,69,69	0
56	MG	1a	1670	1/1	0.95	0.29	64,64,64,64	0
56	MG	1A	3981	1/1	0.95	0.08	27,27,27,27	0
56	MG	1A	3230	1/1	0.95	0.22	52,52,52,52	0
56	MG	1a	1673	1/1	0.95	0.10	48,48,48,48	0
56	MG	1A	3462	1/1	0.95	0.06	53,53,53,53	0
56	MG	1A	3855	1/1	0.95	0.08	32,32,32,32	0
56	MG	1A	3628	1/1	0.95	0.11	46,46,46,46	0
56	MG	2A	3009	1/1	0.95	0.23	66,66,66,66	0
56	MG	2a	1625	1/1	0.95	0.07	97,97,97,97	0
56	MG	2A	3010	1/1	0.95	0.18	55,55,55,55	0
56	MG	1A	3538	1/1	0.95	0.09	45,45,45,45	0
56	MG	1A	3796	1/1	0.96	0.18	51,51,51,51	0
56	MG	1A	3902	1/1	0.96	0.11	74,74,74,74	0
56	MG	1a	1651	1/1	0.96	0.18	51,51,51,51	0
56	MG	1A	3186	1/1	0.96	0.06	50,50,50,50	0
56	MG	1A	3037	1/1	0.96	0.14	28,28,28,28	0
56	MG	2A	3457	1/1	0.96	0.13	60,60,60,60	0
56	MG	2A	3458	1/1	0.96	0.09	37,37,37,37	0
56	MG	1A	4024	1/1	0.96	0.12	38,38,38,38	0
56	MG	1A	3531	1/1	0.96	0.07	42,42,42,42	0
56	MG	2A	3461	1/1	0.96	0.17	72,72,72,72	0
56	MG	2A	3124	1/1	0.96	0.09	48,48,48,48	0
56	MG	2A	3463	1/1	0.96	0.06	37,37,37,37	0
56	MG	1A	3473	1/1	0.96	0.15	48,48,48,48	0
56	MG	1A	3908	1/1	0.96	0.09	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1Q	201	1/1	0.96	0.17	42,42,42,42	0
56	MG	2a	1645	1/1	0.96	0.30	56,56,56,56	0
56	MG	1Q	202	1/1	0.96	0.07	55,55,55,55	0
56	MG	2A	3668	1/1	0.96	0.13	57,57,57,57	0
56	MG	1A	3801	1/1	0.96	0.10	38,38,38,38	0
56	MG	2A	3469	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3533	1/1	0.96	0.26	40,40,40,40	0
56	MG	2A	3673	1/1	0.96	0.17	67,67,67,67	0
56	MG	1A	3911	1/1	0.96	0.06	58,58,58,58	0
56	MG	1A	3115	1/1	0.96	0.22	44,44,44,44	0
56	MG	1A	3161	1/1	0.96	0.31	39,39,39,39	0
56	MG	1A	3477	1/1	0.96	0.11	59,59,59,59	0
56	MG	1R	204	1/1	0.96	0.32	45,45,45,45	0
56	MG	1A	3229	1/1	0.96	0.23	42,42,42,42	0
56	MG	1A	3479	1/1	0.96	0.25	35,35,35,35	0
56	MG	2A	3481	1/1	0.96	0.09	39,39,39,39	0
56	MG	1A	3613	1/1	0.96	0.07	22,22,22,22	0
56	MG	1A	4038	1/1	0.96	0.08	40,40,40,40	0
56	MG	1A	3304	1/1	0.96	0.28	57,57,57,57	0
56	MG	1A	3081	1/1	0.96	0.13	39,39,39,39	0
56	MG	2A	3689	1/1	0.96	0.08	43,43,43,43	0
56	MG	2A	3486	1/1	0.96	0.16	47,47,47,47	0
56	MG	2A	3691	1/1	0.96	0.25	59,59,59,59	0
56	MG	1A	3483	1/1	0.96	0.28	42,42,42,42	0
56	MG	2A	3693	1/1	0.96	0.05	43,43,43,43	0
56	MG	1U	202	1/1	0.96	0.16	41,41,41,41	0
56	MG	1t	201	1/1	0.96	0.15	67,67,67,67	0
56	MG	1a	1676	1/1	0.96	0.41	77,77,77,77	0
56	MG	2A	3698	1/1	0.96	0.14	50,50,50,50	0
56	MG	2A	3699	1/1	0.96	0.11	57,57,57,57	0
56	MG	2A	3148	1/1	0.96	0.16	60,60,60,60	0
56	MG	2A	3494	1/1	0.96	0.11	37,37,37,37	0
56	MG	1A	3191	1/1	0.96	0.20	41,41,41,41	0
56	MG	1A	3430	1/1	0.96	0.27	65,65,65,65	0
56	MG	1A	3097	1/1	0.96	0.06	42,42,42,42	0
56	MG	1U	207	1/1	0.96	0.12	39,39,39,39	0
56	MG	1A	3816	1/1	0.96	0.08	21,21,21,21	0
56	MG	2A	3314	1/1	0.96	0.13	71,71,71,71	0
56	MG	1A	3714	1/1	0.96	0.09	53,53,53,53	0
56	MG	1A	3715	1/1	0.96	0.09	22,22,22,22	0
56	MG	2A	3505	1/1	0.96	0.12	43,43,43,43	0
56	MG	1A	3193	1/1	0.96	0.25	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3158	1/1	0.96	0.14	71,71,71,71	0
56	MG	1A	3820	1/1	0.96	0.07	22,22,22,22	0
56	MG	2A	3509	1/1	0.96	0.09	36,36,36,36	0
56	MG	1A	3821	1/1	0.96	0.15	30,30,30,30	0
56	MG	1A	3194	1/1	0.96	0.41	37,37,37,37	0
56	MG	1W	206	1/1	0.96	0.08	45,45,45,45	0
56	MG	1A	3011	1/1	0.96	0.10	45,45,45,45	0
56	MG	2A	3721	1/1	0.96	0.09	44,44,44,44	0
56	MG	2A	3514	1/1	0.96	0.17	62,62,62,62	0
56	MG	2A	3723	1/1	0.96	0.06	45,45,45,45	0
56	MG	1X	101	1/1	0.96	0.29	44,44,44,44	0
56	MG	1X	102	1/1	0.96	0.14	46,46,46,46	0
56	MG	1X	103	1/1	0.96	0.08	53,53,53,53	0
56	MG	2A	3002	1/1	0.96	0.28	53,53,53,53	0
56	MG	1A	3623	1/1	0.96	0.10	38,38,38,38	0
56	MG	1A	3270	1/1	0.96	0.13	60,60,60,60	0
56	MG	2A	3731	1/1	0.96	0.19	62,62,62,62	0
56	MG	1A	3137	1/1	0.96	0.08	42,42,42,42	0
56	MG	1A	3722	1/1	0.96	0.08	38,38,38,38	0
56	MG	1A	3627	1/1	0.96	0.06	51,51,51,51	0
56	MG	1A	3438	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	3725	1/1	0.96	0.07	46,46,46,46	0
56	MG	2A	3011	1/1	0.96	0.07	48,48,48,48	0
56	MG	1B	205	1/1	0.96	0.09	53,53,53,53	0
56	MG	2A	3740	1/1	0.96	0.15	70,70,70,70	0
56	MG	1A	3629	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	3630	1/1	0.96	0.08	41,41,41,41	0
56	MG	2A	3530	1/1	0.96	0.13	62,62,62,62	0
56	MG	2A	3745	1/1	0.96	0.07	43,43,43,43	0
56	MG	2A	3016	1/1	0.96	0.14	46,46,46,46	0
56	MG	2A	3747	1/1	0.96	0.07	61,61,61,61	0
56	MG	2A	3017	1/1	0.96	0.15	63,63,63,63	0
56	MG	2A	3749	1/1	0.96	0.15	65,65,65,65	0
56	MG	2A	3750	1/1	0.96	0.15	67,67,67,67	0
56	MG	1A	3041	1/1	0.96	0.06	35,35,35,35	0
56	MG	1B	209	1/1	0.96	0.06	55,55,55,55	0
56	MG	2A	3535	1/1	0.96	0.16	62,62,62,62	0
56	MG	1A	3633	1/1	0.96	0.14	53,53,53,53	0
56	MG	1A	3314	1/1	0.96	0.10	59,59,59,59	0
56	MG	2A	3345	1/1	0.96	0.39	66,66,66,66	0
56	MG	1A	3139	1/1	0.96	0.20	46,46,46,46	0
56	MG	1A	3085	1/1	0.96	0.21	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3736	1/1	0.96	0.07	46,46,46,46	0
56	MG	1A	3737	1/1	0.96	0.09	32,32,32,32	0
56	MG	1A	3123	1/1	0.96	0.21	42,42,42,42	0
56	MG	11	105	1/1	0.96	0.08	62,62,62,62	0
56	MG	1A	3086	1/1	0.96	0.13	38,38,38,38	0
56	MG	1A	3562	1/1	0.96	0.17	43,43,43,43	0
56	MG	2A	3032	1/1	0.96	0.08	55,55,55,55	0
56	MG	2A	3196	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3742	1/1	0.96	0.07	37,37,37,37	0
56	MG	2A	3034	1/1	0.96	0.18	57,57,57,57	0
56	MG	1B	220	1/1	0.96	0.08	39,39,39,39	0
56	MG	1A	3282	1/1	0.96	0.12	48,48,48,48	0
56	MG	1A	3206	1/1	0.96	0.08	42,42,42,42	0
56	MG	1A	3567	1/1	0.96	0.07	52,52,52,52	0
56	MG	2A	3557	1/1	0.96	0.18	68,68,68,68	0
56	MG	1A	3643	1/1	0.96	0.06	34,34,34,34	0
56	MG	1A	3644	1/1	0.96	0.06	26,26,26,26	0
56	MG	1a	1723	1/1	0.96	0.15	58,58,58,58	0
56	MG	2A	3562	1/1	0.96	0.13	42,42,42,42	0
56	MG	2A	3563	1/1	0.96	0.12	40,40,40,40	0
56	MG	1A	3960	1/1	0.96	0.05	34,34,34,34	0
56	MG	1a	1725	1/1	0.96	0.13	56,56,56,56	0
56	MG	1A	3042	1/1	0.96	0.19	37,37,37,37	0
56	MG	1a	1727	1/1	0.96	0.11	41,41,41,41	0
56	MG	2a	1753	1/1	0.96	0.15	83,83,83,83	0
56	MG	1A	3962	1/1	0.96	0.05	28,28,28,28	0
56	MG	1A	3647	1/1	0.96	0.06	49,49,49,49	0
56	MG	17	101	1/1	0.96	0.05	34,34,34,34	0
56	MG	1A	3964	1/1	0.96	0.07	49,49,49,49	0
56	MG	17	103	1/1	0.96	0.18	47,47,47,47	0
56	MG	17	104	1/1	0.96	0.08	48,48,48,48	0
56	MG	2a	1760	1/1	0.96	0.24	71,71,71,71	0
56	MG	1a	1735	1/1	0.96	0.21	45,45,45,45	0
56	MG	2A	3378	1/1	0.96	0.16	63,63,63,63	0
56	MG	2A	3379	1/1	0.96	0.40	52,52,52,52	0
56	MG	17	105	1/1	0.96	0.14	62,62,62,62	0
56	MG	2A	3381	1/1	0.96	0.07	59,59,59,59	0
56	MG	1A	3966	1/1	0.96	0.11	42,42,42,42	0
56	MG	1A	3853	1/1	0.96	0.08	28,28,28,28	0
56	MG	18	103	1/1	0.96	0.15	44,44,44,44	0
56	MG	1A	3754	1/1	0.96	0.06	56,56,56,56	0
56	MG	1A	3756	1/1	0.96	0.09	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3060	1/1	0.96	0.06	37,37,37,37	0
56	MG	1D	301	1/1	0.96	0.09	44,44,44,44	0
56	MG	1A	3650	1/1	0.96	0.05	26,26,26,26	0
56	MG	1D	306	1/1	0.96	0.11	46,46,46,46	0
56	MG	2E	306	1/1	0.96	0.26	67,67,67,67	0
56	MG	1A	3503	1/1	0.96	0.23	51,51,51,51	0
56	MG	2A	3590	1/1	0.96	0.07	49,49,49,49	0
56	MG	2A	3591	1/1	0.96	0.15	65,65,65,65	0
56	MG	1a	1747	1/1	0.96	0.18	49,49,49,49	0
56	MG	2A	3066	1/1	0.96	0.11	55,55,55,55	0
56	MG	1A	3449	1/1	0.96	0.06	44,44,44,44	0
56	MG	1A	3074	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3173	1/1	0.96	0.09	43,43,43,43	0
56	MG	1A	3404	1/1	0.96	0.07	46,46,46,46	0
56	MG	1a	1607	1/1	0.96	0.06	59,59,59,59	0
56	MG	1E	301	1/1	0.96	0.21	47,47,47,47	0
56	MG	1A	3663	1/1	0.96	0.09	34,34,34,34	0
56	MG	2Q	201	1/1	0.96	0.10	66,66,66,66	0
56	MG	2A	3075	1/1	0.96	0.08	58,58,58,58	0
56	MG	2Q	203	1/1	0.96	0.09	68,68,68,68	0
56	MG	1a	1611	1/1	0.96	0.08	62,62,62,62	0
56	MG	1A	3575	1/1	0.96	0.26	59,59,59,59	0
56	MG	1A	3665	1/1	0.96	0.09	23,23,23,23	0
56	MG	2A	3241	1/1	0.96	0.16	56,56,56,56	0
56	MG	1A	3406	1/1	0.96	0.21	52,52,52,52	0
56	MG	1a	1615	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	3985	1/1	0.96	0.06	57,57,57,57	0
56	MG	2A	3410	1/1	0.96	0.07	38,38,38,38	0
56	MG	1a	1617	1/1	0.96	0.05	47,47,47,47	0
56	MG	1E	308	1/1	0.96	0.13	45,45,45,45	0
56	MG	2A	3612	1/1	0.96	0.10	38,38,38,38	0
56	MG	1A	3043	1/1	0.96	0.18	39,39,39,39	0
56	MG	1A	3175	1/1	0.96	0.18	37,37,37,37	0
56	MG	1A	3672	1/1	0.96	0.10	32,32,32,32	0
56	MG	1A	3366	1/1	0.96	0.11	54,54,54,54	0
56	MG	1A	3580	1/1	0.96	0.08	27,27,27,27	0
56	MG	23	101	1/1	0.96	0.13	68,68,68,68	0
56	MG	23	102	1/1	0.96	0.13	59,59,59,59	0
56	MG	2A	3089	1/1	0.96	0.11	60,60,60,60	0
56	MG	27	101	1/1	0.96	0.23	67,67,67,67	0
56	MG	1A	3149	1/1	0.96	0.34	51,51,51,51	0
56	MG	1A	3076	1/1	0.96	0.15	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3679	1/1	0.96	0.10	37,37,37,37	0
56	MG	2A	3093	1/1	0.96	0.16	40,40,40,40	0
56	MG	1A	3516	1/1	0.96	0.17	42,42,42,42	0
56	MG	1a	1773	1/1	0.96	0.09	52,52,52,52	0
56	MG	1A	3585	1/1	0.96	0.09	29,29,29,29	0
56	MG	1A	3412	1/1	0.96	0.27	49,49,49,49	0
56	MG	1A	3077	1/1	0.96	0.13	45,45,45,45	0
56	MG	1A	3887	1/1	0.96	0.07	44,44,44,44	0
56	MG	2A	3629	1/1	0.96	0.10	59,59,59,59	0
56	MG	2A	3631	1/1	0.96	0.17	46,46,46,46	0
56	MG	1F	308	1/1	0.96	0.16	52,52,52,52	0
56	MG	1A	3588	1/1	0.96	0.07	54,54,54,54	0
56	MG	1A	3294	1/1	0.96	0.08	46,46,46,46	0
56	MG	1A	3590	1/1	0.96	0.24	58,58,58,58	0
56	MG	1G	201	1/1	0.96	0.13	47,47,47,47	0
56	MG	1G	202	1/1	0.96	0.19	62,62,62,62	0
56	MG	1A	3111	1/1	0.96	0.09	39,39,39,39	0
56	MG	1A	4008	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	3790	1/1	0.96	0.26	38,38,38,38	0
56	MG	1A	3465	1/1	0.96	0.18	39,39,39,39	0
56	MG	1A	3155	1/1	0.96	0.24	47,47,47,47	0
56	MG	1A	3374	1/1	0.96	0.12	34,34,34,34	0
56	MG	1A	3044	1/1	0.96	0.08	40,40,40,40	0
56	MG	2A	3646	1/1	0.96	0.09	39,39,39,39	0
56	MG	2A	3443	1/1	0.96	0.15	61,61,61,61	0
56	MG	1A	3899	1/1	0.96	0.06	48,48,48,48	0
57	K	1A	3520	1/1	0.96	0.20	85,85,85,85	0
56	MG	1A	3185	1/1	0.96	0.12	39,39,39,39	0
56	MG	2A	3446	1/1	0.96	0.12	42,42,42,42	0
56	MG	2A	3448	1/1	0.96	0.15	69,69,69,69	0
59	ZN	2n	501	1/1	0.96	0.06	107,107,107,107	0
56	MG	1A	3728	1/1	0.97	0.06	42,42,42,42	0
56	MG	1A	3273	1/1	0.97	0.17	50,50,50,50	0
56	MG	1A	3991	1/1	0.97	0.06	46,46,46,46	0
56	MG	1A	3096	1/1	0.97	0.17	44,44,44,44	0
56	MG	1A	3480	1/1	0.97	0.11	38,38,38,38	0
56	MG	1A	3815	1/1	0.97	0.14	48,48,48,48	0
56	MG	1A	3996	1/1	0.97	0.05	41,41,41,41	0
56	MG	1A	3657	1/1	0.97	0.06	32,32,32,32	0
56	MG	2P	202	1/1	0.97	0.06	65,65,65,65	0
56	MG	1a	1777	1/1	0.97	0.10	64,64,64,64	0
56	MG	1A	3071	1/1	0.97	0.13	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3679	1/1	0.97	0.06	54,54,54,54	0
56	MG	1A	3660	1/1	0.97	0.06	35,35,35,35	0
56	MG	2A	3681	1/1	0.97	0.04	63,63,63,63	0
56	MG	1D	304	1/1	0.97	0.06	42,42,42,42	0
56	MG	2A	3057	1/1	0.97	0.24	54,54,54,54	0
56	MG	1A	3662	1/1	0.97	0.07	28,28,28,28	0
56	MG	2a	1722	1/1	0.97	0.34	54,54,54,54	0
56	MG	2A	3685	1/1	0.97	0.06	51,51,51,51	0
56	MG	1A	3593	1/1	0.97	0.05	40,40,40,40	0
56	MG	1A	3209	1/1	0.97	0.07	45,45,45,45	0
56	MG	2A	3179	1/1	0.97	0.07	68,68,68,68	0
56	MG	1D	309	1/1	0.97	0.16	32,32,32,32	0
56	MG	1A	3210	1/1	0.97	0.10	48,48,48,48	0
56	MG	1A	3279	1/1	0.97	0.24	38,38,38,38	0
56	MG	1A	3485	1/1	0.97	0.18	62,62,62,62	0
56	MG	1A	3743	1/1	0.97	0.06	27,27,27,27	0
56	MG	2A	3558	1/1	0.97	0.11	40,40,40,40	0
56	MG	1A	3668	1/1	0.97	0.11	31,31,31,31	0
56	MG	1A	3916	1/1	0.97	0.05	45,45,45,45	0
56	MG	1A	3669	1/1	0.97	0.18	46,46,46,46	0
56	MG	1A	3670	1/1	0.97	0.06	38,38,38,38	0
56	MG	1E	306	1/1	0.97	0.12	42,42,42,42	0
56	MG	2A	3071	1/1	0.97	0.16	62,62,62,62	0
56	MG	1A	3393	1/1	0.97	0.18	66,66,66,66	0
56	MG	2A	3703	1/1	0.97	0.07	71,71,71,71	0
56	MG	1A	3354	1/1	0.97	0.14	48,48,48,48	0
56	MG	1A	3439	1/1	0.97	0.24	46,46,46,46	0
56	MG	1A	3543	1/1	0.97	0.19	40,40,40,40	0
56	MG	1A	3923	1/1	0.97	0.07	27,27,27,27	0
56	MG	1A	3116	1/1	0.97	0.14	34,34,34,34	0
56	MG	1a	1801	1/1	0.97	0.19	64,64,64,64	0
56	MG	1A	3755	1/1	0.97	0.22	64,64,64,64	0
56	MG	1A	3098	1/1	0.97	0.15	27,27,27,27	0
56	MG	1A	3284	1/1	0.97	0.12	47,47,47,47	0
56	MG	1A	3606	1/1	0.97	0.04	27,27,27,27	0
56	MG	1E	317	1/1	0.97	0.11	60,60,60,60	0
56	MG	1F	301	1/1	0.97	0.11	44,44,44,44	0
56	MG	1A	3760	1/1	0.97	0.04	45,45,45,45	0
56	MG	1A	3159	1/1	0.97	0.19	38,38,38,38	0
56	MG	1A	3214	1/1	0.97	0.09	56,56,56,56	0
56	MG	1A	3015	1/1	0.97	0.11	40,40,40,40	0
56	MG	1F	306	1/1	0.97	0.19	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3019	1/1	0.97	0.32	55,55,55,55	0
56	MG	2A	3584	1/1	0.97	0.12	66,66,66,66	0
56	MG	2A	3451	1/1	0.97	0.11	68,68,68,68	0
56	MG	2a	1761	1/1	0.97	0.16	64,64,64,64	0
56	MG	2A	3452	1/1	0.97	0.15	46,46,46,46	0
56	MG	1A	3612	1/1	0.97	0.13	36,36,36,36	0
56	MG	1A	3289	1/1	0.97	0.18	32,32,32,32	0
56	MG	1A	3120	1/1	0.97	0.18	41,41,41,41	0
56	MG	2A	3456	1/1	0.97	0.07	37,37,37,37	0
56	MG	1F	311	1/1	0.97	0.08	47,47,47,47	0
56	MG	1A	3405	1/1	0.97	0.05	49,49,49,49	0
56	MG	1A	3689	1/1	0.97	0.05	22,22,22,22	0
56	MG	1A	3054	1/1	0.97	0.15	42,42,42,42	0
56	MG	1a	1709	1/1	0.97	0.13	44,44,44,44	0
56	MG	2A	3099	1/1	0.97	0.11	53,53,53,53	0
56	MG	1A	3849	1/1	0.97	0.09	56,56,56,56	0
56	MG	1w	101	1/1	0.97	0.09	57,57,57,57	0
56	MG	1A	3555	1/1	0.97	0.13	38,38,38,38	0
56	MG	2A	3741	1/1	0.97	0.06	27,27,27,27	0
56	MG	1A	4041	1/1	0.97	0.07	39,39,39,39	0
56	MG	1A	3063	1/1	0.97	0.11	45,45,45,45	0
56	MG	1A	3852	1/1	0.97	0.10	31,31,31,31	0
56	MG	1A	3557	1/1	0.97	0.14	40,40,40,40	0
56	MG	1A	3031	1/1	0.97	0.17	27,27,27,27	0
56	MG	1N	204	1/1	0.97	0.07	48,48,48,48	0
56	MG	1a	1610	1/1	0.97	0.10	29,29,29,29	0
56	MG	2A	3473	1/1	0.97	0.07	46,46,46,46	0
56	MG	2A	3110	1/1	0.97	0.14	45,45,45,45	0
56	MG	1A	3778	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3078	1/1	0.97	0.15	35,35,35,35	0
56	MG	2A	3477	1/1	0.97	0.10	51,51,51,51	0
56	MG	1A	3329	1/1	0.97	0.07	51,51,51,51	0
56	MG	1A	3145	1/1	0.97	0.21	37,37,37,37	0
56	MG	1A	3331	1/1	0.97	0.06	51,51,51,51	0
56	MG	1A	4051	1/1	0.97	0.11	71,71,71,71	0
56	MG	2a	1793	1/1	0.97	0.10	67,67,67,67	0
56	MG	1A	3033	1/1	0.97	0.41	30,30,30,30	0
56	MG	1a	1618	1/1	0.97	0.05	61,61,61,61	0
56	MG	1P	201	1/1	0.97	0.28	40,40,40,40	0
56	MG	1a	1728	1/1	0.97	0.09	41,41,41,41	0
56	MG	2A	3487	1/1	0.97	0.10	39,39,39,39	0
56	MG	1P	202	1/1	0.97	0.24	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3863	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	3007	1/1	0.97	0.05	41,41,41,41	0
56	MG	1A	3785	1/1	0.97	0.08	61,61,61,61	0
56	MG	1A	3565	1/1	0.97	0.20	41,41,41,41	0
56	MG	1A	3702	1/1	0.97	0.11	50,50,50,50	0
56	MG	1A	3460	1/1	0.97	0.11	45,45,45,45	0
56	MG	1A	3705	1/1	0.97	0.06	20,20,20,20	0
56	MG	1A	3107	1/1	0.97	0.23	41,41,41,41	0
56	MG	1B	202	1/1	0.97	0.31	64,64,64,64	0
56	MG	1A	3108	1/1	0.97	0.30	42,42,42,42	0
56	MG	1A	3632	1/1	0.97	0.10	56,56,56,56	0
56	MG	2A	3370	1/1	0.97	0.17	46,46,46,46	0
56	MG	1R	203	1/1	0.97	0.22	46,46,46,46	0
56	MG	2A	3503	1/1	0.97	0.10	41,41,41,41	0
56	MG	2A	3504	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3093	1/1	0.97	0.13	29,29,29,29	0
56	MG	1A	3418	1/1	0.97	0.26	43,43,43,43	0
56	MG	1A	3013	1/1	0.97	0.21	31,31,31,31	0
56	MG	1A	3880	1/1	0.97	0.09	52,52,52,52	0
56	MG	1A	3466	1/1	0.97	0.17	38,38,38,38	0
56	MG	1A	3199	1/1	0.97	0.19	28,28,28,28	0
56	MG	1A	3152	1/1	0.97	0.09	40,40,40,40	0
56	MG	1A	3422	1/1	0.97	0.21	43,43,43,43	0
56	MG	1A	3023	1/1	0.97	0.08	20,20,20,20	0
56	MG	2A	3382	1/1	0.97	0.23	47,47,47,47	0
56	MG	1A	3203	1/1	0.97	0.05	22,22,22,22	0
56	MG	1A	3204	1/1	0.97	0.04	36,36,36,36	0
56	MG	2A	3264	1/1	0.97	0.13	54,54,54,54	0
56	MG	2D	302	1/1	0.97	0.10	49,49,49,49	0
56	MG	1A	3524	1/1	0.97	0.09	38,38,38,38	0
56	MG	2A	3147	1/1	0.97	0.14	44,44,44,44	0
56	MG	1A	3525	1/1	0.97	0.22	45,45,45,45	0
56	MG	1U	208	1/1	0.97	0.37	43,43,43,43	0
56	MG	1A	3978	1/1	0.97	0.10	45,45,45,45	0
56	MG	2A	3151	1/1	0.97	0.08	53,53,53,53	0
56	MG	1A	3979	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3343	1/1	0.97	0.19	33,33,33,33	0
56	MG	1A	3239	1/1	0.97	0.26	32,32,32,32	0
56	MG	1V	204	1/1	0.97	0.20	39,39,39,39	0
56	MG	1A	3649	1/1	0.97	0.09	37,37,37,37	0
56	MG	1A	3177	1/1	0.97	0.15	32,32,32,32	0
56	MG	1W	203	1/1	0.97	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
56	MG	1A	3178	1/1	0.97	0.15	28,28,28,28	0
56	MG	1A	3652	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3988	1/1	0.97	0.10	46,46,46,46	0
56	MG	2F	301	1/1	0.97	0.07	49,49,49,49	0
56	MG	1A	3604	1/1	0.98	0.08	26,26,26,26	0
56	MG	1D	303	1/1	0.98	0.10	27,27,27,27	0
56	MG	1A	3432	1/1	0.98	0.12	42,42,42,42	0
56	MG	2A	3717	1/1	0.98	0.12	44,44,44,44	0
56	MG	1D	305	1/1	0.98	0.14	36,36,36,36	0
56	MG	15	105	1/1	0.98	0.15	36,36,36,36	0
56	MG	1A	3112	1/1	0.98	0.14	41,41,41,41	0
56	MG	1A	3573	1/1	0.98	0.15	19,19,19,19	0
56	MG	2A	3543	1/1	0.98	0.07	40,40,40,40	0
56	MG	2A	3130	1/1	0.98	0.16	44,44,44,44	0
56	MG	2A	3374	1/1	0.98	0.14	28,28,28,28	0
56	MG	1A	4040	1/1	0.98	0.04	33,33,33,33	0
56	MG	2A	3726	1/1	0.98	0.08	55,55,55,55	0
56	MG	1A	3264	1/1	0.98	0.15	45,45,45,45	0
56	MG	1A	3345	1/1	0.98	0.42	33,33,33,33	0
56	MG	1A	3645	1/1	0.98	0.09	27,27,27,27	0
56	MG	2A	3638	1/1	0.98	0.06	58,58,58,58	0
56	MG	1A	3367	1/1	0.98	0.18	29,29,29,29	0
56	MG	2A	3551	1/1	0.98	0.04	45,45,45,45	0
56	MG	1A	3984	1/1	0.98	0.07	57,57,57,57	0
56	MG	1A	3514	1/1	0.98	0.14	42,42,42,42	0
56	MG	2A	3735	1/1	0.98	0.11	46,46,46,46	0
56	MG	1A	3648	1/1	0.98	0.03	25,25,25,25	0
56	MG	1A	3515	1/1	0.98	0.21	43,43,43,43	0
56	MG	1A	3179	1/1	0.98	0.09	36,36,36,36	0
56	MG	1A	3233	1/1	0.98	0.09	66,66,66,66	0
56	MG	1U	201	1/1	0.98	0.15	35,35,35,35	0
56	MG	1a	1746	1/1	0.98	0.10	53,53,53,53	0
56	MG	1A	3234	1/1	0.98	0.26	41,41,41,41	0
56	MG	1A	3012	1/1	0.98	0.04	30,30,30,30	0
56	MG	1A	3738	1/1	0.98	0.07	38,38,38,38	0
56	MG	1A	3993	1/1	0.98	0.15	30,30,30,30	0
56	MG	1U	206	1/1	0.98	0.18	44,44,44,44	0
56	MG	1a	1752	1/1	0.98	0.04	64,64,64,64	0
56	MG	1A	3654	1/1	0.98	0.04	28,28,28,28	0
56	MG	1A	3069	1/1	0.98	0.11	22,22,22,22	0
56	MG	1A	4057	1/1	0.98	0.19	61,61,61,61	0
56	MG	1A	3032	1/1	0.98	0.17	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1V	201	1/1	0.98	0.42	34,34,34,34	0
56	MG	1A	3889	1/1	0.98	0.04	18,18,18,18	0
56	MG	1A	3396	1/1	0.98	0.10	51,51,51,51	0
56	MG	1A	3658	1/1	0.98	0.09	30,30,30,30	0
56	MG	1V	206	1/1	0.98	0.15	61,61,61,61	0
56	MG	1A	4000	1/1	0.98	0.07	26,26,26,26	0
56	MG	1A	3160	1/1	0.98	0.22	44,44,44,44	0
56	MG	1A	3010	1/1	0.98	0.05	38,38,38,38	0
56	MG	1W	204	1/1	0.98	0.17	41,41,41,41	0
56	MG	1A	3072	1/1	0.98	0.07	16,16,16,16	0
56	MG	2A	3493	1/1	0.98	0.10	41,41,41,41	0
56	MG	2A	3670	1/1	0.98	0.06	65,65,65,65	0
56	MG	1A	3747	1/1	0.98	0.05	25,25,25,25	0
56	MG	1A	3021	1/1	0.98	0.12	35,35,35,35	0
56	MG	2A	3766	1/1	0.98	0.04	51,51,51,51	0
56	MG	2A	3166	1/1	0.98	0.09	35,35,35,35	0
56	MG	1A	3625	1/1	0.98	0.05	37,37,37,37	0
56	MG	1A	3153	1/1	0.98	0.14	46,46,46,46	0
56	MG	1A	3752	1/1	0.98	0.06	30,30,30,30	0
56	MG	1A	3592	1/1	0.98	0.07	27,27,27,27	0
56	MG	1A	4010	1/1	0.98	0.09	55,55,55,55	0
56	MG	1A	3276	1/1	0.98	0.12	30,30,30,30	0
56	MG	1A	3475	1/1	0.98	0.20	45,45,45,45	0
56	MG	2A	3014	1/1	0.98	0.08	53,53,53,53	0
56	MG	1A	3450	1/1	0.98	0.12	61,61,61,61	0
56	MG	1A	3227	1/1	0.98	0.15	41,41,41,41	0
56	MG	1A	3758	1/1	0.98	0.06	48,48,48,48	0
56	MG	10	101	1/1	0.98	0.10	54,54,54,54	0
56	MG	1A	4017	1/1	0.98	0.12	49,49,49,49	0
56	MG	2A	3020	1/1	0.98	0.10	29,29,29,29	0
56	MG	1a	1633	1/1	0.98	0.12	27,27,27,27	0
56	MG	1A	3144	1/1	0.98	0.11	40,40,40,40	0
56	MG	1A	3005	1/1	0.98	0.09	49,49,49,49	0
56	MG	1A	3535	1/1	0.98	0.11	42,42,42,42	0
56	MG	2A	3025	1/1	0.98	0.08	44,44,44,44	0
56	MG	1A	3762	1/1	0.98	0.08	25,25,25,25	0
56	MG	1A	3536	1/1	0.98	0.10	46,46,46,46	0
56	MG	1A	3675	1/1	0.98	0.05	29,29,29,29	0
56	MG	1A	3965	1/1	0.98	0.08	46,46,46,46	0
56	MG	2A	3697	1/1	0.98	0.20	68,68,68,68	0
56	MG	1A	3280	1/1	0.98	0.33	43,43,43,43	0
56	MG	1A	3677	1/1	0.98	0.04	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3436	1/1	0.98	0.10	60,60,60,60	0
56	MG	1A	3860	1/1	0.98	0.07	36,36,36,36	0
56	MG	1A	3767	1/1	0.98	0.08	29,29,29,29	0
56	MG	1A	4030	1/1	0.98	0.19	54,54,54,54	0
56	MG	1A	3862	1/1	0.98	0.08	54,54,54,54	0
56	MG	1a	1795	1/1	0.98	0.04	55,55,55,55	0
56	MG	1A	3971	1/1	0.98	0.04	62,62,62,62	0
56	MG	13	101	1/1	0.98	0.11	45,45,45,45	0
56	MG	1A	3281	1/1	0.98	0.31	41,41,41,41	0
56	MG	1A	3864	1/1	0.98	0.12	38,38,38,38	0
56	MG	1A	3215	1/1	0.98	0.14	46,46,46,46	0
58	WC9	1A	4061	34/34	0.98	0.06	21,28,31,33	0
58	WC9	2A	3772	34/34	0.98	0.07	36,44,47,52	0
56	MG	2A	3447	1/1	0.98	0.06	43,43,43,43	0
59	ZN	2Y	501	1/1	0.98	0.04	96,96,96,96	0
56	MG	1a	1652	1/1	0.98	0.12	54,54,54,54	0
56	MG	1P	206	1/1	0.98	0.05	43,43,43,43	0
60	SF4	2d	302	8/8	0.98	0.05	70,77,82,85	0
56	MG	1A	3882	1/1	0.99	0.04	65,65,65,65	0
56	MG	1A	3014	1/1	0.99	0.11	34,34,34,34	0
56	MG	1A	3109	1/1	0.99	0.04	42,42,42,42	0
56	MG	1A	3982	1/1	0.99	0.04	50,50,50,50	0
56	MG	1A	3140	1/1	0.99	0.07	25,25,25,25	0
56	MG	1A	3905	1/1	0.99	0.04	54,54,54,54	0
56	MG	1A	3748	1/1	0.99	0.03	48,48,48,48	0
56	MG	1A	3584	1/1	0.99	0.04	45,45,45,45	0
56	MG	1A	3084	1/1	0.99	0.12	42,42,42,42	0
56	MG	1A	3947	1/1	0.99	0.03	57,57,57,57	0
56	MG	1A	3222	1/1	0.99	0.14	45,45,45,45	0
56	MG	1A	3872	1/1	0.99	0.02	26,26,26,26	0
56	MG	2A	3480	1/1	0.99	0.07	38,38,38,38	0
56	MG	1A	3873	1/1	0.99	0.03	31,31,31,31	0
56	MG	1V	205	1/1	0.99	0.21	56,56,56,56	0
56	MG	1A	3566	1/1	0.99	0.25	39,39,39,39	0
56	MG	1A	3610	1/1	0.99	0.03	20,20,20,20	0
56	MG	1A	3768	1/1	0.99	0.07	24,24,24,24	0
56	MG	1A	3068	1/1	0.99	0.12	30,30,30,30	0
56	MG	1A	4018	1/1	0.99	0.08	34,34,34,34	0
59	ZN	1Y	203	1/1	0.99	0.02	67,67,67,67	0
56	MG	1A	3047	1/1	0.99	0.07	41,41,41,41	0
59	ZN	1n	102	1/1	0.99	0.03	65,65,65,65	0
56	MG	2A	3008	1/1	0.99	0.04	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3661	1/1	0.99	0.03	27,27,27,27	0
59	ZN	26	501	1/1	0.99	0.03	68,68,68,68	0
59	ZN	29	501	1/1	0.99	0.03	78,78,78,78	0
56	MG	1A	3200	1/1	0.99	0.05	34,34,34,34	0
60	SF4	1d	302	8/8	0.99	0.04	62,72,73,73	0
56	MG	1A	3009	1/1	0.99	0.03	30,30,30,30	0
59	ZN	16	102	1/1	1.00	0.03	48,48,48,48	0
59	ZN	19	102	1/1	1.00	0.06	52,52,52,52	0
56	MG	1A	4013	1/1	1.00	0.07	36,36,36,36	0
56	MG	2A	3630	1/1	1.00	0.03	35,35,35,35	0
56	MG	1A	3704	1/1	1.00	0.07	28,28,28,28	0
59	ZN	25	102	1/1	1.00	0.03	59,59,59,59	0
56	MG	1A	3727	1/1	1.00	0.03	28,28,28,28	0
56	MG	1A	3734	1/1	1.00	0.04	42,42,42,42	0
56	MG	1A	3867	1/1	1.00	0.09	45,45,45,45	0
56	MG	1A	3892	1/1	1.00	0.03	34,34,34,34	0
59	ZN	15	108	1/1	1.00	0.02	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.