



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 01:19 am BST

PDB ID : 5WIS  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with methymycin and bound to mRNA and A-, P- and E-site tRNAs at 2.7Å resolution  
Authors : Almutairi, M.M.; Svetlov, M.S.; Hansen, D.A.; Khabibullina, N.F.; Klepacki, D.; Kang, H.Y.; Sherman, D.H.; Vazquez-Laslop, N.; Polikanov, Y.S.; Mankin, A.S.  
Deposited on : 2017-07-20  
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](mailto: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 ⓘ symbol.

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

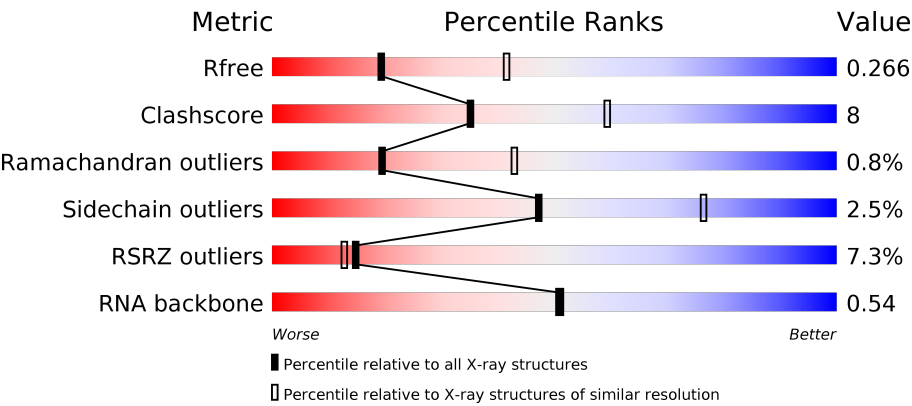
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 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 <sub>free</sub>	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	<div><div>64%28%7%</div><div>%</div></div>
1	2A	2915	<div><div>58%32%6%</div><div>%</div></div>
2	1B	121	<div><div>64%30%</div><div>%</div></div>
2	2B	121	<div><div>52%38%9%</div><div>4%</div></div>

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



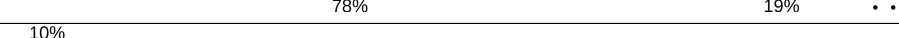


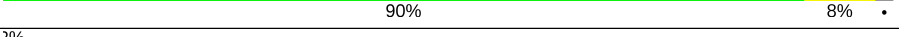

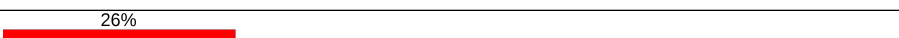


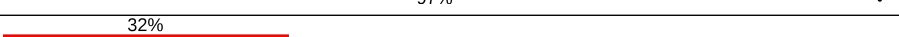




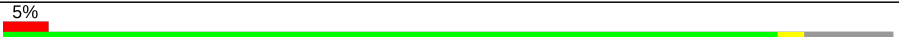






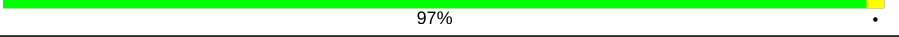

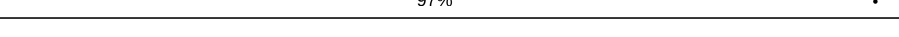
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Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25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

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

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

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Mol	Chain	Length	Quality of chain
53	1v	24	
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
56	MG	10	105	-	-	-	X
56	MG	1A	3366	-	-	-	X
56	MG	1A	3399	-	-	-	X
56	MG	1A	3440	-	-	-	X
56	MG	1A	3480	-	-	-	X
56	MG	1A	3968	-	-	-	X
56	MG	1A	3984	-	-	-	X
56	MG	1A	4011	-	-	-	X
56	MG	1A	4034	-	-	-	X
56	MG	1U	204	-	-	-	X
56	MG	1a	1766	-	-	-	X
56	MG	2A	3088	-	-	-	X
56	MG	2A	3236	-	-	-	X
56	MG	2A	3242	-	-	-	X
56	MG	2A	3243	-	-	-	X
56	MG	2A	3266	-	-	-	X
56	MG	2A	3283	-	-	-	X
56	MG	2A	3293	-	-	-	X
56	MG	2A	3327	-	-	-	X
56	MG	2A	3333	-	-	-	X
56	MG	2A	3343	-	-	-	X
56	MG	2A	3395	-	-	-	X
56	MG	2A	3402	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	2A	3416	-	-	-	X
56	MG	2A	3493	-	-	-	X
56	MG	2A	3705	-	-	-	X
56	MG	2A	3766	-	-	-	X
56	MG	2A	3812	-	-	-	X
56	MG	2Q	3004	-	-	-	X
56	MG	2a	1603	-	-	-	X
56	MG	2a	1629	-	-	-	X



## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 301023 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	C	N	O	S	0	0	0
			933	588	171	170	4			

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

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

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

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

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

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

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

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

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

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

- 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 mRNA.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total 1592	C 713	N 285	O 518	P 74	S 2	0	0	0
54	1y	74	Total 1585	C 707	N 285	O 518	P 74	S 1	0	0	0
54	2w	72	Total 1544	C 690	N 278	O 502	P 72	S 2	0	0	0
54	2y	73	Total 1565	C 698	N 283	O 510	P 73	S 1	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	8	Total	Mg	0	0
			8	8		
56	17	3	Total	Mg	0	0
			3	3		
56	2d	1	Total	Mg	0	0
			1	1		
56	1T	1	Total	Mg	0	0
			1	1		
56	1N	6	Total	Mg	0	0
			6	6		
56	20	3	Total	Mg	0	0
			3	3		
56	18	3	Total	Mg	0	0
			3	3		
56	1o	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2W	3	Total 3	Mg 3	0	0
56	1Y	3	Total 3	Mg 3	0	0
56	13	3	Total 3	Mg 3	0	0
56	1f	2	Total 2	Mg 2	0	0
56	1P	4	Total 4	Mg 4	0	0
56	2B	21	Total 21	Mg 21	0	0
56	1q	1	Total 1	Mg 1	0	0
56	23	3	Total 3	Mg 3	0	0
56	1E	12	Total 12	Mg 12	0	0
56	1b	2	Total 2	Mg 2	0	0
56	2l	3	Total 3	Mg 3	0	0
56	2F	4	Total 4	Mg 4	0	0
56	16	3	Total 3	Mg 3	0	0
56	28	1	Total 1	Mg 1	0	0
56	2e	1	Total 1	Mg 1	0	0
56	1W	7	Total 7	Mg 7	0	0
56	1A	1146	Total 1146	Mg 1146	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1n	1	Total 1	Mg 1	0	0
56	1X	5	Total 5	Mg 5	0	0
56	12	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1y	4	Total 4	Mg 4	0	0
56	1S	3	Total 3	Mg 3	0	0
56	25	4	Total 4	Mg 4	0	0
56	2T	2	Total 2	Mg 2	0	0
56	1D	12	Total 12	Mg 12	0	0
56	2N	1	Total 1	Mg 1	0	0
56	1e	2	Total 2	Mg 2	0	0
56	2G	1	Total 1	Mg 1	0	0
56	1I	1	Total 1	Mg 1	0	0
56	2f	2	Total 2	Mg 2	0	0
56	1V	3	Total 3	Mg 3	0	0
56	2X	2	Total 2	Mg 2	0	0
56	1w	11	Total 11	Mg 11	0	0
56	26	1	Total 1	Mg 1	0	0
56	1a	229	Total 229	Mg 229	0	0
56	2Q	4	Total 4	Mg 4	0	0
56	15	2	Total 2	Mg 2	0	0
56	1x	16	Total 16	Mg 16	0	0
56	2j	2	Total 2	Mg 2	0	0
56	1R	2	Total 2	Mg 2	0	0
56	1s	1	Total 1	Mg 1	0	0

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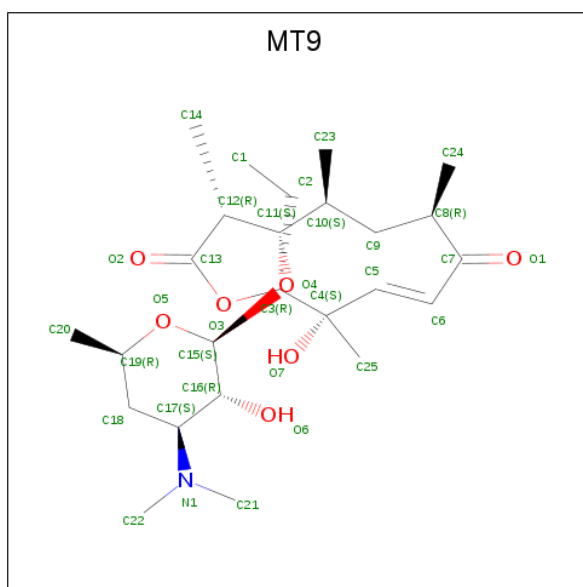
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1m	1	Total Mg 1 1	0	0
56	2U	5	Total Mg 5 5	0	0
56	1G	5	Total Mg 5 5	0	0
56	2O	1	Total Mg 1 1	0	0
56	1l	4	Total Mg 4 4	0	0
56	1d	1	Total Mg 1 1	0	0
56	2r	1	Total Mg 1 1	0	0
56	1H	1	Total Mg 1 1	0	0
56	2g	1	Total Mg 1 1	0	0
56	2Y	1	Total Mg 1 1	0	0
56	2w	9	Total Mg 9 9	0	0
56	1v	1	Total Mg 1 1	0	0
56	2x	6	Total Mg 6 6	0	0
56	2R	2	Total Mg 2 2	0	0
56	1Z	4	Total Mg 4 4	0	0
56	2D	4	Total Mg 4 4	0	0
56	2q	3	Total Mg 3 3	0	0
56	2v	3	Total Mg 3 3	0	0
56	1U	6	Total Mg 6 6	0	0
56	1O	8	Total Mg 8 8	0	0
56	1r	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	19	1	Total 1	Mg 1	0	0
56	1l	3	Total 3	Mg 3	0	0
56	2V	2	Total 2	Mg 2	0	0
56	1F	8	Total 8	Mg 8	0	0
56	10	9	Total 9	Mg 9	0	0
56	2t	1	Total 1	Mg 1	0	0
56	1Q	5	Total 5	Mg 5	0	0
56	2A	903	Total 903	Mg 903	0	0
56	1h	1	Total 1	Mg 1	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	1B	36	Total 36	Mg 36	0	0
56	2y	7	Total 7	Mg 7	0	0
56	27	1	Total 1	Mg 1	0	0
56	2a	244	Total 244	Mg 244	0	0

- Molecule 57 is (3R,4S,5S,7R,9E,11S,12R)-12-ethyl-11-hydroxy-3,5,7,11-tetramethyl-2,8-dioxooxacyclododec-9-en-4-yl 3,4,6-trideoxy-3-(dimethylamino)-beta-D-xylo-hexopyranoside (three-letter code: MT9) (formula: C<sub>25</sub>H<sub>43</sub>N O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	1A	1	Total	C	N	O	0	0
			33	25	1	7		
57	2A	1	Total	C	N	O	0	0
			33	25	1	7		

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	29	1	Total	Zn	0	0
			1	1		

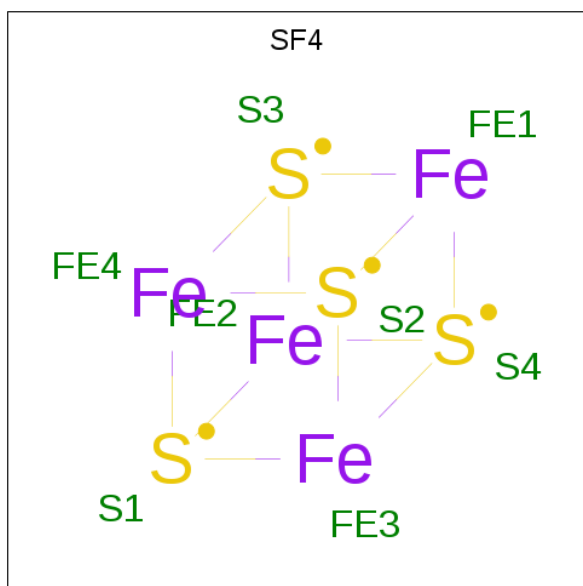
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	19	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	2n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1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

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	2243	Total O 2243 2243	0	0
61	1B	69	Total O 69 69	0	0
61	1D	26	Total O 26 26	0	0
61	1E	28	Total O 28 28	0	0
61	1F	19	Total O 19 19	0	0
61	1G	6	Total O 6 6	0	0
61	1H	2	Total O 2 2	0	0
61	1I	2	Total O 2 2	0	0
61	1N	6	Total O 6 6	0	0
61	1O	7	Total O 7 7	0	0
61	1P	20	Total O 20 20	0	0
61	1Q	15	Total O 15 15	0	0
61	1R	12	Total O 12 12	0	0
61	1S	5	Total O 5 5	0	0
61	1T	10	Total O 10 10	0	0
61	1U	16	Total O 16 16	0	0
61	1V	10	Total O 10 10	0	0
61	1W	6	Total O 6 6	0	0
61	1X	6	Total O 6 6	0	0
61	1Y	4	Total O 4 4	0	0
61	1Z	1	Total O 1 1	0	0
61	10	11	Total O 11 11	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	11	12	Total 12	O 12	0	0
61	12	3	Total 3	O 3	0	0
61	13	5	Total 5	O 5	0	0
61	14	1	Total 1	O 1	0	0
61	15	4	Total 4	O 4	0	0
61	16	2	Total 2	O 2	0	0
61	17	9	Total 9	O 9	0	0
61	18	13	Total 13	O 13	0	0
61	1a	460	Total 460	O 460	0	0
61	1b	1	Total 1	O 1	0	0
61	1d	1	Total 1	O 1	0	0
61	1f	1	Total 1	O 1	0	0
61	1g	1	Total 1	O 1	0	0
61	1l	9	Total 9	O 9	0	0
61	1m	1	Total 1	O 1	0	0
61	1o	1	Total 1	O 1	0	0
61	1p	1	Total 1	O 1	0	0
61	1q	4	Total 4	O 4	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	5	Total 5	O 5	0	0
61	1w	22	Total 22	O 22	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1x	16	Total 16	O 16	0	0
61	1y	2	Total 2	O 2	0	0
61	2A	1395	Total 1395	O 1395	0	0
61	2B	28	Total 28	O 28	0	0
61	2D	25	Total 25	O 25	0	0
61	2E	15	Total 15	O 15	0	0
61	2F	14	Total 14	O 14	0	0
61	2I	4	Total 4	O 4	0	0
61	2N	1	Total 1	O 1	0	0
61	2O	1	Total 1	O 1	0	0
61	2P	14	Total 14	O 14	0	0
61	2Q	2	Total 2	O 2	0	0
61	2R	3	Total 3	O 3	0	0
61	2T	6	Total 6	O 6	0	0
61	2U	4	Total 4	O 4	0	0
61	2V	1	Total 1	O 1	0	0
61	2W	3	Total 3	O 3	0	0
61	2X	4	Total 4	O 4	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	2	Total 2	O 2	0	0
61	20	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	21	14	Total 14	O 14	0	0
61	22	2	Total 2	O 2	0	0
61	23	1	Total 1	O 1	0	0
61	25	5	Total 5	O 5	0	0
61	27	3	Total 3	O 3	0	0
61	28	4	Total 4	O 4	0	0
61	29	1	Total 1	O 1	0	0
61	2a	381	Total 381	O 381	0	0
61	2e	2	Total 2	O 2	0	0
61	2g	1	Total 1	O 1	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	4	Total 4	O 4	0	0
61	2l	6	Total 6	O 6	0	0
61	2o	3	Total 3	O 3	0	0
61	2p	3	Total 3	O 3	0	0
61	2q	1	Total 1	O 1	0	0
61	2r	1	Total 1	O 1	0	0
61	2t	2	Total 2	O 2	0	0
61	2u	1	Total 1	O 1	0	0
61	2v	1	Total 1	O 1	0	0
61	2w	3	Total 3	O 3	0	0

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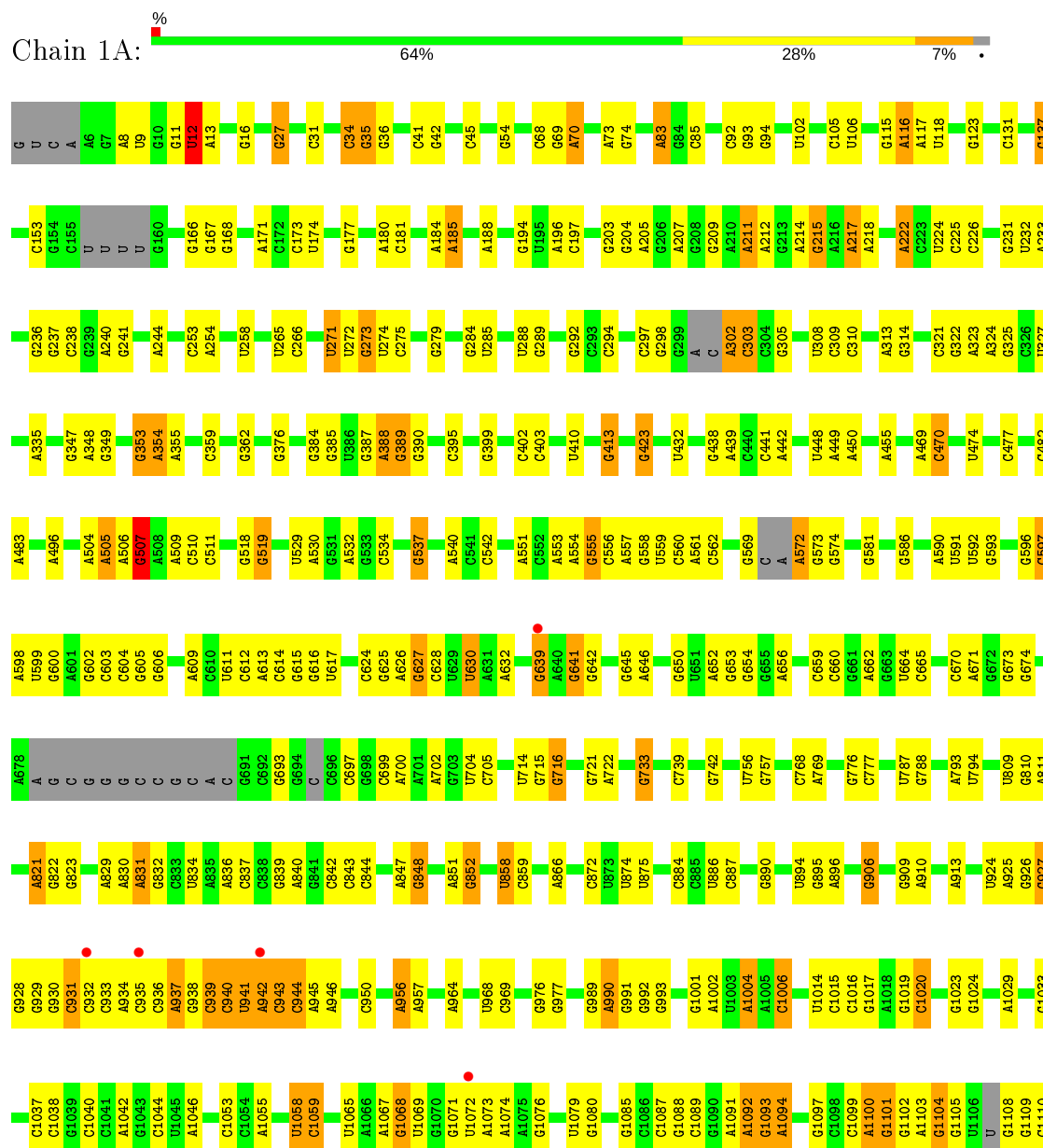
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2x	8	Total	O	0	0
			8	8		
61	2y	19	Total	O	0	0
			19	19		

### 3 Residue-property plots

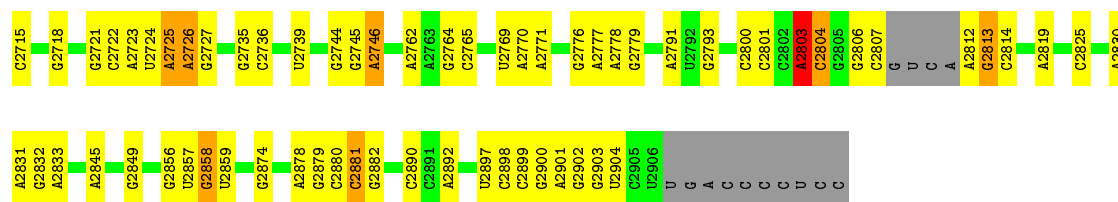
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

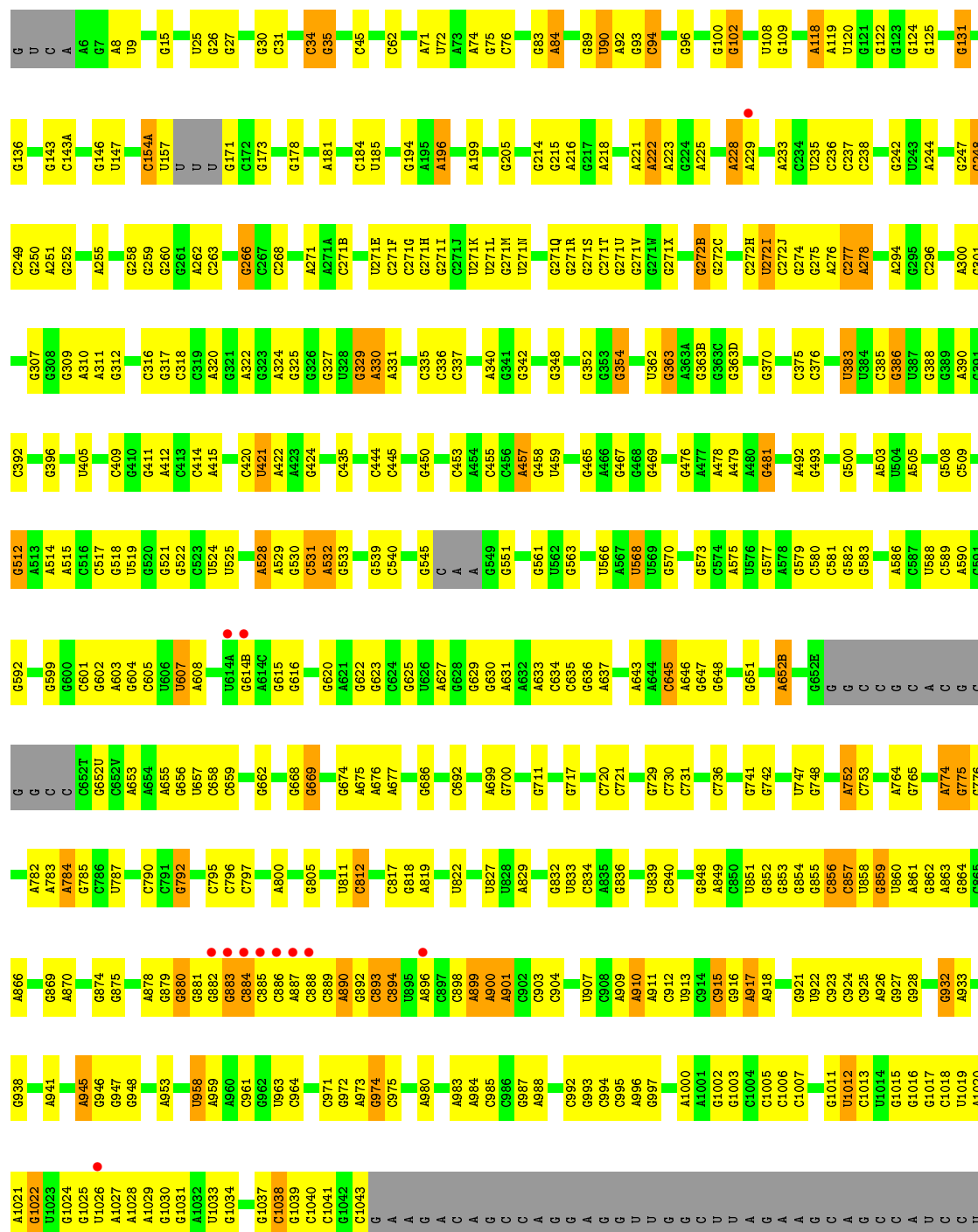




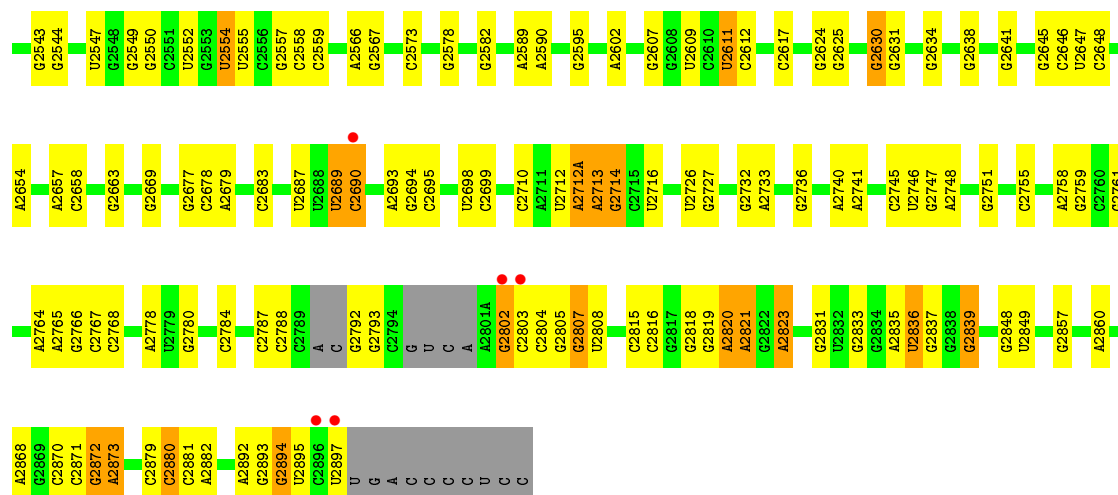




# • Molecule 1: 23S ribosomal RNA

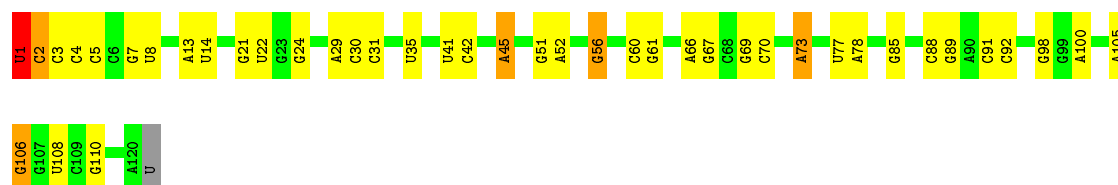






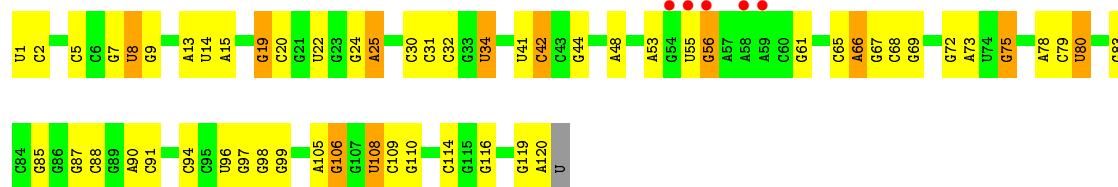
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 64% 30%



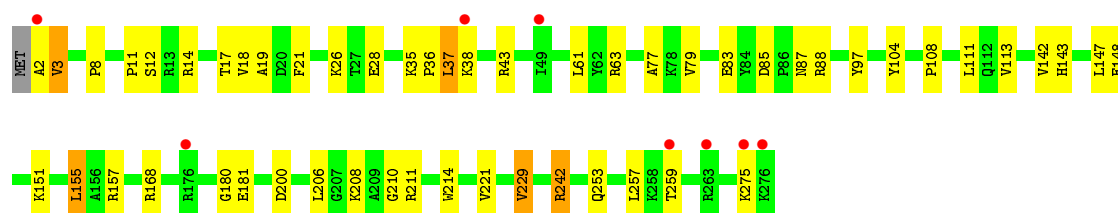
• Molecule 2: 5S Ribosomal RNA

Chain 2B: 4% 52% 38% 9%



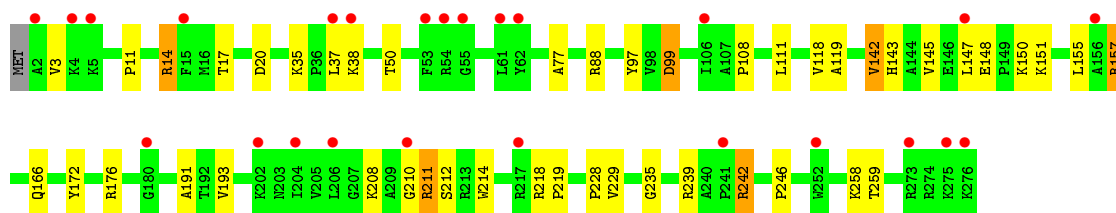
• Molecule 3: 50S ribosomal protein L2

Chain 1D: 3% 80% 17%



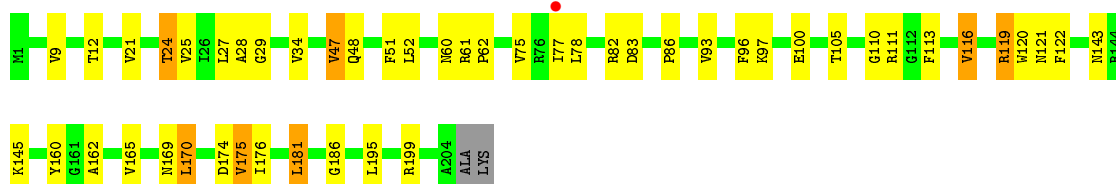
• Molecule 3: 50S ribosomal protein L2

Chain 2D: 9% 83% 14%



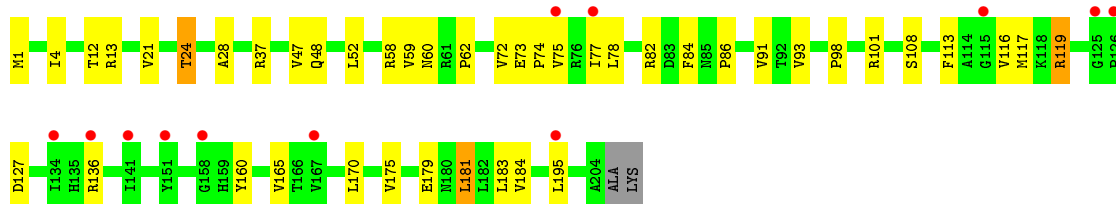
- Molecule 4: 50S ribosomal protein L3

Chain 1E: 75% 20% ..



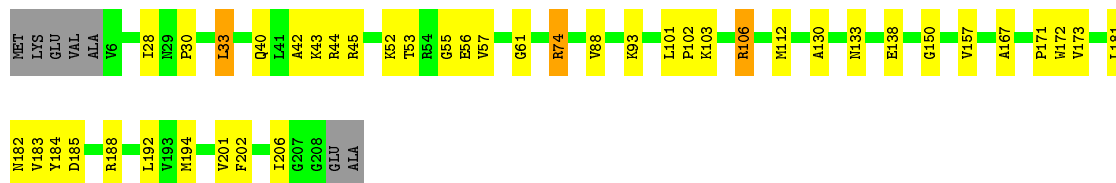
- Molecule 4: 50S ribosomal protein L3

Chain 2E: 6% 78% 20% ..



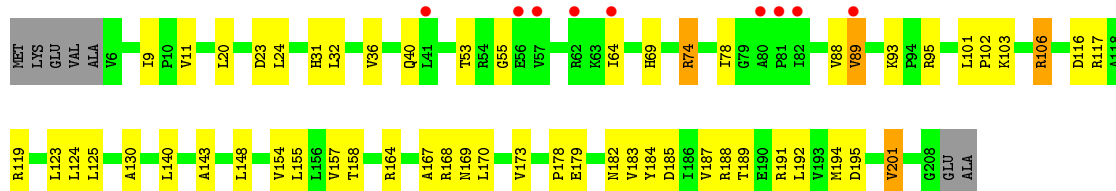
- Molecule 5: 50S ribosomal protein L4

Chain 1F: 77% 19% ..

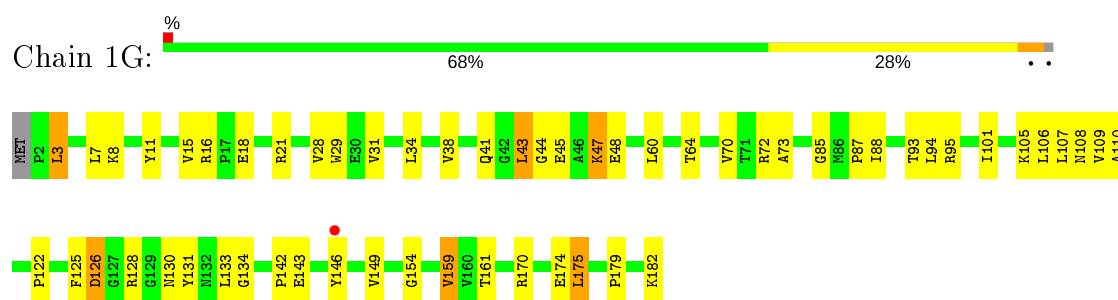


- Molecule 5: 50S ribosomal protein L4

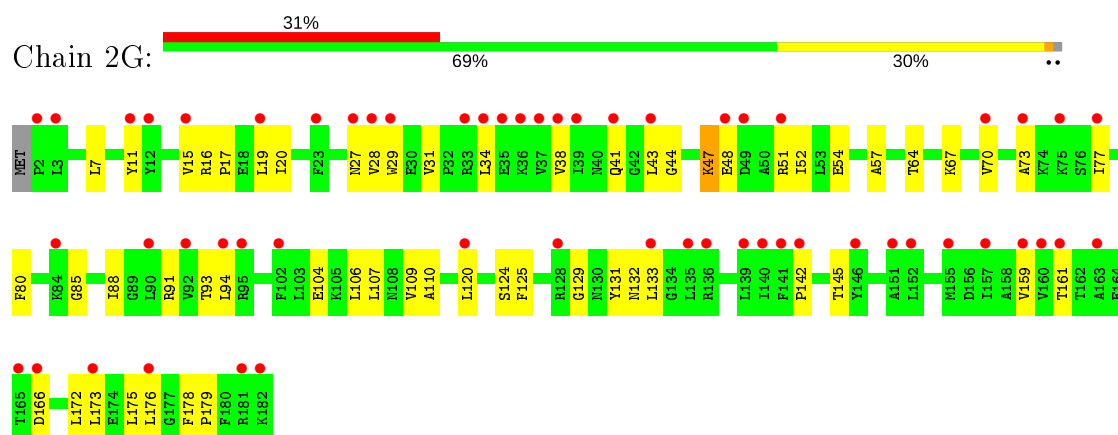
Chain 2F: 4% 70% 25% ..



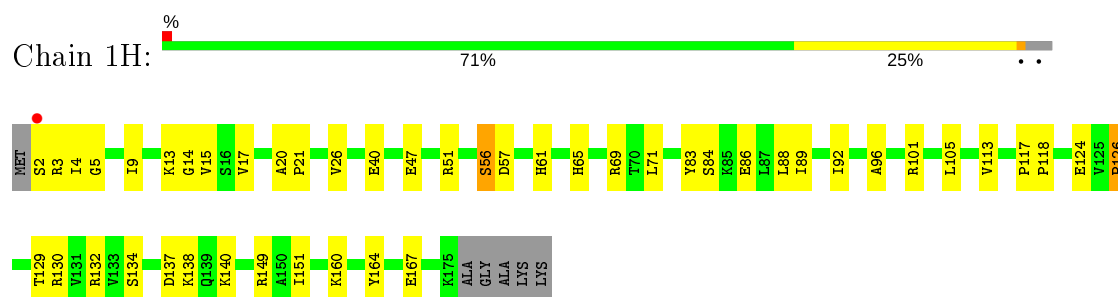
- Molecule 6: 50S ribosomal protein L5



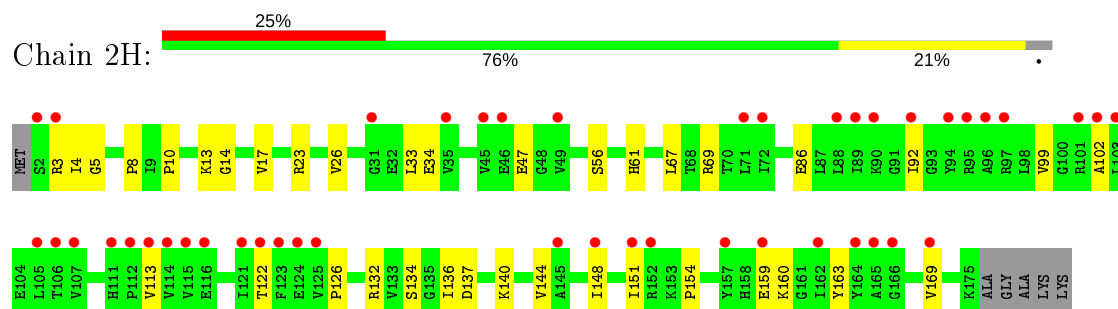
• Molecule 6: 50S ribosomal protein L5



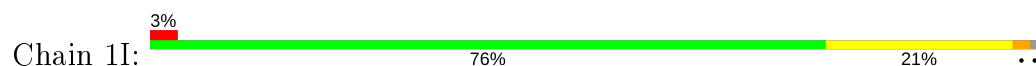
• Molecule 7: 50S ribosomal protein L6

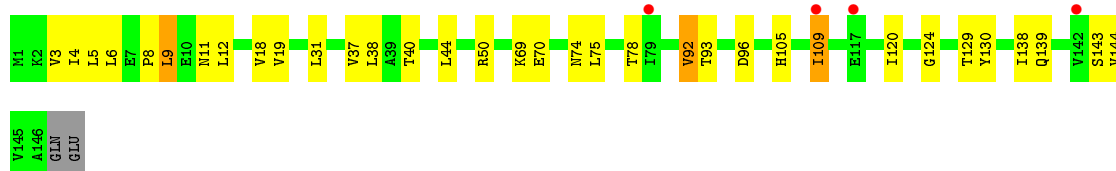


• Molecule 7: 50S ribosomal protein L6

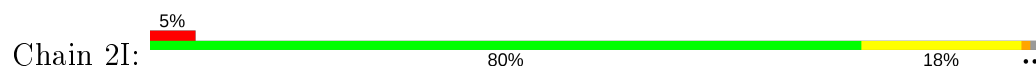


• Molecule 8: 50S ribosomal protein L9

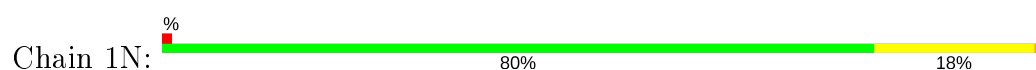




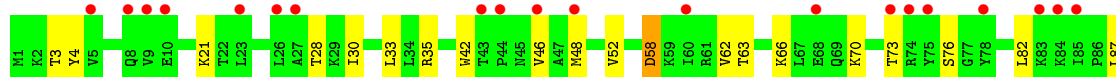
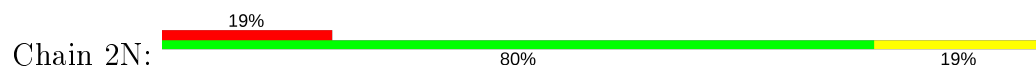
- Molecule 8: 50S ribosomal protein L9



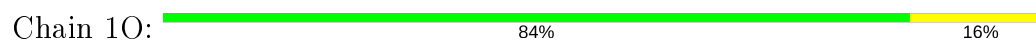
- Molecule 9: 50S ribosomal protein L13



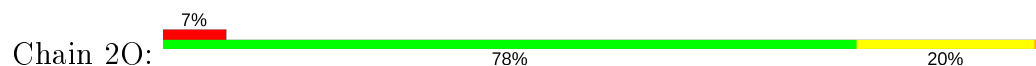
- Molecule 9: 50S ribosomal protein L13



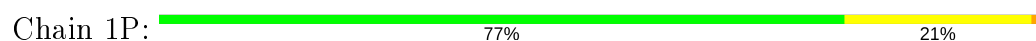
- Molecule 10: 50S ribosomal protein L14

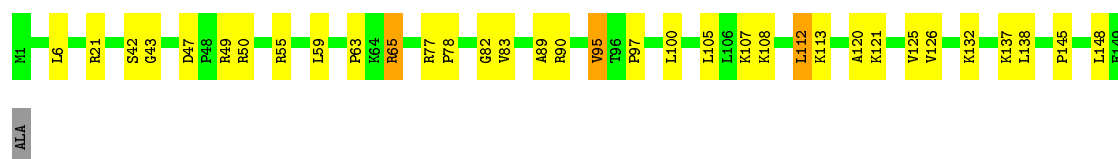


- Molecule 10: 50S ribosomal protein L14

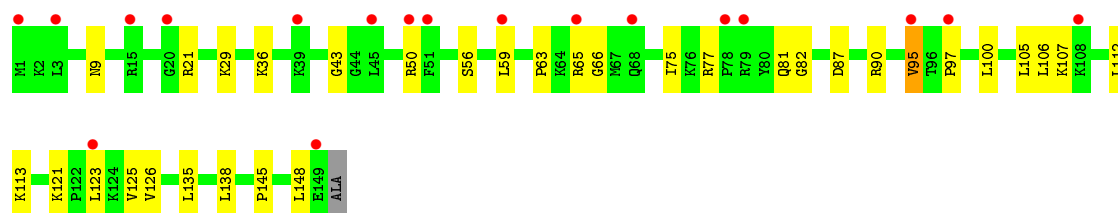
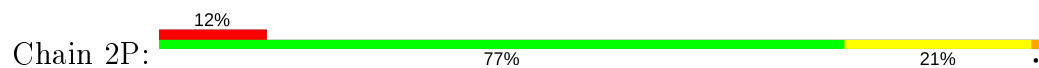


- Molecule 11: 50S ribosomal protein L15

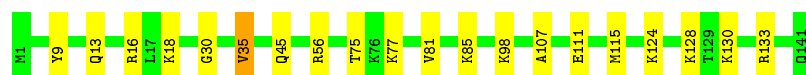
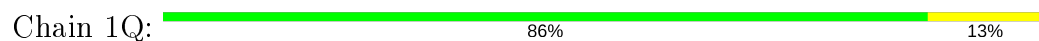




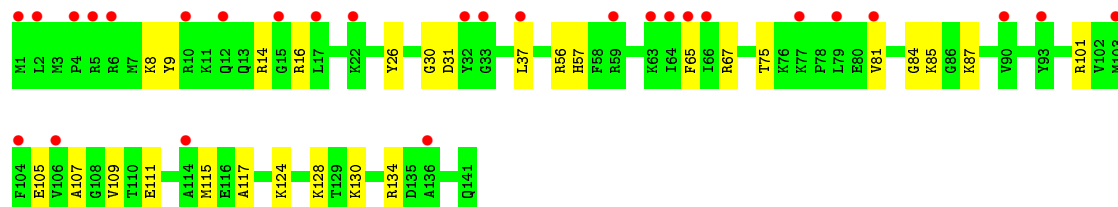
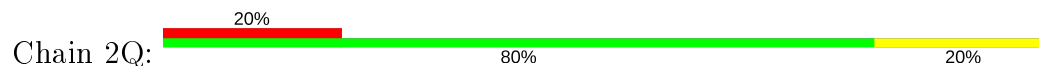
- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16



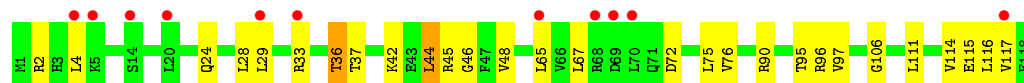
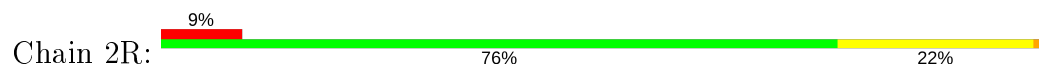
- Molecule 12: 50S ribosomal protein L16



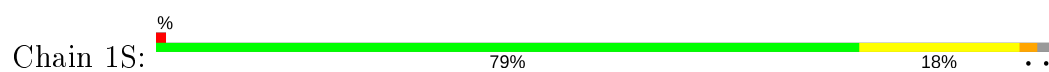
- Molecule 13: 50S ribosomal protein L17



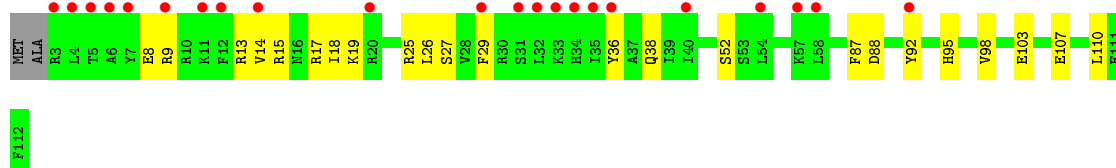
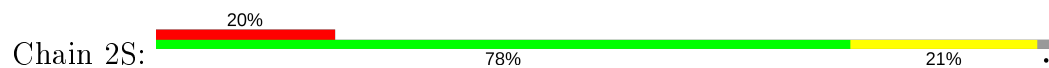
- Molecule 13: 50S ribosomal protein L17



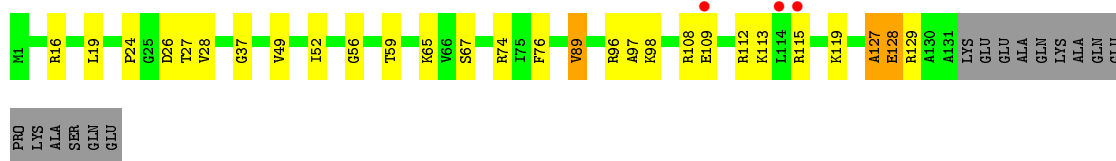
- Molecule 14: 50S ribosomal protein L18



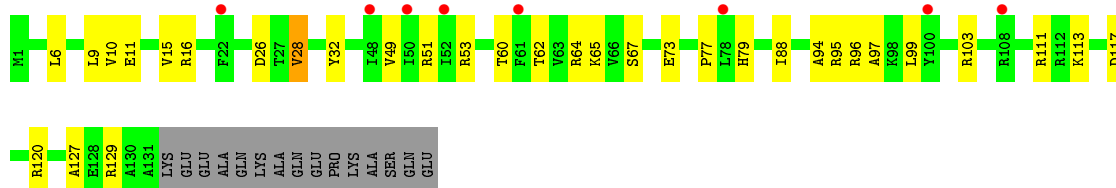
- Molecule 14: 50S ribosomal protein L18



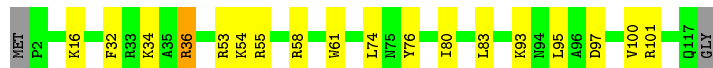
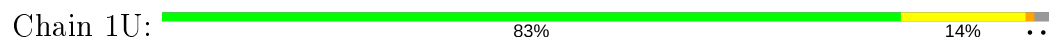
- Molecule 15: 50S ribosomal protein L19



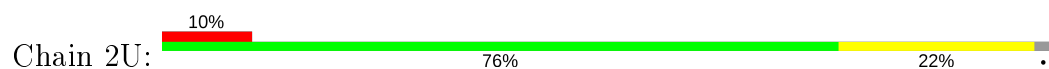
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20




- Molecule 16: 50S ribosomal protein L20

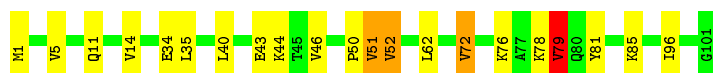





GLY

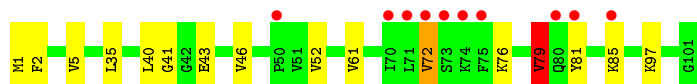
- Molecule 17: 50S ribosomal protein L21

Chain 1V:  79% 17% ..




- Molecule 17: 50S ribosomal protein L21

Chain 2V:  10% 84% 14% ..




- Molecule 18: 50S ribosomal protein L22

Chain 1W:  % 79% 19% ..




- Molecule 18: 50S ribosomal protein L22

Chain 2W:  3% 79% 20% ..




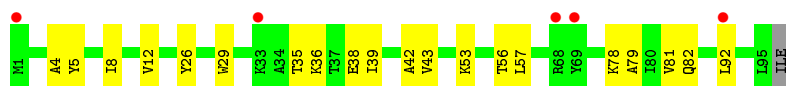
- Molecule 19: 50S ribosomal protein L23

Chain 1X:  2% 85% 13% ..



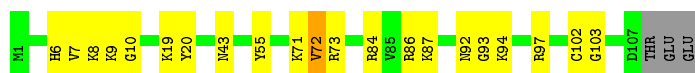
- Molecule 19: 50S ribosomal protein L23

Chain 2X:  5% 78% 21% ..

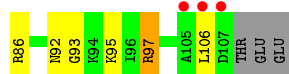
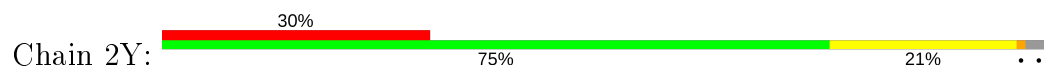


- Molecule 20: 50S ribosomal protein L24

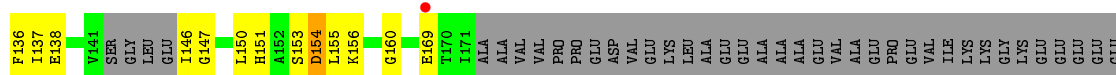
Chain 1Y:  78% 18% ..



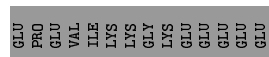
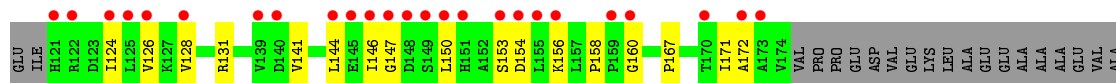
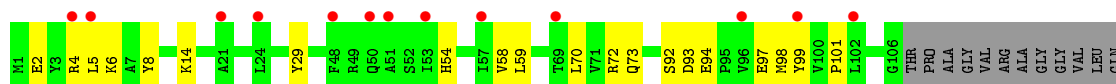
- Molecule 20: 50S ribosomal protein L24



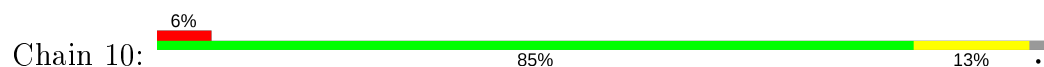
- Molecule 21: 50S ribosomal protein L25



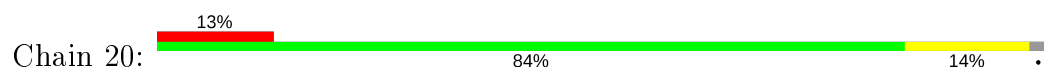
- Molecule 21: 50S ribosomal protein L25



- Molecule 22: 50S ribosomal protein L27

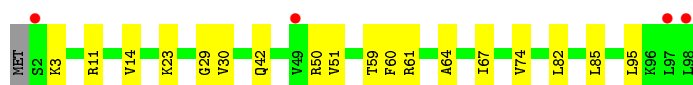
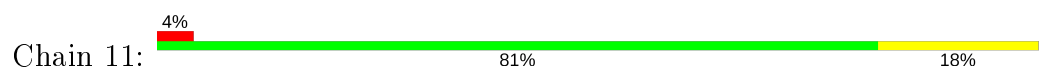


- Molecule 22: 50S ribosomal protein L27

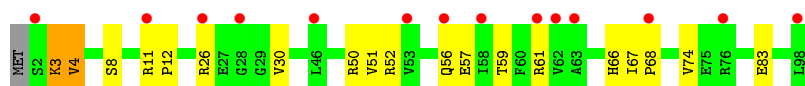
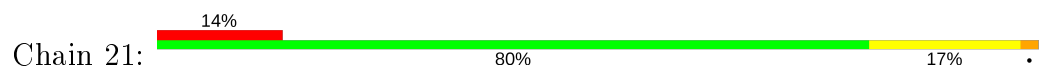




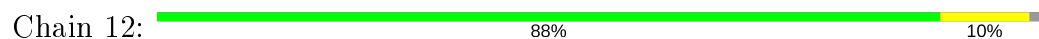
- Molecule 23: 50S ribosomal protein L28



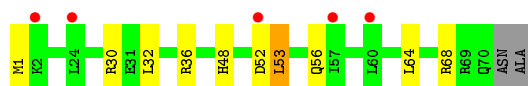
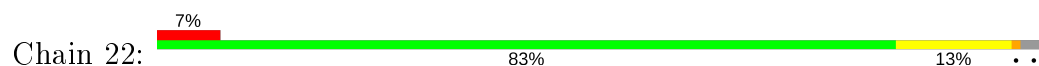
- Molecule 23: 50S ribosomal protein L28



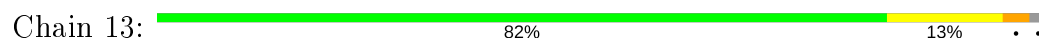
- Molecule 24: 50S ribosomal protein L29



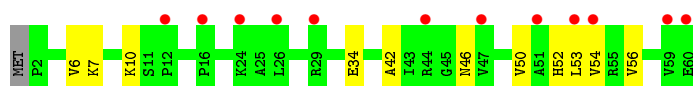
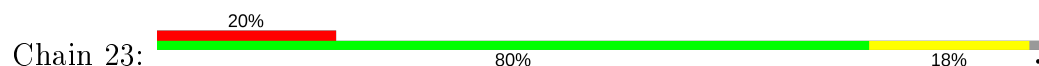
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



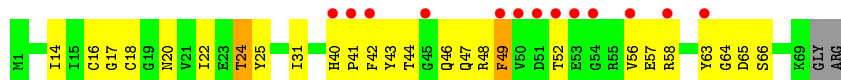
- Molecule 25: 50S ribosomal protein L30



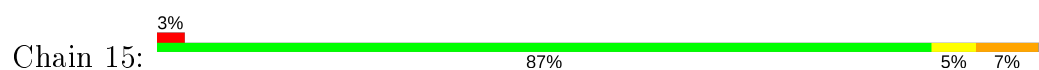
- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



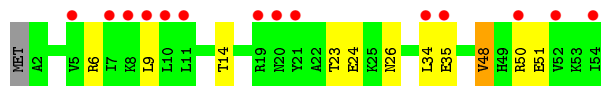
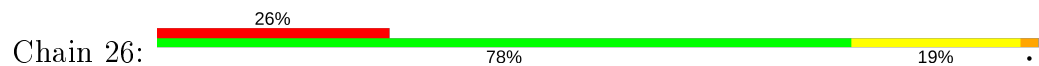
- Molecule 27: 50S ribosomal protein L32



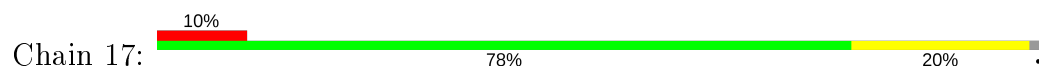
- Molecule 28: 50S ribosomal protein L33



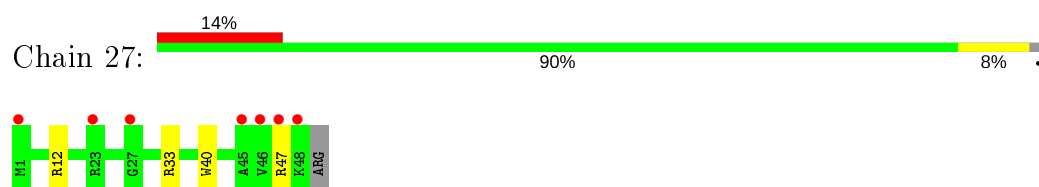
- Molecule 28: 50S ribosomal protein L33



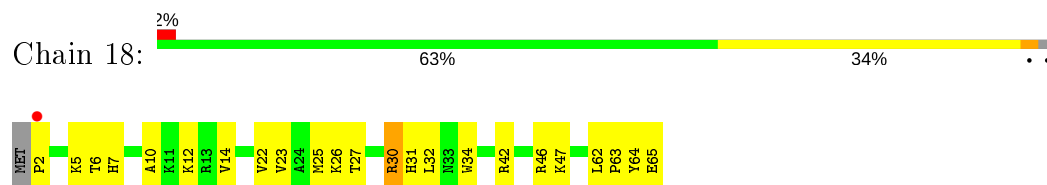
- Molecule 29: 50S ribosomal protein L34



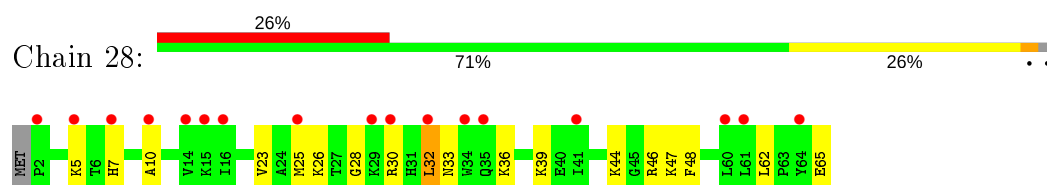
- Molecule 29: 50S ribosomal protein L34



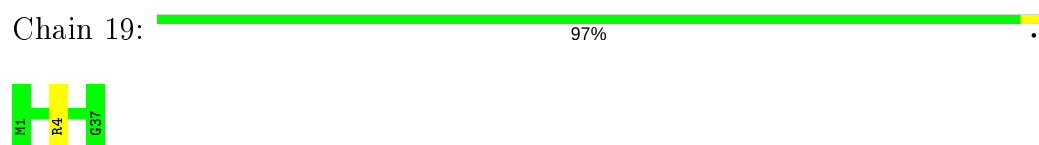
- Molecule 30: 50S ribosomal protein L35



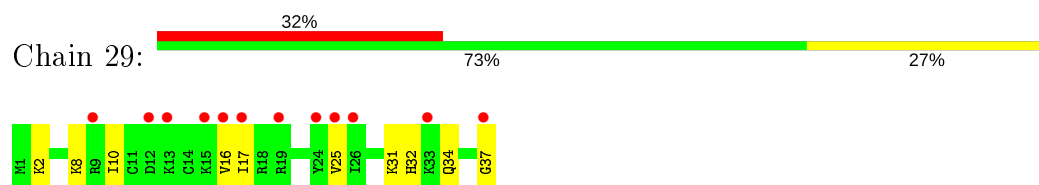
- Molecule 30: 50S ribosomal protein L35



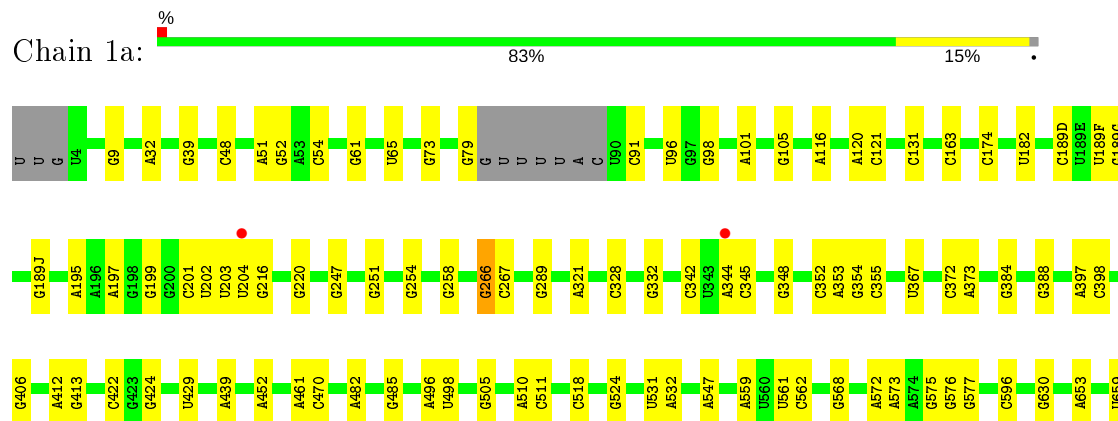
- Molecule 31: 50S ribosomal protein L36

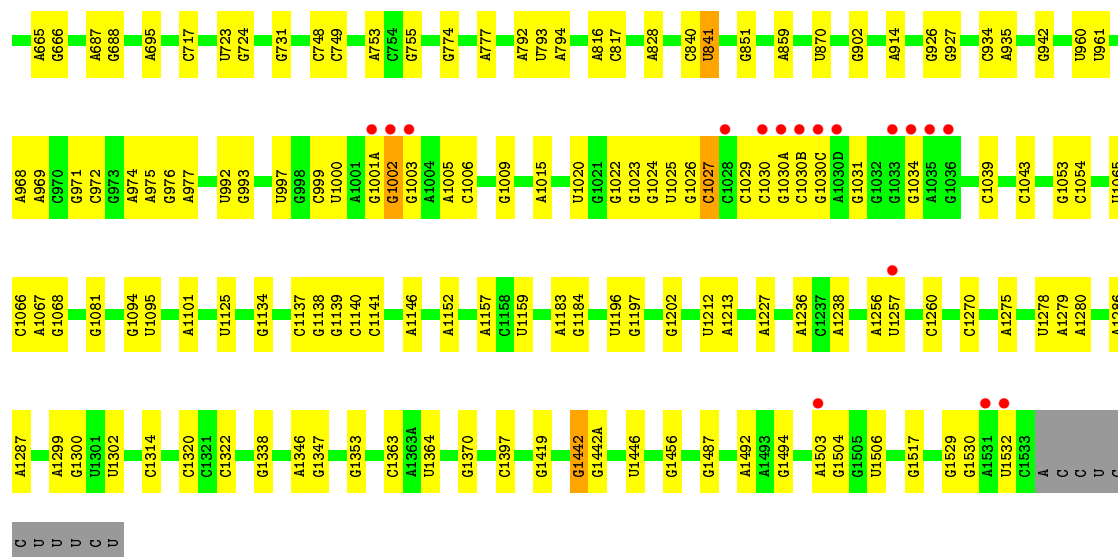


- Molecule 31: 50S ribosomal protein L36

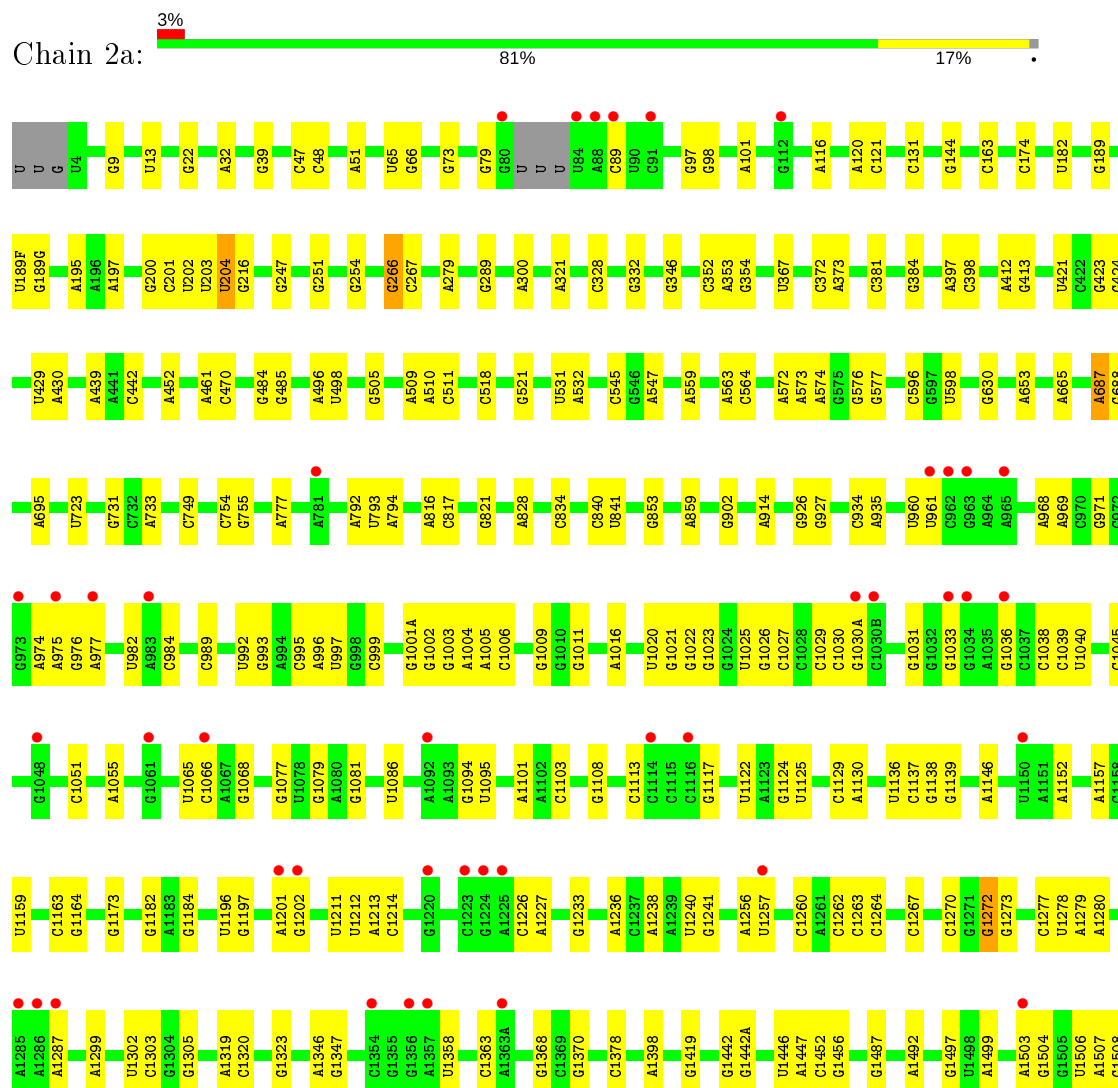


- Molecule 32: 16S Ribosomal RNA

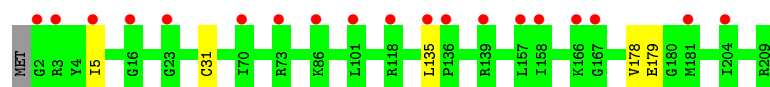




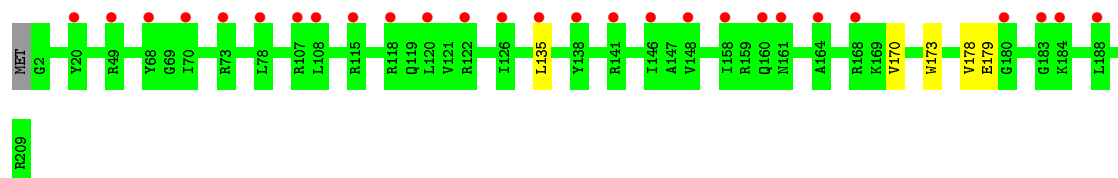
• Molecule 32: 16S Ribosomal RNA







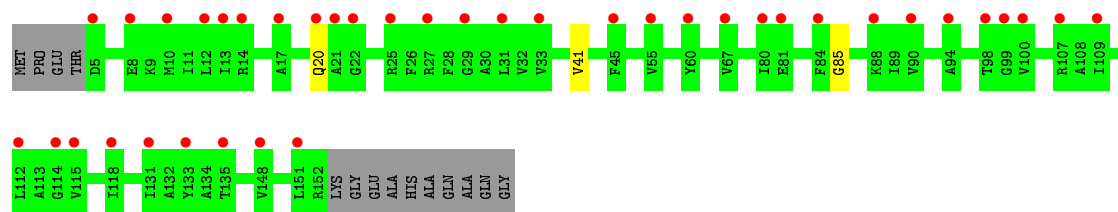
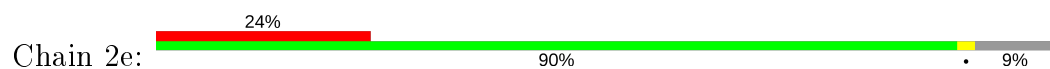
- Molecule 35: 30S ribosomal protein S4



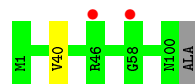
- Molecule 36: 30S ribosomal protein S5



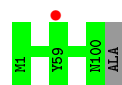
- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6

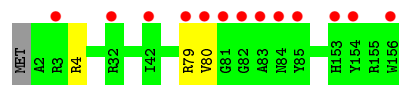


- Molecule 37: 30S ribosomal protein S6

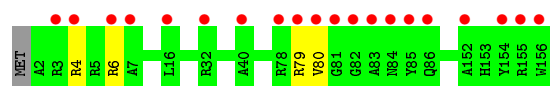


- Molecule 38: 30S ribosomal protein S7





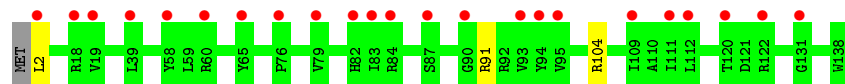
- Molecule 38: 30S ribosomal protein S7



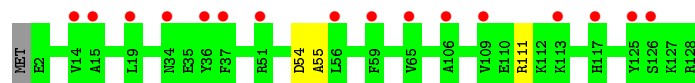
- Molecule 39: 30S ribosomal protein S8



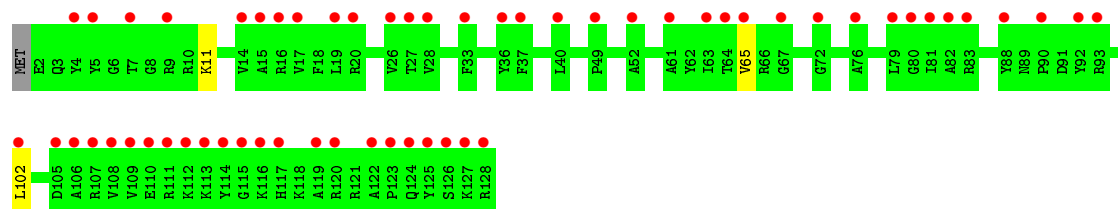
- Molecule 39: 30S ribosomal protein S8



- Molecule 40: 30S ribosomal protein S9

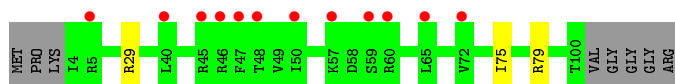


- Molecule 40: 30S ribosomal protein S9

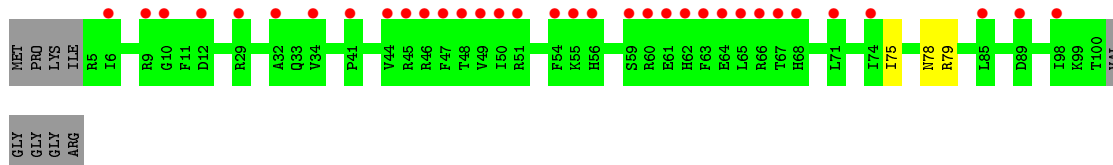
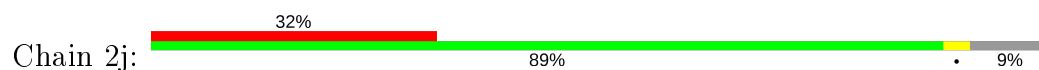


- Molecule 41: 30S ribosomal protein S10

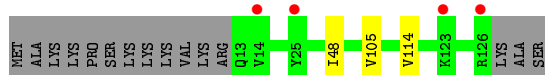
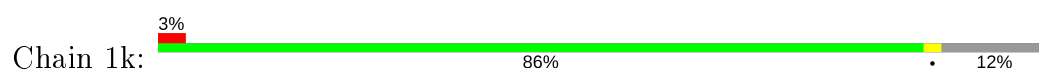




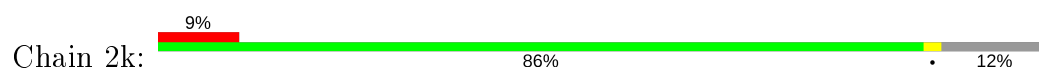
- Molecule 41: 30S ribosomal protein S10



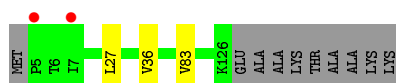
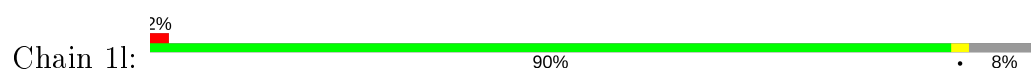
- Molecule 42: 30S ribosomal protein S11



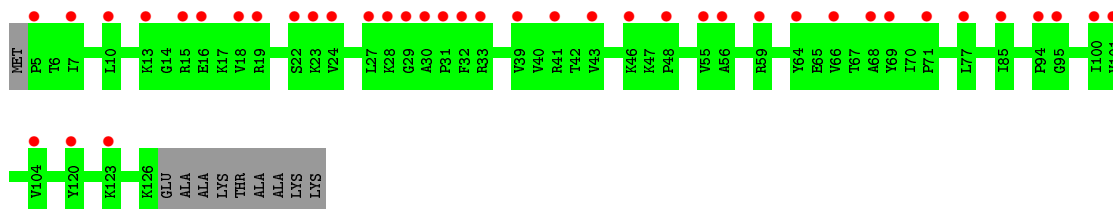
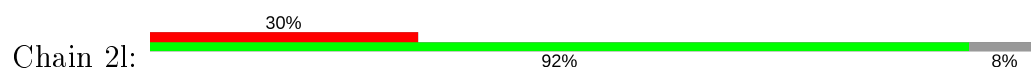
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S12

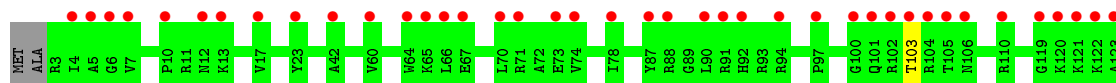


- Molecule 44: 30S ribosomal protein S13

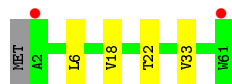
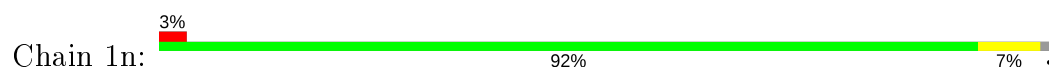




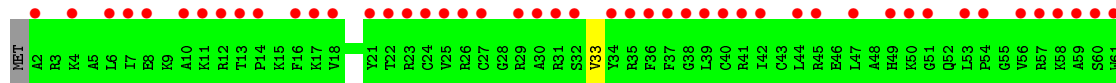
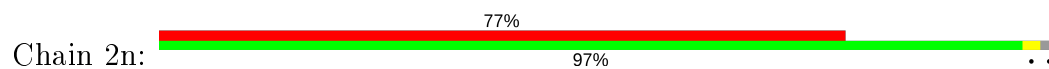
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



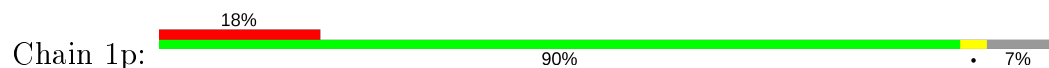
- Molecule 46: 30S ribosomal protein S15

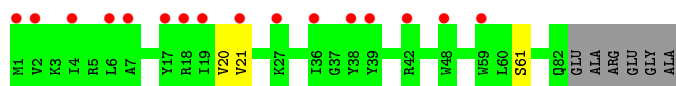


- Molecule 46: 30S ribosomal protein S15

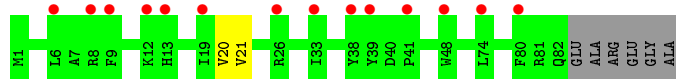
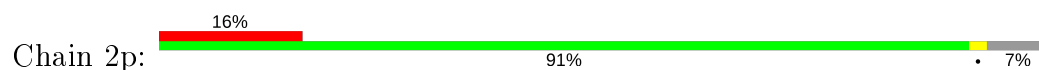


- Molecule 47: 30S ribosomal protein S16

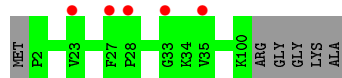




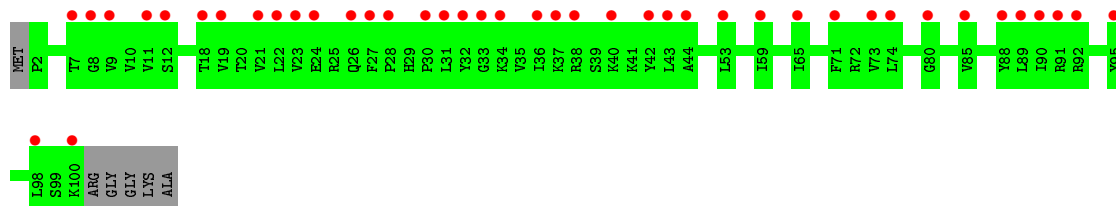
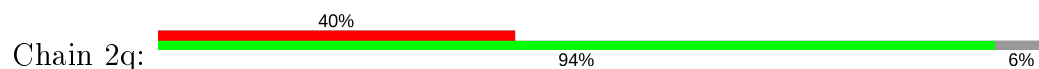
- Molecule 47: 30S ribosomal protein S16



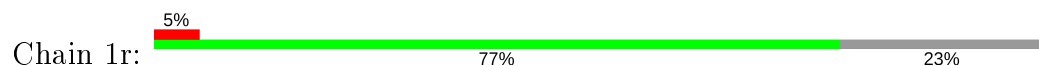
- Molecule 48: 30S ribosomal protein S17



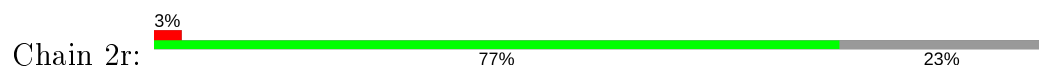
- Molecule 48: 30S ribosomal protein S17



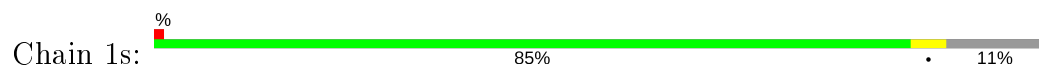
- Molecule 49: 30S ribosomal protein S18

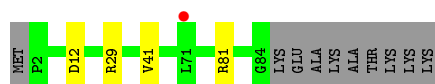


- Molecule 49: 30S ribosomal protein S18

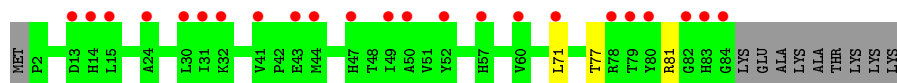
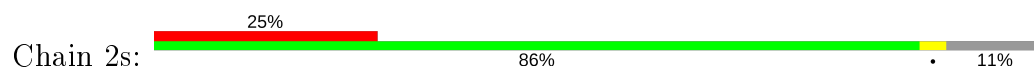


- Molecule 50: 30S ribosomal protein S19

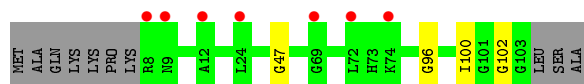
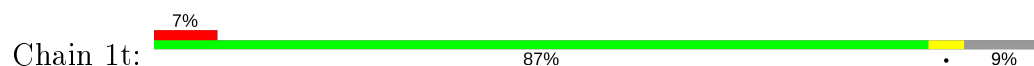




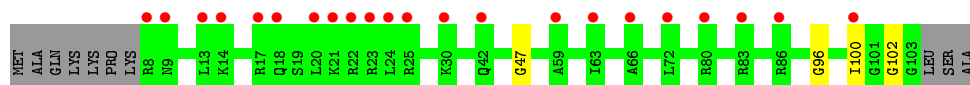
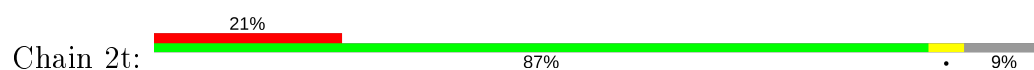
- Molecule 50: 30S ribosomal protein S19



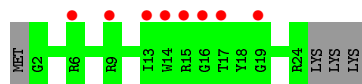
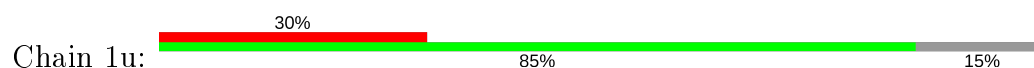
- Molecule 51: 30S ribosomal protein S20



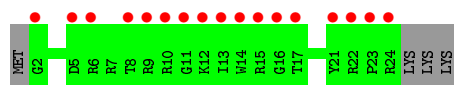
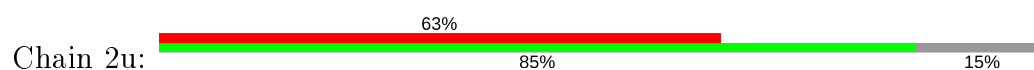
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



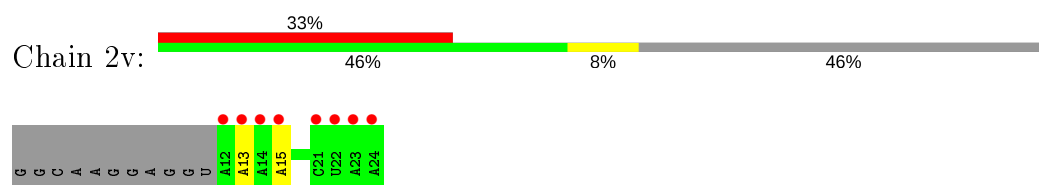
- Molecule 52: 30S ribosomal protein Thx



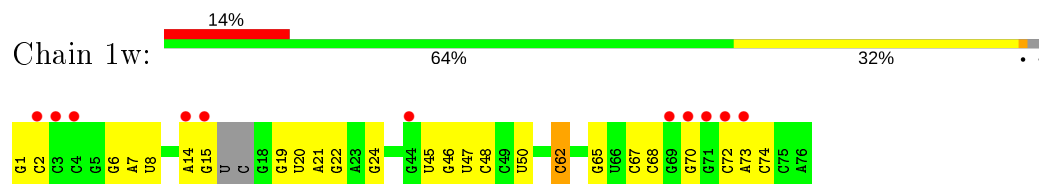
- Molecule 53: mRNA



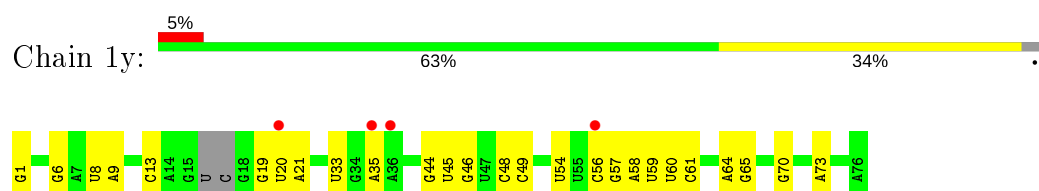
- Molecule 53: mRNA



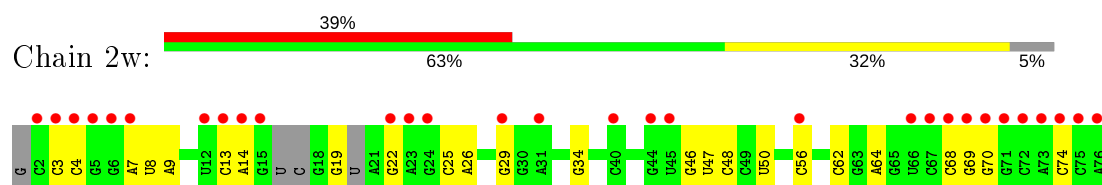
- Molecule 54: A-site and E-site tRNAs



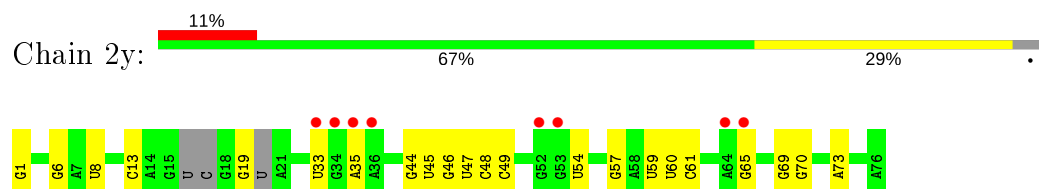
- Molecule 54: A-site and E-site tRNAs



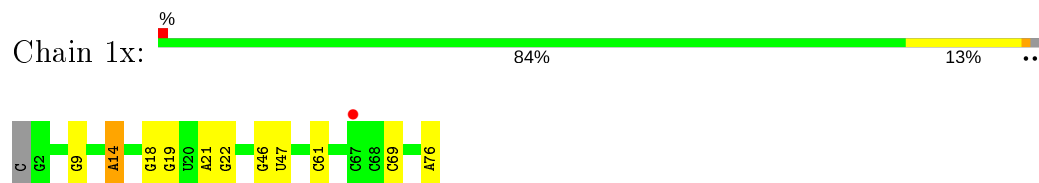
- Molecule 54: A-site and E-site tRNAs



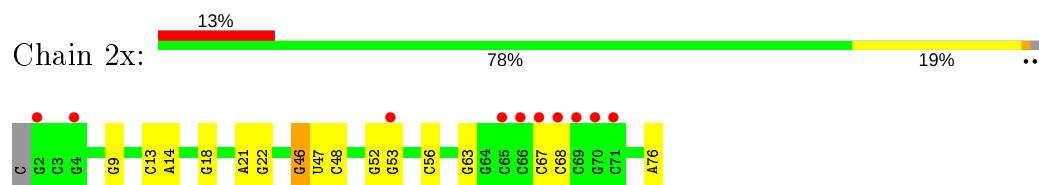
- Molecule 54: A-site and E-site tRNAs



- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.62Å 448.78Å 622.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	255.77 – 2.70 255.77 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (255.77-2.70) 98.9 (255.77-2.70)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, $R_{free}$	0.222 , 0.266 0.222 , 0.266	Depositor DCC
$R_{free}$ test set	78357 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.2	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 56.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	301023	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: 5MU, ZN, MT9, OMG, 2MU, MIA, SF4, 0TD, MG, 2MA, M2G, 2MG, 5MC, UR3, MA6, 4OC, 4SU, 7MG, K, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1A	0.48	0/69009	0.93	57/107712 (0.1%)
1	2A	0.37	0/67293	0.84	30/105034 (0.0%)
2	1B	0.43	1/2882 (0.0%)	0.84	0/4494
2	2B	0.40	1/2879 (0.0%)	0.84	1/4487 (0.0%)
3	1D	0.36	0/2186	0.56	0/2944
3	2D	0.31	0/2186	0.52	0/2944
4	1E	0.33	0/1592	0.58	0/2149
4	2E	0.30	0/1592	0.50	0/2149
5	1F	0.32	0/1619	0.52	0/2193
5	2F	0.29	0/1615	0.48	0/2188
6	1G	0.31	0/1448	0.48	0/1957
6	2G	0.29	0/1453	0.47	0/1963
7	1H	0.31	0/1356	0.50	0/1834
7	2H	0.27	0/1356	0.46	0/1834
8	1I	0.28	0/1112	0.47	0/1514
8	2I	0.27	0/1079	0.47	0/1475
9	1N	0.33	0/1144	0.52	0/1543
9	2N	0.28	0/1144	0.47	0/1543
10	1O	0.33	0/943	0.53	0/1269
10	2O	0.31	0/943	0.50	0/1269
11	1P	0.32	0/1152	0.55	0/1533
11	2P	0.30	0/1152	0.51	0/1533
12	1Q	0.35	0/1143	0.51	0/1527
12	2Q	0.29	0/1143	0.47	0/1527
13	1R	0.32	0/982	0.55	0/1312
13	2R	0.27	0/982	0.48	0/1312
14	1S	0.31	0/883	0.51	0/1176
14	2S	0.29	0/880	0.47	0/1172
15	1T	0.32	0/1105	0.51	0/1477
15	2T	0.28	0/1097	0.47	0/1468
16	1U	0.36	0/977	0.53	0/1301



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.28	0/977	0.43	0/1301
17	1V	0.38	1/782 (0.1%)	0.56	0/1049
17	2V	0.29	0/782	0.52	0/1049
18	1W	0.34	0/897	0.55	0/1205
18	2W	0.30	0/897	0.47	0/1205
19	1X	0.36	0/764	0.55	0/1025
19	2X	0.28	0/764	0.48	0/1025
20	1Y	0.33	0/819	0.53	0/1095
20	2Y	0.31	0/819	0.50	0/1095
21	1Z	0.30	0/1267	0.51	0/1717
21	2Z	0.29	0/1299	0.50	0/1763
22	10	0.33	0/662	0.55	0/881
22	20	0.29	0/662	0.49	0/881
23	11	0.34	0/762	0.51	0/1014
23	21	0.30	0/762	0.51	0/1014
24	12	0.30	0/590	0.43	0/781
24	22	0.27	0/590	0.39	0/781
25	13	0.33	0/474	0.51	0/635
25	23	0.29	0/469	0.45	0/630
26	14	0.34	0/565	0.64	1/761 (0.1%)
26	24	0.31	0/545	0.54	0/737
27	15	0.32	0/469	0.57	1/635 (0.2%)
27	25	0.31	0/469	0.50	0/635
28	16	0.32	0/460	0.53	0/613
28	26	0.26	0/456	0.51	0/608
29	17	0.33	0/426	0.52	0/561
29	27	0.30	0/426	0.50	0/561
30	18	0.33	0/525	0.56	0/691
30	28	0.28	0/525	0.48	0/691
31	19	0.32	0/310	0.54	0/407
31	29	0.29	0/310	0.50	0/407
32	1a	0.35	0/35795	0.85	25/55864 (0.0%)
32	2a	0.34	2/35886 (0.0%)	0.87	28/56005 (0.0%)
33	1b	0.28	0/1881	0.47	0/2542
33	2b	0.28	0/1860	0.45	0/2518
34	1c	0.28	0/1572	0.45	0/2126
34	2c	0.27	0/1566	0.45	0/2119
35	1d	0.28	0/1685	0.47	0/2262
35	2d	0.27	0/1704	0.46	0/2284
36	1e	0.30	0/1145	0.49	0/1543
36	2e	0.29	0/1149	0.49	0/1548
37	1f	0.29	0/823	0.45	0/1115
37	2f	0.29	0/829	0.45	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.27	0/1250	0.43	0/1679
38	2g	0.27	0/1254	0.41	0/1683
39	1h	0.28	0/1108	0.47	0/1494
39	2h	0.27	0/1108	0.45	0/1494
40	1i	0.29	0/1002	0.51	0/1346
40	2i	0.29	0/997	0.50	0/1343
41	1j	0.27	0/722	0.46	0/982
41	2j	0.27	0/727	0.47	0/988
42	1k	0.27	0/844	0.47	0/1145
42	2k	0.27	0/848	0.46	0/1149
43	1l	0.29	0/937	0.50	0/1260
43	2l	0.29	0/937	0.51	0/1260
44	1m	0.28	0/969	0.49	0/1302
44	2m	0.28	0/961	0.48	0/1291
45	1n	0.30	0/501	0.46	0/664
45	2n	0.28	0/501	0.45	0/664
46	1o	0.27	0/739	0.45	0/985
46	2o	0.26	0/739	0.44	0/985
47	1p	0.27	0/697	0.50	0/939
47	2p	0.28	0/693	0.49	0/935
48	1q	0.27	0/836	0.46	0/1117
48	2q	0.27	0/836	0.46	0/1117
49	1r	0.28	0/560	0.48	0/746
49	2r	0.26	0/560	0.46	0/746
50	1s	0.27	0/667	0.52	0/900
50	2s	0.27	0/661	0.51	0/893
51	1t	0.27	0/730	0.42	0/965
51	2t	0.25	0/729	0.42	0/965
52	1u	0.26	0/203	0.46	0/266
52	2u	0.29	0/203	0.49	0/266
53	1v	0.34	0/310	0.81	0/480
53	2v	0.42	0/310	0.82	0/480
54	1w	0.50	1/1606 (0.1%)	1.06	2/2497 (0.1%)
54	1y	0.48	1/1606 (0.1%)	1.02	5/2497 (0.2%)
54	2w	0.45	0/1556	1.02	0/2418
54	2y	0.50	1/1583 (0.1%)	1.02	4/2459 (0.2%)
55	1x	0.49	0/1725	1.07	10/2689 (0.4%)
55	2x	0.42	0/1725	1.01	4/2689 (0.1%)
All	All	0.38	8/316686 (0.0%)	0.80	168/474113 (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
6	1G	0	1
26	14	0	1
26	24	0	2
33	2b	0	1
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	1	G	OP3-P	-10.39	1.48	1.61
54	1y	1	G	OP3-P	-10.26	1.48	1.61
2	2B	1	U	OP3-P	-10.19	1.49	1.61
2	1B	1	U	OP3-P	-10.15	1.49	1.61
54	1w	1	G	OP3-P	-9.98	1.49	1.61
32	2a	1272	G	N1-C2	-8.87	1.30	1.37
32	2a	1272	G	C6-N1	-8.82	1.33	1.39
17	1V	34	GLU	C-N	-5.13	1.22	1.34

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	C5-C6-O6	20.98	141.19	128.60
32	2a	1272	G	N3-C2-N2	20.30	134.11	119.90
32	2a	1263	C	N1-C2-O2	20.06	130.93	118.90
32	2a	1272	G	N1-C2-N2	-17.02	100.88	116.20
32	2a	1272	G	N1-C6-O6	-13.01	112.09	119.90
1	1A	1132	A	N1-C6-N6	-12.71	110.97	118.60
32	2a	1272	G	C6-N1-C2	12.30	132.48	125.10
32	2a	1263	C	N3-C2-O2	-11.96	113.53	121.90
32	2a	1263	C	C2-N3-C4	11.24	125.52	119.90
1	1A	1121	C	N1-C2-O2	10.20	125.02	118.90
1	1A	1109	G	C5-C6-O6	10.12	134.67	128.60
2	2B	80	U	O4'-C1'-N1	10.07	116.26	108.20
32	2a	1272	G	C5-C6-N1	-9.64	106.68	111.50
1	1A	1121	C	C2-N3-C4	9.42	124.61	119.90
32	2a	1263	C	C5-C6-N1	8.81	125.41	121.00
1	1A	2189	U	C2-N1-C1'	8.34	127.71	117.70
1	2A	2136	C	N1-C2-O2	8.32	123.89	118.90
1	1A	2627	U	O5'-P-OP1	-8.00	98.50	105.70
32	1a	1027	C	C5-C4-N4	7.98	125.79	120.20
1	1A	1109	G	C6-N1-C2	7.91	129.85	125.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	14	A	C4-C5-C6	7.72	120.86	117.00
32	1a	1027	C	N3-C4-C5	-7.63	118.85	121.90
1	1A	1020	C	N1-C2-O2	-7.62	114.33	118.90
32	1a	1034	G	N3-C2-N2	7.61	125.23	119.90
55	1x	14	A	C5-N7-C8	7.61	107.70	103.90
1	1A	1121	C	C5-C4-N4	7.61	125.53	120.20
1	1A	537	G	O4'-C1'-N9	7.48	114.18	108.20
1	1A	1132	A	C5-C6-N6	7.45	129.66	123.70
32	2a	1263	C	C2-N1-C1'	7.41	126.95	118.80
32	1a	1027	C	N3-C2-O2	-7.40	116.72	121.90
55	1x	14	A	C4-C5-C6	7.39	120.69	117.00
54	2y	33	U	C2-N1-C1'	7.35	126.52	117.70
1	1A	1109	G	N3-C2-N2	7.34	125.04	119.90
1	1A	848	G	O5'-P-OP2	-7.25	99.17	105.70
32	2a	254	G	O5'-P-OP1	-7.22	99.20	105.70
54	1y	56	C	N1-C2-O2	7.21	123.23	118.90
1	1A	834	U	O5'-P-OP1	-7.18	99.23	105.70
32	2a	1263	C	C6-N1-C2	-7.08	117.47	120.30
1	1A	1985	U	C2-N1-C1'	7.04	126.15	117.70
1	1A	1020	C	C2-N1-C1'	-7.04	111.06	118.80
32	2a	1272	G	C2-N3-C4	-6.95	108.42	111.90
54	1y	33	U	C2-N1-C1'	6.94	126.03	117.70
1	1A	215	G	O4'-C1'-N9	6.92	113.73	108.20
1	2A	2140	C	C2-N1-C1'	6.84	126.32	118.80
32	2a	1272	G	C4-N9-C1'	6.80	135.34	126.50
32	1a	1034	G	N9-C4-C5	-6.71	102.72	105.40
32	2a	1272	G	C8-N9-C1'	-6.68	118.32	127.00
1	1A	2189	U	N1-C2-O2	6.61	127.43	122.80
32	1a	1030(B)	C	C2-N1-C1'	6.55	126.01	118.80
1	2A	2149	G	N3-C4-N9	6.50	129.90	126.00
1	1A	894	U	C2-N1-C1'	6.50	125.49	117.70
32	1a	1002	G	C4-N9-C1'	6.41	134.83	126.50
32	1a	1027	C	C6-N1-C2	-6.40	117.74	120.30
55	2x	14	A	C5-N7-C8	6.38	107.09	103.90
32	1a	1027	C	C6-N1-C1'	6.33	128.40	120.80
1	1A	1020	C	C6-N1-C1'	6.18	128.21	120.80
54	1y	33	U	N1-C2-O2	6.12	127.09	122.80
1	2A	2689	U	P-O3'-C3'	6.11	127.03	119.70
1	2A	1313	U	C2-N1-C1'	6.10	125.02	117.70
54	2y	33	U	N1-C2-O2	6.09	127.07	122.80
55	1x	22	G	N1-C6-O6	-6.09	116.25	119.90
1	1A	2189	U	N3-C2-O2	-6.08	117.94	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	22	G	C8-N9-C1'	6.07	134.89	127.00
32	2a	754	C	C2-N1-C1'	6.07	125.48	118.80
32	2a	1263	C	C4-C5-C6	-6.04	114.38	117.40
32	1a	1034	G	C6-N1-C2	6.03	128.72	125.10
1	1A	1121	C	N3-C2-O2	-6.01	117.69	121.90
1	2A	2139	C	C2-N1-C1'	5.98	125.38	118.80
32	1a	266	G	P-O3'-C3'	5.96	126.85	119.70
55	2x	14	A	C5-C6-N1	-5.94	114.73	117.70
1	2A	2136	C	N3-C2-O2	-5.94	117.74	121.90
1	1A	1128	U	N3-C4-O4	-5.91	115.26	119.40
55	1x	14	A	C5-C6-N1	-5.91	114.75	117.70
54	1y	58	A	C2-N3-C4	5.89	113.55	110.60
1	2A	2473	U	C2-N1-C1'	5.89	124.77	117.70
1	1A	410	U	O4'-C1'-N1	5.88	112.91	108.20
1	1A	2566	U	O5'-P-OP1	-5.85	100.43	105.70
32	2a	1263	C	C5-C4-N4	5.83	124.28	120.20
1	1A	1128	U	N3-C4-C5	5.79	118.07	114.60
1	1A	1109	G	C5-C6-N1	-5.77	108.61	111.50
32	1a	1002	G	C8-N9-C1'	-5.76	119.51	127.00
32	1a	1442	G	N3-C4-C5	-5.75	125.73	128.60
55	1x	46	G	C6-N1-C2	-5.75	121.65	125.10
55	1x	22	G	C4-N9-C1'	-5.73	119.05	126.50
1	2A	2174	C	N1-C2-O2	5.71	122.33	118.90
1	2A	2248	C	O5'-P-OP2	-5.69	100.58	105.70
26	14	64	GLY	N-CA-C	5.65	127.23	113.10
1	1A	2858	G	O4'-C1'-N9	5.65	112.72	108.20
55	1x	22	G	C4-C5-C6	-5.61	115.43	118.80
32	1a	1002	G	N3-C4-N9	5.61	129.37	126.00
1	1A	572	A	P-O3'-C3'	5.58	126.40	119.70
1	2A	1992	G	P-O3'-C3'	5.58	126.40	119.70
1	1A	2189	U	C5-C6-N1	5.58	125.49	122.70
1	1A	31	C	O5'-P-OP1	-5.57	100.68	105.70
32	2a	266	G	N3-C4-C5	-5.56	125.82	128.60
32	1a	1030(B)	C	N1-C2-O2	5.56	122.24	118.90
55	1x	22	G	N3-C4-N9	-5.55	122.67	126.00
1	1A	410	U	C2-N1-C1'	-5.54	111.05	117.70
1	1A	1359	U	N3-C2-O2	-5.53	118.33	122.20
1	1A	1398	U	O5'-P-OP1	-5.52	100.73	105.70
32	1a	1034	G	N3-C4-N9	5.50	129.30	126.00
1	1A	1219	A	P-O3'-C3'	5.50	126.30	119.70
32	1a	1442	G	N3-C4-N9	5.47	129.28	126.00
1	2A	228	A	P-O3'-C3'	5.47	126.26	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	46	G	C6-N1-C2	-5.46	121.82	125.10
55	1x	22	G	C6-C5-N7	5.45	133.67	130.40
54	1w	62	C	C2-N1-C1'	5.45	124.79	118.80
1	2A	2689	U	N3-C2-O2	-5.45	118.39	122.20
1	1A	2014	G	P-O3'-C3'	5.44	126.23	119.70
32	2a	1263	C	N3-C4-N4	-5.42	114.21	118.00
32	2a	266	G	P-O3'-C3'	5.41	126.19	119.70
27	15	58	LEU	CA-CB-CG	5.40	127.72	115.30
1	1A	2881	C	O5'-P-OP2	-5.40	100.84	105.70
1	1A	1222	A	O5'-P-OP1	-5.38	100.86	105.70
1	2A	2140	C	N3-C2-O2	-5.37	118.14	121.90
1	1A	840	A	O5'-P-OP2	-5.37	100.87	105.70
32	1a	1030(B)	C	C6-N1-C2	-5.37	118.15	120.30
1	2A	1698	A	O4'-C1'-N9	5.35	112.48	108.20
1	2A	783	A	C2-N3-C4	5.35	113.27	110.60
32	2a	687	A	P-O3'-C3'	5.34	126.11	119.70
1	2A	383	U	O4'-C1'-N1	5.33	112.47	108.20
32	1a	1034	G	C4-C5-N7	5.33	112.93	110.80
1	2A	512	G	O4'-C1'-N9	5.33	112.46	108.20
1	1A	2015	U	O5'-P-OP1	-5.32	100.91	105.70
1	1A	1109	G	N1-C6-O6	-5.32	116.71	119.90
1	2A	752	A	P-O3'-C3'	5.31	126.08	119.70
32	2a	1263	C	N1-C2-N3	-5.31	115.48	119.20
54	2y	33	U	N3-C2-O2	-5.29	118.49	122.20
1	2A	1530	C	P-O3'-C3'	5.28	126.04	119.70
32	2a	65	U	P-O3'-C3'	5.28	126.03	119.70
1	2A	2140	C	N1-C2-O2	5.27	122.06	118.90
1	1A	821	A	C8-N9-C4	-5.26	103.70	105.80
32	1a	254	G	O5'-P-OP1	-5.24	100.98	105.70
1	2A	2149	G	N9-C4-C5	-5.21	103.32	105.40
54	1y	64	A	C5-C6-N6	5.21	127.86	123.70
32	2a	204	U	C2-N1-C1'	5.20	123.94	117.70
1	1A	1462	G	O4'-C1'-N9	5.20	112.36	108.20
32	1a	841	U	C5-C6-N1	5.20	125.30	122.70
1	2A	2492	U	O5'-P-OP1	-5.20	101.02	105.70
32	1a	266	G	O4'-C1'-N9	-5.18	104.06	108.20
54	1w	22	G	N1-C6-O6	5.18	123.01	119.90
1	2A	645	C	N1-C2-O2	5.17	122.00	118.90
1	1A	1128	U	C2-N3-C4	-5.17	123.90	127.00
32	1a	748	C	P-O3'-C3'	5.17	125.90	119.70
32	1a	1002	G	N3-C4-C5	-5.16	126.02	128.60
1	1A	2803	A	C2-N3-C4	5.16	113.18	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2189	U	C6-N1-C1'	-5.15	113.99	121.20
1	2A	645	C	C2-N1-C1'	5.15	124.46	118.80
1	1A	1219	A	OP1-P-O3'	5.14	116.52	105.20
1	2A	2167	U	N1-C2-O2	5.14	126.40	122.80
1	1A	12	U	C2-N1-C1'	5.14	123.87	117.70
1	1A	2565	G	N3-C4-C5	-5.13	126.03	128.60
1	2A	2167	U	N3-C2-O2	-5.13	118.61	122.20
32	1a	1067	A	P-O3'-C3'	5.12	125.85	119.70
1	1A	590	A	O5'-P-OP1	-5.12	101.09	105.70
1	2A	528	A	P-O3'-C3'	5.12	125.84	119.70
1	1A	989	G	C4-N9-C1'	5.12	133.15	126.50
1	1A	1221	G	OP1-P-O3'	5.11	116.44	105.20
54	2y	47	U	C2-N1-C1'	5.11	123.83	117.70
1	1A	1121	C	N3-C4-N4	-5.10	114.43	118.00
1	1A	137	G	N3-C4-N9	5.09	129.06	126.00
32	2a	563	A	O4'-C1'-N9	5.08	112.27	108.20
1	1A	505	A	O4'-C1'-N9	5.04	112.23	108.20
1	1A	507	G	O4'-C1'-N9	5.03	112.23	108.20
1	2A	528	A	OP1-P-O3'	5.03	116.27	105.20
1	2A	2061	G	O5'-P-OP2	-5.02	101.18	105.70
32	2a	1201	A	P-O3'-C3'	5.02	125.72	119.70
1	1A	1359	U	O4'-C1'-N1	5.01	112.21	108.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	63	TYR	Peptide
6	1G	126	ASP	Peptide
26	24	56	VAL	Peptide
26	24	63	TYR	Peptide
33	2b	9	GLU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31193	617	0
1	2A	60322	0	30421	732	0
2	1B	2577	0	1305	30	0
2	2B	2575	0	1303	35	0
3	1D	2136	0	2218	48	0
3	2D	2136	0	2218	47	0
4	1E	1559	0	1618	34	0
4	2E	1559	0	1618	28	0
5	1F	1584	0	1625	33	0
5	2F	1580	0	1619	35	0
6	1G	1423	0	1436	39	0
6	2G	1428	0	1438	40	0
7	1H	1330	0	1407	30	0
7	2H	1330	0	1407	21	0
8	1I	1097	0	1140	22	0
8	2I	1064	0	1082	15	0
9	1N	1117	0	1184	20	0
9	2N	1117	0	1184	20	0
10	1O	933	0	996	9	0
10	2O	933	0	996	18	0
11	1P	1135	0	1212	29	0
11	2P	1135	0	1212	25	0
12	1Q	1122	0	1179	17	0
12	2Q	1122	0	1179	22	0
13	1R	968	0	1033	20	0
13	2R	968	0	1033	18	0
14	1S	873	0	927	13	0
14	2S	870	0	923	15	0
15	1T	1091	0	1151	20	0
15	2T	1083	0	1136	24	0
16	1U	959	0	1019	14	0
16	2U	959	0	1019	22	0
17	1V	771	0	830	13	0
17	2V	771	0	830	11	0
18	1W	886	0	940	13	0
18	2W	886	0	940	15	0
19	1X	750	0	814	9	0
19	2X	750	0	814	14	0
20	1Y	806	0	881	18	0
20	2Y	806	0	881	18	0
21	1Z	1240	0	1240	25	0
21	2Z	1271	0	1273	23	0
22	10	653	0	674	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	653	0	674	13	0
23	11	755	0	826	11	0
23	21	755	0	826	17	0
24	12	588	0	643	3	0
24	22	588	0	643	8	0
25	13	469	0	518	5	0
25	23	464	0	514	7	0
26	14	552	0	533	14	0
26	24	532	0	503	13	0
27	15	455	0	465	5	0
27	25	455	0	465	5	0
28	16	453	0	473	9	0
28	26	449	0	469	9	0
29	17	418	0	467	5	0
29	27	418	0	467	4	0
30	18	517	0	582	22	0
30	28	517	0	582	16	0
31	19	307	0	335	0	0
31	29	307	0	335	6	0
32	1a	32246	0	16295	0	0
32	2a	32327	0	16339	0	0
33	1b	1846	0	1867	0	0
33	2b	1825	0	1828	0	0
34	1c	1548	0	1535	0	0
34	2c	1542	0	1517	0	0
35	1d	1655	0	1672	0	0
35	2d	1674	0	1714	0	0
36	1e	1129	0	1185	0	0
36	2e	1133	0	1191	0	0
37	1f	810	0	804	0	0
37	2f	816	0	808	0	0
38	1g	1231	0	1238	0	0
38	2g	1235	0	1249	0	0
39	1h	1088	0	1126	0	0
39	2h	1088	0	1126	0	0
40	1i	983	0	986	0	0
40	2i	978	0	966	0	0
41	1j	709	0	650	0	0
41	2j	714	0	672	0	0
42	1k	829	0	825	0	0
42	2k	833	0	836	0	0
43	1l	932	0	981	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	932	0	981	0	0
44	1m	958	0	1002	0	0
44	2m	950	0	988	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0
46	1o	728	0	760	0	0
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	677	0	686	0	0
48	1q	823	0	891	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	652	0	662	0	0
50	2s	646	0	644	0	0
51	1t	728	0	798	0	0
51	2t	727	0	796	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1v	277	0	140	0	0
53	2v	277	0	140	0	0
54	1w	1592	0	819	0	0
54	1y	1585	0	804	0	0
54	2w	1544	0	788	0	0
54	2y	1565	0	795	0	0
55	1x	1625	0	828	0	0
55	2x	1625	0	828	0	0
56	10	9	0	0	0	0
56	11	4	0	0	0	0
56	12	2	0	0	0	0
56	13	3	0	0	0	0
56	15	2	0	0	0	0
56	16	3	0	0	0	0
56	17	3	0	0	0	0
56	18	3	0	0	0	0
56	19	1	0	0	0	0
56	1A	1146	0	0	0	0
56	1B	36	0	0	0	0
56	1D	12	0	0	0	0
56	1E	12	0	0	0	0
56	1F	8	0	0	0	0
56	1G	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1H	1	0	0	0	0
56	1I	1	0	0	0	0
56	1N	6	0	0	0	0
56	1O	8	0	0	0	0
56	1P	4	0	0	0	0
56	1Q	5	0	0	0	0
56	1R	2	0	0	0	0
56	1S	3	0	0	0	0
56	1T	1	0	0	0	0
56	1U	6	0	0	0	0
56	1V	3	0	0	0	0
56	1W	7	0	0	0	0
56	1X	5	0	0	0	0
56	1Y	3	0	0	0	0
56	1Z	4	0	0	0	0
56	1a	229	0	0	0	0
56	1b	2	0	0	0	0
56	1d	1	0	0	0	0
56	1e	2	0	0	0	0
56	1f	2	0	0	0	0
56	1h	1	0	0	0	0
56	1l	3	0	0	0	0
56	1m	1	0	0	0	0
56	1n	1	0	0	0	0
56	1o	1	0	0	0	0
56	1q	1	0	0	0	0
56	1r	1	0	0	0	0
56	1s	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	1	0	0	0	0
56	1w	11	0	0	0	0
56	1x	16	0	0	0	0
56	1y	4	0	0	0	0
56	20	3	0	0	0	0
56	23	3	0	0	0	0
56	25	4	0	0	0	0
56	26	1	0	0	0	0
56	27	1	0	0	0	0
56	28	1	0	0	0	0
56	2A	903	0	0	0	0
56	2B	21	0	0	0	0
56	2D	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2E	8	0	0	0	0
56	2F	4	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	2Q	4	0	0	0	0
56	2R	2	0	0	0	0
56	2T	2	0	0	0	0
56	2U	5	0	0	0	0
56	2V	2	0	0	0	0
56	2W	3	0	0	0	0
56	2X	2	0	0	0	0
56	2Y	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	244	0	0	0	0
56	2d	1	0	0	0	0
56	2e	1	0	0	0	0
56	2f	2	0	0	0	0
56	2g	1	0	0	0	0
56	2j	2	0	0	0	0
56	2l	3	0	0	0	0
56	2q	3	0	0	0	0
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	3	0	0	0	0
56	2w	9	0	0	0	0
56	2x	6	0	0	0	0
56	2y	7	0	0	0	0
57	1A	33	0	43	1	0
57	2A	33	0	43	1	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	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
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0
61	10	11	0	0	1	0
61	11	12	0	0	0	0
61	12	3	0	0	0	0
61	13	5	0	0	1	0
61	14	1	0	0	0	0
61	15	4	0	0	0	0
61	16	2	0	0	0	0
61	17	9	0	0	0	0
61	18	13	0	0	2	0
61	1A	2243	0	0	54	0
61	1B	69	0	0	1	0
61	1D	26	0	0	2	0
61	1E	28	0	0	6	0
61	1F	19	0	0	1	0
61	1G	6	0	0	3	0
61	1H	2	0	0	0	0
61	1I	2	0	0	0	0
61	1N	6	0	0	2	0
61	1O	7	0	0	0	0
61	1P	20	0	0	2	0
61	1Q	15	0	0	0	0
61	1R	12	0	0	0	0
61	1S	5	0	0	0	0
61	1T	10	0	0	1	0
61	1U	16	0	0	0	0
61	1V	10	0	0	1	0
61	1W	6	0	0	0	0
61	1X	6	0	0	1	0
61	1Y	4	0	0	0	0
61	1Z	1	0	0	0	0
61	1a	460	0	0	0	0
61	1b	1	0	0	0	0
61	1d	1	0	0	0	0
61	1f	1	0	0	0	0
61	1g	1	0	0	0	0
61	1l	9	0	0	0	0
61	1m	1	0	0	0	0
61	1o	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6l	1p	1	0	0	0	0
6l	1q	4	0	0	0	0
6l	1u	1	0	0	0	0
6l	1v	5	0	0	0	0
6l	1w	22	0	0	0	0
6l	1x	16	0	0	0	0
6l	1y	2	0	0	0	0
6l	20	4	0	0	0	0
6l	21	14	0	0	0	0
6l	22	2	0	0	0	0
6l	23	1	0	0	0	0
6l	25	5	0	0	1	0
6l	27	3	0	0	0	0
6l	28	4	0	0	0	0
6l	29	1	0	0	0	0
6l	2A	1395	0	0	72	0
6l	2B	28	0	0	0	0
6l	2D	25	0	0	0	0
6l	2E	15	0	0	1	0
6l	2F	14	0	0	0	0
6l	2I	4	0	0	0	0
6l	2N	1	0	0	0	0
6l	2O	1	0	0	0	0
6l	2P	14	0	0	2	0
6l	2Q	2	0	0	1	0
6l	2R	3	0	0	0	0
6l	2T	6	0	0	0	0
6l	2U	4	0	0	0	0
6l	2V	1	0	0	0	0
6l	2W	3	0	0	0	0
6l	2X	4	0	0	1	0
6l	2Y	1	0	0	0	0
6l	2Z	2	0	0	0	0
6l	2a	381	0	0	0	0
6l	2e	2	0	0	0	0
6l	2g	1	0	0	0	0
6l	2i	1	0	0	0	0
6l	2j	4	0	0	0	0
6l	2l	6	0	0	0	0
6l	2o	3	0	0	0	0
6l	2p	3	0	0	0	0
6l	2q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2r	1	0	0	0	0
61	2t	2	0	0	0	0
61	2u	1	0	0	0	0
61	2v	1	0	0	0	0
61	2w	3	0	0	0	0
61	2x	8	0	0	0	0
61	2y	19	0	0	0	0
All	All	301023	0	196772	2146	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (2146) 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:1128:U:H3	1:1A:1132:A:N6	1.27	1.29
1:2A:2138:C:N4	1:2A:2153:G:H1	1.48	1.09
1:2A:1002:G:H1	1:2A:1038:C:N4	42.43	1.05
1:1A:1128:U:O4	1:1A:1132:A:N1	1.88	1.04
1:1A:2158:C:N4	1:1A:2177:G:H1	1.57	1.01
1:1A:2149:G:H1	1:1A:2183:C:H42	1.01	0.99
1:2A:2099:U:H3	1:2A:2190:G:H1	0.99	0.97
1:2A:2129:C:N4	1:2A:2159:G:H1	1.61	0.97
1:1A:2149:G:H1	1:1A:2183:C:N4	1.62	0.95
1:2A:76:C:H42	1:2A:93:G:H1	27.11	0.95
1:1A:1004:A:N6	1:1A:1037:C:N3	55.45	0.94
1:1A:2158:C:H42	1:1A:2177:G:H1	1.05	0.93
1:1A:656:A:OP1	11:1P:65:ARG:NH1	2.02	0.92
1:2A:2121:G:H1	1:2A:2177:C:H42	1.17	0.92
1:2A:2136:C:N4	1:2A:2155:G:H1	1.68	0.91
22:20:10:THR:HG22	22:20:12:ASN:H	1.34	0.91
1:1A:2143:G:H1	1:1A:2199:C:H42	1.15	0.91
1:2A:2345:G:H4'	1:2A:2346:A:H5''	1.53	0.90
1:2A:1422:G:H5''	10:2O:48:PRO:HB3	100.05	0.90
1:1A:303:C:H42	1:1A:385:G:H1	1.19	0.90
1:2A:76:C:N4	1:2A:93:G:H1	26.30	0.89
1:1A:2440:G:OP1	61:1A:4201:HOH:O	1.89	0.88
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.38	0.88
1:2A:2127:G:N1	1:2A:2161:C:C4	2.41	0.88
1:2A:2127:G:C6	1:2A:2161:C:N4	2.41	0.88
1:1A:2160:C:H42	1:1A:2175:G:H1	1.19	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2158:C:N3	1:1A:2177:G:N2	2.22	0.87
1:2A:2807:G:N1	1:2A:2893:G:O6	2.08	0.86
1:2A:1002:G:N2	1:2A:1038:C:N3	41.81	0.85
1:2A:2129:C:H42	1:2A:2159:G:H1	0.87	0.85
1:2A:2127:G:C2	1:2A:2161:C:N3	2.45	0.84
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.10	0.84
1:2A:83:G:H1	1:2A:102:G:HO2'	1.26	0.84
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.60	0.84
1:1A:1100:A:N6	1:1A:1151:U:H3	1.75	0.84
1:2A:2589:A:OP1	61:2A:4001:HOH:O	1.95	0.84
1:2A:1002:G:H1	1:2A:1038:C:H42	42.71	0.83
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.60	0.83
1:1A:1111:U:O2	1:1A:1119:A:N6	2.11	0.83
12:2Q:85:LYS:HG2	22:20:7:LEU:HB3	1.60	0.83
1:1A:1105:G:H1	1:1A:1125:C:H42	1.26	0.83
1:2A:266:G:H5''	1:2A:268:C:H41	11.50	0.83
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.60	0.82
1:2A:2127:G:C2	1:2A:2161:C:C4	2.67	0.82
1:2A:1204:A:H2	1:2A:1241:A:H62	1.25	0.82
1:2A:1311:G:H2'	29:27:47:ARG:HH22	1.43	0.82
11:1P:100:LEU:HD12	11:1P:112:LEU:HD11	1.59	0.82
1:1A:2160:C:N4	1:1A:2175:G:H1	1.78	0.81
1:2A:854:G:H2'	1:2A:855:G:H8	1.45	0.81
1:1A:11:G:H2'	1:1A:12:U:H5''	1.62	0.81
1:2A:2127:G:N2	1:2A:2161:C:C2	2.49	0.81
1:1A:927:G:H2'	1:1A:928:G:H8	1.46	0.81
1:2A:882:G:H1	1:2A:894:C:H42	1.29	0.81
15:1T:16:ARG:HH21	15:1T:19:LEU:HD21	1.45	0.80
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.62	0.80
1:2A:2138:C:N3	1:2A:2153:G:N2	2.26	0.80
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.65	0.79
1:2A:450:G:O6	61:2A:4017:HOH:O	2.00	0.79
1:2A:2355:C:H1'	22:20:39:ARG:HH21	1.46	0.79
15:1T:112:ARG:HG3	15:1T:115:ARG:HH21	1.47	0.78
1:1A:1006:C:H42	1:1A:1023:G:H1	21.11	0.78
1:2A:424:G:N7	61:2A:4041:HOH:O	2.17	0.77
1:2A:1648:C:OP1	61:2A:4014:HOH:O	2.01	0.77
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.18	0.77
1:1A:2158:C:N4	1:1A:2177:G:N1	2.23	0.77
1:2A:2625:G:O6	61:2A:4018:HOH:O	2.03	0.77
1:1A:2143:G:H1	1:1A:2199:C:N4	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:23:6:VAL:HG13	25:23:56:VAL:HG22	1.68	0.76
1:2A:1671:U:OP2	61:2A:4002:HOH:O	2.02	0.76
1:1A:1140:U:H1'	1:1A:1143:U:H5	1.51	0.76
1:2A:2126:A:N6	1:2A:2162:G:O2'	2.19	0.76
1:2A:335:C:H4'	20:2Y:73:ARG:HD3	1.67	0.76
1:1A:1104:G:N2	1:1A:1126:C:N3	2.35	0.75
1:1A:2185:C:OP1	1:1A:2187:G:N2	2.19	0.75
26:24:46:GLN:HE21	26:24:48:ARG:HE	1.34	0.75
1:2A:1038:C:H42	1:2A:1117:G:H1	1.33	0.75
1:1A:2529:C:OP1	61:1A:4251:HOH:O	2.04	0.75
1:1A:2146:G:H1	1:1A:2196:C:H42	1.31	0.75
5:1F:53:THR:HG22	5:1F:56:GLU:HG3	1.69	0.75
22:10:11:ARG:O	22:10:14:ARG:NH2	2.18	0.75
5:1F:101:LEU:O	5:1F:106:ARG:NH1	2.20	0.75
1:1A:1104:G:H1	1:1A:1126:C:H42	1.28	0.75
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.20	0.74
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.69	0.74
1:1A:1006:C:N3	1:1A:1023:G:N2	22.64	0.74
11:1P:42:SER:O	61:1P:301:HOH:O	2.04	0.74
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.33	0.74
1:2A:1530:C:O2'	1:2A:1531:C:O5'	2.05	0.74
1:2A:2677:G:N3	61:2A:4049:HOH:O	2.20	0.74
4:2E:119:ARG:HD2	4:2E:160:TYR:HB2	1.68	0.74
4:1E:110:GLY:O	61:1E:401:HOH:O	2.05	0.74
18:2W:25:ARG:NH2	18:2W:74:ALA:O	2.19	0.74
1:1A:1202:A:OP1	16:1U:55:ARG:NH1	2.20	0.74
1:1A:2124:U:H3	1:1A:2209:G:H1	1.32	0.74
11:1P:89:ALA:O	11:1P:121:LYS:NZ	2.19	0.74
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.68	0.74
1:2A:2502:G:N7	61:2A:4054:HOH:O	2.20	0.74
1:2A:1566:A:OP1	3:2D:211:ARG:NH1	2.21	0.74
1:1A:2121:U:H3	1:1A:2212:G:H1	1.33	0.74
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.23	0.73
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.23	0.73
1:1A:1151:U:H2'	1:1A:1152:G:H8	1.53	0.73
1:1A:2122:G:H1	1:1A:2211:U:H3	1.36	0.73
15:1T:98:LYS:NZ	61:1T:8101:HOH:O	2.21	0.73
1:1A:2227:G:H3'	1:1A:2228:G:C8	2.23	0.73
1:2A:2657:A:O3'	7:2H:160:LYS:NZ	2.22	0.73
1:1A:928:G:N2	1:1A:943:C:O2	2.21	0.73
1:1A:2164:C:N3	1:1A:2171:G:O6	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:765:G:H1	1:2A:812:C:HO2'	83.65	0.72
1:1A:2128:G:H1	1:1A:2205:C:H42	1.35	0.72
1:2A:2121:G:H1	1:2A:2177:C:N4	1.87	0.72
1:1A:1221:G:N2	1:1A:1223:C:OP2	2.22	0.72
1:1A:1848:G:OP1	3:1D:88:ARG:NH2	2.22	0.72
1:2A:300:A:OP1	20:2Y:86:ARG:NH2	2.23	0.72
1:2A:1568:G:N7	61:2A:4071:HOH:O	2.23	0.71
1:1A:1104:G:H1	1:1A:1126:C:N4	1.88	0.71
1:1A:1516:A:OP2	61:1A:4252:HOH:O	2.08	0.71
9:2N:70:LYS:HD3	9:2N:87:LEU:HD12	1.72	0.71
1:1A:1100:A:N6	1:1A:1151:U:N3	2.37	0.71
1:2A:692:C:O2'	3:2D:38:LYS:NZ	2.24	0.71
1:1A:2205:C:H2'	1:1A:2206:G:H8	1.55	0.71
5:2F:101:LEU:O	5:2F:106:ARG:NH1	2.22	0.71
1:1A:1101:G:H1	1:1A:1150:C:H42	1.38	0.71
1:1A:1814:A:N7	61:1A:4297:HOH:O	2.24	0.71
1:1A:2849:G:H5'	13:1R:46:GLY:HA2	1.73	0.71
1:2A:296:C:O3'	20:2Y:95:LYS:NZ	2.23	0.71
1:1A:359:C:H4'	20:1Y:73:ARG:HD3	1.72	0.71
1:2A:1355:G:O6	61:2A:4019:HOH:O	2.05	0.71
1:2A:1356:G:OP2	61:2A:4023:HOH:O	2.09	0.71
1:2A:1603:A:OP1	61:2A:4020:HOH:O	2.08	0.71
1:2A:2287:A:H62	1:2A:2344:U:H3	1.37	0.71
1:2A:731:C:OP2	61:2A:4022:HOH:O	2.09	0.71
1:1A:2149:G:N2	1:1A:2183:C:N3	2.35	0.70
1:2A:2736:G:N2	1:2A:2768:C:O2	2.20	0.70
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.72	0.70
17:1V:78:LYS:O	61:1V:301:HOH:O	2.08	0.70
1:1A:1099:C:H42	1:1A:1152:G:H1	1.38	0.70
23:21:50:ARG:HG2	23:21:59:THR:HG22	1.73	0.70
26:24:24:THR:OG1	26:24:25:TYR:N	2.23	0.70
13:2R:67:LEU:HD13	13:2R:76:VAL:HG21	1.72	0.70
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.73	0.70
1:1A:2695:C:O2	10:1O:70:LYS:NZ	2.17	0.70
1:2A:1689:A:H62	1:2A:1698:A:H2	1.38	0.70
1:2A:677:A:OP1	61:2A:4021:HOH:O	2.08	0.70
1:1A:1151:U:H2'	1:1A:1152:G:C8	2.26	0.70
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.24	0.69
1:2A:1783:A:OP2	61:2A:4025:HOH:O	2.10	0.69
1:2A:775:G:O3'	61:2A:4024:HOH:O	2.10	0.69
1:1A:1785:C:H5	15:1T:96:ARG:HH21	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:119:ARG:HD2	4:1E:160:TYR:HB2	1.74	0.69
1:1A:1540:A:OP1	61:1A:4253:HOH:O	2.11	0.69
1:2A:582:G:OP2	61:2A:4027:HOH:O	2.11	0.69
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.55	0.69
1:2A:1441:G:O2'	61:2A:4026:HOH:O	2.10	0.69
1:2A:882:G:H2'	1:2A:883:G:H8	1.58	0.69
1:2A:2595:G:N7	61:2A:4079:HOH:O	2.24	0.69
1:1A:1055:A:OP2	9:1N:37:LYS:NZ	2.19	0.69
1:1A:2288:G:N7	61:1A:4307:HOH:O	2.26	0.69
1:1A:294:C:H42	1:1A:390:G:H1	1.41	0.68
1:1A:929:G:H1	1:1A:940:C:H42	1.41	0.68
1:2A:1434:A:H61	1:2A:1558:A:H62	1.41	0.68
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.75	0.68
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.26	0.68
1:2A:131:G:OP1	61:2A:4028:HOH:O	2.11	0.68
1:1A:1044:C:OP1	61:1A:4254:HOH:O	2.11	0.68
1:2A:2136:C:N4	1:2A:2155:G:N1	2.40	0.68
1:2A:1696:G:N7	61:2A:4082:HOH:O	2.24	0.68
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.27	0.68
1:2A:89:G:H3'	1:2A:90:U:H5''	1.75	0.68
1:2A:2152:G:C2	1:2A:2153:G:H1'	2.29	0.68
1:2A:1754:C:H5	15:2T:96:ARG:HH21	1.42	0.68
1:2A:2129:C:N3	1:2A:2159:G:N2	2.35	0.68
1:1A:2177:G:H3'	1:1A:2178:G:H8	1.60	0.67
1:1A:542:C:OP1	27:15:16:ARG:NH2	2.27	0.67
15:1T:24:PRO:HD3	15:1T:52:ILE:HD12	1.76	0.67
1:2A:2524:G:N7	61:2A:4095:HOH:O	2.26	0.67
1:1A:1684:A:OP1	61:1A:4255:HOH:O	2.12	0.67
1:1A:325:G:OP2	20:1Y:84:ARG:NH2	2.27	0.67
23:21:51:VAL:HG11	23:21:74:VAL:HG21	1.77	0.67
1:2A:643:A:N1	1:2A:2369:A:O2'	2.26	0.67
21:2Z:153:SER:HB3	21:2Z:167:PRO:HB3	1.75	0.67
1:2A:2138:C:H42	1:2A:2153:G:H1	0.72	0.67
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.75	0.67
1:1A:2286:A:OP2	61:1A:4258:HOH:O	2.13	0.67
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.76	0.67
1:1A:1346:U:H4'	1:1A:1347:A:H5''	1.76	0.67
1:1A:2718:G:N7	61:1A:4323:HOH:O	2.28	0.67
1:2A:2837:G:N7	61:2A:4108:HOH:O	2.28	0.67
18:1W:4:LYS:HD2	18:1W:6:ILE:HD11	1.77	0.67
4:2E:127:ASP:OD2	61:2E:401:HOH:O	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2641:A:O2'	1:1A:2642:G:OP2	2.12	0.66
1:2A:2171:A:N3	1:2A:2172:U:N3	2.43	0.66
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.10	0.66
5:2F:116:ASP:OD1	5:2F:119:ARG:NH2	2.28	0.66
1:1A:2297:C:OP2	28:16:6:ARG:NH1	2.28	0.66
1:2A:476:G:OP1	61:2A:4029:HOH:O	2.12	0.66
1:2A:2049:G:N7	61:2A:4112:HOH:O	2.28	0.66
1:1A:1115:A:H4'	1:1A:1116:A:H8	1.60	0.66
1:1A:555:G:N1	1:1A:2045:G:OP1	2.26	0.66
61:1E:401:HOH:O	13:1R:3:HIS:NE2	2.28	0.66
1:2A:818:G:OP2	61:2A:4030:HOH:O	2.13	0.66
17:2V:40:LEU:HB2	17:2V:46:VAL:HG22	1.77	0.66
1:1A:1117:G:H1'	1:1A:1135:G:H2'	1.77	0.66
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.27	0.66
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.29	0.66
1:1A:1500:A:OP2	61:1A:4259:HOH:O	2.13	0.66
1:1A:848:G:O6	5:1F:53:THR:OG1	2.13	0.66
1:2A:586:A:H5'	5:2F:89:VAL:HG21	1.78	0.66
1:1A:2595:G:OP2	61:1A:4256:HOH:O	2.13	0.66
1:1A:2419:G:OP1	61:1A:4257:HOH:O	2.13	0.66
1:2A:2148:G:H2'	1:2A:2149:G:H8	1.61	0.66
1:1A:1110:C:N3	1:1A:1120:G:O6	2.29	0.65
1:1A:2157:A:H5'	1:1A:2182:G:H4'	1.78	0.65
1:1A:1140:U:H1'	1:1A:1143:U:C5	2.31	0.65
1:1A:92:C:H2'	1:1A:93:G:H8	3.04	0.65
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.79	0.65
3:1D:242:ARG:H	3:1D:242:ARG:HH11	1.43	0.65
1:2A:2144:U:H1'	1:2A:2148:G:N2	2.12	0.65
1:2A:861:A:N3	2:2B:79:C:O2'	2.29	0.65
1:1A:232:U:OP1	30:18:6:THR:OG1	2.14	0.65
19:2X:57:LEU:HD11	19:2X:78:LYS:HE2	1.78	0.65
1:1A:1004:A:H5''	1:1A:1024:G:H1	27.67	0.65
1:1A:1697:G:OP2	61:1A:4260:HOH:O	2.13	0.65
1:1A:2832:G:OP2	61:1E:401:HOH:O	2.13	0.65
12:1Q:18:LYS:O	12:1Q:98:LYS:NZ	2.17	0.65
1:2A:2849:U:OP2	15:2T:95:ARG:NH1	2.30	0.65
19:1X:57:LEU:HD11	19:1X:78:LYS:HE2	1.78	0.65
24:22:32:LEU:HB2	24:22:53:LEU:HD22	1.79	0.65
1:2A:1119:C:H2'	1:2A:1120:G:C8	3.38	0.65
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.28	0.65
31:29:16:VAL:HG22	31:29:25:VAL:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:72:U:OP1	61:2A:4032:HOH:O	2.14	0.65
1:2A:994:C:H3'	16:2U:54:LYS:HE3	1.79	0.65
25:13:7:LYS:HB2	25:13:34:GLU:HG3	1.79	0.65
1:1A:2801:C:OP1	4:1E:61:ARG:NH2	2.30	0.65
6:1G:126:ASP:HB3	6:1G:128:ARG:H	1.60	0.65
1:2A:2448:A:OP1	61:2A:4031:HOH:O	2.14	0.65
1:2A:34:C:H2'	1:2A:35:G:H8	4.28	0.65
1:2A:568:U:H5'	1:2A:945:A:N1	2.12	0.65
1:1A:943:C:N3	1:1A:944:C:N4	2.45	0.64
4:1E:162:ALA:O	61:1E:402:HOH:O	2.14	0.64
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.80	0.64
1:2A:1007:C:N3	1:2A:1022:G:O6	16.75	0.64
1:2A:2042:A:OP1	61:2A:4034:HOH:O	2.14	0.64
1:2A:2882:A:OP1	13:2R:96:ARG:NH1	2.31	0.64
1:1A:2397:C:OP1	61:1A:4262:HOH:O	2.15	0.64
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.78	0.64
1:2A:1783:A:HO2'	1:2A:2607:G:HO2'	1.45	0.64
5:2F:40:GLN:NE2	5:2F:182:ASN:HB2	2.12	0.64
1:1A:347:G:C8	5:1F:171:PRO:HG3	2.32	0.64
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.14	0.64
10:2O:73:ASP:OD2	15:2T:32:TYR:OH	2.11	0.64
1:1A:1105:G:H1	1:1A:1125:C:N4	1.96	0.64
1:1A:2166:U:H3	1:1A:2169:G:H22	1.46	0.64
7:2H:23:ARG:NH1	7:2H:34:GLU:OE1	2.31	0.64
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.32	0.64
1:2A:711:G:N2	1:2A:720:C:O2	2.18	0.64
1:2A:925:C:H2'	1:2A:926:A:H8	1.63	0.64
2:1B:51:G:OP2	61:1B:3101:HOH:O	2.15	0.64
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.61	0.64
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.63	0.64
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.30	0.64
1:2A:987:G:H1	1:2A:1218:C:H42	46.53	0.64
1:1A:1517:G:N3	1:1A:1941:A:O2'	112.35	0.64
1:2A:882:G:H2'	1:2A:883:G:C8	2.33	0.64
1:1A:1513:G:HO2'	1:1A:1593:C:HO2'	1.42	0.63
1:1A:2735:G:OP2	61:1A:4264:HOH:O	2.15	0.63
6:1G:125:PHE:O	61:1G:3101:HOH:O	2.14	0.63
1:2A:2136:C:H42	1:2A:2155:G:H1	1.43	0.63
1:2A:2404:C:O3'	11:2P:77:ARG:NH2	2.31	0.63
1:2A:2759:G:OP2	61:2A:4036:HOH:O	2.15	0.63
1:1A:1717:C:OP1	61:1A:4263:HOH:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2710:C:N4	61:2A:4133:HOH:O	2.31	0.63
1:2A:900:A:O2'	1:2A:901:A:OP1	2.15	0.63
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.33	0.63
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.30	0.63
1:2A:974:G:OP1	1:2A:1187:G:O2'	2.15	0.63
1:1A:2112:G:O6	61:1A:4261:HOH:O	2.14	0.63
18:1W:25:ARG:NH2	18:1W:74:ALA:O	2.30	0.63
8:1I:12:LEU:HD22	8:1I:19:VAL:HG21	1.80	0.63
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.17	0.63
1:2A:76:C:N3	1:2A:93:G:N2	28.95	0.63
1:1A:2669:A:O3'	7:1H:160:LYS:NZ	2.32	0.63
1:2A:987:G:O2'	1:2A:1000:A:N3	2.31	0.63
2:2B:22:U:H3	2:2B:61:G:H22	1.46	0.63
20:2Y:77:PRO:HD2	20:2Y:106:LEU:HD23	1.80	0.63
1:1A:646:A:OP2	11:1P:108:LYS:NZ	2.32	0.63
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	1.81	0.63
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.32	0.63
7:1H:86:GLU:OE2	7:1H:132:ARG:NH2	2.31	0.63
18:1W:73:ALA:HB3	18:1W:106:ILE:HD12	1.79	0.63
1:2A:2165:G:H2'	1:2A:2166:G:O4'	1.99	0.63
6:2G:11:TYR:HA	6:2G:15:VAL:HB	1.79	0.63
8:1I:31:LEU:HD21	8:1I:38:LEU:HD23	1.81	0.62
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.16	0.62
1:1A:1829:U:H5'	3:1D:259:THR:HG22	1.81	0.62
17:1V:5:VAL:HG21	17:1V:35:LEU:HD23	1.80	0.62
1:2A:2141:G:O6	1:2A:2150:U:O2	2.17	0.62
1:2A:1971:A:OP1	61:2A:4038:HOH:O	2.16	0.62
1:2A:236:C:H2'	1:2A:237:C:C6	2.34	0.62
1:2A:852:G:H2'	1:2A:853:G:H8	1.63	0.62
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.14	0.62
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.00	0.62
7:1H:84:SER:OG	7:1H:132:ARG:NH1	2.32	0.62
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.35	0.62
1:2A:625:G:N7	11:2P:107:LYS:NZ	2.40	0.62
14:2S:15:ARG:HB3	14:2S:19:LYS:HE3	1.81	0.62
1:1A:85:C:H4'	1:1A:102:U:H1'	1.81	0.62
6:1G:41:GLN:HB3	6:1G:43:LEU:HD13	1.80	0.62
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.17	0.62
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.82	0.62
1:1A:231:G:C8	30:18:5:LYS:HG2	2.35	0.62
1:1A:890:G:O2'	1:1A:906:G:O6	46.43	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1762:A:N1	61:2A:4135:HOH:O	2.31	0.62
1:2A:2218:U:H1'	23:21:52:ARG:HH12	1.64	0.62
1:2A:330:A:H2	1:2A:1210:A:HO2'	1.46	0.62
1:1A:2177:G:H3'	1:1A:2178:G:C8	2.35	0.62
1:2A:2136:C:N3	1:2A:2155:G:N2	2.38	0.62
1:1A:1435:G:H2'	1:1A:1436:U:C6	3.20	0.61
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.34	0.61
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.64	0.61
1:2A:860:U:H1'	1:2A:2268:A:H5'	1.81	0.61
1:2A:878:A:H61	1:2A:899:A:H1'	1.66	0.61
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.00	0.61
7:2H:122:THR:HB	7:2H:134:SER:HB2	1.81	0.61
6:1G:3:LEU:O	6:1G:8:LYS:NZ	2.24	0.61
7:1H:17:VAL:HG22	7:1H:26:VAL:HG22	1.82	0.61
1:2A:646:A:H2'	1:2A:647:G:O4'	2.00	0.61
17:2V:46:VAL:HG23	17:2V:52:VAL:HG11	1.82	0.61
1:2A:84:A:H5'	20:2Y:8:LYS:HG2	1.80	0.61
1:1A:2178:G:H2'	1:1A:2179:G:C2	2.35	0.61
1:2A:307:G:H21	1:2A:330:A:H62	1.48	0.61
1:1A:2156:A:OP2	1:1A:2178:G:N2	2.33	0.61
1:1A:2658:C:OP2	1:1A:2745:G:O2'	2.17	0.61
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.33	0.61
1:1A:1633:A:H2'	1:1A:1634:C:C6	2.35	0.61
1:2A:2127:G:C5	1:2A:2161:C:N4	2.69	0.61
1:2A:276:A:H5''	1:2A:277:C:H5'	1.82	0.61
1:2A:764:A:H5'	3:2D:210:GLY:HA2	1.83	0.61
1:1A:1827:U:H2'	1:1A:1828:C:C6	2.36	0.61
1:1A:302:A:H2'	1:1A:303:C:C6	2.36	0.61
5:1F:167:ALA:HB1	5:1F:173:VAL:HG11	1.83	0.61
1:2A:1970:A:OP1	61:2A:4038:HOH:O	2.16	0.61
1:2A:2128:C:N3	1:2A:2160:G:O6	2.33	0.61
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.82	0.61
1:2A:2280:G:N7	61:2A:4132:HOH:O	2.31	0.61
1:2A:1826:G:H4'	3:2D:242:ARG:HH21	1.66	0.61
1:1A:2153:G:N2	1:1A:2180:A:N1	2.49	0.60
1:1A:2340:A:H2'	1:1A:2341:G:C8	2.36	0.60
1:2A:194:G:N7	61:2A:4137:HOH:O	2.31	0.60
1:1A:1475:G:H2'	1:1A:1476:C:C6	2.36	0.60
2:1B:14:U:OP2	2:1B:70:C:O2'	2.17	0.60
1:2A:1218:C:H42	1:2A:1231:G:H1	1.49	0.60
1:2A:2148:G:H2'	1:2A:2149:G:C8	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.35	0.60
1:2A:674:G:H2'	1:2A:675:A:H8	4.97	0.60
13:1R:33:ARG:HG2	13:1R:115:GLU:HB3	1.84	0.60
21:1Z:72:ARG:NH2	21:1Z:97:GLU:O	2.34	0.60
1:2A:122:G:N3	61:2A:4138:HOH:O	2.32	0.60
9:2N:58:ASP:N	9:2N:58:ASP:OD1	2.31	0.60
23:11:3:LYS:HB2	23:11:61:ARG:HH12	1.64	0.60
1:1A:2762:A:OP1	7:1H:3:ARG:NH1	2.34	0.60
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.83	0.60
1:2A:1119:C:H2'	1:2A:1120:G:H8	2.62	0.60
1:2A:1310:G:H1	1:2A:1327:C:H42	26.41	0.60
1:2A:2127:G:C6	1:2A:2161:C:C4	2.88	0.60
57:2A:3897:MT9:H5	57:2A:3897:MT9:H9	1.84	0.60
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.15	0.60
1:2A:2871:C:N4	61:2A:4160:HOH:O	2.34	0.60
26:14:53:GLU:HB2	26:14:55:ARG:H	1.66	0.60
26:14:56:VAL:HB	26:14:60:GLN:HG3	1.83	0.60
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.36	0.60
1:1A:153:C:H42	1:1A:168:G:H1	25.37	0.60
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.36	0.60
1:1A:1071:G:C4	1:1A:1180:C:H1'	2.37	0.60
1:1A:166:G:H2'	1:1A:167:G:H8	3.56	0.60
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.74	0.60
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.66	0.60
6:1G:143:GLU:O	26:14:28:LYS:NZ	2.35	0.59
2:1B:1:U:O2'	2:1B:2:C:OP1	2.19	0.59
1:2A:2317:C:N4	1:2A:2318:G:O6	2.35	0.59
2:2B:91:C:OP2	12:2Q:16:ARG:NH1	2.35	0.59
1:1A:2133:C:N3	1:1A:2167:C:O2'	2.31	0.59
1:1A:2205:C:H2'	1:1A:2206:G:C8	2.37	0.59
1:1A:2495:C:N3	12:1Q:124:LYS:NZ	2.50	0.59
1:1A:968:U:H2'	1:1A:969:C:C6	2.37	0.59
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.84	0.59
1:1A:1006:C:N4	1:1A:1023:G:N1	22.15	0.59
1:1A:1211:U:H2'	1:1A:1212:C:C6	2.36	0.59
1:1A:2564:2MU:O5'	1:1A:2564:2MU:H6	2.03	0.59
12:1Q:16:ARG:HG3	12:1Q:18:LYS:HG3	1.84	0.59
1:1A:946:A:O2'	1:1A:1333:A:N3	123.69	0.59
5:2F:103:LYS:HA	5:2F:106:ARG:HG3	1.84	0.59
1:1A:2164:C:O2	1:1A:2171:G:N1	2.27	0.59
7:1H:56:SER:OG	7:1H:57:ASP:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.37	0.59
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.37	0.59
26:14:57:GLU:HB3	26:14:58:ARG:HD2	1.85	0.59
1:1A:1087:C:H42	1:1A:1160:G:H1	1.50	0.59
1:1A:2150:C:H42	1:1A:2182:G:H1	1.47	0.59
1:2A:662:G:O2'	1:2A:836:G:OP1	26.26	0.59
28:26:34:LEU:HB2	28:26:51:GLU:HB3	1.85	0.59
1:2A:1633:G:OP2	61:2A:4040:HOH:O	2.17	0.59
1:1A:1104:G:N1	1:1A:1126:C:N4	2.39	0.59
1:2A:2278:A:OP2	22:20:12:ASN:ND2	2.35	0.59
1:1A:153:C:N4	1:1A:168:G:H1	25.30	0.59
1:1A:16:G:N2	61:1A:4292:HOH:O	2.22	0.59
1:1A:2290:A:OP2	22:10:12:ASN:ND2	2.33	0.59
21:2Z:4:ARG:HG2	21:2Z:58:VAL:HB	1.84	0.59
1:1A:1305:G:N2	1:1A:1331:G:H1'	39.95	0.58
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.84	0.58
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.21	0.58
1:1A:2146:G:H1	1:1A:2196:C:N4	2.00	0.58
6:1G:109:VAL:HG11	26:14:14:ILE:HG21	1.86	0.58
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.85	0.58
1:1A:1817:A:H1'	1:1A:1960:A:N6	2.18	0.58
1:2A:859:G:N2	1:2A:917:A:OP2	2.35	0.58
17:2V:72:VAL:HG13	17:2V:85:LYS:HB3	1.85	0.58
1:1A:2128:G:H1	1:1A:2205:C:N4	2.02	0.58
21:1Z:91:LEU:HD23	21:1Z:130:PRO:HB3	1.86	0.58
6:2G:179:PRO:HB2	26:24:42:PHE:HE2	1.67	0.58
1:1A:1219:A:H4'	1:1A:1220:U:OP1	2.02	0.58
1:2A:1021:A:H62	1:2A:1141:U:H3	1.51	0.58
1:2A:2144:U:H1'	1:2A:2148:G:H22	1.67	0.58
1:2A:984:A:H5''	1:2A:985:C:H5	1.68	0.58
7:2H:86:GLU:OE2	7:2H:132:ARG:NH2	2.36	0.58
1:1A:927:G:H2'	1:1A:928:G:C8	2.33	0.58
3:1D:85:ASP:OD2	3:1D:88:ARG:NH1	2.29	0.58
6:1G:38:VAL:HG22	6:1G:93:THR:HG23	1.83	0.58
9:1N:43:THR:HB	9:1N:48:MET:HE1	1.85	0.58
14:1S:61:ASN:HB3	14:1S:64:GLU:HB2	1.86	0.58
18:2W:12:ILE:O	18:2W:101:SER:OG	2.21	0.58
25:23:10:LYS:HB3	25:23:53:LEU:HA	1.86	0.58
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.17	0.58
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.39	0.58
6:2G:17:PRO:HA	6:2G:20:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:18:23:VAL:HG11	30:18:47:LYS:HD3	1.86	0.58
4:2E:59:VAL:HG21	4:2E:74:PRO:HB3	1.86	0.58
4:2E:77:ILE:HD13	4:2E:195:LEU:HD22	1.85	0.58
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.84	0.58
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.37	0.58
1:1A:1810:U:OP2	61:1A:4267:HOH:O	2.17	0.58
5:1F:56:GLU:OE1	5:1F:93:LYS:NZ	2.36	0.58
1:1A:2247:G:N7	61:1A:4349:HOH:O	2.32	0.57
1:2A:1826:G:H4'	3:2D:242:ARG:NH2	2.19	0.57
1:1A:2744:G:OP1	4:1E:169:ASN:ND2	2.36	0.57
4:1E:48:GLN:NE2	4:1E:78:LEU:HD23	2.19	0.57
6:1G:73:ALA:HB3	6:1G:85:GLY:H	1.68	0.57
1:1A:2013:U:H2'	1:1A:2014:G:H5''	1.87	0.57
1:1A:606:G:N2	1:1A:632:A:N7	49.75	0.57
1:2A:2379:G:O2'	14:2S:17:ARG:NH2	2.37	0.57
1:2A:668:G:H5'	1:2A:669:G:OP2	2.04	0.57
1:1A:1971:G:O6	61:1A:4265:HOH:O	2.16	0.57
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.85	0.57
18:2W:18:ARG:HG2	18:2W:76:VAL:HB	1.86	0.57
28:16:10:LEU:HG	28:16:54:ILE:HG13	1.86	0.57
30:28:23:VAL:HG11	30:28:47:LYS:HD3	1.86	0.57
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.40	0.57
1:2A:1639:U:H2'	1:2A:1640:C:H5''	1.85	0.57
1:2A:62:C:H42	1:2A:93:G:H1	1.52	0.57
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.87	0.57
1:1A:1059:C:OP2	61:1A:4270:HOH:O	2.17	0.57
1:1A:1404:G:OP2	61:1A:4268:HOH:O	2.17	0.57
2:1B:92:C:OP1	21:1Z:79:ARG:NH1	2.37	0.57
1:1A:1076:G:OP2	12:1Q:128:LYS:NZ	2.38	0.57
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.85	0.57
1:1A:1452:U:H2'	1:1A:1453:C:C6	2.39	0.57
1:1A:2175:G:H2'	1:1A:2176:G:C8	2.40	0.57
1:1A:2255:U:OP1	61:1A:4272:HOH:O	2.18	0.57
1:2A:923:C:H2'	1:2A:924:C:C6	2.40	0.57
1:2A:973:A:OP2	61:2A:4039:HOH:O	2.17	0.57
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.39	0.57
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.05	0.57
11:2P:36:LYS:O	61:2P:201:HOH:O	2.18	0.57
15:2T:65:LYS:HE3	15:2T:67:SER:HB2	1.87	0.57
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.40	0.57
1:2A:1034:G:O6	61:2A:4033:HOH:O	2.14	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.87	0.56
1:1A:1898:A:H2'	1:1A:1899:A:C8	2.39	0.56
1:1A:2324:U:H5'	6:1G:88:ILE:HD11	1.87	0.56
11:1P:59:LEU:HD21	30:18:10:ALA:HA	1.87	0.56
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.40	0.56
1:2A:2502:G:OP1	61:2A:4042:HOH:O	2.17	0.56
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.86	0.56
29:17:46:VAL:HG13	29:17:48:LYS:HE3	1.87	0.56
1:1A:271:U:H1'	8:1I:50:ARG:HE	1.70	0.56
1:2A:1024:G:HO2'	1:2A:1144:G:HO2'	1.51	0.56
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.40	0.56
27:25:2:ALA:N	61:25:201:HOH:O	2.37	0.56
30:18:6:THR:HG23	30:18:64:TYR:HD2	1.71	0.56
1:1A:1058:U:O4	9:1N:28:THR:HG21	2.05	0.56
1:1A:1085:G:H1	1:1A:1162:C:H42	1.53	0.56
1:2A:1253:A:OP1	61:2A:4043:HOH:O	2.18	0.56
1:2A:2590:A:O3'	3:2D:239:ARG:NH2	2.38	0.56
1:2A:1693:U:H1'	3:2D:14:ARG:NH2	2.21	0.56
1:1A:1069:U:OP2	61:1A:4274:HOH:O	2.18	0.56
1:1A:1159:U:H2'	1:1A:1160:G:C8	2.41	0.56
16:1U:97:ASP:OD1	16:1U:101:ARG:NH1	2.39	0.56
1:2A:309:G:N3	1:2A:329:G:O2'	2.36	0.56
21:2Z:154:ASP:N	21:2Z:154:ASP:OD1	2.38	0.56
1:1A:2892:A:OP1	13:1R:96:ARG:NH1	2.38	0.56
25:23:7:LYS:NZ	25:23:34:GLU:OE1	2.32	0.56
30:28:28:GLY:O	30:28:36:LYS:NZ	2.38	0.56
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.40	0.56
1:2A:822:U:OP2	61:2A:4044:HOH:O	2.18	0.56
1:1A:1425:A:H4'	1:1A:1426:G:OP2	2.05	0.56
1:1A:1995:G:OP1	61:1A:4271:HOH:O	2.17	0.56
19:1X:88:LYS:HE2	19:1X:93:GLU:HG3	1.86	0.56
1:2A:2375:G:N2	1:2A:2378:A:OP2	2.37	0.56
12:1Q:35:VAL:HG13	12:1Q:130:LYS:HB3	1.87	0.56
16:2U:29:SER:OG	16:2U:30:LYS:NZ	2.37	0.56
1:1A:976:G:H5'	1:1A:1358:U:O2'	103.31	0.56
1:1A:2289:G:OP2	22:10:10:THR:HG21	2.06	0.56
1:2A:136:G:H1	1:2A:143(A):C:H42	1.52	0.56
1:2A:2624:G:N7	61:2A:4148:HOH:O	2.33	0.56
1:1A:1699:A:OP1	13:1R:8:ARG:NH1	2.39	0.56
1:1A:2159:C:H2'	1:1A:2160:C:C6	2.41	0.56
1:1A:2339:A:H2'	1:1A:2340:A:C8	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.39	0.56
1:1A:1091:A:H5'	1:1A:1092:A:H5'	1.88	0.56
1:1A:1402:G:OP2	61:1A:4269:HOH:O	2.17	0.56
1:1A:173:C:H2'	1:1A:174:U:C6	2.41	0.56
1:1A:2160:C:N3	1:1A:2175:G:N2	2.49	0.56
1:2A:2223:G:OP1	3:2D:172:TYR:OH	2.23	0.56
1:2A:258:G:H2'	1:2A:259:G:H8	2.51	0.56
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.30	0.56
1:1A:1232:G:H5''	17:1V:81:TYR:CE1	2.42	0.55
1:1A:131:C:O2	1:1A:231:G:N2	72.17	0.55
1:1A:1405:A:H2'	1:1A:1406:A:H5'	1.87	0.55
17:1V:46:VAL:HG23	17:1V:52:VAL:HG11	1.88	0.55
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.24	0.55
1:1A:166:G:H2'	1:1A:167:G:C8	3.88	0.55
1:1A:238:C:O2	30:18:12:LYS:NZ	2.36	0.55
1:1A:673:G:H2'	1:1A:674:G:C8	3.12	0.55
6:1G:64:THR:HB	6:1G:94:LEU:HD21	1.88	0.55
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.39	0.55
1:2A:1693:U:H1'	3:2D:14:ARG:HH22	1.70	0.55
1:2A:2116:G:N2	1:2A:2162:G:OP1	2.39	0.55
14:2S:92:TYR:HB3	14:2S:98:VAL:HG21	1.88	0.55
23:21:83:GLU:N	23:21:83:GLU:OE1	2.40	0.55
1:2A:465:G:OP1	29:27:12:ARG:NH2	2.39	0.55
3:2D:242:ARG:H	3:2D:242:ARG:HH11	1.53	0.55
3:2D:242:ARG:HD3	3:2D:246:PRO:HG3	1.87	0.55
6:2G:28:VAL:O	6:2G:31:VAL:HG12	2.06	0.55
1:1A:1123:A:H2'	1:1A:1124:U:H4'	1.88	0.55
1:1A:215:G:H21	1:1A:217:A:H62	1.54	0.55
1:1A:2389:A:H2'	1:1A:2390:A:C8	2.42	0.55
1:1A:2859:U:H4'	1:1A:2878:A:C2	2.42	0.55
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.88	0.55
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.42	0.55
1:2A:251:A:C5	1:2A:252:G:H1'	2.42	0.55
1:2A:839:U:H2'	1:2A:840:C:C6	2.42	0.55
11:1P:126:VAL:HG12	11:1P:148:LEU:HD23	1.88	0.55
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	1.87	0.55
1:1A:1006:C:N4	1:1A:1023:G:H1	21.70	0.55
1:1A:1816:A:OP2	61:1A:4275:HOH:O	2.18	0.55
1:1A:2897:U:H2'	1:1A:2898:C:C6	2.42	0.55
3:1D:242:ARG:NH1	61:1D:403:HOH:O	2.39	0.55
1:1A:950:C:O2'	21:1Z:169:GLU:OE2	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1027:A:C2	1:2A:2488:A:H5'	2.41	0.55
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.89	0.55
1:2A:2313:C:H5''	6:2G:91:ARG:HD3	1.89	0.55
1:1A:739:C:O2'	3:1D:38:LYS:NZ	2.34	0.55
1:1A:843:C:H2'	1:1A:844:C:C6	2.41	0.55
1:2A:2096:U:H3	1:2A:2193:G:H1	1.55	0.55
1:2A:2638:G:P	4:2E:82:ARG:HH12	2.30	0.55
1:2A:531:C:OP1	1:2A:561:G:N1	2.39	0.55
1:2A:923:C:H2'	1:2A:924:C:H6	1.71	0.55
6:2G:131:TYR:HE2	6:2G:133:LEU:HD23	1.70	0.55
6:2G:41:GLN:HB3	6:2G:43:LEU:HD13	1.89	0.55
13:1R:28:LEU:HD23	13:1R:48:VAL:HG21	1.88	0.55
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.06	0.55
30:18:6:THR:HG22	30:18:63:PRO:HD2	1.89	0.54
1:1A:776:G:C8	3:1D:208:LYS:HD2	2.42	0.54
4:1E:111:ARG:HG3	4:1E:111:ARG:HH11	1.73	0.54
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.72	0.54
2:2B:24:G:H4'	2:2B:25:A:C8	2.42	0.54
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.71	0.54
3:2D:17:THR:O	3:2D:211:ARG:NH2	2.40	0.54
2:1B:24:G:N7	2:1B:56:G:H2'	2.21	0.54
8:1I:5:LEU:HD11	8:1I:19:VAL:HG22	1.89	0.54
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.69	0.54
1:1A:1099:C:N4	1:1A:1152:G:H1	2.04	0.54
1:1A:2262:G:OP1	12:1Q:85:LYS:NZ	2.35	0.54
18:1W:71:VAL:HA	18:1W:107:LEU:HD12	1.88	0.54
1:1A:321:C:H5''	20:1Y:87:LYS:HG3	1.90	0.54
1:2A:1452:A:OP2	61:2A:4047:HOH:O	2.18	0.54
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.42	0.54
1:1A:704:U:H2'	1:1A:705:C:C6	2.43	0.54
1:2A:880:G:H2'	1:2A:881:G:H8	1.72	0.54
1:2A:1818:U:H2'	3:2D:157:ARG:HD2	1.89	0.54
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	1.88	0.54
1:1A:2317:A:H5''	6:1G:134:GLY:HA3	1.90	0.54
1:2A:1286:A:C8	1:2A:1287:A:H4'	8.17	0.54
1:2A:775:G:N3	61:2A:4157:HOH:O	2.33	0.54
1:1A:1556:A:H3'	1:1A:1557:A:H8	1.73	0.54
8:1I:69:LYS:HG3	8:1I:138:ILE:HG12	1.89	0.54
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.41	0.54
5:2F:155:LEU:HB2	5:2F:189:THR:HG21	1.88	0.54
5:2F:32:LEU:O	5:2F:36:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1108:G:P	1:1A:1116:A:H1'	2.48	0.54
1:1A:167:G:H2'	1:1A:168:G:C8	3.14	0.54
1:1A:273:G:O2'	1:1A:274:U:H5''	2.08	0.54
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.88	0.54
1:1A:83:A:H5''	20:1Y:8:LYS:HG2	1.90	0.54
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.90	0.54
1:2A:2502:G:H5''	1:2A:2503:2MA:H5''	1.89	0.54
1:1A:1874:C:H5'	3:1D:253:GLN:OE1	2.07	0.54
4:1E:111:ARG:HD2	4:1E:160:TYR:CD2	2.43	0.54
1:1A:2800:C:H1'	4:1E:62:PRO:HG3	1.88	0.54
4:2E:12:THR:HG22	4:2E:13:ARG:H	1.73	0.54
5:2F:143:ALA:HB1	5:2F:148:LEU:HB2	1.90	0.54
9:2N:62:VAL:HG22	9:2N:66:LYS:HD2	1.89	0.54
10:2O:68:GLU:OE1	10:2O:78:ARG:NH1	2.39	0.54
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.90	0.54
1:1A:2442:A:H2'	1:1A:2442:A:N3	2.23	0.54
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	1.89	0.54
17:1V:43:GLU:N	17:1V:43:GLU:OE1	2.38	0.54
18:1W:86:LEU:HD22	18:1W:96:ILE:HD11	1.88	0.54
1:2A:987:G:H1	1:2A:1218:C:N4	46.16	0.54
1:2A:247:G:H4'	1:2A:386:G:C5	2.42	0.54
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.90	0.54
1:2A:605:C:O2	1:2A:657:U:O2'	2.20	0.54
15:2T:127:ALA:C	15:2T:129:ARG:H	2.10	0.54
20:2Y:92:ASN:N	20:2Y:93:GLY:HA2	2.22	0.54
1:1A:1004:A:C5'	1:1A:1024:G:H1	27.56	0.54
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.43	0.54
1:2A:857:C:OP1	22:20:69:PHE:HD2	1.91	0.54
10:1O:64:ARG:HD2	10:1O:79:PHE:CD1	2.43	0.53
1:1A:1201:A:OP1	16:1U:55:ARG:HD2	2.08	0.53
1:1A:2147:G:N1	1:1A:2194:U:OP1	2.24	0.53
1:2A:848:G:N9	1:2A:933:A:H8	2.07	0.53
1:1A:1810:U:H2'	61:1A:4297:HOH:O	2.09	0.53
6:1G:126:ASP:HB2	6:1G:130:ASN:H	1.74	0.53
1:2A:1007:C:O2	1:2A:1022:G:N1	18.40	0.53
1:2A:1147:C:H2'	1:2A:1148:A:H8	1.73	0.53
1:1A:2008:A:OP2	61:1A:4277:HOH:O	2.19	0.53
1:2A:1833:U:O2'	1:2A:1969:A:N1	2.40	0.53
1:2A:1423:G:H2'	1:2A:1424:G:H8	1.72	0.53
1:2A:817:C:N4	1:2A:1529:G:O6	112.06	0.53
1:2A:918:A:C2	2:2B:80:U:H4'	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1785:C:H5	15:1T:96:ARG:NH2	2.07	0.53
1:2A:1152:C:H2'	1:2A:1153:C:H6	1.73	0.53
1:2A:1530:C:H1'	1:2A:1531:C:OP1	2.09	0.53
1:2A:2126:A:N3	1:2A:2127:G:H1'	2.24	0.53
1:2A:988:A:N7	61:2A:4159:HOH:O	2.34	0.53
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.91	0.53
25:13:30:ARG:NH1	61:13:5001:HOH:O	2.22	0.53
1:1A:1053:C:H5''	9:1N:35:ARG:HH11	1.73	0.53
1:1A:1154:U:H2'	1:1A:1155:C:O4'	2.09	0.53
1:2A:2203:U:O4'	3:2D:151:LYS:HE2	2.09	0.53
3:2D:11:PRO:O	3:2D:14:ARG:HG3	2.09	0.53
5:2F:140:LEU:HD11	5:2F:170:LEU:HD11	1.90	0.53
7:2H:159:GLU:HG3	7:2H:169:VAL:HG11	1.90	0.53
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.08	0.53
28:16:8:LYS:HD3	30:18:34:TRP:CD2	2.44	0.53
1:1A:2328:C:O2'	6:1G:128:ARG:NH2	2.42	0.53
8:1I:4:ILE:HG12	8:1I:18:VAL:HG22	1.91	0.53
1:2A:854:G:H2'	1:2A:855:G:C8	2.35	0.53
1:2A:903:C:H2'	1:2A:904:C:C6	2.43	0.53
11:2P:100:LEU:HD12	11:2P:112:LEU:HD11	1.91	0.53
1:1A:776:G:C6	3:1D:208:LYS:HB2	2.44	0.53
1:2A:1031:G:H5''	31:29:8:LYS:HE3	1.91	0.53
1:2A:2250:G:OP1	12:2Q:85:LYS:NZ	2.41	0.53
2:2B:24:G:N7	2:2B:56:G:H2'	2.24	0.53
1:1A:704:U:H2'	1:1A:705:C:H6	1.75	0.52
1:2A:2127:G:C2	1:2A:2161:C:C2	2.93	0.52
1:1A:1037:C:H2'	1:1A:1038:C:H6	1.96	0.52
1:1A:1040:C:OP2	16:1U:54:LYS:NZ	2.38	0.52
1:1A:1566:U:H2'	1:1A:1567:G:O4'	2.09	0.52
1:1A:1740:U:H1'	3:1D:14:ARG:NH2	2.25	0.52
1:1A:2044:U:O2'	1:1A:2629:C:H5'	2.08	0.52
1:1A:611:U:H2'	1:1A:612:C:C6	2.44	0.52
4:1E:60:ASN:ND2	4:1E:62:PRO:HD2	2.24	0.52
20:1Y:7:VAL:HG21	20:1Y:72:VAL:HG12	1.90	0.52
20:1Y:92:ASN:N	20:1Y:93:GLY:HA2	2.25	0.52
1:2A:518:G:H2'	1:2A:519:U:C6	2.45	0.52
22:10:10:THR:HG22	22:10:12:ASN:H	1.75	0.52
1:1A:1535:U:HO2'	1:1A:1536:A:H8	1.58	0.52
1:1A:1720:U:OP1	61:1A:4280:HOH:O	2.19	0.52
1:1A:1912:A:OP2	61:1A:4281:HOH:O	2.19	0.52
13:1R:12:ARG:O	13:1R:17:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2498:C:H3'	61:2A:4006:HOH:O	2.09	0.52
1:1A:2642:G:H2'	1:1A:2643:G:C8	2.44	0.52
1:1A:2803:A:H5'	1:1A:2902:G:H21	1.74	0.52
1:2A:851:U:O2'	25:23:42:ALA:O	2.27	0.52
1:2A:2031:A:N3	1:2A:2455:G:O2'	2.37	0.52
1:2A:322:A:H5'	1:2A:340:A:H1'	1.91	0.52
1:2A:833:U:H2'	1:2A:834:C:C6	3.08	0.52
1:1A:1634:C:H2'	1:1A:1635:C:H6	1.75	0.52
1:1A:1834:A:O2'	3:1D:259:THR:HG21	2.10	0.52
6:1G:45:GLU:OE2	61:1G:3102:HOH:O	2.19	0.52
1:2A:2291:U:H2'	1:2A:2292:C:H6	1.73	0.52
1:2A:93:G:H2'	1:2A:94:C:C6	2.45	0.52
1:1A:1992:A:OP1	61:1A:4278:HOH:O	2.19	0.52
1:1A:931:C:H42	1:1A:938:G:H1	1.58	0.52
7:1H:89:ILE:O	7:1H:129:THR:OG1	2.27	0.52
7:1H:4:ILE:O	7:1H:69:ARG:HD2	2.09	0.52
15:1T:127:ALA:C	15:1T:129:ARG:H	2.12	0.52
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.27	0.52
7:2H:3:ARG:NH1	7:2H:5:GLY:H	2.08	0.52
1:2A:2641:G:H5''	9:2N:76:SER:HB3	1.91	0.52
23:21:8:SER:HB3	23:21:66:HIS:CD2	2.44	0.52
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.09	0.52
1:2A:2128:C:O2	1:2A:2160:G:N1	2.38	0.52
1:2A:453:C:O2	1:2A:457:A:O2'	2.28	0.52
10:2O:1:MET:HG3	10:2O:67:LYS:HG2	1.92	0.52
16:2U:104:GLN:NE2	16:2U:105:VAL:HG23	2.25	0.52
1:1A:265:U:H2'	1:1A:266:C:C6	2.45	0.52
9:1N:133:GLN:N	9:1N:133:GLN:OE1	2.41	0.52
1:2A:581:C:H2'	1:2A:582:G:C8	2.44	0.52
1:2A:796:C:H2'	1:2A:797:C:C6	2.45	0.52
3:2D:77:ALA:HB2	3:2D:97:TYR:CD1	2.45	0.52
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.91	0.52
8:2I:5:LEU:HD11	8:2I:19:VAL:HG22	1.91	0.52
1:1A:1159:U:H2'	1:1A:1160:G:H8	1.74	0.52
3:1D:26:LYS:HD3	3:1D:83:GLU:OE2	2.10	0.52
10:1O:120:GLU:HG2	10:1O:122:LEU:HG	1.92	0.52
1:2A:531:C:H4'	1:2A:532:A:H5''	1.92	0.52
1:2A:601:C:O2	1:2A:605:C:H4'	2.09	0.52
10:2O:80:ASP:OD2	15:2T:64:ARG:NH2	2.43	0.52
1:1A:2182:G:O6	1:1A:2183:C:N4	2.43	0.52
1:1A:2303:U:H2'	1:1A:2304:C:C6	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:641:G:OP2	5:1F:43:LYS:NZ	2.33	0.52
1:1A:847:A:OP1	1:1A:847:A:H8	1.93	0.52
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.92	0.52
26:24:18:CYS:SG	26:24:20:ASN:HB2	2.50	0.52
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.44	0.52
1:2A:2524:G:O6	61:2A:4045:HOH:O	2.18	0.52
6:2G:44:GLY:N	6:2G:88:ILE:O	2.43	0.52
1:1A:1320:A:N3	1:1A:1343:C:H1'	2.26	0.51
1:1A:2255:U:H2'	1:1A:2256:U:C6	2.45	0.51
1:1A:236:G:H4'	1:1A:413:G:C5	2.44	0.51
1:1A:2453:C:OP2	1:1A:2598:C:O2'	2.25	0.51
1:1A:559:U:H2'	1:1A:560:C:C6	2.45	0.51
12:1Q:81:VAL:HB	22:10:7:LEU:HD21	1.91	0.51
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.33	0.51
23:21:50:ARG:HD2	23:21:57:GLU:OE2	2.09	0.51
1:2A:1011:G:H1	1:2A:1018:C:H42	17.92	0.51
1:2A:1364:G:OP2	23:21:61:ARG:NH1	2.43	0.51
1:2A:2238:G:H5''	61:2A:4887:HOH:O	2.09	0.51
4:2E:4:ILE:HD12	4:2E:91:VAL:HG12	1.91	0.51
28:16:9:LEU:HD13	28:16:51:GLU:HB2	1.91	0.51
1:1A:1037:C:H2'	1:1A:1038:C:C6	2.70	0.51
1:1A:1405:A:H2	1:1A:1418:U:O4	1.93	0.51
1:1A:2880:C:H2'	1:1A:2881:C:O4'	2.10	0.51
1:1A:591:U:O5'	1:1A:990:A:N6	2.43	0.51
3:1D:2:ALA:HB1	3:1D:200:ASP:OD2	2.10	0.51
4:1E:77:ILE:HD13	4:1E:195:LEU:HD22	1.92	0.51
26:24:41:PRO:HG3	26:24:49:PHE:CZ	2.45	0.51
1:2A:918:A:O2'	2:2B:97:G:N2	2.42	0.51
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.10	0.51
6:2G:7:LEU:HD13	6:2G:104:GLU:HA	1.91	0.51
6:2G:11:TYR:O	6:2G:16:ARG:HB2	2.10	0.51
1:1A:395:C:OP2	61:1A:4276:HOH:O	2.19	0.51
1:1A:714:U:O2	30:18:2:PRO:HD2	2.10	0.51
1:1A:721:G:O2'	5:1F:74:ARG:HD3	2.10	0.51
24:22:1:MET:SD	24:22:56:GLN:NE2	2.84	0.51
1:2A:2820:A:C5	13:2R:4:LEU:HD11	2.46	0.51
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.45	0.51
1:2A:2712(A):A:OP2	61:2A:4046:HOH:O	2.18	0.51
13:2R:96:ARG:NH2	13:2R:117:VAL:HG13	2.26	0.51
1:1A:2476:C:H1'	61:1A:5905:HOH:O	2.11	0.51
3:1D:19:ALA:HB3	3:1D:21:PHE:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:37:LEU:HD13	3:1D:87:ASN:ND2	2.24	0.51
6:1G:34:LEU:HD23	6:1G:161:THR:HG22	1.91	0.51
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.93	0.51
18:1W:97:LYS:HE2	18:1W:99:ARG:NH2	2.26	0.51
26:24:14:ILE:HB	26:24:22:ILE:HB	1.90	0.51
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.39	0.51
1:2A:2315:G:H2'	1:2A:2316:C:H6	1.76	0.51
1:2A:336:C:H2'	1:2A:337:C:C6	2.91	0.51
1:2A:492:A:H2'	1:2A:493:G:O4'	2.10	0.51
2:2B:98:G:H3'	2:2B:99:G:H8	1.74	0.51
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HE2	1.92	0.51
1:1A:957:A:H2'	12:1Q:9:TYR:OH	2.10	0.51
1:1A:1040:C:OP1	16:1U:53:ARG:NH2	2.43	0.51
18:1W:78:GLU:OE2	18:1W:99:ARG:NH1	2.42	0.51
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.74	0.51
27:15:33:CYS:HB2	27:15:40:LYS:HD3	1.92	0.51
1:2A:1213:A:N3	1:2A:1238:G:O2'	2.38	0.51
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.11	0.51
1:2A:2303:G:O2'	6:2G:132:ASN:ND2	2.41	0.51
7:2H:137:ASP:HB3	7:2H:140:LYS:HB3	1.92	0.51
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.46	0.51
1:1A:1711:A:OP1	61:1A:4283:HOH:O	2.20	0.51
1:1A:181:C:OP1	61:1A:4282:HOH:O	2.19	0.51
1:1A:2801:C:O2'	1:1A:2819:A:N3	2.38	0.51
1:1A:925:A:N6	1:1A:945:A:O2'	2.41	0.51
7:1H:3:ARG:HH11	7:1H:4:ILE:H	1.57	0.51
11:1P:97:PRO:HD3	11:1P:126:VAL:O	2.11	0.51
28:26:9:LEU:HD13	28:26:51:GLU:HB2	1.93	0.51
31:29:2:LYS:NZ	31:29:31:LYS:O	2.39	0.51
1:2A:248:G:OP1	61:2A:4048:HOH:O	2.19	0.51
1:2A:774:A:N3	1:2A:774:A:H2'	2.26	0.51
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.45	0.51
22:10:4:LYS:NZ	61:10:201:HOH:O	2.43	0.51
29:17:12:ARG:NH2	29:17:44:PRO:HB3	2.26	0.51
1:2A:1300:U:H4'	1:2A:1301:A:H5''	1.92	0.51
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.23	0.51
8:2I:3:VAL:HG12	8:2I:38:LEU:HA	1.92	0.51
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.92	0.51
21:2Z:92:SER:OG	21:2Z:94:GLU:OE1	2.23	0.51
1:1A:1093:G:O2'	1:1A:1094:A:O5'	2.29	0.51
1:1A:292:G:N7	1:1A:305:G:N2	28.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:505:A:N3	1:1A:507:G:H5''	2.25	0.51
1:1A:831:A:N6	3:1D:229:VAL:HG11	2.26	0.51
17:1V:50:PRO:HG2	17:1V:51:VAL:HG12	1.93	0.51
1:2A:34:C:H2'	1:2A:35:G:C8	5.12	0.51
2:2B:83:G:H1	2:2B:94:C:H42	1.59	0.51
1:1A:1410:G:P	23:11:3:LYS:HG3	2.50	0.50
1:1A:1494:G:HO2'	1:1A:1934:A:HO2'	126.37	0.50
1:1A:2702:C:OP1	13:1R:17:ARG:NH2	2.40	0.50
1:1A:787:U:H2'	1:1A:788:G:C8	2.46	0.50
1:1A:886:U:H2'	1:1A:887:C:C6	2.46	0.50
1:1A:939:C:H2'	1:1A:940:C:C6	2.46	0.50
1:2A:2376:A:H3'	1:2A:2377:A:H8	1.76	0.50
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.12	0.50
24:12:22:GLU:OE2	24:12:68:ARG:NH2	2.44	0.50
1:1A:2661:U:H2'	1:1A:2662:U:C6	2.45	0.50
1:2A:2286:A:H4'	1:2A:2287:A:O4'	2.11	0.50
1:2A:307:G:N1	1:2A:310:A:OP2	2.42	0.50
1:1A:1121:C:C2'	1:1A:1122:C:H5'	2.41	0.50
1:1A:1233:U:H4'	17:1V:79:VAL:HG22	1.92	0.50
1:1A:1898:A:H2'	1:1A:1899:A:H8	1.76	0.50
1:1A:510:C:H2'	1:1A:511:C:C6	2.46	0.50
1:2A:2104:G:H1	1:2A:2185:C:H42	1.58	0.50
3:2D:148:GLU:OE1	3:2D:151:LYS:NZ	2.36	0.50
10:2O:68:GLU:HB3	10:2O:78:ARG:HB2	1.94	0.50
11:2P:95:VAL:HG13	11:2P:125:VAL:HA	1.93	0.50
1:1A:1255:A:H5''	1:1A:1257:G:O4'	2.11	0.50
1:1A:1960:A:OP2	61:1A:4279:HOH:O	2.19	0.50
1:2A:2419:U:H5''	30:28:33:ASN:HB2	1.93	0.50
1:2A:1002:G:N3	1:2A:1003:G:H1'	2.88	0.50
1:2A:1651:G:H2'	1:2A:1652:A:O4'	2.12	0.50
1:2A:392:C:H5''	1:2A:409:C:H5''	1.93	0.50
1:2A:518:G:H5'	18:2W:18:ARG:CZ	2.42	0.50
1:1A:116:A:H61	1:1A:313:A:H1'	39.60	0.50
1:1A:1634:C:H2'	1:1A:1635:C:C6	2.47	0.50
1:1A:1679:A:N6	61:1A:4205:HOH:O	2.41	0.50
1:1A:1921:G:N3	1:1A:1921:G:H2'	2.26	0.50
30:28:26:LYS:HD2	30:28:48:PHE:CD2	2.47	0.50
1:2A:1125:G:H5'	31:29:37:GLY:HA2	1.94	0.50
1:2A:2127:G:N1	1:2A:2161:C:C5	2.79	0.50
1:2A:855:G:H2'	1:2A:856:C:C6	2.46	0.50
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:3:ARG:HH11	7:2H:4:ILE:H	1.59	0.50
1:1A:2045:G:H5'	1:1A:2629:C:H4'	1.94	0.50
6:1G:41:GLN:HG2	6:1G:154:GLY:O	2.12	0.50
1:2A:2314:C:H2'	1:2A:2315:G:C8	2.47	0.50
1:2A:271(B):C:H42	1:2A:271(V):G:H1	1.59	0.50
26:14:58:ARG:O	26:14:61:ARG:HB3	2.11	0.50
1:1A:2549:U:H2'	1:1A:2550:C:C6	2.46	0.50
5:1F:150:GLY:HA2	5:1F:172:TRP:CD2	2.47	0.50
27:25:16:ARG:HG3	27:25:17:ASP:N	2.26	0.50
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.26	0.50
1:2A:2557:G:H2'	1:2A:2558:C:H6	1.77	0.50
1:2A:910:A:N1	1:2A:2277:G:H1'	2.26	0.50
2:2B:66:A:H61	2:2B:109:C:H5''	1.77	0.50
1:1A:895:G:H2'	1:1A:896:A:C8	2.47	0.50
1:2A:1028:A:H2'	1:2A:1029:A:C8	2.47	0.50
1:2A:2164:C:H3'	1:2A:2165:G:O4'	2.12	0.50
1:2A:218:A:C2	1:2A:235:U:H4'	2.47	0.50
1:2A:2552:2MU:H6	1:2A:2552:2MU:O5'	2.12	0.50
1:2A:479:A:N3	1:2A:481:G:H5''	2.27	0.50
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.12	0.50
1:1A:1101:G:H1	1:1A:1150:C:N4	2.07	0.50
1:1A:928:G:H3'	1:1A:929:G:H8	1.77	0.50
1:2A:1899:G:N3	1:2A:1899:G:H2'	2.26	0.50
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.11	0.50
9:2N:42:TRP:HA	9:2N:48:MET:SD	2.52	0.50
13:2R:97:VAL:HG22	13:2R:114:VAL:HG22	1.92	0.50
16:2U:97:ASP:OD1	16:2U:101:ARG:NH1	2.45	0.50
20:2Y:38:ILE:HD11	20:2Y:66:PRO:HG3	1.93	0.50
1:1A:2162:C:H2'	1:1A:2163:G:C8	2.45	0.49
7:1H:40:GLU:OE1	7:1H:61:HIS:NE2	2.44	0.49
7:1H:9:ILE:HD11	7:1H:69:ARG:HG2	1.94	0.49
22:20:11:ARG:O	22:20:14:ARG:NH2	2.40	0.49
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.47	0.49
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.93	0.49
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.93	0.49
1:1A:2130:C:H2'	1:1A:2131:U:H6	1.76	0.49
1:1A:956:A:N1	1:1A:2289:G:H1'	2.28	0.49
1:1A:553:A:O2'	1:1A:554:A:H5'	2.13	0.49
1:1A:909:G:H2'	1:1A:910:A:O4'	2.12	0.49
2:1B:41:U:H5	6:1G:70:VAL:H	1.60	0.49
1:2A:1268:A:H2'	1:2A:1269:A:C8	3.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.47	0.49
15:2T:73:GLU:OE2	15:2T:103:ARG:NE	2.45	0.49
1:1A:1809:U:H2'	1:1A:1815:A:N6	2.26	0.49
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.95	0.49
15:1T:26:ASP:O	15:1T:49:VAL:HG22	2.11	0.49
1:2A:262:A:H2'	1:2A:263:C:O4'	2.12	0.49
1:2A:566:U:H5''	11:2P:29:LYS:HE3	1.94	0.49
1:1A:574:G:O2'	1:1A:1265:A:N3	2.38	0.49
7:1H:88:LEU:HD23	7:1H:130:ARG:HG3	1.94	0.49
1:1A:1139:G:H3'	1:1A:1140:U:H5''	1.93	0.49
1:1A:2459:G:OP2	61:1A:4285:HOH:O	2.20	0.49
3:1D:242:ARG:O	61:1D:401:HOH:O	2.20	0.49
1:2A:184:C:H2'	1:2A:185:U:C6	2.48	0.49
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.94	0.49
1:2A:993:G:OP1	16:2U:50:ARG:HD2	2.13	0.49
1:1A:1501:U:O2'	1:1A:1502:G:N7	2.41	0.49
1:1A:2175:G:H2'	1:1A:2176:G:H8	1.77	0.49
1:2A:2022:U:OP2	27:25:15:ARG:NH2	2.46	0.49
1:2A:729:G:C6	3:2D:208:LYS:HB2	2.48	0.49
3:2D:118:VAL:HG22	3:2D:119:ALA:H	1.77	0.49
7:2H:144:VAL:O	7:2H:148:ILE:HG13	2.13	0.49
11:2P:87:ASP:O	11:2P:90:ARG:NH1	2.46	0.49
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.95	0.49
4:1E:119:ARG:HG2	4:1E:120:TRP:NE1	2.27	0.49
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.27	0.49
1:2A:658:C:H2'	1:2A:659:C:C6	2.48	0.49
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.95	0.49
12:2Q:57:HIS:HD2	12:2Q:117:ALA:HB2	1.78	0.49
1:1A:302:A:O2'	1:1A:303:C:OP1	2.27	0.49
1:2A:1589:C:H2'	1:2A:1590:U:C6	2.48	0.49
1:2A:2168:G:H8	1:2A:2170:A:N7	2.11	0.49
15:2T:26:ASP:O	15:2T:49:VAL:HG22	2.13	0.49
1:1A:2348:A:H61	22:10:43:THR:CG2	2.25	0.49
14:1S:20:ARG:NH2	22:10:51:VAL:O	2.45	0.49
1:1A:1388:A:OP2	61:1A:4284:HOH:O	2.20	0.49
1:1A:2203:G:O2'	1:1A:2204:G:OP1	2.29	0.49
1:2A:964:C:O2'	1:2A:2273:A:N3	2.36	0.49
1:2A:2848:G:C8	15:2T:97:ALA:HB2	2.48	0.49
1:1A:2825:C:H5'	27:15:29:THR:HG21	1.94	0.49
1:1A:1074:A:N6	1:1A:1171:G:H2'	2.28	0.49
1:1A:2314:G:H2'	1:1A:2315:G:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1459:G:N7	61:2A:4167:HOH:O	2.35	0.49
1:2A:1607:C:N4	1:2A:1622:G:OP2	2.42	0.49
1:2A:927:G:H2'	1:2A:928:G:O4'	2.12	0.49
1:2A:973:A:H8	1:2A:973:A:OP1	1.95	0.49
30:18:30:ARG:O	61:18:201:HOH:O	2.20	0.48
1:1A:2130:C:H2'	1:1A:2131:U:C6	2.48	0.48
1:1A:2193:A:O2'	1:1A:2194:U:H5''	2.13	0.48
1:1A:449:A:H2'	1:1A:450:A:C8	2.48	0.48
1:1A:439:A:C8	1:1A:496:A:C6	75.66	0.48
1:2A:1006:C:H2'	1:2A:1007:C:C6	3.14	0.48
1:2A:2405:G:H5'	11:2P:75:ILE:HD13	1.95	0.48
1:2A:2815:C:H2'	1:2A:2816:C:C6	2.48	0.48
1:2A:467:G:OP1	29:27:33:ARG:HD2	2.13	0.48
1:2A:521:G:H2'	1:2A:522:G:H8	1.78	0.48
3:2D:145:VAL:HG13	3:2D:191:ALA:HB2	1.94	0.48
4:1E:24:THR:HG22	4:1E:186:GLY:O	2.13	0.48
8:1I:130:TYR:O	8:1I:138:ILE:N	2.45	0.48
13:1R:33:ARG:HH21	13:1R:113:LEU:HD22	1.79	0.48
1:2A:839:U:H1'	1:2A:1191:G:H1'	1.94	0.48
1:2A:2258:C:O2'	1:2A:2427:C:OP2	2.30	0.48
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.48	0.48
1:2A:588:U:H2'	1:2A:589:C:C6	2.48	0.48
1:2A:629:G:H2'	1:2A:630:G:O4'	2.50	0.48
1:2A:947:G:H2'	1:2A:948:G:C8	2.49	0.48
17:2V:5:VAL:HG21	17:2V:35:LEU:HD23	1.94	0.48
18:1W:65:LEU:HD12	18:1W:68:ARG:HE	1.78	0.48
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.48	0.48
1:2A:2133:G:O2'	1:2A:2157:G:N2	2.46	0.48
1:2A:354:G:N2	1:2A:388:G:O2'	66.54	0.48
1:2A:582:G:H2'	1:2A:583:G:C8	2.49	0.48
3:2D:14:ARG:HB3	3:2D:14:ARG:HE	1.42	0.48
1:1A:1001:G:H5''	12:1Q:77:LYS:HD2	1.96	0.48
1:1A:1466:U:O2'	1:1A:1467:G:OP1	2.30	0.48
1:1A:2018:C:H4'	1:1A:2019:G:OP1	2.12	0.48
1:1A:2123:G:H2'	1:1A:2124:U:C6	2.49	0.48
1:1A:2148:A:N3	1:1A:2149:G:H1'	2.28	0.48
1:1A:327:U:O4	61:1A:4273:HOH:O	2.18	0.48
1:1A:605:G:H2'	1:1A:606:G:C8	2.48	0.48
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.49	0.48
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.13	0.48
1:2A:236:C:H2'	1:2A:237:C:H6	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:370:G:OP2	61:2A:4051:HOH:O	2.20	0.48
1:2A:911:A:OP1	61:2A:4053:HOH:O	2.20	0.48
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.78	0.48
1:1A:207:A:C2	1:1A:224:U:H4'	2.49	0.48
1:1A:2299:A:O2'	1:1A:2301:G:N7	2.39	0.48
1:1A:2327:G:H2'	1:1A:2328:C:C6	2.49	0.48
1:1A:929:G:H1	1:1A:940:C:N4	2.09	0.48
2:1B:1:U:H2'	2:1B:2:C:H6	1.78	0.48
3:1D:11:PRO:O	3:1D:14:ARG:HG3	2.13	0.48
7:1H:126:PRO:HB2	7:1H:130:ARG:HH21	1.78	0.48
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.12	0.48
8:1I:93:THR:H	8:1I:96:ASP:HB2	1.78	0.48
21:1Z:8:TYR:HB2	21:1Z:38:TYR:CE2	2.49	0.48
1:2A:2271:G:OP1	22:20:18:ALA:HB1	2.14	0.48
28:26:34:LEU:H	28:26:51:GLU:HG2	1.79	0.48
1:2A:2166:G:H3'	1:2A:2167:U:H5''	1.95	0.48
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.95	0.48
1:2A:312:G:H4'	1:2A:331:A:N3	2.28	0.48
2:2B:66:A:N6	2:2B:109:C:H5''	2.27	0.48
20:2Y:13:VAL:HB	20:2Y:72:VAL:HG13	1.94	0.48
1:1A:1405:A:C2	1:1A:1418:U:O4	2.67	0.48
1:1A:1494:G:O2'	1:1A:1934:A:O2'	126.53	0.48
1:1A:1312:G:O2'	1:1A:2034:G:O6	2.24	0.48
9:1N:35:ARG:HH21	9:1N:42:TRP:HZ2	1.61	0.48
13:1R:103:ARG:HD3	13:1R:108:GLY:O	2.14	0.48
13:1R:44:LEU:HD22	13:1R:48:VAL:HG23	1.94	0.48
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.49	0.48
2:2B:42:C:O2'	6:2G:67:LYS:O	2.13	0.48
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.49	0.48
1:2A:84:A:H5''	20:2Y:8:LYS:HE3	1.94	0.48
1:1A:2291:G:O6	22:10:14:ARG:HG3	2.13	0.48
1:1A:2832:G:N7	61:1A:4360:HOH:O	2.35	0.48
15:1T:112:ARG:HG3	15:1T:115:ARG:NH2	2.24	0.48
1:2A:2298:A:N6	1:2A:2318:G:C8	2.81	0.48
1:2A:514:A:N3	1:2A:581:C:O2'	2.42	0.48
1:2A:674:G:O2'	5:2F:74:ARG:HD3	2.14	0.48
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.95	0.48
1:1A:2343:G:O2'	1:1A:2348:A:N1	2.44	0.48
1:1A:606:G:N3	1:1A:632:A:N6	52.87	0.48
1:2A:1474:C:H2'	1:2A:1475:G:C8	2.48	0.48
1:2A:1506:C:H2'	1:2A:1507:A:H5'	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:500:G:N1	1:2A:503:A:OP2	2.45	0.48
2:2B:15:A:OP2	2:2B:69:G:N2	2.46	0.48
10:2O:15:GLY:O	10:2O:47:ILE:HG12	2.13	0.48
1:1A:2346:G:H5'	14:1S:9:ARG:HG2	1.96	0.48
1:1A:2576:A:C2	1:1A:2659:U:H4'	2.49	0.48
1:1A:348:A:N6	1:1A:362:G:O2'	2.47	0.48
7:1H:101:ARG:NH1	7:1H:117:PRO:HG2	2.29	0.48
1:1A:2391:G:O2'	14:1S:17:ARG:NH2	2.47	0.48
1:2A:1390:U:H2'	1:2A:1391:U:C6	3.27	0.48
1:2A:1639:U:C2'	1:2A:1640:C:H5'	2.43	0.48
1:2A:878:A:N6	1:2A:899:A:O2'	2.47	0.48
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	1.96	0.48
21:2Z:150:LEU:O	21:2Z:171:ILE:HG13	2.14	0.48
30:18:26:LYS:HG2	30:18:46:ARG:O	2.14	0.48
1:1A:1068:G:OP2	1:1A:1068:G:H8	6.77	0.48
1:1A:2168:C:H4'	1:1A:2169:G:C4	2.48	0.48
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.59	0.48
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	1.96	0.48
16:2U:107:ALA:O	16:2U:111:GLU:HG2	2.14	0.48
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.14	0.48
1:1A:1214:G:H1	1:1A:1226:C:H42	1.62	0.47
1:1A:1323:G:H2'	1:1A:1324:A:C8	2.96	0.47
1:1A:2457:G:OP1	5:1F:74:ARG:NH2	2.43	0.47
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.49	0.47
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.49	0.47
1:2A:1662:C:O2'	1:2A:2687:U:OP1	2.31	0.47
1:2A:928:G:H8	1:2A:928:G:O5'	1.97	0.47
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.47	0.47
12:2Q:31:ASP:HA	12:2Q:134:ARG:NH1	2.29	0.47
1:1A:1014:U:H2'	1:1A:1015:C:C6	2.48	0.47
8:1I:129:THR:HG22	8:1I:139:GLN:HE22	1.79	0.47
1:2A:1364:G:P	23:21:3:LYS:HG3	2.54	0.47
1:2A:2320:A:H2'	1:2A:2320:A:N3	2.30	0.47
1:2A:2611:U:OP1	61:2A:4055:HOH:O	2.20	0.47
1:2A:2698:U:H2'	1:2A:2699:C:C6	2.49	0.47
1:2A:884:C:H3'	1:2A:885:C:H6	1.80	0.47
7:2H:4:ILE:O	7:2H:69:ARG:HD2	2.14	0.47
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.14	0.47
12:2Q:84:GLY:N	61:2Q:3101:HOH:O	2.47	0.47
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.46	0.47
1:1A:1001:G:H2'	1:1A:1002:A:H2'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2745:G:H3'	1:1A:2746:A:O4'	2.13	0.47
1:1A:211:A:H5''	1:1A:448:U:OP1	2.15	0.47
1:1A:212:A:O4'	1:1A:449:A:H5'	2.13	0.47
1:1A:597:C:N3	4:1E:145:LYS:NZ	2.61	0.47
3:1D:18:VAL:HG12	3:1D:211:ARG:HH12	1.78	0.47
1:2A:1474:C:H2'	1:2A:1475:G:H8	1.80	0.47
1:2A:2099:U:O2	1:2A:2190:G:N2	2.32	0.47
1:2A:736:C:H5''	61:2A:5160:HOH:O	2.15	0.47
1:2A:963:U:OP2	61:2A:4008:HOH:O	2.20	0.47
15:2T:94:ALA:HB1	15:2T:99:LEU:HD21	1.96	0.47
1:1A:1825:U:H2'	1:1A:1826:C:C6	2.49	0.47
5:1F:40:GLN:NE2	5:1F:182:ASN:HB2	2.29	0.47
6:1G:43:LEU:HB3	6:1G:44:GLY:H	1.54	0.47
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.14	0.47
1:2A:848:G:H2'	1:2A:849:A:C8	2.48	0.47
10:2O:86:ILE:HG22	10:2O:94:ARG:HD3	1.97	0.47
14:2S:36:TYR:HD1	14:2S:52:SER:HB2	1.80	0.47
1:1A:1133:G:H2'	1:1A:1135:G:C8	2.49	0.47
1:1A:1701:A:H1'	1:1A:2833:A:H5'	1.96	0.47
1:1A:630:U:OP1	5:1F:102:PRO:HA	2.14	0.47
1:1A:742:G:OP1	1:1A:1426:G:O2'	2.23	0.47
5:1F:61:GLY:O	61:1F:401:HOH:O	2.20	0.47
11:1P:47:ASP:OD2	11:1P:49:ARG:NH2	2.40	0.47
23:21:3:LYS:HB2	23:21:61:ARG:HH12	1.79	0.47
1:2A:1007:C:N3	1:2A:1022:G:C6	17.05	0.47
1:2A:2151:G:H2'	1:2A:2152:G:H8	1.79	0.47
1:2A:2393:A:H5''	11:2P:63:PRO:HB3	1.95	0.47
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	1.97	0.47
1:1A:1288:A:N3	1:1A:1352:C:O2'	95.77	0.47
1:1A:2074:G:H4'	4:1E:143:ASN:O	2.14	0.47
1:1A:2162:C:H2'	1:1A:2163:G:H8	1.79	0.47
1:1A:225:C:H2'	1:1A:226:C:C6	2.49	0.47
1:1A:2285:A:H2'	1:1A:2286:A:C8	2.49	0.47
1:1A:348:A:H2'	1:1A:349:G:O4'	2.14	0.47
1:1A:625:G:O2'	1:1A:702:A:N6	2.47	0.47
1:2A:1038:C:N4	1:2A:1117:G:H1	2.05	0.47
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.14	0.47
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.49	0.47
1:2A:579:G:H2'	1:2A:580:C:C6	2.50	0.47
1:2A:890:A:H2'	1:2A:892:G:H8	1.80	0.47
18:2W:17:VAL:HG11	18:2W:103:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1094:A:N1	1:1A:1158:G:O2'	2.43	0.47
1:1A:1654:A:H1'	1:1A:1656:A:OP2	2.15	0.47
1:1A:1841:A:H2'	1:1A:1842:G:O4'	2.15	0.47
1:1A:2701:U:H4'	1:1A:2702:C:H5'	1.97	0.47
2:1B:77:U:OP1	21:1Z:19:ARG:NH2	2.46	0.47
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.96	0.47
1:2A:2119:A:N6	1:2A:2171:A:C6	2.82	0.47
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.78	0.47
1:2A:994:C:OP2	16:2U:54:LYS:NZ	2.47	0.47
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	1.97	0.47
1:1A:1239:A:H62	1:1A:1299:A:N6	21.22	0.47
1:1A:1324:A:OP1	13:1R:36:THR:HG23	2.15	0.47
8:1I:3:VAL:HG12	8:1I:38:LEU:HA	1.96	0.47
11:1P:90:ARG:NH1	11:1P:105:LEU:HD11	2.29	0.47
21:1Z:136:PHE:O	21:1Z:137:ILE:HG13	2.15	0.47
1:2A:2137:C:N3	1:2A:2155:G:C6	2.82	0.47
19:2X:26:TYR:HB3	19:2X:92:LEU:HD22	1.96	0.47
21:2Z:6:LYS:HE3	21:2Z:8:TYR:CE2	2.50	0.47
1:1A:1899:A:H5''	1:1A:1900:G:OP2	2.14	0.47
4:1E:97:LYS:HE2	4:1E:97:LYS:HB3	1.78	0.47
7:1H:96:ALA:HB2	7:1H:105:LEU:HD23	1.97	0.47
1:2A:2328:A:H2'	1:2A:2329:G:H8	1.77	0.47
1:2A:222:A:H5''	1:2A:421:U:OP1	2.15	0.47
1:2A:729:G:O5'	3:2D:208:LYS:NZ	2.46	0.47
6:2G:7:LEU:HD11	6:2G:107:LEU:HD12	1.97	0.47
9:2N:96:GLU:H	9:2N:96:GLU:CD	2.18	0.47
15:2T:51:ARG:HG2	15:2T:62:THR:HB	1.97	0.47
17:2V:2:PHE:CZ	17:2V:41:GLY:HA3	2.49	0.47
1:1A:2348:A:H61	22:10:43:THR:HG21	1.80	0.47
30:18:42:ARG:HD2	61:18:202:HOH:O	2.14	0.47
1:1A:1218:G:O2'	1:1A:1219:A:O4'	2.33	0.47
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.96	0.47
24:22:64:LEU:O	24:22:68:ARG:HG2	2.15	0.47
1:2A:118:A:N3	1:2A:178:G:H1'	2.30	0.47
1:2A:2114:A:N6	1:2A:2115:G:H21	2.13	0.47
1:2A:2377:A:H2'	1:2A:2378:A:C8	2.50	0.47
1:2A:833:U:H2'	1:2A:834:C:H6	2.59	0.47
1:2A:8:A:H2'	1:2A:9:U:H6	1.80	0.47
4:2E:117:MET:SD	4:2E:136:ARG:NE	2.81	0.47
21:2Z:156:LYS:HE3	21:2Z:158:PRO:HD3	1.96	0.47
1:1A:1935:A:H4'	1:1A:1936:C:H5''	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:196:A:H2'	1:1A:197:C:O4'	2.13	0.47
1:1A:722:A:C8	1:1A:851:A:C6	3.03	0.47
3:1D:208:LYS:HG3	3:1D:210:GLY:H	1.80	0.47
10:1O:68:GLU:OE1	10:1O:78:ARG:NH1	2.48	0.47
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.50	0.47
12:2Q:85:LYS:HD3	22:20:7:LEU:HD13	1.97	0.47
18:2W:67:ASP:N	18:2W:67:ASP:OD1	2.37	0.47
1:1A:2482:G:OP1	12:1Q:56:ARG:NH2	2.47	0.46
4:1E:111:ARG:HD2	4:1E:160:TYR:CE2	2.50	0.46
2:1B:8:U:O3'	14:1S:25:ARG:NH2	2.48	0.46
2:1B:73:A:N1	21:1Z:34:ASN:ND2	2.63	0.46
22:20:69:PHE:HE1	22:20:79:VAL:HG13	1.80	0.46
30:28:33:ASN:HA	30:28:36:LYS:HD2	1.98	0.46
1:2A:2156:G:H2'	1:2A:2157:G:C4	2.50	0.46
2:2B:105:A:HO2'	21:2Z:29:TYR:HD1	1.59	0.46
5:2F:164:ARG:O	5:2F:168:ARG:HB2	2.14	0.46
1:1A:1974:A:C6	1:1A:1975:A:N1	2.83	0.46
1:1A:2149:G:N1	1:1A:2183:C:N4	2.44	0.46
1:1A:2227:G:H5''	1:1A:2228:G:N7	2.30	0.46
1:1A:83:A:C5'	20:1Y:8:LYS:HG2	2.45	0.46
2:1B:13:A:N1	2:1B:69:G:O2'	2.39	0.46
6:1G:11:TYR:HA	6:1G:15:VAL:HB	1.97	0.46
1:2A:1141:U:OP2	9:2N:63:THR:OG1	2.27	0.46
6:2G:15:VAL:HG13	6:2G:175:LEU:HD23	1.97	0.46
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.64	0.46
21:2Z:146:ILE:HA	21:2Z:147:GLY:HA2	1.55	0.46
12:1Q:85:LYS:HG2	22:10:7:LEU:HB3	1.96	0.46
1:1A:2366:G:H21	22:10:36:ILE:HD11	1.81	0.46
1:1A:659:C:H2'	1:1A:660:C:C6	2.51	0.46
2:1B:2:C:H2'	2:1B:3:C:H6	1.80	0.46
3:1D:18:VAL:HG12	3:1D:211:ARG:NH1	2.31	0.46
6:1G:41:GLN:OE1	6:1G:60:LEU:HD22	2.15	0.46
9:1N:91:LEU:HA	9:1N:91:LEU:HD23	1.82	0.46
17:1V:72:VAL:HG13	17:1V:85:LYS:HB3	1.97	0.46
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.63	0.46
23:21:11:ARG:HG3	23:21:12:PRO:HD2	1.97	0.46
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.50	0.46
1:2A:2369:A:H2'	1:2A:2370:G:C8	2.51	0.46
1:2A:2658:C:H5'	7:2H:160:LYS:HZ2	1.80	0.46
1:2A:892:G:H3'	1:2A:893:C:C5'	2.45	0.46
18:2W:78:GLU:OE2	18:2W:99:ARG:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1314:A:H2'	1:1A:1315:A:O4'	2.15	0.46
1:1A:1827:U:H2'	1:1A:1828:C:H6	1.80	0.46
2:1B:1:U:HO2'	2:1B:2:C:P	2.36	0.46
5:1F:184:TYR:O	5:1F:188:ARG:HG3	2.15	0.46
9:1N:20:GLY:HA2	9:1N:61:ARG:HG2	1.97	0.46
18:1W:58:ALA:HB1	18:1W:64:MET:HB2	1.97	0.46
26:24:64:GLY:O	26:24:66:SER:N	2.45	0.46
28:26:14:THR:HG21	28:26:48:VAL:HG13	1.98	0.46
1:2A:271(G):C:H2'	1:2A:271(H):G:H8	1.81	0.46
1:2A:300:A:O2'	1:2A:318:C:O2	2.33	0.46
21:2Z:6:LYS:HE3	21:2Z:8:TYR:HE2	1.79	0.46
1:1A:1371:G:OP1	1:1A:1694:G:O2'	2.28	0.46
1:1A:180:A:H2'	1:1A:181:C:C6	2.51	0.46
1:1A:2482:G:O6	1:1A:2488:A:O2'	2.23	0.46
1:1A:2638:C:H2'	1:1A:2639:G:O4'	2.15	0.46
3:1D:35:LYS:HB2	3:1D:36:PRO:HD2	1.97	0.46
15:1T:109:GLU:O	15:1T:113:LYS:HG2	2.16	0.46
1:2A:2029:G:H2'	1:2A:2031:A:OP1	2.15	0.46
1:2A:2131:G:N7	1:2A:2133:G:N2	2.62	0.46
1:2A:478:A:N1	1:2A:500:G:H4'	2.31	0.46
1:2A:656:G:H2'	1:2A:657:U:O4'	2.15	0.46
6:2G:173:LEU:HB3	6:2G:178:PHE:CD2	2.51	0.46
1:1A:1475:G:H2'	1:1A:1476:C:H6	1.80	0.46
1:1A:1572:G:C6	1:1A:1573:G:C2	3.03	0.46
1:1A:937:A:H2'	1:1A:938:G:O4'	2.15	0.46
16:1U:34:LYS:HD3	16:1U:34:LYS:HA	1.51	0.46
1:2A:1383:C:O2	61:2A:4035:HOH:O	2.14	0.46
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.14	0.46
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.15	0.46
1:2A:272(B):G:H2'	1:2A:272(C):G:C8	2.50	0.46
1:2A:652(B):A:H61	1:2A:655:A:H1'	1.81	0.46
19:2X:35:THR:HG22	19:2X:38:GLU:H	1.81	0.46
1:1A:2283:G:OP1	22:10:18:ALA:HB1	2.16	0.46
1:1A:2150:C:H2'	1:1A:2151:C:O4'	2.16	0.46
1:1A:240:A:C5	1:1A:241:G:H1'	2.50	0.46
1:1A:715:G:H5'	1:1A:716:G:OP2	2.16	0.46
2:1B:78:A:C2	2:1B:100:A:C4	3.03	0.46
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.31	0.46
1:2A:2167:U:H3'	1:2A:2168:G:H21	1.81	0.46
1:2A:2447:G:N2	1:2A:2450:A:OP2	2.48	0.46
1:2A:602:G:O2'	1:2A:655:A:N6	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1033:G:O2'	1:1A:1046:A:N3	2.42	0.46
1:1A:2190:G:C6	1:1A:2193:A:C8	3.04	0.46
1:1A:2364:A:N6	1:1A:2377:G:O2'	2.48	0.46
1:1A:185:A:O2'	1:1A:852:G:O6	2.24	0.46
4:1E:174:ASP:OD1	4:1E:175:VAL:N	2.48	0.46
5:1F:101:LEU:HB3	5:1F:106:ARG:HD3	1.97	0.46
11:1P:112:LEU:HD23	11:1P:113:LYS:N	2.31	0.46
6:2G:109:VAL:HG11	26:24:14:ILE:HG21	1.97	0.46
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.51	0.46
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.16	0.46
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.16	0.46
1:2A:581:C:H2'	1:2A:582:G:H8	1.80	0.46
1:2A:839:U:H2'	1:2A:840:C:H6	1.79	0.46
1:2A:863:A:H2'	1:2A:864:G:C8	2.51	0.46
1:2A:912:C:OP1	12:2Q:8:LYS:NZ	2.35	0.46
2:2B:55:U:H1'	6:2G:29:TRP:CD1	2.50	0.46
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	1.97	0.46
11:2P:43:GLY:HA3	61:2P:203:HOH:O	2.14	0.46
1:1A:1653:C:H4'	1:1A:1654:A:O5'	2.16	0.46
1:1A:2879:G:H2'	1:1A:2880:C:O4'	2.15	0.46
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.51	0.46
1:2A:1037:G:H2'	1:2A:1038:C:O4'	2.16	0.46
1:2A:196:A:N3	1:2A:196:A:H2'	2.31	0.46
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.13	0.46
13:2R:44:LEU:HD22	13:2R:48:VAL:HG23	1.97	0.46
1:1A:1121:C:H2'	1:1A:1122:C:H5'	1.98	0.46
1:1A:1132:A:N3	1:1A:1132:A:H5''	2.30	0.46
1:1A:1199:C:H2'	1:1A:1200:G:O4'	2.16	0.46
1:1A:650:G:N7	11:1P:107:LYS:NZ	2.55	0.46
6:1G:15:VAL:HG22	6:1G:175:LEU:HB3	1.97	0.46
1:2A:1660:C:H2'	1:2A:1661:G:H8	1.80	0.46
1:2A:1754:C:H5	15:2T:96:ARG:NH2	2.12	0.46
1:2A:1857:G:C6	1:2A:1858:G:N1	2.84	0.46
1:2A:900:A:HO2'	1:2A:901:A:P	2.38	0.46
12:2Q:30:GLY:HA2	12:2Q:107:ALA:HB2	1.98	0.46
12:2Q:65:PHE:HB2	12:2Q:105:GLU:HB2	1.97	0.46
1:2A:1155:A:OP1	16:2U:55:ARG:HD2	2.16	0.46
1:1A:1140:U:O2'	1:1A:1141:A:N7	2.31	0.45
16:1U:58:ARG:HA	16:1U:61:TRP:CE3	2.51	0.45
28:26:23:THR:OG1	28:26:24:GLU:N	2.48	0.45
1:2A:2191:G:H2'	1:2A:2192:G:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:272(H):C:H2'	1:2A:272(I):U:C6	2.51	0.45
1:2A:2645:G:N2	1:2A:2767:C:OP2	2.50	0.45
1:2A:390:A:N6	61:2A:4293:HOH:O	2.48	0.45
13:2R:72:ASP:HB3	13:2R:75:LEU:HB3	1.97	0.45
15:2T:16:ARG:HD3	15:2T:79:HIS:HA	1.98	0.45
30:18:23:VAL:HG13	30:18:47:LYS:HB3	1.98	0.45
1:1A:2023:A:H2'	1:1A:2024:G:C8	2.51	0.45
1:1A:645:G:N3	1:1A:645:G:H5'	2.30	0.45
1:1A:884:C:N4	61:1A:4490:HOH:O	2.48	0.45
4:1E:121:ASN:ND2	61:1E:407:HOH:O	2.49	0.45
5:1F:103:LYS:HA	5:1F:106:ARG:HG3	1.98	0.45
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.97	0.45
15:1T:56:GLY:O	15:1T:59:THR:HG22	2.17	0.45
26:24:40:HIS:O	26:24:44:THR:HG22	2.15	0.45
1:2A:1422:G:O3'	10:2O:49:ARG:NH1	99.99	0.45
1:2A:1968:G:OP1	61:2A:4056:HOH:O	2.21	0.45
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.50	0.45
1:2A:2558:C:H2'	1:2A:2559:C:O4'	2.17	0.45
1:2A:271(Q):G:H2'	1:2A:271(R):G:C8	2.51	0.45
1:2A:748:G:C8	18:2W:89:ALA:HB1	2.51	0.45
13:2R:33:ARG:HG2	13:2R:115:GLU:CB	2.47	0.45
1:1A:551:A:O2'	1:1A:2065:C:O2	2.30	0.45
1:1A:2650:G:P	4:1E:82:ARG:HH12	2.39	0.45
1:1A:2225:U:O4'	3:1D:151:LYS:HE2	2.16	0.45
5:1F:102:PRO:O	5:1F:106:ARG:HG2	2.16	0.45
13:1R:33:ARG:HG2	13:1R:115:GLU:CB	2.45	0.45
1:1A:1785:C:H5''	15:1T:113:LYS:HE2	1.99	0.45
19:1X:35:THR:HG22	19:1X:38:GLU:H	1.82	0.45
1:2A:1782:C:H1'	1:2A:2609:U:H5''	1.99	0.45
1:2A:2857:G:N2	1:2A:2860:A:OP2	2.48	0.45
1:2A:882:G:H1	1:2A:894:C:N4	2.06	0.45
2:2B:105:A:H5'	2:2B:106:G:OP2	2.17	0.45
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.51	0.45
1:1A:1115:A:H2'	1:1A:1119:A:N7	2.30	0.45
1:1A:599:U:H2'	1:1A:600:G:C8	2.51	0.45
2:1B:45:A:O4'	6:1G:95:ARG:NH1	2.50	0.45
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.97	0.45
30:28:26:LYS:HG2	30:28:46:ARG:O	2.16	0.45
1:2A:2012:G:OP1	18:2W:11:ARG:NH2	2.48	0.45
1:2A:274:G:H2'	1:2A:275:G:C8	2.52	0.45
20:2Y:7:VAL:HG21	20:2Y:72:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:15:16:ARG:HG3	27:15:17:ASP:N	2.31	0.45
1:1A:1314:A:C2	1:1A:2035:A:C4	3.05	0.45
21:1Z:31:ARG:NH1	21:1Z:94:GLU:OE2	2.49	0.45
30:28:26:LYS:HB2	30:28:44:LYS:O	2.17	0.45
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.51	0.45
1:2A:1580:A:H3'	1:2A:1581:G:H8	1.81	0.45
1:2A:8:A:H2'	1:2A:9:U:C6	2.51	0.45
5:2F:178:PRO:HB2	5:2F:201:VAL:HG21	1.98	0.45
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.32	0.45
20:2Y:8:LYS:HG3	20:2Y:97:ARG:NH1	2.31	0.45
1:1A:1683:C:H2'	1:1A:1684:A:C8	2.51	0.45
1:1A:2724:U:O2'	1:1A:2725:A:OP2	2.29	0.45
1:1A:2812:A:H1'	1:1A:2904:U:H1'	1.99	0.45
1:1A:945:A:N3	1:1A:945:A:H2'	2.32	0.45
3:1D:180:GLY:HA3	3:1D:275:LYS:HG2	1.97	0.45
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.99	0.45
18:1W:46:PHE:O	18:1W:50:VAL:HG23	2.17	0.45
1:2A:1442:G:N3	1:2A:1442:G:H2'	2.90	0.45
1:2A:1593:G:H2'	1:2A:1594:G:H8	1.78	0.45
1:2A:2461:C:H2'	1:2A:2462:U:C6	2.51	0.45
1:2A:2461:C:H2'	1:2A:2462:U:H6	1.81	0.45
1:2A:2557:G:H2'	1:2A:2558:C:C6	2.51	0.45
26:14:34:GLU:OE1	26:14:34:GLU:N	2.45	0.45
30:18:23:VAL:CG1	30:18:47:LYS:HD3	2.46	0.45
1:1A:215:G:N2	1:1A:217:A:H62	2.14	0.45
1:1A:2227:G:H5''	1:1A:2228:G:C5	2.52	0.45
1:1A:2602:A:H2'	1:1A:2603:C:C6	2.51	0.45
57:1A:4113:MT9:H9	57:1A:4113:MT9:H5	1.99	0.45
1:1A:941:U:O2'	1:1A:942:A:OP1	2.30	0.45
2:1B:2:C:H2'	2:1B:3:C:C6	2.51	0.45
5:1F:185:ASP:OD1	5:1F:188:ARG:NH1	2.42	0.45
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.52	0.45
25:23:46:ASN:O	25:23:50:VAL:HG22	2.17	0.45
1:2A:2100:G:H2'	1:2A:2101:G:H8	1.81	0.45
1:2A:2176:A:H2'	1:2A:2177:C:H6	1.81	0.45
1:2A:2291:U:OP1	1:2A:2380:C:O2'	2.34	0.45
1:2A:258:G:H2'	1:2A:259:G:C8	3.22	0.45
1:2A:524:U:H2'	1:2A:525:U:C6	2.51	0.45
1:2A:631:A:H1'	11:2P:66:GLY:HA2	1.99	0.45
4:2E:179:GLU:HG3	15:2T:9:LEU:HD21	1.99	0.45
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:13:8:LEU:HG	25:13:31:LEU:HD23	1.98	0.45
1:1A:1108:G:H1	1:1A:1123:A:H61	1.65	0.45
1:1A:1530:G:OP1	1:1A:1530:G:H4'	4.86	0.45
1:1A:2198:A:H2'	1:1A:2199:C:C6	2.52	0.45
1:1A:41:C:H2'	1:1A:42:G:O4'	2.16	0.45
8:1I:130:TYR:N	8:1I:138:ILE:O	2.35	0.45
11:1P:120:ALA:HB2	11:1P:137:LYS:HB3	1.98	0.45
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.63	0.45
1:2A:1882:C:H5''	23:21:26:ARG:NH2	2.32	0.45
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.17	0.45
1:2A:2164:C:C4	1:2A:2165:G:H1'	2.51	0.45
1:2A:2787:C:H2'	1:2A:2788:C:H6	1.82	0.45
1:2A:993:G:H2'	1:2A:993:G:N3	3.08	0.45
1:2A:2848:G:H8	15:2T:97:ALA:HB2	1.81	0.45
1:1A:1141:A:C8	1:1A:1142:A:C8	3.05	0.45
1:1A:1087:C:N4	1:1A:1160:G:H1	2.14	0.45
8:1I:70:GLU:O	8:1I:74:ASN:HB2	2.16	0.45
5:1F:33:LEU:HB3	11:1P:6:LEU:HD21	1.99	0.45
13:1R:96:ARG:HG2	13:1R:115:GLU:HG2	1.99	0.45
17:1V:40:LEU:HB2	17:1V:46:VAL:HG22	1.97	0.45
1:2A:1385:G:O2'	1:2A:1396:U:O2	2.31	0.45
1:2A:1427:A:H4'	1:2A:1428:C:O5'	2.17	0.45
1:2A:2386:C:H2'	1:2A:2387:U:C6	2.52	0.45
1:2A:2061:G:H5''	1:2A:2503:2MA:C2	2.47	0.45
1:2A:848:G:C4	1:2A:933:A:H8	2.35	0.45
6:2G:77:ILE:HG22	6:2G:80:PHE:H	1.82	0.45
13:2R:36:THR:HG22	13:2R:37:THR:H	1.82	0.45
21:2Z:54:HIS:CD2	21:2Z:101:PRO:HG3	2.52	0.45
1:1A:1385:G:H5''	19:1X:16:LYS:HD3	1.99	0.45
1:1A:34:C:H5''	1:1A:35:G:OP2	2.16	0.45
2:1B:31:C:H4'	6:1G:29:TRP:CH2	2.52	0.45
3:1D:108:PRO:HD2	3:1D:111:LEU:HD22	1.99	0.45
2:1B:7:G:H5'	14:1S:29:PHE:CE2	2.52	0.45
1:2A:2131:G:H1	1:2A:2158:A:H62	1.65	0.45
1:2A:747:U:O2	1:2A:2014:A:H1'	2.17	0.45
1:1A:2602:A:H2'	1:1A:2603:C:H6	1.81	0.44
1:1A:624:C:O2'	1:1A:628:C:OP1	2.28	0.44
3:1D:79:VAL:HG12	3:1D:113:VAL:HA	1.99	0.44
5:1F:202:PHE:CZ	5:1F:206:ILE:HD13	2.53	0.44
21:1Z:154:ASP:OD1	21:1Z:154:ASP:N	2.50	0.44
30:28:62:LEU:HB3	30:28:65:GLU:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1015:G:H2'	1:2A:1016:G:C8	2.42	0.44
1:2A:1607:C:H5''	1:2A:1608:A:H5'	1.99	0.44
1:2A:1752:C:H2'	1:2A:1753:G:C8	2.52	0.44
1:2A:2065:C:H2'	1:2A:2066:C:C6	2.52	0.44
1:2A:829:A:N7	1:2A:2248:C:H5'	2.32	0.44
1:2A:2261:C:H1'	1:2A:2388:A:N3	2.32	0.44
1:2A:2611:U:H6	1:2A:2611:U:H5'	1.83	0.44
7:2H:99:VAL:N	7:2H:102:ALA:O	2.48	0.44
1:2A:1012:U:O4	9:2N:28:THR:HG21	2.17	0.44
10:2O:7:TYR:CZ	10:2O:44:LYS:HG3	2.52	0.44
3:1D:211:ARG:HG3	3:1D:214:TRP:CZ3	2.52	0.44
4:1E:96:PHE:HA	4:1E:100:GLU:OE1	2.18	0.44
6:1G:146:TYR:O	6:1G:149:VAL:HG12	2.18	0.44
12:1Q:45:GLN:N	12:1Q:45:GLN:OE1	2.47	0.44
15:1T:24:PRO:HA	15:1T:49:VAL:HG23	1.98	0.44
21:1Z:128:VAL:HG23	21:1Z:160:GLY:O	2.17	0.44
12:2Q:81:VAL:HB	22:20:7:LEU:HD21	2.00	0.44
1:2A:2420:C:P	30:28:33:ASN:H	2.39	0.44
1:2A:30:G:H2'	1:2A:31:C:C6	2.53	0.44
1:2A:274:G:C2	1:2A:363:G:C6	3.05	0.44
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.38	0.44
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.50	0.44
1:1A:2699:U:H2'	1:1A:2700:U:O4'	2.16	0.44
7:1H:83:TYR:CE2	7:1H:138:LYS:HB2	2.52	0.44
1:2A:1882:C:H5''	23:21:26:ARG:HH21	1.83	0.44
1:2A:2128:C:N3	1:2A:2160:G:C6	2.86	0.44
1:2A:2369:A:H2'	1:2A:2370:G:H8	1.82	0.44
1:2A:383:U:H2'	1:2A:385:C:H5	1.82	0.44
1:2A:855:G:H1	1:2A:922:U:H3	1.65	0.44
2:2B:68:C:H2'	2:2B:69:G:H8	1.83	0.44
4:2E:98:PRO:HD3	4:2E:175:VAL:HG12	1.98	0.44
5:2F:158:THR:HB	5:2F:195:ASP:HB2	1.99	0.44
2:2B:75:G:H1	21:2Z:73:GLN:NE2	2.16	0.44
1:1A:1355:G:H2'	1:1A:1356:G:C8	3.77	0.44
1:1A:388:A:H2'	1:1A:389:G:C8	2.53	0.44
1:1A:602:G:H2'	1:1A:603:C:C6	2.52	0.44
1:1A:616:G:C6	1:1A:617:U:C4	3.05	0.44
4:1E:29:GLY:HA3	61:1E:406:HOH:O	2.16	0.44
9:1N:46:VAL:HG23	9:1N:48:MET:CE	2.47	0.44
1:2A:2831:G:OP1	4:2E:58:ARG:NH2	2.46	0.44
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:907:U:O2'	12:2Q:101:ARG:NH2	2.49	0.44
23:11:23:LYS:HB3	23:11:29:GLY:HA3	2.00	0.44
1:1A:1546:G:H2'	1:1A:1547:C:C6	2.53	0.44
1:1A:2416:C:O3'	11:1P:77:ARG:NH2	2.51	0.44
12:1Q:30:GLY:HA2	12:1Q:107:ALA:HB2	1.99	0.44
1:2A:1221(A):C:C2	1:2A:1229:G:C2	3.06	0.44
1:2A:675:A:H2'	1:2A:676:A:C8	3.16	0.44
2:2B:34:U:O4	2:2B:44:G:O2'	2.32	0.44
4:2E:1:MET:O	4:2E:84:PHE:HB2	2.17	0.44
28:16:13:CYS:SG	28:16:47:THR:HG21	2.58	0.44
1:1A:1111:U:H5''	1:1A:1112:U:OP2	2.18	0.44
1:1A:1411:A:OP2	23:11:3:LYS:HG2	2.18	0.44
1:1A:1627:A:H8	1:1A:1627:A:OP2	2.01	0.44
1:1A:2155:G:H21	1:1A:2156:A:H62	1.65	0.44
6:1G:7:LEU:HD11	6:1G:107:LEU:HD12	2.00	0.44
7:1H:3:ARG:NH1	7:1H:4:ILE:H	2.15	0.44
23:21:67:ILE:N	23:21:68:PRO:HD2	2.33	0.44
25:23:6:VAL:HG22	25:23:56:VAL:HG13	2.00	0.44
26:24:57:GLU:CB	26:24:58:ARG:HD2	2.47	0.44
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.52	0.44
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.52	0.44
1:2A:2893:G:H5''	1:2A:2894:G:O4'	2.18	0.44
1:2A:589:C:H2'	1:2A:590:A:C8	2.53	0.44
3:2D:147:LEU:HD13	3:2D:155:LEU:HD11	2.00	0.44
8:2I:93:THR:H	8:2I:96:ASP:HB2	1.82	0.44
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	1.99	0.44
27:15:16:ARG:NH1	27:15:17:ASP:OD1	2.49	0.44
21:1Z:92:SER:OG	21:1Z:94:GLU:OE1	2.36	0.44
1:2A:2117:A:O2'	1:2A:2118:U:H5''	2.17	0.44
1:2A:2155:G:C5	1:2A:2156:G:H1'	2.52	0.44
1:2A:2312:U:H5'	6:2G:88:ILE:HD11	2.00	0.44
1:2A:2454:G:O6	61:2A:4050:HOH:O	2.20	0.44
1:2A:2483:C:N3	12:2Q:124:LYS:NZ	2.60	0.44
1:2A:2758:A:C4	7:2H:67:LEU:HD21	2.53	0.44
1:2A:2872:G:O2'	1:2A:2873:A:H5'	2.18	0.44
5:2F:179:GLU:OE1	5:2F:179:GLU:N	2.50	0.44
5:2F:40:GLN:HE22	5:2F:182:ASN:HB2	1.82	0.44
7:2H:17:VAL:HG22	7:2H:26:VAL:HG22	2.00	0.44
1:1A:1016:C:H2'	1:1A:1017:G:O4'	2.18	0.44
1:1A:1136:U:N3	1:1A:1148:C:H1'	2.32	0.44
3:1D:242:ARG:N	3:1D:242:ARG:HH11	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:51:PHE:O	4:1E:75:VAL:HG13	2.17	0.44
5:1F:112:MET:HB2	5:1F:112:MET:HE2	1.74	0.44
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.18	0.44
9:1N:70:LYS:HD3	9:1N:87:LEU:HD12	1.99	0.44
19:1X:12:VAL:HG21	19:1X:27:THR:HG22	2.00	0.44
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.53	0.44
1:2A:1448:G:N7	61:2A:4172:HOH:O	2.36	0.44
1:2A:2118:U:N3	1:2A:2149:G:H1'	2.33	0.44
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.32	0.44
1:2A:532:A:H2'	1:2A:532:A:N3	2.51	0.44
1:2A:2831:G:P	4:2E:58:ARG:HH21	2.40	0.44
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.17	0.44
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.65	0.44
11:2P:121:LYS:O	11:2P:123:LEU:N	2.51	0.44
1:1A:1110:C:H2'	1:1A:1111:U:O4'	2.18	0.44
1:1A:1356:G:OP2	29:17:9:ARG:NE	2.50	0.44
1:1A:1418:U:H2'	1:1A:1419:A:O4'	2.18	0.44
1:1A:768:C:H2'	1:1A:769:A:C8	2.53	0.44
1:1A:1830:G:O2'	3:1D:181:GLU:OE2	2.27	0.44
3:1D:61:LEU:O	3:1D:63:ARG:NH1	2.50	0.44
8:1I:6:LEU:HD11	8:1I:37:VAL:HG23	1.98	0.44
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.18	0.44
14:1S:65:VAL:O	14:1S:69:VAL:HG12	2.18	0.44
22:20:24:LYS:O	22:20:25:ARG:NH1	2.38	0.44
1:2A:892:G:H3'	1:2A:893:C:H5''	2.00	0.44
2:2B:13:A:O2'	2:2B:14:U:H3'	2.18	0.44
2:2B:56:G:OP1	6:2G:27:ASN:ND2	2.51	0.44
1:2A:1022:G:N7	9:2N:66:LYS:HE2	2.33	0.44
13:2R:95:THR:HG22	13:2R:116:LEU:HD23	1.99	0.44
15:2T:113:LYS:HA	15:2T:113:LYS:HD2	1.90	0.44
16:2U:69:CYS:HB3	16:2U:74:LEU:HD12	2.00	0.44
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.99	0.44
19:2X:5:TYR:CZ	24:22:30:ARG:HB2	2.53	0.44
28:16:38:LYS:HE3	28:16:38:LYS:HB3	1.69	0.43
1:1A:1246:C:N4	61:1A:4478:HOH:O	2.46	0.43
1:1A:1417:G:H2'	1:1A:1418:U:H5	1.83	0.43
1:1A:1473:A:H4'	1:1A:1474:C:O4'	2.18	0.43
1:1A:2430:A:H2'	1:1A:2431:U:C6	2.53	0.43
1:1A:809:U:H5''	61:1A:4314:HOH:O	2.17	0.43
1:1A:821:A:H2'	1:1A:821:A:N3	2.33	0.43
2:1B:66:A:H61	2:1B:108:U:H2'	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:119:ARG:HG2	4:1E:120:TRP:CE2	2.53	0.43
1:2A:2497:A:OP1	61:2A:4057:HOH:O	2.21	0.43
1:2A:2512:C:H2'	1:2A:2513:G:O4'	2.18	0.43
1:2A:2803:C:H2'	1:2A:2804:C:C6	2.53	0.43
1:2A:2823:A:OP1	4:2E:113:PHE:HB2	2.18	0.43
1:2A:647:G:H8	1:2A:647:G:O5'	2.00	0.43
8:2I:65:ALA:O	8:2I:69:LYS:N	2.49	0.43
11:2P:126:VAL:HG12	11:2P:148:LEU:HD23	1.99	0.43
1:1A:11:G:C2'	1:1A:12:U:H5''	2.43	0.43
1:1A:1639:G:H2'	1:1A:1640:G:C8	2.54	0.43
1:1A:1847:G:O6	3:1D:35:LYS:NZ	2.51	0.43
1:1A:2054:G:OP2	1:1A:2466:G:O2'	2.33	0.43
1:1A:2343:G:O2'	22:10:43:THR:HG22	2.17	0.43
1:1A:510:C:H2'	1:1A:511:C:H6	1.83	0.43
1:1A:653:G:H2'	1:1A:654:G:C8	2.53	0.43
4:1E:82:ARG:HG3	4:1E:83:ASP:N	2.32	0.43
6:1G:18:GLU:OE2	6:1G:21:ARG:NH1	2.51	0.43
21:1Z:17:ALA:HA	21:1Z:20:ARG:HH21	1.84	0.43
1:2A:1637:A:O2'	61:2A:4061:HOH:O	2.21	0.43
1:2A:2184:G:H2'	1:2A:2185:C:C6	2.52	0.43
1:2A:124:G:N2	1:2A:237:C:O2	57.74	0.43
1:2A:1490:A:O2'	3:2D:99:ASP:OD1	2.35	0.43
8:2I:81:VAL:O	8:2I:146:ALA:HA	2.18	0.43
1:1A:1617:A:H2'	1:1A:1618:A:C8	2.54	0.43
1:1A:1954:A:H2'	1:1A:1955:G:O4'	2.19	0.43
1:1A:2155:G:N2	1:1A:2156:A:H62	2.16	0.43
1:1A:2679:C:H2'	1:1A:2680:G:O4'	2.18	0.43
1:1A:297:C:H2'	1:1A:298:G:H8	1.83	0.43
1:1A:324:A:OP1	20:1Y:86:ARG:NH2	2.51	0.43
4:1E:9:VAL:HG22	4:1E:25:VAL:HB	1.99	0.43
23:21:4:VAL:HG11	23:21:11:ARG:HH21	1.82	0.43
1:2A:1496:A:OP2	1:2A:1496:A:H8	2.01	0.43
1:2A:2059:A:O3'	5:2F:69:HIS:HA	2.18	0.43
1:2A:884:C:N3	1:2A:893:C:O2'	2.47	0.43
1:2A:893:C:H2'	1:2A:894:C:C5	2.53	0.43
1:2A:910:A:H2'	1:2A:911:A:C8	2.53	0.43
2:2B:87:G:N2	2:2B:90:A:OP2	2.41	0.43
22:10:43:THR:HG23	22:10:43:THR:O	2.19	0.43
2:1B:91:C:OP2	12:1Q:16:ARG:NH1	2.51	0.43
5:1F:133:ASN:N	5:1F:138:GLU:OE1	2.34	0.43
9:1N:61:ARG:HD3	9:1N:61:ARG:HA	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.54	0.43
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.17	0.43
1:2A:1913:A:H4'	1:2A:1914:C:O5'	2.18	0.43
1:2A:2137:C:O2'	1:2A:2138:C:OP2	2.33	0.43
1:2A:271(T):C:H2'	1:2A:271(U):G:H8	1.83	0.43
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.83	0.43
1:2A:320:A:H4'	1:2A:322:A:N7	2.33	0.43
1:2A:741:G:H2'	1:2A:742:G:O4'	2.66	0.43
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.54	0.43
1:1A:1112:U:N3	1:1A:1115:A:OP2	2.51	0.43
1:1A:1262:C:H2'	1:1A:1263:C:C6	3.55	0.43
1:1A:1391:C:H2'	1:1A:1392:G:H8	1.84	0.43
1:1A:1744:G:OP2	1:1A:1745:A:O2'	2.23	0.43
1:1A:2298:A:H4'	1:1A:2299:A:O4'	2.18	0.43
1:1A:322:G:H5''	1:1A:323:A:OP1	2.19	0.43
3:1D:14:ARG:HB3	3:1D:14:ARG:HE	1.59	0.43
3:1D:83:GLU:OE1	3:1D:104:TYR:OH	2.23	0.43
6:1G:122:PRO:HG3	6:1G:182:LYS:H	1.83	0.43
6:1G:45:GLU:CD	6:1G:45:GLU:H	2.22	0.43
7:1H:149:ARG:HD2	7:1H:164:TYR:CE2	2.54	0.43
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.18	0.43
1:2A:570:G:H2'	1:2A:2030:A:C5	2.53	0.43
1:2A:2150:U:H2'	1:2A:2151:G:C8	2.53	0.43
1:2A:2151:G:H2'	1:2A:2152:G:C8	2.54	0.43
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.53	0.43
1:2A:250:G:C6	1:2A:251:A:C6	3.06	0.43
1:2A:320:A:H4'	1:2A:322:A:C8	2.53	0.43
1:2A:884:C:H3'	1:2A:885:C:C6	2.54	0.43
1:2A:971:C:H2'	1:2A:972:G:O4'	2.19	0.43
11:2P:138:LEU:HD23	11:2P:145:PRO:HB3	2.00	0.43
20:2Y:8:LYS:HG3	20:2Y:97:ARG:HH11	1.84	0.43
1:1A:1285:G:H2'	1:1A:1286:U:O4'	2.18	0.43
1:1A:27:G:N2	1:1A:537:G:H1'	2.34	0.43
1:1A:8:A:H2'	1:1A:9:U:H6	1.83	0.43
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.34	0.43
1:1A:2331:G:N1	14:1S:3:ARG:HA	2.33	0.43
16:1U:93:LYS:NZ	17:1V:11:GLN:O	2.49	0.43
1:2A:1007:C:H5''	9:2N:35:ARG:NH1	2.33	0.43
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.60	0.43
1:2A:1260:G:C6	1:2A:1261:C:C4	3.06	0.43
1:2A:1779:U:OP2	61:2A:4059:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2140:C:H2'	1:2A:2141:G:H5'	2.00	0.43
1:2A:2492:U:H2'	1:2A:2493:U:C6	2.54	0.43
1:2A:652(B):A:N6	1:2A:655:A:H1'	2.33	0.43
21:2Z:128:VAL:HG23	21:2Z:160:GLY:O	2.18	0.43
1:1A:1210:G:H2'	1:1A:1211:U:C6	2.54	0.43
1:1A:1552:C:H2'	1:1A:1553:A:H8	1.83	0.43
1:1A:992:G:H2'	1:1A:993:G:C8	2.53	0.43
2:1B:14:U:O3'	2:1B:108:U:O2'	2.36	0.43
1:2A:2161:C:H2'	1:2A:2162:G:O4'	2.18	0.43
1:2A:2438:U:O2'	1:2A:2440:C:OP1	2.30	0.43
1:2A:458:G:O2'	1:2A:469:G:O6	2.31	0.43
2:2B:24:G:H4'	2:2B:25:A:N7	2.34	0.43
3:2D:142:VAL:HG23	3:2D:193:VAL:HA	2.01	0.43
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	2.01	0.43
9:2N:123:TYR:CE2	9:2N:129:PRO:HD2	2.53	0.43
1:1A:1550:C:H2'	1:1A:1551:C:C6	2.53	0.43
1:1A:2203:G:HO2'	1:1A:2204:G:P	2.41	0.43
1:1A:2764:G:C4	7:1H:2:SER:HA	2.53	0.43
1:1A:68:C:H2'	1:1A:69:G:C8	2.54	0.43
2:1B:60:C:C2	2:1B:61:G:C8	3.07	0.43
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.54	0.43
1:2A:1423:G:H2'	1:2A:1424:G:C8	2.53	0.43
1:2A:2532:G:N2	1:2A:2663:G:O2'	2.51	0.43
1:2A:27:G:N2	1:2A:512:G:H1'	2.33	0.43
1:2A:855:G:C6	1:2A:856:C:N4	2.87	0.43
1:2A:90:U:H1'	1:2A:92:A:C8	2.54	0.43
4:2E:48:GLN:NE2	4:2E:78:LEU:HD23	2.34	0.43
11:2P:90:ARG:NH1	11:2P:105:LEU:HD11	2.33	0.43
18:2W:15:ARG:O	18:2W:19:LEU:HD13	2.18	0.43
20:2Y:37:VAL:HG21	20:2Y:72:VAL:HG21	2.01	0.43
21:2Z:5:LEU:O	21:2Z:59:LEU:HA	2.18	0.43
1:1A:1093:G:H2'	1:1A:1156:G:H22	1.83	0.43
1:1A:1821:C:H2'	1:1A:1822:A:C5	2.54	0.43
1:1A:2150:C:N4	1:1A:2182:G:H1	2.14	0.43
1:1A:2053:A:C6	1:1A:2510:C:H1'	2.54	0.43
28:26:34:LEU:N	28:26:51:GLU:HG2	2.33	0.43
1:2A:2111:C:C4	1:2A:2118:U:C4	3.07	0.43
1:2A:2141:G:H2'	1:2A:2142:C:O4'	2.18	0.43
1:2A:2473:U:H2'	1:2A:2473:U:O2	2.18	0.43
1:2A:765:G:N1	1:2A:812:C:O2'	83.85	0.43
5:2F:154:VAL:HG22	5:2F:191:ARG:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:124:SER:HB2	6:2G:131:TYR:CE1	2.54	0.43
6:2G:54:GLU:HA	6:2G:57:ALA:HB3	2.00	0.43
4:2E:183:LEU:HD21	15:2T:10:VAL:HG11	2.01	0.43
1:1A:2149:G:HO2'	1:1A:2195:A:H2	1.66	0.43
1:1A:2803:A:H5''	1:1A:2804:C:H5''	2.00	0.43
1:1A:2054:G:H1'	4:1E:145:LYS:HD3	2.01	0.43
7:1H:124:GLU:HG3	7:1H:132:ARG:HB3	2.00	0.43
10:1O:63:VAL:HG12	10:1O:106:LEU:HD11	2.00	0.43
1:2A:1138:G:C6	1:2A:1140:C:H1'	6.49	0.43
1:2A:1218:C:N4	1:2A:1231:G:H1	2.14	0.43
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.34	0.43
1:2A:2494:G:C4	1:2A:2495:G:C8	3.07	0.43
1:2A:271(R):G:H2'	1:2A:271(S):G:H8	1.84	0.43
1:2A:479:A:O2'	1:2A:481:G:H5'	2.18	0.43
1:2A:675:A:H2'	1:2A:676:A:H8	3.07	0.43
1:2A:921:G:C6	1:2A:922:U:C4	3.07	0.43
5:2F:9:ILE:HG21	5:2F:125:LEU:HD13	2.01	0.43
9:2N:73:THR:OG1	9:2N:82:LEU:HD11	2.18	0.43
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.19	0.43
23:11:51:VAL:HG11	23:11:74:VAL:HG21	2.01	0.42
26:14:40:HIS:O	26:14:44:THR:HG22	2.19	0.42
1:1A:1478:C:H2'	1:1A:1479:U:O4'	2.19	0.42
1:1A:2152:U:H2'	1:1A:2180:A:N1	2.34	0.42
1:1A:2858:G:C8	15:1T:97:ALA:HB2	2.54	0.42
9:1N:63:THR:HB	61:1N:303:HOH:O	2.19	0.42
20:1Y:6:HIS:CD2	20:1Y:6:HIS:H	2.36	0.42
21:1Z:39:VAL:HG21	21:1Z:44:PHE:HB2	2.01	0.42
28:26:35:GLU:OE2	28:26:50:ARG:NH1	2.52	0.42
1:2A:108:U:H2'	1:2A:109:G:C8	2.54	0.42
1:2A:1614:A:P	1:2A:1614:A:H8	2.41	0.42
1:2A:2408:U:H2'	1:2A:2409:G:C8	2.54	0.42
1:2A:223:A:O2'	1:2A:420:C:O2	2.36	0.42
2:2B:41:U:H5	6:2G:70:VAL:H	1.66	0.42
6:2G:64:THR:HG22	6:2G:94:LEU:HD11	2.02	0.42
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.54	0.42
11:2P:135:LEU:HA	11:2P:135:LEU:HD23	1.85	0.42
12:2Q:26:TYR:O	12:2Q:67:ARG:NH1	2.39	0.42
20:2Y:55:TYR:CZ	20:2Y:61:ILE:HG21	2.54	0.42
1:1A:1071:G:O2'	61:1A:4274:HOH:O	2.20	0.42
1:1A:1128:U:C4	1:1A:1132:A:N1	2.77	0.42
1:1A:2519:C:H2'	1:1A:2520:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:842:C:H2'	1:1A:843:C:C6	2.54	0.42
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	2.00	0.42
5:1F:42:ALA:O	5:1F:45:ARG:HB2	2.19	0.42
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	2.01	0.42
8:1I:124:GLY:H	8:1I:144:VAL:HG23	1.84	0.42
9:1N:73:THR:OG1	9:1N:82:LEU:HD11	2.19	0.42
11:1P:47:ASP:N	11:1P:47:ASP:OD1	4.20	0.42
1:2A:1152:C:H2'	1:2A:1153:C:C6	2.53	0.42
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.54	0.42
1:2A:958:U:H5''	12:2Q:14:ARG:HD3	2.01	0.42
1:2A:862:G:O2'	2:2B:78:A:N3	2.52	0.42
3:2D:20:ASP:N	3:2D:20:ASP:OD1	2.49	0.42
4:2E:170:LEU:HB3	4:2E:184:VAL:CG2	2.49	0.42
6:2G:73:ALA:HB3	6:2G:85:GLY:H	1.84	0.42
25:13:10:LYS:HE3	25:13:15:TYR:OH	2.19	0.42
6:1G:108:ASN:HB3	26:14:22:ILE:HD13	2.00	0.42
1:1A:2421:G:C6	1:1A:2422:G:C5	3.07	0.42
1:1A:308:U:H2'	1:1A:309:C:C6	2.55	0.42
1:1A:540:A:H1'	1:1A:604:C:H1'	2.02	0.42
7:1H:117:PRO:HA	7:1H:118:PRO:HD3	1.92	0.42
1:2A:1169:G:N2	1:2A:1181:C:N3	2.67	0.42
1:2A:570:G:H2'	1:2A:2030:A:N7	2.34	0.42
1:2A:2144:U:O2'	1:2A:2147:G:O6	2.35	0.42
1:2A:324:A:H2'	1:2A:325:G:O4'	2.18	0.42
1:2A:532:A:N6	1:2A:1206:G:O2'	62.83	0.42
1:1A:1150:C:H2'	1:1A:1151:U:C6	2.53	0.42
1:1A:309:C:H2'	1:1A:310:C:C6	2.53	0.42
1:2A:1310:G:H1	1:2A:1327:C:N4	26.85	0.42
1:2A:1496:A:N3	1:2A:1577:C:O2'	2.51	0.42
1:2A:1805:U:O2	3:2D:50:THR:HB	2.19	0.42
1:2A:2106:G:H5''	1:2A:2107:C:OP2	2.19	0.42
1:2A:2678:C:H2'	1:2A:2679:A:O4'	2.20	0.42
2:2B:96:U:OP1	21:2Z:14:LYS:NZ	2.47	0.42
5:2F:123:LEU:HD12	5:2F:124:LEU:H	1.84	0.42
9:2N:21:LYS:NZ	9:2N:140:VAL:OXT	2.44	0.42
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.53	0.42
1:1A:1112:U:H2'	1:1A:1114:G:OP2	2.19	0.42
1:1A:1756:U:H2'	1:1A:1757:C:C6	2.54	0.42
1:1A:1938:A:H2'	1:1A:1939:PSU:O4'	2.20	0.42
1:1A:2327:G:H2'	1:1A:2328:C:H6	1.83	0.42
1:1A:2382:G:H2'	1:1A:2383:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2658:C:H2'	1:1A:2659:U:O4'	2.20	0.42
1:1A:2691:A:H4'	4:1E:165:VAL:HG11	2.02	0.42
1:1A:581:G:OP1	9:1N:111:PRO:HD2	2.20	0.42
15:1T:65:LYS:HE3	15:1T:67:SER:HB2	2.01	0.42
1:2A:1235:G:C6	1:2A:1236:G:N1	2.87	0.42
1:2A:787:U:OP2	61:2A:4058:HOH:O	2.21	0.42
3:2D:228:PRO:HD3	3:2D:235:GLY:N	2.35	0.42
4:2E:60:ASN:CG	4:2E:62:PRO:HD2	2.40	0.42
7:2H:8:PRO:O	7:2H:10:PRO:HD3	2.19	0.42
14:2S:103:GLU:O	14:2S:107:GLU:N	2.49	0.42
1:1A:1403:U:H2'	1:1A:1404:G:O4'	2.19	0.42
1:1A:284:G:C2	1:1A:285:U:O4	2.73	0.42
4:1E:170:LEU:HA	4:1E:170:LEU:HD12	1.86	0.42
4:1E:176:ILE:HB	4:1E:181:LEU:HB2	2.00	0.42
8:1I:78:THR:HA	8:1I:143:SER:HG	1.85	0.42
9:1N:109:LYS:HE2	61:1N:304:HOH:O	2.20	0.42
11:1P:132:LYS:HB2	11:1P:132:LYS:HE2	1.83	0.42
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.55	0.42
21:1Z:93:ASP:CB	21:1Z:131:ARG:HH22	2.33	0.42
21:1Z:103:ARG:O	21:1Z:138:GLU:HA	2.20	0.42
21:1Z:155:LEU:HD12	21:1Z:155:LEU:HA	1.90	0.42
1:2A:517:C:OP1	27:25:16:ARG:NH2	2.52	0.42
30:28:62:LEU:HB3	30:28:65:GLU:CG	2.50	0.42
1:2A:1011:G:H1	1:2A:1018:C:N4	18.18	0.42
1:2A:1473:G:C6	1:2A:1474:C:C4	3.08	0.42
1:2A:1551:C:H2'	1:2A:1552:G:O4'	2.20	0.42
1:2A:2051:A:H5'	1:2A:2578:G:O4'	2.20	0.42
1:2A:272(B):G:H2'	1:2A:272(C):G:H8	1.84	0.42
2:2B:19:G:H2'	2:2B:20:C:O4'	2.19	0.42
1:1A:1529:G:H4'	1:1A:1530:G:OP2	4.54	0.42
1:1A:1882:U:H2'	1:1A:1883:C:O4'	2.19	0.42
1:1A:2376:C:H2'	1:1A:2377:G:O4'	2.20	0.42
1:1A:561:A:H2'	1:1A:562:C:C6	2.54	0.42
15:1T:108:ARG:HG3	15:1T:109:GLU:N	2.34	0.42
17:1V:1:MET:HE1	17:1V:44:LYS:H	1.84	0.42
1:2A:1005:C:H2'	1:2A:1006:C:H6	1.83	0.42
1:2A:1115:G:H2'	1:2A:1116:C:O4'	2.20	0.42
1:2A:1231:G:H2'	1:2A:1232:G:C8	2.55	0.42
1:2A:1463:C:H2'	1:2A:1464:C:H6	1.84	0.42
1:2A:146:G:H2'	1:2A:147:U:C6	2.55	0.42
1:2A:1665:A:H4'	10:2O:67:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2156:G:H2'	1:2A:2157:G:C2	2.55	0.42
1:2A:2547:U:O2	10:2O:23:ARG:NH1	2.50	0.42
1:2A:322:A:C5	1:2A:340:A:C2	3.07	0.42
1:2A:515:A:H1'	1:2A:581:C:H1'	2.00	0.42
1:2A:800:A:OP1	1:2A:800:A:H8	2.03	0.42
2:2B:7:G:H5'	14:2S:29:PHE:CE2	2.54	0.42
1:2A:2784:C:H1'	4:2E:37:ARG:NH1	2.35	0.42
10:2O:53:LYS:N	10:2O:56:ASP:OD2	2.46	0.42
21:2Z:72:ARG:HD3	21:2Z:72:ARG:HA	1.83	0.42
24:12:41:ILE:HG13	24:12:43:GLN:HG3	2.02	0.42
25:13:4:LEU:O	25:13:36:VAL:HA	2.20	0.42
1:1A:1102:G:H5''	1:1A:1103:A:O4'	2.19	0.42
1:1A:354:A:HO2'	1:1A:355:A:H8	1.66	0.42
2:1B:88:C:H2'	2:1B:89:G:O4'	2.20	0.42
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.55	0.42
11:1P:50:ARG:HD3	30:18:7:HIS:HD2	1.79	0.42
1:1A:2849:G:N2	13:1R:91:GLN:O	2.46	0.42
16:1U:16:LYS:HE2	16:1U:16:LYS:HB3	1.79	0.42
19:1X:57:LEU:HA	61:1X:3102:HOH:O	2.20	0.42
20:1Y:92:ASN:HB3	20:1Y:94:LYS:N	2.35	0.42
30:28:32:LEU:O	30:28:36:LYS:HE3	2.20	0.42
1:2A:1002:G:C2	1:2A:1003:G:H1'	2.76	0.42
1:2A:2180:U:H2'	1:2A:2181:G:O4'	2.19	0.42
1:2A:2815:C:H2'	1:2A:2816:C:H6	1.84	0.42
1:2A:238:C:O2'	1:2A:608:A:N3	2.48	0.42
1:2A:622:G:H2'	1:2A:623:G:H8	1.84	0.42
1:2A:864:G:N2	1:2A:913:U:C2	2.88	0.42
2:2B:66:A:N6	2:2B:108:U:H3'	2.34	0.42
3:2D:166:GLN:NE2	3:2D:176:ARG:HH21	2.18	0.42
6:2G:120:LEU:HD12	6:2G:178:PHE:HB3	2.01	0.42
1:2A:1007:C:H5''	9:2N:35:ARG:HH11	1.85	0.42
23:11:82:LEU:HA	23:11:85:LEU:HD12	2.00	0.42
30:18:6:THR:CG2	30:18:63:PRO:HD2	2.50	0.42
1:1A:794:U:O2	1:1A:2036:A:H1'	2.19	0.42
1:1A:613:A:H2'	1:1A:614:C:O4'	2.20	0.42
1:1A:858:U:H2'	11:1P:21:ARG:HA	2.02	0.42
1:1A:930:G:H2'	1:1A:931:C:H5	1.84	0.42
1:1A:639:G:N2	5:1F:44:ARG:O	2.52	0.42
6:1G:101:ILE:HG22	6:1G:105:LYS:HE2	2.01	0.42
1:2A:1257:C:H2'	1:2A:1258:C:C6	2.55	0.42
1:2A:2164:C:C5	1:2A:2165:G:H1'	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:238:C:C2	1:2A:260:G:C2	3.08	0.42
1:2A:275:G:H2'	1:2A:276:A:O4'	2.20	0.42
6:2G:129:GLY:O	6:2G:161:THR:OG1	2.37	0.42
2:2B:31:C:H4'	6:2G:29:TRP:CH2	2.55	0.42
8:2I:61:ARG:HD3	8:2I:61:ARG:HA	1.83	0.42
10:2O:24:VAL:HG12	10:2O:33:ALA:HB2	2.02	0.42
13:2R:42:LYS:HB3	13:2R:45:ARG:NH2	2.34	0.42
17:2V:1:MET:HG3	17:2V:41:GLY:O	2.20	0.42
26:14:24:THR:OG1	26:14:25:TYR:N	2.53	0.42
1:1A:1686:U:H4'	1:1A:2711:C:H4'	2.02	0.42
1:1A:2087:C:H2'	1:1A:2088:C:C6	2.54	0.42
1:1A:225:C:H2'	1:1A:226:C:H6	1.84	0.42
1:1A:2702:C:N4	1:1A:2726:A:H1'	2.34	0.42
1:1A:2856:G:H2'	1:1A:2857:U:O4'	2.20	0.42
1:1A:384:G:H2'	1:1A:385:G:C8	2.55	0.42
1:1A:756:U:H2'	1:1A:757:G:C8	2.54	0.42
11:1P:95:VAL:HG13	11:1P:125:VAL:HA	2.01	0.42
21:1Z:93:ASP:HB3	21:1Z:131:ARG:HH22	1.84	0.42
1:2A:1003:G:N2	1:2A:1153:C:C2	2.88	0.42
1:2A:1434:A:H2'	1:2A:1435:G:C8	2.54	0.42
1:2A:2287:A:N6	1:2A:2344:U:H3	2.11	0.42
1:2A:2400:G:H2'	1:2A:2401:U:H6	1.85	0.42
1:2A:2549:G:H2'	1:2A:2550:G:H8	1.85	0.42
1:2A:266:G:H2'	1:2A:266:G:N3	3.02	0.42
1:2A:2747:G:O6	1:2A:2755:C:H5''	2.20	0.42
1:2A:518:G:H2'	1:2A:519:U:H6	1.84	0.42
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.35	0.42
1:2A:2295:C:H5	14:2S:13:ARG:HH12	1.67	0.42
1:1A:1121:C:O2	1:1A:1122:C:H2'	2.19	0.41
1:1A:1532:A:H2'	1:1A:1533:G:C8	2.55	0.41
1:1A:1640:G:H2'	1:1A:1641:G:O4'	2.19	0.41
1:1A:2227:G:OP2	1:1A:2227:G:H4'	2.20	0.41
1:1A:2672:A:H2'	1:1A:2673:G:O4'	2.19	0.41
1:1A:2735:G:H2'	1:1A:2736:C:C6	2.54	0.41
1:1A:1097:G:H4'	1:1A:2765:C:H4'	2.02	0.41
1:1A:532:A:N6	1:1A:1206:G:O2'	80.03	0.41
1:1A:872:C:O2	11:1P:55:ARG:NH1	2.50	0.41
3:1D:147:LEU:HD13	3:1D:155:LEU:HD11	2.01	0.41
1:1A:1829:U:H5'	3:1D:259:THR:CG2	2.47	0.41
9:1N:21:LYS:NZ	9:1N:140:VAL:OXT	2.42	0.41
16:1U:32:PHE:CZ	16:1U:36:ARG:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:21:52:ARG:HD3	23:21:56:GLN:O	2.19	0.41
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.52	0.41
1:2A:1355:G:H2'	1:2A:1356:G:O4'	2.38	0.41
1:2A:1411:C:H42	1:2A:1591:G:H1	1.67	0.41
1:2A:2647:U:H2'	1:2A:2648:C:C6	2.55	0.41
1:2A:995:C:O2	9:2N:3:THR:OG1	2.35	0.41
3:2D:211:ARG:HG3	3:2D:214:TRP:CE3	2.55	0.41
4:2E:24:THR:HG23	4:2E:184:VAL:HG13	2.01	0.41
14:2S:26:LEU:HD22	14:2S:87:PHE:HD1	1.86	0.41
16:2U:102:GLU:HG3	17:2V:2:PHE:CE2	2.55	0.41
1:1A:1464:G:O2'	1:1A:1627:A:N6	2.52	0.41
1:1A:177:G:H5'	23:11:14:VAL:HG21	2.02	0.41
1:1A:185:A:H2'	1:1A:185:A:N3	2.36	0.41
1:1A:2021:C:H4'	1:1A:2736:C:O2	2.19	0.41
1:1A:2108:U:H2'	1:1A:2109:G:C8	2.55	0.41
1:1A:209:G:O2'	1:1A:222:A:N3	2.44	0.41
1:1A:2460:A:OP1	61:1A:4209:HOH:O	2.22	0.41
1:1A:2627:U:H2'	1:1A:2628:C:H6	1.85	0.41
1:1A:2812:A:H5''	1:1A:2813:G:C8	2.55	0.41
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.55	0.41
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.20	0.41
24:22:1:MET:N	24:22:52:ASP:OD1	2.53	0.41
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.21	0.41
1:2A:1973:G:H2'	1:2A:1974:C:C6	2.55	0.41
1:2A:2123:G:H2'	1:2A:2124:G:C8	2.55	0.41
1:2A:2274:A:C5	1:2A:2276:G:C8	3.08	0.41
1:2A:2335:A:C8	1:2A:2337:G:C5	3.07	0.41
1:2A:2740:A:H2'	1:2A:2741:A:C8	2.55	0.41
1:2A:322:A:OP1	5:2F:168:ARG:HD2	2.20	0.41
1:2A:720:C:H2'	1:2A:721:C:H6	1.84	0.41
1:2A:992:C:OP1	16:2U:47:TYR:OH	2.27	0.41
1:2A:2820:A:OP2	13:2R:2:ARG:NH2	2.53	0.41
16:2U:34:LYS:HA	16:2U:34:LYS:HD3	1.61	0.41
16:2U:74:LEU:HD21	16:2U:110:VAL:HG13	2.02	0.41
29:17:29:LYS:O	29:17:33:ARG:HB2	2.20	0.41
1:1A:1091:A:H1'	1:1A:1093:G:N3	2.35	0.41
1:1A:2136:A:H2'	1:1A:2137:G:O4'	2.20	0.41
1:1A:2776:G:OP2	61:1A:4291:HOH:O	2.22	0.41
1:1A:402:C:H2'	1:1A:403:C:C6	2.56	0.41
3:1D:26:LYS:NZ	3:1D:28:GLU:O	2.44	0.41
10:1O:24:VAL:HG12	10:1O:33:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2032:G:H5''	18:1W:42:ARG:HB2	2.02	0.41
1:2A:2117:A:H1'	1:2A:2119:A:OP2	2.20	0.41
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.85	0.41
1:2A:312:G:H4'	1:2A:331:A:C2	2.55	0.41
1:2A:630:G:N2	1:2A:633:A:OP2	2.46	0.41
1:2A:784:A:N6	3:2D:229:VAL:HG11	2.35	0.41
4:2E:72:VAL:HG12	4:2E:73:GLU:O	2.21	0.41
18:2W:36:LEU:HD13	18:2W:48:ALA:HA	2.02	0.41
19:2X:56:THR:O	61:2X:201:HOH:O	2.22	0.41
1:1A:1151:U:C2	1:1A:1152:G:N7	2.88	0.41
1:1A:2143:G:N2	1:1A:2199:C:N3	2.51	0.41
1:1A:233:A:C2	1:1A:244:A:C4	3.09	0.41
3:1D:206:LEU:HA	3:1D:211:ARG:HE	1.86	0.41
1:1A:1834:A:H4'	3:1D:259:THR:HG23	2.02	0.41
3:1D:3:VAL:HG13	3:1D:17:THR:HB	2.03	0.41
5:1F:28:ILE:O	5:1F:30:PRO:HD3	2.20	0.41
5:1F:52:LYS:HD3	5:1F:56:GLU:O	2.20	0.41
8:1I:8:PRO:O	8:1I:9:LEU:HD12	2.20	0.41
14:1S:5:THR:OG1	14:1S:8:GLU:HG2	2.19	0.41
20:1Y:19:LYS:HE3	20:1Y:20:TYR:CE2	2.55	0.41
28:26:50:ARG:HE	28:26:50:ARG:HB2	1.76	0.41
1:2A:2114:A:H62	1:2A:2115:G:H21	1.68	0.41
1:2A:2154:G:H2'	1:2A:2155:G:H5'	2.01	0.41
1:2A:2031:A:C6	1:2A:2498:C:H1'	2.56	0.41
1:2A:635:C:H2'	1:2A:636:G:O4'	2.20	0.41
6:2G:142:PRO:HB2	26:24:31:ILE:HG21	2.01	0.41
7:2H:33:LEU:HD21	7:2H:136:ILE:HG13	2.02	0.41
24:12:1:MET:HB3	24:12:5:GLU:OE1	2.19	0.41
26:14:53:GLU:O	26:14:56:VAL:HG13	2.20	0.41
1:1A:2143:G:H2'	1:1A:2144:U:C6	2.55	0.41
1:1A:2398:C:H2'	1:1A:2399:U:C6	2.56	0.41
1:1A:2874:G:OP1	15:1T:119:LYS:HD2	2.20	0.41
5:1F:106:ARG:H	5:1F:106:ARG:HG2	1.54	0.41
7:1H:149:ARG:HH11	7:1H:164:TYR:HE2	1.66	0.41
9:1N:22:THR:HA	9:1N:61:ARG:O	2.21	0.41
10:1O:115:VAL:HG13	10:1O:121:VAL:HG21	2.03	0.41
21:1Z:24:LEU:HD12	21:1Z:25:PRO:HD2	2.01	0.41
22:20:69:PHE:CE1	22:20:79:VAL:HG22	2.55	0.41
1:2A:1364:G:C8	23:21:3:LYS:HD2	2.55	0.41
25:23:52:HIS:CD2	25:23:53:LEU:HG	2.56	0.41
26:24:16:CYS:SG	26:24:17:GLY:N	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1147:C:H2'	1:2A:1148:A:C8	2.54	0.41
1:2A:1419:A:C8	1:2A:1421:G:C6	3.08	0.41
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.55	0.41
1:2A:2099:U:O4	1:2A:2190:G:O6	2.39	0.41
1:2A:1889:A:N1	1:2A:2234:G:H1'	2.35	0.41
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.49	0.41
5:2F:11:VAL:HG21	5:2F:20:LEU:HB2	2.02	0.41
8:2I:129:THR:HA	8:2I:138:ILE:O	2.21	0.41
12:2Q:31:ASP:HA	12:2Q:134:ARG:HH11	1.84	0.41
13:2R:44:LEU:HD23	13:2R:44:LEU:HA	1.90	0.41
23:11:60:PHE:HE1	23:11:95:LEU:HD11	1.86	0.41
26:14:16:CYS:SG	26:14:17:GLY:N	2.94	0.41
1:1A:105:C:H2'	1:1A:106:U:H6	1.84	0.41
1:1A:1316:C:H5''	1:1A:1317:G:O5'	2.20	0.41
1:1A:1465:A:C8	1:1A:1467:G:C6	3.09	0.41
1:1A:1857:G:H4'	3:1D:242:ARG:NH2	2.36	0.41
1:1A:2183:C:O2'	1:1A:2184:G:H8	2.03	0.41
1:1A:664:U:H2'	1:1A:665:C:C6	2.56	0.41
6:1G:170:ARG:NH2	6:1G:174:GLU:OE2	2.54	0.41
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.36	0.41
8:1I:109:ILE:HD12	8:1I:109:ILE:HA	1.77	0.41
1:2A:1199:U:H2'	1:2A:1200:C:C6	2.55	0.41
1:2A:1754:C:N3	1:2A:2716:U:O2'	2.47	0.41
1:2A:1941:C:C5	1:2A:1942:5MC:HM52	2.56	0.41
1:2A:414:C:H2'	1:2A:415:A:C8	2.56	0.41
1:2A:911:A:H2'	12:2Q:9:TYR:OH	2.19	0.41
1:2A:925:C:H2'	1:2A:926:A:C8	2.48	0.41
5:2F:23:ASP:O	5:2F:24:LEU:HD12	2.21	0.41
5:2F:93:LYS:O	5:2F:95:ARG:HG3	2.20	0.41
6:2G:51:ARG:HA	6:2G:51:ARG:HD3	1.88	0.41
10:2O:63:VAL:HG23	10:2O:64:ARG:HG3	2.02	0.41
1:2A:811:U:H2'	11:2P:21:ARG:HA	2.03	0.41
16:2U:76:TYR:CE2	16:2U:80:ILE:HG13	2.56	0.41
17:2V:97:LYS:HA	17:2V:97:LYS:HD2	1.93	0.41
21:2Z:93:ASP:CB	21:2Z:131:ARG:HH22	2.34	0.41
21:2Z:70:LEU:HA	21:2Z:70:LEU:HD23	1.85	0.41
1:1A:1085:G:H1	1:1A:1162:C:N4	2.17	0.41
1:1A:1088:G:C6	1:1A:1089:C:C4	3.09	0.41
1:1A:1305:G:H22	1:1A:1331:G:H1'	40.22	0.41
1:1A:2306:C:H5''	14:1S:10:ARG:HD2	2.03	0.41
1:1A:2661:U:H2'	1:1A:2662:U:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2721:G:H2'	1:1A:2722:C:C6	2.55	0.41
1:1A:1343:C:OP1	1:1A:2722:C:H4'	2.21	0.41
1:1A:423:G:H1'	23:11:42:GLN:HB3	2.03	0.41
1:1A:441:C:H2'	1:1A:442:A:C8	2.56	0.41
19:1X:43:VAL:HG21	19:1X:81:VAL:HG11	2.03	0.41
23:21:8:SER:HB3	23:21:66:HIS:NE2	2.36	0.41
1:2A:1786:A:C4	1:2A:1938:A:C6	3.09	0.41
1:2A:2065:C:H2'	1:2A:2066:C:H6	1.85	0.41
1:2A:2525:G:C2	1:2A:2539:C:N3	2.89	0.41
1:2A:244:A:C2	1:2A:255:A:C4	3.09	0.41
1:2A:277:C:O2'	1:2A:278:A:OP1	2.32	0.41
1:2A:817:C:O2'	1:2A:839:U:H5''	2.20	0.41
1:2A:890:A:N6	1:2A:893:C:O2	2.54	0.41
1:2A:898:C:H2'	1:2A:899:A:H5'	2.02	0.41
4:2E:108:SER:HB3	4:2E:165:VAL:HG21	2.03	0.41
15:2T:28:VAL:HG23	15:2T:88:ILE:HD13	2.03	0.41
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	2.03	0.41
21:2Z:98:MET:O	21:2Z:126:VAL:N	2.52	0.41
1:1A:1338:U:H2'	1:1A:1339:C:C6	2.56	0.41
1:1A:1765:U:H2'	1:1A:1766:G:O4'	2.21	0.41
1:1A:2040:G:N3	16:1U:34:LYS:NZ	2.67	0.41
1:1A:2368:C:H2'	1:1A:2369:U:O4'	2.21	0.41
1:1A:2562:G:OP1	61:1A:4288:HOH:O	2.21	0.41
1:1A:469:A:H1'	1:1A:1246:C:O4'	2.20	0.41
1:1A:470:C:H6	1:1A:470:C:H2'	3.90	0.41
1:1A:592:U:C4	1:1A:593:G:C6	3.09	0.41
13:1R:36:THR:HG22	13:1R:37:THR:H	1.84	0.41
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.21	0.41
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.56	0.41
1:2A:1021:A:H3'	1:2A:1021:A:H8	1.85	0.41
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.55	0.41
1:2A:1463:C:H2'	1:2A:1464:C:C6	2.56	0.41
1:2A:154(A):C:H42	1:2A:171:G:H1	1.68	0.41
1:2A:2378:A:O5'	1:2A:2378:A:H8	2.03	0.41
1:2A:2821:A:OP2	61:2A:4060:HOH:O	2.21	0.41
1:2A:945:A:C4	1:2A:2448:A:C2	3.09	0.41
3:2D:242:ARG:N	3:2D:242:ARG:HH11	2.17	0.41
4:2E:101:ARG:HA	4:2E:101:ARG:HD3	1.92	0.41
6:2G:34:LEU:HD23	6:2G:161:THR:HG22	2.02	0.41
1:1A:1554:A:O2'	1:1A:1555:C:H5''	2.21	0.41
1:1A:1793:A:H2'	61:1A:5820:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1940:A:H8	1:1A:1940:A:OP2	2.04	0.41
1:1A:253:C:O2'	1:1A:254:A:H2'	2.21	0.41
1:1A:699:C:H2'	1:1A:700:A:O4'	2.21	0.41
1:1A:886:U:H1'	1:1A:1236:G:H1'	2.03	0.41
1:1A:956:A:C5	12:1Q:13:GLN:HG3	2.56	0.41
5:1F:181:LEU:HA	5:1F:181:LEU:HD12	1.89	0.41
6:1G:16:ARG:NH2	6:1G:28:VAL:O	2.48	0.41
15:1T:127:ALA:O	15:1T:128:GLU:HG2	2.21	0.41
1:1A:70:A:N7	19:1X:31:HIS:HE1	2.19	0.41
1:2A:1021:A:H3'	1:2A:1021:A:C8	2.56	0.41
1:2A:1316:U:H2'	1:2A:1317:A:H8	1.86	0.41
1:2A:1530:C:HO2'	1:2A:1531:C:P	2.41	0.41
6:2G:19:LEU:HD11	6:2G:172:LEU:HD13	2.02	0.41
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	2.03	0.41
16:2U:74:LEU:HD13	16:2U:79:PHE:HB2	2.03	0.41
16:2U:92:ARG:HA	16:2U:95:LEU:HB2	2.01	0.41
20:2Y:39:VAL:HB	20:2Y:42:VAL:HB	2.02	0.41
1:1A:1073:A:N3	61:1A:4385:HOH:O	2.37	0.41
1:1A:1103:A:C2	1:1A:1104:G:H1'	2.56	0.41
1:1A:1103:A:N6	1:1A:1133:G:OP2	2.54	0.41
1:1A:1276:C:H2'	1:1A:1277:G:C8	2.55	0.41
1:1A:1550:C:H2'	1:1A:1551:C:H6	1.86	0.41
1:1A:1702:A:H3'	1:1A:1703:C:C6	2.55	0.41
1:1A:518:G:H2'	1:1A:519:G:O4'	2.20	0.41
2:1B:1:U:O2'	2:1B:2:C:P	2.79	0.41
20:1Y:92:ASN:HB3	20:1Y:94:LYS:HG2	2.02	0.41
21:1Z:138:GLU:H	21:1Z:156:LYS:NZ	2.19	0.41
1:2A:1865:G:OP1	61:2A:4064:HOH:O	2.22	0.41
1:2A:2136:C:HO2'	1:2A:2137:C:H6	1.68	0.41
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.56	0.41
1:2A:858:U:O2	1:2A:2268:A:H2'	2.21	0.41
1:2A:2499:C:O2	61:2A:4052:HOH:O	2.20	0.41
1:2A:2694:G:C6	1:2A:2695:C:C4	3.08	0.41
1:2A:2881:C:H2'	1:2A:2882:A:O4'	2.21	0.41
1:2A:459:U:H4'	29:27:40:TRP:CZ3	2.55	0.41
1:2A:699:A:H2'	1:2A:700:G:O4'	2.21	0.41
14:2S:8:GLU:HG2	14:2S:8:GLU:H	1.61	0.41
11:1P:63:PRO:HG2	30:18:25:MET:HB2	2.03	0.41
1:1A:1073:A:C2	1:1A:2500:A:H5'	2.56	0.41
1:1A:1258:A:H1'	1:1A:1284:G:N3	2.36	0.41
1:1A:2122:G:H2'	1:1A:2123:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2314:G:C2	1:1A:2327:G:C2	3.09	0.41
1:1A:2899:C:H2'	1:1A:2900:G:O4'	2.21	0.41
1:1A:313:A:H2'	1:1A:314:G:O4'	2.21	0.41
1:2A:2080:G:H2'	1:2A:2081:C:H6	1.85	0.41
1:2A:2110:G:H3'	1:2A:2111:C:H5'	2.03	0.41
1:2A:2121:G:N2	1:2A:2177:C:N3	2.56	0.41
1:2A:2287:A:O2'	1:2A:2288:A:H5''	2.21	0.41
1:2A:25:U:C4	1:2A:26:G:C6	3.09	0.41
1:2A:2802:G:H2'	1:2A:2803:C:O4'	2.20	0.41
2:2B:68:C:H2'	2:2B:69:G:C8	2.56	0.41
3:2D:228:PRO:HD3	3:2D:235:GLY:CA	2.51	0.41
4:2E:181:LEU:HD12	4:2E:181:LEU:HA	1.89	0.41
8:2I:73:GLU:HG3	8:2I:138:ILE:HG23	2.02	0.41
5:2F:31:HIS:HB2	11:2P:9:ASN:OD1	2.21	0.41
21:2Z:97:GLU:HA	21:2Z:126:VAL:O	2.20	0.41
1:1A:1742:G:H1'	3:1D:8:PRO:O	2.22	0.40
1:1A:2050:U:H2'	1:1A:2051:G:O4'	2.21	0.40
1:1A:2807:C:H42	1:1A:2813:G:H22	1.69	0.40
1:1A:504:A:C6	1:1A:506:A:C6	3.08	0.40
2:1B:29:A:C2	2:1B:30:C:C2	3.08	0.40
5:1F:202:PHE:O	5:1F:206:ILE:HG12	2.21	0.40
12:1Q:111:GLU:O	12:1Q:115:MET:HG2	2.21	0.40
18:1W:64:MET:HE2	18:1W:109:GLU:HG3	2.04	0.40
20:1Y:7:VAL:HG21	20:1Y:72:VAL:CG1	2.49	0.40
1:2A:2365:G:O6	30:28:39:LYS:HE3	2.21	0.40
1:2A:2745:C:H2'	1:2A:2746:U:O4'	2.21	0.40
6:2G:15:VAL:HG21	6:2G:176:LEU:HD23	2.02	0.40
8:2I:38:LEU:H	8:2I:38:LEU:HG	1.61	0.40
9:2N:121:LYS:HD3	9:2N:130:HIS:CE1	2.56	0.40
11:2P:81:GLN:HB3	11:2P:106:LEU:HD12	2.03	0.40
1:2A:1288:U:O4	13:2R:106:GLY:HA3	2.21	0.40
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.54	0.40
15:2T:26:ASP:OD1	15:2T:120:ARG:NH2	2.51	0.40
19:2X:36:LYS:HA	19:2X:39:ILE:HD12	2.02	0.40
19:2X:56:THR:HG22	19:2X:79:ALA:HB2	2.03	0.40
28:16:11:LEU:HA	28:16:11:LEU:HD23	1.81	0.40
1:1A:1217:G:H3'	1:1A:1218:G:H5'	2.02	0.40
1:1A:1740:U:H1'	3:1D:14:ARG:HH22	1.84	0.40
1:1A:1913:G:C6	1:1A:1914:C:C4	3.09	0.40
1:1A:2142:G:O2'	1:1A:2143:G:H5'	2.21	0.40
1:1A:294:C:N4	1:1A:390:G:H1	2.15	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:964:A:H5''	2:1B:98:G:O2'	2.22	0.40
11:1P:43:GLY:HA3	61:1P:301:HOH:O	2.21	0.40
11:1P:77:ARG:HB2	11:1P:78:PRO:HD2	2.02	0.40
21:1Z:150:LEU:HG	21:1Z:151:HIS:N	2.35	0.40
1:2A:909:A:O2'	1:2A:910:A:H5'	2.21	0.40
3:2D:150:LYS:N	3:2D:150:LYS:HD2	2.36	0.40
4:2E:48:GLN:HE21	4:2E:78:LEU:HB3	1.86	0.40
8:2I:4:ILE:HD11	8:2I:44:LEU:HD12	2.04	0.40
12:2Q:56:ARG:HD2	12:2Q:56:ARG:HA	1.87	0.40
14:2S:29:PHE:HD2	14:2S:36:TYR:HD2	1.69	0.40
1:2A:445:C:OP1	16:2U:2:PRO:HA	2.21	0.40
1:2A:1151:G:H4'	16:2U:81:HIS:CD2	2.57	0.40
18:2W:6:ILE:HG22	18:2W:8:ARG:HG3	2.03	0.40
30:18:14:VAL:HG13	30:18:22:VAL:HG13	2.03	0.40
1:1A:1842:G:N7	61:1A:4388:HOH:O	2.37	0.40
1:1A:2314:G:H2'	1:1A:2315:G:C8	2.56	0.40
1:1A:627:G:C6	1:1A:628:C:C4	3.08	0.40
1:1A:776:G:O2'	1:1A:810:G:H4'	2.21	0.40
1:1A:929:G:H22	1:1A:940:C:N4	2.20	0.40
2:1B:21:G:H2'	2:1B:22:U:O4'	2.21	0.40
7:1H:56:SER:HB3	7:1H:61:HIS:ND1	2.37	0.40
13:1R:72:ASP:HB3	13:1R:75:LEU:HB3	2.03	0.40
15:1T:27:THR:HG22	15:1T:89:VAL:HG13	2.03	0.40
18:1W:64:MET:CE	18:1W:109:GLU:HG3	2.51	0.40
20:1Y:6:HIS:HE1	20:1Y:72:VAL:O	2.05	0.40
1:1A:353:G:OP2	20:1Y:71:LYS:HE2	2.22	0.40
31:29:10:ILE:HD12	31:29:32:HIS:HA	2.02	0.40
1:2A:271:A:N6	1:2A:271(X):G:H1'	2.36	0.40
1:2A:2819:G:H2'	1:2A:2821:A:N7	2.36	0.40
1:2A:539:G:H2'	1:2A:540:C:C6	2.57	0.40
1:2A:795:C:OP2	61:2A:4063:HOH:O	2.22	0.40
5:2F:155:LEU:HD22	5:2F:185:ASP:O	2.21	0.40
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.21	0.40
1:1A:1138:C:C2'	1:1A:1139:G:H5'	2.52	0.40
1:1A:1554:A:O2'	1:1A:1555:C:OP1	2.29	0.40
1:1A:2104:A:H2'	1:1A:2105:G:O4'	2.22	0.40
1:1A:733:G:H8	29:17:6:GLN:O	2.04	0.40
2:1B:4:C:H2'	2:1B:5:C:O4'	2.21	0.40
6:1G:133:LEU:HA	61:1G:3103:HOH:O	2.21	0.40
7:1H:113:VAL:HG11	7:1H:151:ILE:HG21	2.03	0.40
13:1R:98:LEU:HD23	13:1R:98:LEU:HA	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2X:5:TYR:CE2	24:22:30:ARG:HB2	2.57	0.40
1:2A:1508:A:H4'	1:2A:1509(A):A:C5	2.57	0.40
1:2A:1845:G:OP1	3:2D:258:LYS:NZ	2.40	0.40
1:2A:2366:A:H2'	1:2A:2367:G:O4'	2.21	0.40
1:2A:2552:2MU:H2'	1:2A:2554:U:OP2	2.21	0.40
1:2A:2792:G:N3	1:2A:2792:G:H2'	2.36	0.40
1:2A:375:C:H2'	1:2A:376:C:C6	2.56	0.40
1:2A:729:G:C8	3:2D:208:LYS:HD2	2.56	0.40
1:2A:932:G:H4'	1:2A:933:A:O5'	2.21	0.40
12:2Q:75:THR:HG21	12:2Q:87:LYS:HE3	2.04	0.40
1:1A:1006:C:N3	1:1A:1023:G:C2	22.41	0.40
1:1A:1053:C:OP1	9:1N:37:LYS:NZ	2.52	0.40
1:1A:1149:A:O5'	1:1A:1149:A:H8	2.05	0.40
1:1A:1684:A:H4'	1:1A:2723:A:O2'	2.22	0.40
1:1A:2418:U:H2'	1:1A:2418:U:OP2	2.22	0.40
1:1A:2504:U:H2'	1:1A:2505:U:C6	2.57	0.40
1:1A:507:G:C4	1:1A:532:A:C2	3.10	0.40
3:1D:79:VAL:CG1	3:1D:113:VAL:HA	2.51	0.40
1:1A:1615:G:H5''	3:1D:61:LEU:HD13	2.04	0.40
1:2A:1411:C:H5''	1:2A:1412:A:OP2	2.22	0.40
1:2A:1481:U:H2'	1:2A:1482:G:C8	6.58	0.40
1:2A:242:G:C8	30:28:5:LYS:HG2	2.57	0.40
1:2A:2690:C:N4	1:2A:2713:A:H1'	2.37	0.40
1:2A:784:A:C8	1:2A:792:G:C5	3.09	0.40
1:2A:915:C:H3'	1:2A:916:G:H8	1.86	0.40
2:2B:7:G:H2'	2:2B:8:U:O4'	2.21	0.40
5:2F:117:ARG:NH2	5:2F:187:VAL:HA	2.36	0.40
8:2I:47:LEU:HD23	8:2I:47:LEU:HA	1.88	0.40
9:2N:103:VAL:O	9:2N:107:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	259 (95%)	13 (5%)	1 (0%)	34	60
3	2D	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	34	60
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	29	54
4	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	29	54
5	1F	201/210 (96%)	192 (96%)	8 (4%)	1 (0%)	29	54
5	2F	201/210 (96%)	193 (96%)	6 (3%)	2 (1%)	15	37
6	1G	179/182 (98%)	170 (95%)	8 (4%)	1 (1%)	25	50
6	2G	179/182 (98%)	164 (92%)	13 (7%)	2 (1%)	14	34
7	1H	172/180 (96%)	159 (92%)	10 (6%)	3 (2%)	9	23
7	2H	172/180 (96%)	162 (94%)	7 (4%)	3 (2%)	9	23
8	1I	144/148 (97%)	131 (91%)	12 (8%)	1 (1%)	22	46
8	2I	144/148 (97%)	133 (92%)	9 (6%)	2 (1%)	11	28
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
11	1P	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
11	2P	147/150 (98%)	140 (95%)	7 (5%)	0	100	100
12	1Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
12	2Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
14	2S	108/112 (96%)	99 (92%)	9 (8%)	0	100	100
15	1T	129/146 (88%)	124 (96%)	2 (2%)	3 (2%)	6	16
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	37
17	2V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	37
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	15	37
20	2Y	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
21	1Z	148/206 (72%)	136 (92%)	10 (7%)	2 (1%)	11	28
21	2Z	156/206 (76%)	136 (87%)	17 (11%)	3 (2%)	8	20
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	34
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	68 (100%)	0	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	55 (82%)	10 (15%)	2 (3%)	4	10
26	24	67/71 (94%)	53 (79%)	12 (18%)	2 (3%)	4	10
27	15	57/60 (95%)	56 (98%)	1 (2%)	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%)	48 (94%)	3 (6%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	202 (88%)	19 (8%)	8 (4%)	3	8
33	2b	229/256 (90%)	205 (90%)	19 (8%)	5 (2%)	6	17
34	1c	204/239 (85%)	190 (93%)	13 (6%)	1 (0%)	29	54
34	2c	204/239 (85%)	190 (93%)	12 (6%)	2 (1%)	15	37
35	1d	206/209 (99%)	191 (93%)	13 (6%)	2 (1%)	15	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/209 (99%)	192 (93%)	11 (5%)	3 (2%)	10	26
36	1e	146/162 (90%)	136 (93%)	8 (6%)	2 (1%)	11	28
36	2e	146/162 (90%)	135 (92%)	10 (7%)	1 (1%)	22	46
37	1f	98/101 (97%)	95 (97%)	2 (2%)	1 (1%)	15	37
37	2f	98/101 (97%)	98 (100%)	0	0	100	100
38	1g	153/156 (98%)	143 (94%)	8 (5%)	2 (1%)	12	30
38	2g	153/156 (98%)	142 (93%)	8 (5%)	3 (2%)	7	19
39	1h	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
40	1i	125/128 (98%)	112 (90%)	11 (9%)	2 (2%)	9	24
40	2i	125/128 (98%)	116 (93%)	8 (6%)	1 (1%)	19	43
41	1j	95/105 (90%)	85 (90%)	7 (7%)	3 (3%)	4	9
41	2j	94/105 (90%)	82 (87%)	9 (10%)	3 (3%)	4	9
42	1k	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	17	40
42	2k	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	8	21
43	1l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
43	2l	119/132 (90%)	109 (92%)	10 (8%)	0	100	100
44	1m	121/126 (96%)	113 (93%)	8 (7%)	0	100	100
44	2m	120/126 (95%)	111 (92%)	9 (8%)	0	100	100
45	1n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
45	2n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
46	1o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
46	2o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
47	1p	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
47	2p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
48	1q	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
50	1s	81/93 (87%)	73 (90%)	6 (7%)	2 (2%)	5	14
50	2s	81/93 (87%)	71 (88%)	9 (11%)	1 (1%)	13	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2	5
51	2t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2	5
52	1u	21/27 (78%)	21 (100%)	0	0	100	100
52	2u	21/27 (78%)	21 (100%)	0	0	100	100
All	All	11370/12128 (94%)	10694 (94%)	588 (5%)	88 (1%)	19	43

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	47	LYS
7	1H	126	PRO
26	14	55	ARG
33	1b	10	LEU
41	1j	75	ILE
51	1t	100	ILE
5	2F	130	ALA
17	2V	79	VAL
21	2Z	172	ALA
38	2g	6	ARG
41	2j	75	ILE
50	2s	81	ARG
51	2t	100	ILE
33	1b	9	GLU
33	1b	17	PHE
33	1b	22	LYS
40	1i	54	ASP
41	1j	79	ARG
51	1t	96	GLY
5	2F	89	VAL
7	2H	92	ILE
7	2H	126	PRO
33	2b	9	GLU
33	2b	127	ILE
34	2c	156	ARG
42	2k	49	GLY
51	2t	96	GLY
5	1F	130	ALA
7	1H	47	GLU
38	1g	4	ARG
50	1s	81	ARG
6	2G	47	LYS

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Mol	Chain	Res	Type
21	2Z	2	GLU
23	21	3	LYS
26	24	47	GLN
26	24	65	ASP
33	2b	20	GLU
35	2d	173	TRP
38	2g	4	ARG
41	2j	78	ASN
51	2t	47	GLY
51	2t	102	GLY
4	1E	52	LEU
15	1T	127	ALA
15	1T	128	GLU
21	1Z	2	GLU
26	14	57	GLU
33	1b	11	LEU
35	1d	179	GLU
51	1t	102	GLY
4	2E	52	LEU
35	2d	179	GLU
38	2g	80	VAL
40	2i	11	LYS
3	1D	3	VAL
8	1I	11	ASN
21	1Z	153	SER
33	1b	125	PRO
40	1i	55	ALA
41	1j	29	ARG
50	1s	29	ARG
3	2D	3	VAL
7	2H	47	GLU
8	2I	42	SER
8	2I	98	ALA
21	2Z	141	VAL
33	2b	16	HIS
36	2e	85	GLY
41	2j	79	ARG
7	1H	92	ILE
15	1T	37	GLY
36	1e	69	VAL
37	1f	40	VAL
38	1g	80	VAL

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Mol	Chain	Res	Type
51	1t	47	GLY
33	2b	17	PHE
34	1c	66	VAL
17	1V	79	VAL
33	1b	124	SER
35	1d	178	VAL
36	1e	85	GLY
42	1k	105	VAL
6	2G	52	ILE
34	2c	66	VAL
35	2d	178	VAL
20	1Y	55	TYR
33	1b	231	GLU
42	2k	105	VAL

### 5.3.2 Protein sidechains ⓘ

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%)	205 (95%)	10 (5%)	26	54
3	2D	215/218 (99%)	207 (96%)	8 (4%)	34	63
4	1E	164/166 (99%)	152 (93%)	12 (7%)	14	33
4	2E	164/166 (99%)	158 (96%)	6 (4%)	34	63
5	1F	160/166 (96%)	152 (95%)	8 (5%)	24	51
5	2F	159/166 (96%)	153 (96%)	6 (4%)	33	62
6	1G	143/156 (92%)	138 (96%)	5 (4%)	36	65
6	2G	143/156 (92%)	141 (99%)	2 (1%)	67	86
7	1H	144/148 (97%)	139 (96%)	5 (4%)	36	65
7	2H	144/148 (97%)	144 (100%)	0	100	100
8	1I	113/124 (91%)	110 (97%)	3 (3%)	44	74
8	2I	105/124 (85%)	102 (97%)	3 (3%)	42	71
9	1N	118/119 (99%)	111 (94%)	7 (6%)	19	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	2N	118/119 (99%)	115 (98%)	3 (2%)	47	76
10	1O	100/100 (100%)	98 (98%)	2 (2%)	55	81
10	2O	100/100 (100%)	97 (97%)	3 (3%)	41	70
11	1P	115/116 (99%)	111 (96%)	4 (4%)	36	65
11	2P	115/116 (99%)	113 (98%)	2 (2%)	60	84
12	1Q	111/111 (100%)	109 (98%)	2 (2%)	59	83
12	2Q	111/111 (100%)	110 (99%)	1 (1%)	78	92
13	1R	101/101 (100%)	90 (89%)	11 (11%)	6	14
13	2R	101/101 (100%)	95 (94%)	6 (6%)	19	43
14	1S	86/88 (98%)	80 (93%)	6 (7%)	15	35
14	2S	85/88 (97%)	83 (98%)	2 (2%)	49	77
15	1T	115/127 (91%)	113 (98%)	2 (2%)	60	84
15	2T	113/127 (89%)	111 (98%)	2 (2%)	59	83
16	1U	93/94 (99%)	89 (96%)	4 (4%)	29	57
16	2U	93/94 (99%)	93 (100%)	0	100	100
17	1V	80/82 (98%)	75 (94%)	5 (6%)	18	40
17	2V	80/82 (98%)	77 (96%)	3 (4%)	33	62
18	1W	90/92 (98%)	87 (97%)	3 (3%)	38	67
18	2W	90/92 (98%)	89 (99%)	1 (1%)	73	90
19	1X	77/78 (99%)	76 (99%)	1 (1%)	69	87
19	2X	77/78 (99%)	77 (100%)	0	100	100
20	1Y	85/91 (93%)	83 (98%)	2 (2%)	49	77
20	2Y	85/91 (93%)	84 (99%)	1 (1%)	71	88
21	1Z	135/179 (75%)	134 (99%)	1 (1%)	84	94
21	2Z	137/179 (76%)	136 (99%)	1 (1%)	84	94
22	10	65/67 (97%)	64 (98%)	1 (2%)	65	86
22	20	65/67 (97%)	65 (100%)	0	100	100
23	11	80/83 (96%)	78 (98%)	2 (2%)	47	76
23	21	80/83 (96%)	78 (98%)	2 (2%)	47	76
24	12	65/67 (97%)	64 (98%)	1 (2%)	65	86
24	22	65/67 (97%)	64 (98%)	1 (2%)	65	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	13	51/52 (98%)	48 (94%)	3 (6%)	19	43
25	23	50/52 (96%)	49 (98%)	1 (2%)	55	81
26	14	59/63 (94%)	55 (93%)	4 (7%)	16	36
26	24	53/63 (84%)	50 (94%)	3 (6%)	20	44
27	15	50/52 (96%)	45 (90%)	5 (10%)	7	18
27	25	50/52 (96%)	49 (98%)	1 (2%)	55	81
28	16	51/52 (98%)	48 (94%)	3 (6%)	19	43
28	26	50/52 (96%)	49 (98%)	1 (2%)	55	81
29	17	41/42 (98%)	39 (95%)	2 (5%)	25	52
29	27	41/42 (98%)	41 (100%)	0	100	100
30	18	54/55 (98%)	51 (94%)	3 (6%)	21	45
30	28	54/55 (98%)	52 (96%)	2 (4%)	34	63
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	71
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	71
33	1b	192/220 (87%)	192 (100%)	0	100	100
33	2b	187/220 (85%)	179 (96%)	8 (4%)	29	57
34	1c	142/188 (76%)	141 (99%)	1 (1%)	84	94
34	2c	140/188 (74%)	140 (100%)	0	100	100
35	1d	169/181 (93%)	166 (98%)	3 (2%)	59	83
35	2d	173/181 (96%)	171 (99%)	2 (1%)	71	88
36	1e	113/123 (92%)	112 (99%)	1 (1%)	78	92
36	2e	114/123 (93%)	112 (98%)	2 (2%)	59	83
37	1f	84/90 (93%)	84 (100%)	0	100	100
37	2f	85/90 (94%)	85 (100%)	0	100	100
38	1g	119/127 (94%)	118 (99%)	1 (1%)	81	93
38	2g	120/127 (94%)	119 (99%)	1 (1%)	81	93
39	1h	114/119 (96%)	112 (98%)	2 (2%)	59	83
39	2h	114/119 (96%)	111 (97%)	3 (3%)	46	75
40	1i	90/99 (91%)	89 (99%)	1 (1%)	73	90
40	2i	89/99 (90%)	87 (98%)	2 (2%)	52	79
41	1j	66/92 (72%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	2j	69/92 (75%)	69 (100%)	0	100	100
42	1k	82/99 (83%)	80 (98%)	2 (2%)	49	77
42	2k	83/99 (84%)	82 (99%)	1 (1%)	71	88
43	1l	96/108 (89%)	93 (97%)	3 (3%)	40	69
43	2l	96/108 (89%)	96 (100%)	0	100	100
44	1m	93/101 (92%)	91 (98%)	2 (2%)	52	79
44	2m	92/101 (91%)	91 (99%)	1 (1%)	73	90
45	1n	49/50 (98%)	45 (92%)	4 (8%)	11	26
45	2n	49/50 (98%)	48 (98%)	1 (2%)	55	81
46	1o	78/80 (98%)	78 (100%)	0	100	100
46	2o	78/80 (98%)	78 (100%)	0	100	100
47	1p	69/74 (93%)	66 (96%)	3 (4%)	29	57
47	2p	68/74 (92%)	66 (97%)	2 (3%)	42	71
48	1q	94/97 (97%)	94 (100%)	0	100	100
48	2q	94/97 (97%)	94 (100%)	0	100	100
49	1r	59/77 (77%)	59 (100%)	0	100	100
49	2r	59/77 (77%)	59 (100%)	0	100	100
50	1s	69/80 (86%)	67 (97%)	2 (3%)	42	71
50	2s	67/80 (84%)	65 (97%)	2 (3%)	41	70
51	1t	70/82 (85%)	70 (100%)	0	100	100
51	2t	70/82 (85%)	70 (100%)	0	100	100
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9303/10064 (92%)	9073 (98%)	230 (2%)	47	76

All (230) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	37	LEU
3	1D	43	ARG
3	1D	142	VAL
3	1D	155	LEU
3	1D	157	ARG
3	1D	168	ARG

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Mol	Chain	Res	Type
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	257	LEU
4	1E	12	THR
4	1E	21	VAL
4	1E	24	THR
4	1E	27	LEU
4	1E	34	VAL
4	1E	47	VAL
4	1E	113	PHE
4	1E	116	VAL
4	1E	119	ARG
4	1E	170	LEU
4	1E	175	VAL
4	1E	181	LEU
5	1F	33	LEU
5	1F	57	VAL
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	3	LEU
6	1G	31	VAL
6	1G	43	LEU
6	1G	159	VAL
6	1G	175	LEU
7	1H	15	VAL
7	1H	51	ARG
7	1H	56	SER
7	1H	71	LEU
7	1H	134	SER
8	1I	9	LEU
8	1I	92	VAL
8	1I	109	ILE
9	1N	14	VAL
9	1N	33	LEU
9	1N	34	LEU
9	1N	46	VAL
9	1N	48	MET

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Mol	Chain	Res	Type
9	1N	73	THR
9	1N	114	ARG
10	1O	10	VAL
10	1O	22	ILE
11	1P	65	ARG
11	1P	83	VAL
11	1P	95	VAL
11	1P	112	LEU
12	1Q	35	VAL
12	1Q	75	THR
13	1R	6	SER
13	1R	24	GLN
13	1R	29	LEU
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	100	LEU
13	1R	111	LEU
13	1R	114	VAL
14	1S	23	ARG
14	1S	25	ARG
14	1S	36	TYR
14	1S	50	SER
14	1S	69	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	89	VAL
16	1U	36	ARG
16	1U	74	LEU
16	1U	83	LEU
16	1U	95	LEU
17	1V	51	VAL
17	1V	52	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	79	VAL
18	1W	17	VAL
18	1W	23	LEU
18	1W	107	LEU
19	1X	35	THR

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Mol	Chain	Res	Type
20	1Y	72	VAL
20	1Y	97	ARG
21	1Z	154	ASP
22	10	39	ARG
23	11	11	ARG
23	11	30	VAL
24	12	53	LEU
25	13	30	ARG
25	13	34	GLU
25	13	54	VAL
26	14	27	THR
26	14	52	THR
26	14	56	VAL
26	14	65	ASP
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
27	15	40	LYS
27	15	58	LEU
28	16	6	ARG
28	16	48	VAL
28	16	51	GLU
29	17	41	ARG
29	17	43	THR
30	18	30	ARG
30	18	31	HIS
30	18	32	LEU
31	19	4	ARG
34	1c	3	ASN
35	1d	5	ILE
35	1d	31	CYS
35	1d	135	LEU
36	1e	41	VAL
38	1g	79	ARG
39	1h	91	ARG
39	1h	104	ARG
40	1i	111	ARG
42	1k	48	ILE
42	1k	114	VAL
43	1l	27	LEU
43	1l	36	VAL
43	1l	83	VAL

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Mol	Chain	Res	Type
44	1m	47	ASP
44	1m	104	ARG
45	1n	6	LEU
45	1n	18	VAL
45	1n	22	THR
45	1n	33	VAL
47	1p	20	VAL
47	1p	21	VAL
47	1p	61	SER
50	1s	12	ASP
50	1s	41	VAL
3	2D	14	ARG
3	2D	37	LEU
3	2D	99	ASP
3	2D	142	VAL
3	2D	157	ARG
3	2D	211	ARG
3	2D	212	SER
3	2D	242	ARG
4	2E	21	VAL
4	2E	24	THR
4	2E	75	VAL
4	2E	116	VAL
4	2E	119	ARG
4	2E	181	LEU
5	2F	74	ARG
5	2F	88	VAL
5	2F	106	ARG
5	2F	183	VAL
5	2F	192	LEU
5	2F	201	VAL
6	2G	145	THR
6	2G	159	VAL
8	2I	38	LEU
8	2I	127	VAL
8	2I	144	VAL
9	2N	33	LEU
9	2N	46	VAL
9	2N	58	ASP
10	2O	23	ARG
10	2O	24	VAL
10	2O	28	SER

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Mol	Chain	Res	Type
11	2P	56	SER
11	2P	95	VAL
12	2Q	109	VAL
13	2R	24	GLN
13	2R	29	LEU
13	2R	36	THR
13	2R	44	LEU
13	2R	65	LEU
13	2R	111	LEU
14	2S	25	ARG
14	2S	110	LEU
15	2T	28	VAL
15	2T	111	ARG
17	2V	61	VAL
17	2V	72	VAL
17	2V	79	VAL
18	2W	23	LEU
20	2Y	97	ARG
21	2Z	144	LEU
23	21	4	VAL
23	21	30	VAL
24	22	53	LEU
25	23	54	VAL
26	24	24	THR
26	24	49	PHE
26	24	52	THR
27	25	6	VAL
28	26	48	VAL
30	28	30	ARG
30	28	32	LEU
31	29	17	ILE
33	2b	11	LEU
33	2b	19	HIS
33	2b	93	VAL
33	2b	94	ASN
33	2b	124	SER
33	2b	127	ILE
33	2b	154	LEU
33	2b	189	ASP
35	2d	135	LEU
35	2d	170	VAL
36	2e	20	GLN

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Mol	Chain	Res	Type
36	2e	41	VAL
38	2g	79	ARG
39	2h	2	LEU
39	2h	91	ARG
39	2h	104	ARG
40	2i	65	VAL
40	2i	102	LEU
42	2k	41	THR
44	2m	103	THR
45	2n	33	VAL
47	2p	20	VAL
47	2p	21	VAL
50	2s	71	LEU
50	2s	77	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	180	ASN
5	1F	8	GLN
5	1F	69	HIS
8	1I	105	HIS
10	1O	3	GLN
13	1R	31	HIS
16	1U	94	ASN
19	1X	31	HIS
19	1X	82	GLN
21	1Z	73	GLN
21	1Z	75	ASN
24	12	65	ASN
25	13	32	GLN
33	1b	78	GLN
33	1b	94	ASN
33	1b	113	HIS
34	1c	6	HIS
34	1c	37	GLN
34	1c	162	GLN
34	1c	176	HIS
35	1d	77	ASN
35	1d	123	HIS
35	1d	125	HIS
36	1e	78	HIS

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Mol	Chain	Res	Type
38	1g	28	ASN
40	1i	3	GLN
40	1i	58	HIS
40	1i	124	GLN
41	1j	56	HIS
43	1l	99	HIS
44	1m	40	ASN
46	1o	46	HIS
50	1s	69	HIS
50	1s	83	HIS
51	1t	75	ASN
3	2D	166	GLN
4	2E	48	GLN
5	2F	69	HIS
13	2R	24	GLN
15	2T	58	ASN
19	2X	31	HIS
20	2Y	6	HIS
21	2Z	55	HIS
21	2Z	73	GLN
25	23	32	GLN
26	24	46	GLN
33	2b	78	GLN
33	2b	94	ASN
33	2b	113	HIS
35	2d	77	ASN
35	2d	123	HIS
35	2d	125	HIS
36	2e	78	HIS
37	2f	32	ASN
37	2f	73	ASN
37	2f	100	ASN
38	2g	28	ASN
38	2g	148	ASN
40	2i	58	HIS
40	2i	89	ASN
40	2i	124	GLN
41	2j	56	HIS
42	2k	22	HIS
44	2m	12	ASN
46	2o	9	GLN
46	2o	62	GLN

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Mol	Chain	Res	Type
47	2p	16	HIS
49	2r	63	GLN
50	2s	69	HIS
50	2s	83	HIS
51	2t	42	GLN
51	2t	90	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	412 (14%)	34 (1%)
1	2A	2788/2915 (95%)	455 (16%)	22 (0%)
2	1B	120/121 (99%)	11 (9%)	1 (0%)
2	2B	118/121 (97%)	27 (22%)	0
32	1a	1494/1521 (98%)	232 (15%)	0
32	2a	1498/1521 (98%)	263 (17%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	2 (16%)	0
54	1w	71/76 (93%)	23 (32%)	0
54	1y	71/76 (93%)	21 (29%)	0
54	2w	68/76 (89%)	24 (35%)	0
54	2y	69/76 (90%)	19 (27%)	0
55	1x	75/77 (97%)	9 (12%)	0
55	2x	75/77 (97%)	15 (20%)	0
All	All	9332/9620 (97%)	1515 (16%)	57 (0%)

All (1515) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	27	G
1	1A	34	C
1	1A	35	G
1	1A	36	G
1	1A	45	C
1	1A	54	G
1	1A	70	A
1	1A	73	A
1	1A	74	G
1	1A	83	A

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Mol	Chain	Res	Type
1	1A	94	G
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	123	G
1	1A	137	G
1	1A	171	A
1	1A	185	A
1	1A	188	A
1	1A	194	G
1	1A	203	G
1	1A	204	G
1	1A	205	A
1	1A	211	A
1	1A	214	A
1	1A	217	A
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	258	U
1	1A	272	U
1	1A	273	G
1	1A	275	C
1	1A	279	G
1	1A	288	U
1	1A	289	G
1	1A	303	C
1	1A	335	A
1	1A	353	G
1	1A	354	A
1	1A	376	G
1	1A	387	G
1	1A	388	A
1	1A	389	G
1	1A	399	G
1	1A	413	G
1	1A	423	G
1	1A	432	U
1	1A	438	G
1	1A	455	A
1	1A	470	C
1	1A	474	U

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Mol	Chain	Res	Type
1	1A	477	C
1	1A	482	C
1	1A	483	A
1	1A	507	G
1	1A	519	G
1	1A	529	U
1	1A	530	A
1	1A	534	C
1	1A	555	G
1	1A	556	C
1	1A	557	A
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	586	G
1	1A	596	G
1	1A	597	C
1	1A	598	A
1	1A	609	A
1	1A	615	G
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	639	G
1	1A	641	G
1	1A	642	G
1	1A	652	A
1	1A	662	A
1	1A	670	C
1	1A	671	A
1	1A	693	G
1	1A	697	C
1	1A	716	G
1	1A	733	G
1	1A	777	C
1	1A	811	A
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	830	A
1	1A	831	A
1	1A	832	G

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Mol	Chain	Res	Type
1	1A	836	A
1	1A	837	C
1	1A	839	G
1	1A	852	G
1	1A	858	U
1	1A	859	C
1	1A	866	A
1	1A	874	U
1	1A	875	U
1	1A	906	G
1	1A	924	U
1	1A	926	G
1	1A	927	G
1	1A	931	C
1	1A	932	C
1	1A	933	C
1	1A	934	A
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	939	C
1	1A	940	C
1	1A	941	U
1	1A	942	A
1	1A	943	C
1	1A	944	C
1	1A	956	A
1	1A	977	G
1	1A	990	A
1	1A	991	G
1	1A	1004	A
1	1A	1006	C
1	1A	1019	G
1	1A	1020	C
1	1A	1029	A
1	1A	1042	A
1	1A	1058	U
1	1A	1059	C
1	1A	1068	G
1	1A	1072	U
1	1A	1079	U
1	1A	1080	G

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Mol	Chain	Res	Type
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1100	A
1	1A	1101	G
1	1A	1104	G
1	1A	1112	U
1	1A	1113	A
1	1A	1114	G
1	1A	1117	G
1	1A	1119	A
1	1A	1120	G
1	1A	1121	C
1	1A	1122	C
1	1A	1124	U
1	1A	1125	C
1	1A	1129	U
1	1A	1131	A
1	1A	1134	A
1	1A	1135	G
1	1A	1136	U
1	1A	1137	G
1	1A	1139	G
1	1A	1140	U
1	1A	1142	A
1	1A	1147	U
1	1A	1156	G
1	1A	1157	A
1	1A	1158	G
1	1A	1161	G
1	1A	1162	C
1	1A	1174	A
1	1A	1175	A
1	1A	1176	U
1	1A	1180	C
1	1A	1181	G
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1222	A

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Mol	Chain	Res	Type
1	1A	1223	C
1	1A	1256	U
1	1A	1283	A
1	1A	1290	G
1	1A	1294	G
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1346	U
1	1A	1347	A
1	1A	1349	G
1	1A	1391	C
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1426	G
1	1A	1430	A
1	1A	1431	G
1	1A	1432	C
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1491	A
1	1A	1497	G
1	1A	1502	G
1	1A	1514	C
1	1A	1529	G
1	1A	1539	C
1	1A	1540	A
1	1A	1554	A
1	1A	1555	C
1	1A	1556	A
1	1A	1586	G
1	1A	1587	U
1	1A	1605	A
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U

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Mol	Chain	Res	Type
1	1A	1628	G
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1656	A
1	1A	1668	G
1	1A	1694	G
1	1A	1695	C
1	1A	1701	A
1	1A	1711	A
1	1A	1721	G
1	1A	1743	G
1	1A	1747	A
1	1A	1748	A
1	1A	1750	G
1	1A	1767	A
1	1A	1776	G
1	1A	1787	G
1	1A	1793	A
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1811	A
1	1A	1813	C
1	1A	1821	C
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1847	G
1	1A	1860	A
1	1A	1878	A
1	1A	1892	G
1	1A	1899	A
1	1A	1900	G
1	1A	1911	A
1	1A	1922	A
1	1A	1928	G
1	1A	1949	A
1	1A	1951	G
1	1A	1952	G
1	1A	1959	A
1	1A	1960	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	1977	U
1	1A	1985	U
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2015	U
1	1A	2019	G
1	1A	2042	A
1	1A	2045	G
1	1A	2053	A
1	1A	2054	G
1	1A	2055	A
1	1A	2061	C
1	1A	2065	C
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2091	G
1	1A	2132	G
1	1A	2135	U
1	1A	2136	A
1	1A	2137	G
1	1A	2138	G
1	1A	2140	U
1	1A	2143	G
1	1A	2144	U
1	1A	2148	A
1	1A	2149	G
1	1A	2151	C
1	1A	2152	U
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2157	A
1	1A	2158	C
1	1A	2162	C
1	1A	2164	C
1	1A	2166	U
1	1A	2168	C

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Mol	Chain	Res	Type
1	1A	2169	G
1	1A	2172	U
1	1A	2173	G
1	1A	2178	G
1	1A	2179	G
1	1A	2180	A
1	1A	2181	G
1	1A	2187	G
1	1A	2188	G
1	1A	2193	A
1	1A	2194	U
1	1A	2195	A
1	1A	2196	C
1	1A	2200	C
1	1A	2203	G
1	1A	2204	G
1	1A	2206	G
1	1A	2213	G
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A
1	1A	2237	A
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2285	A
1	1A	2292	G
1	1A	2295	C
1	1A	2299	A
1	1A	2306	C
1	1A	2317	A
1	1A	2320	G
1	1A	2332	A
1	1A	2337	G
1	1A	2346	G
1	1A	2348	A
1	1A	2359	C
1	1A	2362	C
1	1A	2366	G

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Mol	Chain	Res	Type
1	1A	2373	A
1	1A	2395	G
1	1A	2397	C
1	1A	2408	G
1	1A	2418	U
1	1A	2422	G
1	1A	2437	A
1	1A	2441	G
1	1A	2442	A
1	1A	2443	U
1	1A	2447	A
1	1A	2451	A
1	1A	2453	C
1	1A	2460	A
1	1A	2480	G
1	1A	2488	A
1	1A	2499	G
1	1A	2514	G
1	1A	2517	G
1	1A	2530	A
1	1A	2541	G
1	1A	2561	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2585	C
1	1A	2594	G
1	1A	2614	A
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2640	C
1	1A	2641	A
1	1A	2642	G
1	1A	2653	G
1	1A	2666	A
1	1A	2701	U
1	1A	2702	C
1	1A	2714	U
1	1A	2715	C
1	1A	2725	A
1	1A	2726	A

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Mol	Chain	Res	Type
1	1A	2727	G
1	1A	2739	U
1	1A	2746	A
1	1A	2770	A
1	1A	2771	A
1	1A	2777	A
1	1A	2778	A
1	1A	2779	G
1	1A	2791	A
1	1A	2793	G
1	1A	2803	A
1	1A	2804	C
1	1A	2806	G
1	1A	2813	G
1	1A	2814	C
1	1A	2830	A
1	1A	2831	A
1	1A	2845	A
1	1A	2882	G
1	1A	2890	C
1	1A	2901	A
1	1A	2903	G
2	1B	2	C
2	1B	35	U
2	1B	42	C
2	1B	45	A
2	1B	52	A
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	85	G
2	1B	106	G
2	1B	110	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	51	A
32	1a	52	G
32	1a	54	C
32	1a	61	G
32	1a	65	U

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Mol	Chain	Res	Type
32	1a	73	G
32	1a	79	G
32	1a	91	C
32	1a	96	U
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	120	A
32	1a	121	C
32	1a	131	C
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(D)	C
32	1a	189(F)	U
32	1a	189(G)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
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
32	1a	344	A
32	1a	345	C
32	1a	348	G
32	1a	352	C
32	1a	353	A

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Mol	Chain	Res	Type
32	1a	354	G
32	1a	355	C
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	388	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	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	510	A
32	1a	511	C
32	1a	518	C
32	1a	524	G
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	562	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	575	G
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	630	G

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Mol	Chain	Res	Type
32	1a	653	A
32	1a	659	U
32	1a	665	A
32	1a	666	G
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	717	C
32	1a	723	U
32	1a	724	G
32	1a	731	G
32	1a	749	C
32	1a	753	A
32	1a	755	G
32	1a	774	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	816	A
32	1a	817	C
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	859	A
32	1a	870	U
32	1a	902	G
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
32	1a	972	C
32	1a	974	A
32	1a	975	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	999	C
32	1a	1000	U
32	1a	1001(A)	G
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1015	A
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1039	C
32	1a	1043	C
32	1a	1053	G
32	1a	1054	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1125	U
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G

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Mol	Chain	Res	Type
32	1a	1140	C
32	1a	1141	C
32	1a	1146	A
32	1a	1152	A
32	1a	1157	A
32	1a	1159	U
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1314	C
32	1a	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G

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Mol	Chain	Res	Type
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
53	1v	14	A
54	1w	2	C
54	1w	6	G
54	1w	7	A
54	1w	8	4SU
54	1w	14	A
54	1w	15	G
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	24	G
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	62	C
54	1w	65	G
54	1w	67	C
54	1w	68	C
54	1w	70	G
54	1w	72	C
54	1w	73	A
54	1w	74	C
55	1x	9	G
55	1x	14	A
55	1x	18	G
55	1x	19	G

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Mol	Chain	Res	Type
55	1x	21	A
55	1x	47	U
55	1x	61	C
55	1x	69	C
55	1x	76	A
54	1y	6	G
54	1y	8	4SU
54	1y	9	A
54	1y	13	C
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	35	A
54	1y	44	G
54	1y	45	U
54	1y	46	7MG
54	1y	48	C
54	1y	49	C
54	1y	54	5MU
54	1y	57	G
54	1y	59	U
54	1y	60	U
54	1y	61	C
54	1y	65	G
54	1y	70	G
54	1y	73	A
1	2A	15	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	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	125	G

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Mol	Chain	Res	Type
1	2A	131	G
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
1	2A	248	G
1	2A	249	C
1	2A	266	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	272(I)	U
1	2A	272(J)	C
1	2A	277	C
1	2A	278	A
1	2A	294	A
1	2A	311	A
1	2A	316	C
1	2A	317	G
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	348	G
1	2A	352	G
1	2A	354	G
1	2A	362	U
1	2A	363	G

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Mol	Chain	Res	Type
1	2A	363(B)	G
1	2A	363(D)	G
1	2A	386	G
1	2A	396	G
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	422	A
1	2A	435	C
1	2A	444	C
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	551	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	592	G
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	648	G
1	2A	651	G

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Mol	Chain	Res	Type
1	2A	652(B)	A
1	2A	652(U)	G
1	2A	653	A
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	832	G
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	870	A
1	2A	874	G
1	2A	875	G
1	2A	879	G
1	2A	880	G
1	2A	883	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	899	A
1	2A	900	A

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Mol	Chain	Res	Type
1	2A	901	A
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	980	A
1	2A	983	A
1	2A	996	A
1	2A	997	G
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	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1040	C
1	2A	1041	C
1	2A	1043	C
1	2A	1114	G
1	2A	1116	C
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1144	G
1	2A	1166	C
1	2A	1169	G
1	2A	1171	G

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Mol	Chain	Res	Type
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1237	A
1	2A	1250	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1284	A
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1314	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	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1411	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1424	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A

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Mol	Chain	Res	Type
1	2A	1493	C
1	2A	1497	U
1	2A	1506	C
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1545	A
1	2A	1547	C
1	2A	1558	A
1	2A	1569	A
1	2A	1578	U
1	2A	1584	C
1	2A	1586	A
1	2A	1588	C
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C
1	2A	1647	G
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	1739	U
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A

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Mol	Chain	Res	Type
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1811	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
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	1931	U
1	2A	1936	A
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1964	G
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2067	G
1	2A	2069	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2A	2096	U
1	2A	2097	C
1	2A	2106	G
1	2A	2109	U
1	2A	2110	G
1	2A	2111	C
1	2A	2116	G
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2134	A
1	2A	2135	A
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2146	C
1	2A	2150	U
1	2A	2154	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2164	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	2178	C
1	2A	2182	G
1	2A	2185	C
1	2A	2189	U

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Mol	Chain	Res	Type
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2239	G
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2294	C
1	2A	2305	A
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2328	A
1	2A	2331	G
1	2A	2334	G
1	2A	2336	A
1	2A	2341	G
1	2A	2346	A
1	2A	2347	C
1	2A	2350	C
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2403	C
1	2A	2406	U
1	2A	2410	G
1	2A	2419	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2431	U
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G

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Mol	Chain	Res	Type
1	2A	2448	A
1	2A	2476	A
1	2A	2490	G
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2530	A
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2582	G
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
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	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	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2780	G
1	2A	2793	G

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Mol	Chain	Res	Type
1	2A	2802	G
1	2A	2807	G
1	2A	2808	U
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2823	A
1	2A	2833	G
1	2A	2835	A
1	2A	2836	U
1	2A	2839	G
1	2A	2872	G
1	2A	2873	A
1	2A	2879	C
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	2B	2	C
2	2B	5	C
2	2B	8	U
2	2B	9	G
2	2B	19	G
2	2B	25	A
2	2B	30	C
2	2B	32	C
2	2B	34	U
2	2B	42	C
2	2B	53	A
2	2B	56	G
2	2B	65	C
2	2B	66	A
2	2B	67	G
2	2B	72	G
2	2B	73	A
2	2B	75	G
2	2B	85	G
2	2B	88	C
2	2B	106	G
2	2B	108	U
2	2B	110	G

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Mol	Chain	Res	Type
2	2B	114	C
2	2B	116	G
2	2B	119	G
2	2B	120	A
32	2a	9	G
32	2a	13	U
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	66	G
32	2a	73	G
32	2a	79	G
32	2a	89	C
32	2a	97	G
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	120	A
32	2a	121	C
32	2a	131	C
32	2a	144	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189	G
32	2a	189(F)	U
32	2a	189(G)	G
32	2a	195	A
32	2a	197	A
32	2a	200	G
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	266	G
32	2a	267	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	279	A
32	2a	289	G
32	2a	300	A
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	346	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	381	C
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
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	518	C
32	2a	521	G
32	2a	531	U
32	2a	532	A
32	2a	545	C

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Mol	Chain	Res	Type
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	577	G
32	2a	596	C
32	2a	598	U
32	2a	630	G
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	723	U
32	2a	731	G
32	2a	733	A
32	2a	749	C
32	2a	755	G
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	834	C
32	2a	840	C
32	2a	841	U
32	2a	853	G
32	2a	859	A
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	960	U
32	2a	961	U

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Mol	Chain	Res	Type
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	982	U
32	2a	984	C
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	996	A
32	2a	997	U
32	2a	999	C
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1033	G
32	2a	1036	G
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1045	C

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Mol	Chain	Res	Type
32	2a	1051	C
32	2a	1055	A
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1079	G
32	2a	1081	G
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1103	C
32	2a	1108	G
32	2a	1113	C
32	2a	1117	G
32	2a	1122	U
32	2a	1124	G
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1163	C
32	2a	1164	G
32	2a	1173	G
32	2a	1182	G
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1214	C
32	2a	1226	C

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Mol	Chain	Res	Type
32	2a	1227	A
32	2a	1233	G
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1262	C
32	2a	1264	C
32	2a	1267	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1299	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1319	A
32	2a	1320	C
32	2a	1323	G
32	2a	1346	A
32	2a	1347	G
32	2a	1358	U
32	2a	1363	C
32	2a	1368	G
32	2a	1370	G
32	2a	1378	C
32	2a	1398	A
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G

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Mol	Chain	Res	Type
32	2a	1487	G
32	2a	1492	A
32	2a	1497	G
32	2a	1499	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	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	15	A
54	2w	3	C
54	2w	4	C
54	2w	7	A
54	2w	8	4SU
54	2w	9	A
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	25	C
54	2w	26	A
54	2w	29	G
54	2w	34	G
54	2w	46	7MG
54	2w	47	U
54	2w	48	C
54	2w	50	U
54	2w	56	C
54	2w	62	C
54	2w	64	A
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	74	C
55	2x	9	G

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Mol	Chain	Res	Type
55	2x	13	C
55	2x	18	G
55	2x	21	A
55	2x	22	G
55	2x	46	G
55	2x	47	U
55	2x	48	C
55	2x	52	G
55	2x	53	G
55	2x	56	C
55	2x	63	G
55	2x	67	C
55	2x	68	C
55	2x	76	A
54	2y	6	G
54	2y	8	4SU
54	2y	13	C
54	2y	19	G
54	2y	35	A
54	2y	44	G
54	2y	45	U
54	2y	46	7MG
54	2y	48	C
54	2y	49	C
54	2y	54	5MU
54	2y	57	G
54	2y	59	U
54	2y	60	U
54	2y	61	C
54	2y	65	G
54	2y	69	G
54	2y	70	G
54	2y	73	A

All (57) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	115	G
1	1A	184	A
1	1A	185	A
1	1A	271	U
1	1A	302	A

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Mol	Chain	Res	Type
1	1A	509	A
1	1A	572	A
1	1A	596	G
1	1A	793	A
1	1A	913	A
1	1A	941	U
1	1A	1065	U
1	1A	1067	A
1	1A	1093	G
1	1A	1124	U
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A
1	1A	1425	A
1	1A	1466	U
1	1A	1554	A
1	1A	1710	C
1	1A	2014	G
1	1A	2156	A
1	1A	2192	A
1	1A	2203	G
1	1A	2205	C
1	1A	2418	U
1	1A	2442	A
1	1A	2641	A
1	1A	2701	U
1	1A	2769	U
2	1B	1	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	620	G
1	2A	752	A
1	2A	774	A
1	2A	827	U
1	2A	856	C
1	2A	900	A

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Mol	Chain	Res	Type
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2689	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
32	MA6	2a	1519	32	19,26,27	1.02	1 (5%)	18,38,41	1.56	3 (16%)
32	2MG	1a	1207	32	19,26,27	1.26	2 (10%)	21,38,41	2.54	9 (42%)
1	2MA	1A	2515	1,56	17,25,26	1.22	2 (11%)	19,37,40	2.02	3 (15%)
32	MA6	2a	1518	32	19,26,27	0.99	1 (5%)	18,38,41	1.72	4 (22%)
1	5MU	1A	1937	1	15,22,23	1.09	1 (6%)	16,32,35	1.81	1 (6%)
54	7MG	2w	46	54	22,26,27	1.80	4 (18%)	28,39,42	2.63	9 (32%)
54	PSU	1w	32	54	17,21,22	1.55	2 (11%)	20,30,33	3.17	6 (30%)
1	PSU	1A	2617	1,56	17,21,22	1.64	4 (23%)	20,30,33	3.16	6 (30%)
32	2MG	2a	1207	32	19,26,27	1.27	2 (10%)	21,38,41	2.21	6 (28%)
1	5MC	1A	1964	1	15,22,23	1.16	1 (6%)	19,32,35	1.42	3 (15%)
1	5MU	2A	1939	1,56	15,22,23	1.08	2 (13%)	16,32,35	1.85	2 (12%)
32	MA6	1a	1519	32	19,26,27	1.05	1 (5%)	18,38,41	1.61	4 (22%)
54	4SU	1w	8	54	14,21,22	1.27	1 (7%)	15,30,33	1.42	2 (13%)
32	5MC	1a	1400	32	15,22,23	1.32	1 (6%)	19,32,35	1.40	3 (15%)
32	UR3	2a	1498	32	14,22,23	0.79	1 (7%)	15,32,35	0.73	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	4OC	1a	1402	32	16,23,24	0.69	0	17,32,35	1.39	1 (5%)
54	4SU	2y	8	54	14,21,22	1.30	2 (14%)	15,30,33	1.57	2 (13%)
54	4SU	2w	8	54	14,21,22	1.27	1 (7%)	15,30,33	1.21	2 (13%)
32	5MC	1a	1407	32	15,22,23	1.29	1 (6%)	19,32,35	1.39	3 (15%)
1	5MU	2A	1915	1	15,22,23	1.07	1 (6%)	16,32,35	1.81	2 (12%)
1	OMG	1A	2263	1,55,56	18,26,27	1.25	2 (11%)	20,38,41	2.12	6 (30%)
55	PSU	1x	55	55,56	17,21,22	1.69	3 (17%)	20,30,33	3.19	6 (30%)
32	7MG	1a	527	32	22,26,27	1.81	4 (18%)	28,39,42	2.66	9 (32%)
55	PSU	2x	55	55	17,21,22	1.57	2 (11%)	20,30,33	3.14	6 (30%)
54	MIA	1w	37	54	24,31,32	2.19	4 (16%)	26,44,47	2.60	9 (34%)
32	5MC	1a	967	32	15,22,23	1.34	1 (6%)	19,32,35	1.30	3 (15%)
1	OMG	2A	2251	1,55	18,26,27	1.14	2 (11%)	20,38,41	2.06	6 (30%)
1	PSU	2A	2605	1	17,21,22	1.57	3 (17%)	20,30,33	3.12	6 (30%)
1	5MC	1A	1984	1	15,22,23	1.29	1 (6%)	19,32,35	1.33	3 (15%)
1	4OC	1A	1942	1	15,22,24	0.68	0	17,31,35	1.52	2 (11%)
32	M2G	2a	966	32	20,27,28	1.39	3 (15%)	22,40,43	2.11	6 (27%)
54	PSU	2y	32	54	17,21,22	1.43	2 (11%)	20,30,33	3.21	5 (25%)
54	4SU	1y	8	54	14,21,22	1.27	1 (7%)	15,30,33	1.61	2 (13%)
54	PSU	1w	39	54	17,21,22	1.67	3 (17%)	20,30,33	3.09	6 (30%)
54	MIA	2y	37	54	18,24,32	1.17	2 (11%)	18,35,47	1.25	2 (11%)
1	PSU	2A	1917	1	17,21,22	1.59	2 (11%)	20,30,33	3.20	6 (30%)
1	5MC	2A	1962	1,56	15,22,23	1.20	1 (6%)	19,32,35	1.46	3 (15%)
54	5MU	2y	54	54	15,22,23	1.09	1 (6%)	16,32,35	2.02	1 (6%)
32	5MC	2a	1407	32	15,22,23	1.24	1 (6%)	19,32,35	1.57	4 (21%)
43	0TD	2l	92	43	4,9,10	3.09	1 (25%)	3,11,13	2.70	1 (33%)
1	2MU	1A	2564	1,56	14,22,24	0.84	1 (7%)	14,31,36	0.86	1 (7%)
32	PSU	2a	516	32	17,21,22	1.50	3 (17%)	20,30,33	3.22	6 (30%)
32	UR3	1a	1498	32	14,22,23	0.85	1 (7%)	15,32,35	0.70	0
54	PSU	2w	39	54	17,21,22	1.44	2 (11%)	20,30,33	3.33	6 (30%)
32	4OC	2a	1402	32	16,23,24	0.67	0	17,32,35	1.68	1 (5%)
1	5MU	1A	1961	1,56	15,22,23	1.11	2 (13%)	16,32,35	1.79	2 (12%)
54	PSU	2y	55	54	17,21,22	1.51	2 (11%)	20,30,33	3.14	6 (30%)
54	PSU	2w	55	54	17,21,22	1.40	2 (11%)	20,30,33	3.33	6 (30%)
32	5MC	2a	1404	32	15,22,23	1.36	1 (6%)	19,32,35	1.33	3 (15%)
54	7MG	1y	46	54	22,26,27	1.85	4 (18%)	28,39,42	3.00	10 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	2A	1911	1	17,21,22	1.58	2 (11%)	20,30,33	3.13	6 (30%)
43	0TD	1l	92	43	4,9,10	3.19	1 (25%)	3,11,13	7.49	1 (33%)
54	7MG	1w	46	54	22,26,27	1.78	4 (18%)	28,39,42	2.86	8 (28%)
54	PSU	1y	32	54	17,21,22	1.43	2 (11%)	20,30,33	3.10	5 (25%)
54	MIA	2w	37	54	20,27,32	1.82	3 (15%)	22,39,47	1.86	7 (31%)
32	PSU	1a	516	32	17,21,22	1.48	4 (23%)	20,30,33	3.08	6 (30%)
55	5MU	2x	54	55	15,22,23	1.06	1 (6%)	16,32,35	1.60	2 (12%)
54	MIA	1y	37	54	18,24,32	1.14	2 (11%)	18,35,47	1.29	2 (11%)
54	5MU	2w	54	54	15,22,23	1.09	1 (6%)	16,32,35	1.97	1 (6%)
55	4SU	1x	8	55	14,21,22	1.49	2 (14%)	15,30,33	2.53	2 (13%)
55	4SU	2x	8	55	14,21,22	1.26	2 (14%)	15,30,33	2.40	2 (13%)
1	2MU	2A	2552	1	14,22,24	0.89	0	14,31,36	0.88	0
54	7MG	2y	46	54	22,26,27	1.85	3 (13%)	28,39,42	3.02	9 (32%)
55	5MU	1x	54	55,56	15,22,23	1.13	1 (6%)	16,32,35	1.94	2 (12%)
1	4OC	2A	1920	1	15,22,24	0.64	0	17,31,35	1.39	2 (11%)
1	PSU	1A	1933	1	17,21,22	1.49	2 (11%)	20,30,33	3.01	6 (30%)
32	5MC	1a	1404	32	15,22,23	1.37	1 (6%)	19,32,35	1.26	3 (15%)
32	MA6	1a	1518	32	19,26,27	0.95	1 (5%)	18,38,41	1.66	4 (22%)
1	5MC	2A	1942	1	15,22,23	1.30	1 (6%)	19,32,35	1.40	3 (15%)
54	PSU	1y	55	54	17,21,22	1.52	2 (11%)	20,30,33	3.11	6 (30%)
55	5MC	2x	32	55	15,22,23	1.27	1 (6%)	19,32,35	1.41	3 (15%)
1	PSU	1A	1939	1	17,21,22	1.43	2 (11%)	20,30,33	3.25	6 (30%)
32	5MC	2a	967	32	15,22,23	1.41	1 (6%)	19,32,35	1.26	3 (15%)
54	PSU	1w	55	54	17,21,22	1.43	2 (11%)	20,30,33	3.34	6 (30%)
54	PSU	2y	39	54	17,21,22	1.49	2 (11%)	20,30,33	3.16	6 (30%)
54	5MU	1y	54	54	15,22,23	1.11	2 (13%)	16,32,35	2.11	1 (6%)
32	M2G	1a	966	32	20,27,28	1.44	3 (15%)	22,40,43	2.25	6 (27%)
32	7MG	2a	527	32,56	22,26,27	1.80	4 (18%)	28,39,42	2.69	9 (32%)
54	5MU	1w	54	54	15,22,23	1.08	2 (13%)	16,32,35	1.83	2 (12%)
32	5MC	2a	1400	32	15,22,23	1.31	1 (6%)	19,32,35	1.34	3 (15%)
1	2MA	2A	2503	1,56	17,25,26	1.30	2 (11%)	19,37,40	1.99	3 (15%)
54	PSU	1y	39	54	17,21,22	1.48	2 (11%)	20,30,33	3.10	5 (25%)
55	5MC	1x	32	55	15,22,23	1.32	1 (6%)	19,32,35	1.55	4 (21%)
54	PSU	2w	32	54	17,21,22	1.52	2 (11%)	20,30,33	3.07	6 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	2a	1519	32	-	5/7/29/30	0/3/3/3
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
1	2MA	1A	2515	1,56	-	2/3/25/26	0/3/3/3
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
1	5MU	1A	1937	1	-	0/5/25/26	0/2/2/2
54	7MG	2w	46	54	-	5/7/37/38	0/3/3/3
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	1,56	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
1	5MC	1A	1964	1	-	0/5/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	0/5/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
54	4SU	1w	8	54	-	0/5/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
32	4OC	1a	1402	32	-	3/9/29/30	0/2/2/2
54	4SU	2y	8	54	-	2/5/25/26	0/2/2/2
54	4SU	2w	8	54	-	1/5/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
1	OMG	1A	2263	1,55,56	-	0/5/27/28	0/3/3/3
55	PSU	1x	55	55,56	-	2/7/25/26	0/2/2/2
32	7MG	1a	527	32	-	2/7/37/38	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/11/33/34	0/3/3/3
32	5MC	1a	967	32	-	0/5/25/26	0/2/2/2
1	OMG	2A	2251	1,55	-	0/5/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1984	1	-	2/5/25/26	0/2/2/2
1	4OC	1A	1942	1	-	1/7/27/30	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	2/5/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	2/3/25/34	0/3/3/3
1	PSU	2A	1917	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	2A	1962	1,56	-	2/5/25/26	0/2/2/2
54	5MU	2y	54	54	-	3/5/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/3/12/14	-
1	2MU	1A	2564	1,56	-	0/7/27/28	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	5/9/29/30	0/2/2/2
1	5MU	1A	1961	1,56	-	0/5/25/26	0/2/2/2
54	PSU	2y	55	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
54	7MG	1y	46	54	-	3/7/37/38	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/3/12/14	-
54	7MG	1w	46	54	-	2/7/37/38	0/3/3/3
54	PSU	1y	32	54	-	1/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/7/29/34	0/3/3/3
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/5/25/26	0/2/2/2
54	MIA	1y	37	54	-	1/3/25/34	0/3/3/3
54	5MU	2w	54	54	-	0/5/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/5/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/5/25/26	0/2/2/2
1	2MU	2A	2552	1	-	0/7/27/28	0/2/2/2
54	7MG	2y	46	54	-	3/7/37/38	0/3/3/3
55	5MU	1x	54	55,56	-	0/5/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/7/27/30	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
32	MA6	1a	1518	32	-	1/7/29/30	0/3/3/3
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/5/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/5/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	3/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	7MG	2a	527	32,56	-	3/7/37/38	0/3/3/3
54	5MU	1w	54	54	-	0/5/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	2/3/25/26	0/3/3/3
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/5/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2

All (150) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C13-C14	7.18	1.53	1.32
54	2w	37	MIA	C2-S10	-6.81	1.69	1.75
54	1w	37	MIA	C2-S10	-6.34	1.70	1.75
43	1l	92	0TD	CB-SB	-6.09	1.69	1.84
43	2l	92	0TD	CB-SB	-5.98	1.69	1.84
32	2a	527	7MG	C6-C5	5.13	1.48	1.41
54	2w	46	7MG	C6-C5	5.11	1.48	1.41
32	2a	967	5MC	C5-C4	5.10	1.49	1.41
55	1x	55	PSU	C5-C1'	-4.95	1.48	1.52
54	1w	39	PSU	C5-C1'	-4.94	1.48	1.52
54	2y	46	7MG	C6-C5	4.91	1.48	1.41
32	2a	1404	5MC	C5-C4	4.88	1.48	1.41
32	1a	1404	5MC	C5-C4	4.88	1.48	1.41
32	1a	967	5MC	C5-C4	4.85	1.48	1.41
54	2y	46	7MG	C5-C4	4.84	1.48	1.39
54	1y	46	7MG	C6-C5	4.83	1.48	1.41
32	1a	527	7MG	C6-C5	4.82	1.48	1.41
54	1y	46	7MG	C5-C4	4.78	1.48	1.39
54	1w	46	7MG	C5-C4	4.71	1.48	1.39
55	1x	32	5MC	C5-C4	4.66	1.48	1.41
32	1a	527	7MG	C5-C4	4.65	1.48	1.39
1	2A	1942	5MC	C5-C4	4.64	1.48	1.41
32	1a	1400	5MC	C5-C4	4.61	1.48	1.41
55	2x	32	5MC	C5-C4	4.58	1.48	1.41
32	2a	1400	5MC	C5-C4	4.58	1.48	1.41
1	1A	1984	5MC	C5-C4	4.58	1.48	1.41
1	1A	2617	PSU	C5-C1'	-4.51	1.48	1.52
1	2A	1917	PSU	C5-C1'	-4.51	1.48	1.52
32	2a	527	7MG	C5-C4	4.46	1.47	1.39
1	2A	2605	PSU	C5-C1'	-4.45	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1407	5MC	C5-C4	4.43	1.48	1.41
54	2w	46	7MG	C5-C4	4.43	1.47	1.39
1	2A	1911	PSU	C5-C1'	-4.35	1.48	1.52
32	2a	1207	2MG	C6-C5	4.34	1.48	1.41
1	2A	2503	2MA	C6-C5	4.31	1.47	1.41
32	1a	966	M2G	C6-C5	4.27	1.48	1.41
32	2a	1407	5MC	C5-C4	4.25	1.48	1.41
32	1a	1207	2MG	C6-C5	4.24	1.48	1.41
54	1w	46	7MG	C6-C5	4.23	1.47	1.41
54	2y	55	PSU	C5-C1'	-4.21	1.48	1.52
32	2a	966	M2G	C6-C5	4.20	1.48	1.41
54	1w	32	PSU	C5-C1'	-4.19	1.48	1.52
55	2x	55	PSU	C5-C1'	-4.16	1.48	1.52
1	2A	1962	5MC	C5-C4	4.15	1.47	1.41
1	1A	1964	5MC	C5-C4	4.13	1.47	1.41
1	1A	2515	2MA	C6-C5	4.10	1.47	1.41
54	2w	8	4SU	C4-S4	-4.01	1.60	1.67
55	1x	8	4SU	C4-S4	-4.00	1.60	1.67
54	1w	8	4SU	C4-S4	-3.99	1.60	1.67
54	1y	55	PSU	C5-C1'	-3.97	1.48	1.52
54	2y	8	4SU	C4-S4	-3.94	1.60	1.67
1	1A	2263	OMG	C6-C5	3.82	1.47	1.41
54	2y	39	PSU	C5-C1'	-3.81	1.49	1.52
54	2w	32	PSU	C5-C1'	-3.80	1.49	1.52
1	2A	2251	OMG	C6-C5	3.78	1.47	1.41
54	1y	8	4SU	C4-S4	-3.78	1.60	1.67
54	2w	55	PSU	C4-C5	3.78	1.49	1.41
54	1y	32	PSU	C4-C5	3.75	1.49	1.41
54	2w	32	PSU	C4-C5	3.75	1.49	1.41
1	1A	1933	PSU	C5-C1'	-3.75	1.49	1.52
32	2a	516	PSU	C4-C5	3.71	1.49	1.41
54	2w	39	PSU	C5-C1'	-3.69	1.49	1.52
55	2x	55	PSU	C4-C5	3.67	1.49	1.41
54	1y	39	PSU	C4-C5	3.66	1.49	1.41
54	2y	32	PSU	C4-C5	3.66	1.49	1.41
55	2x	8	4SU	C4-S4	-3.62	1.60	1.67
54	1w	46	7MG	C5-N7	-3.60	1.33	1.39
32	1a	966	M2G	C2-N2	3.58	1.40	1.34
32	2a	516	PSU	C5-C1'	-3.58	1.49	1.52
54	1y	46	7MG	C5-N7	-3.57	1.33	1.39
54	2y	39	PSU	C4-C5	3.57	1.49	1.41
55	1x	8	4SU	C2-N3	-3.54	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	54	5MU	C4-C5	3.54	1.49	1.41
54	2y	46	7MG	C5-N7	-3.53	1.33	1.39
1	1A	1939	PSU	C5-C1'	-3.48	1.49	1.52
32	1a	516	PSU	C5-C1'	-3.47	1.49	1.52
1	1A	1937	5MU	C4-C5	3.45	1.48	1.41
32	1a	527	7MG	C5-N7	-3.45	1.33	1.39
54	2y	54	5MU	C4-C5	3.45	1.48	1.41
54	1y	39	PSU	C5-C1'	-3.44	1.49	1.52
54	1y	55	PSU	C4-C5	3.44	1.48	1.41
54	1w	32	PSU	C4-C5	3.44	1.48	1.41
54	2w	54	5MU	C4-C5	3.43	1.48	1.41
1	2A	1915	5MU	C4-C5	3.43	1.48	1.41
54	1y	54	5MU	C4-C5	3.43	1.48	1.41
55	2x	54	5MU	C4-C5	3.40	1.48	1.41
54	1w	55	PSU	C5-C1'	-3.37	1.49	1.52
54	1w	55	PSU	C4-C5	3.37	1.48	1.41
32	1a	516	PSU	C4-C5	3.33	1.48	1.41
1	2A	1911	PSU	C4-C5	3.33	1.48	1.41
54	2y	55	PSU	C4-C5	3.28	1.48	1.41
54	1w	54	5MU	C4-C5	3.28	1.48	1.41
1	1A	1933	PSU	C4-C5	3.27	1.48	1.41
1	2A	1917	PSU	C4-C5	3.26	1.48	1.41
55	1x	55	PSU	C4-C5	3.25	1.48	1.41
1	2A	1939	5MU	C4-C5	3.24	1.48	1.41
54	2w	39	PSU	C4-C5	3.22	1.48	1.41
54	2y	32	PSU	C5-C1'	-3.19	1.49	1.52
1	1A	1961	5MU	C4-C5	3.17	1.48	1.41
32	2a	966	M2G	C2-N2	3.17	1.40	1.34
1	1A	2617	PSU	C4-C5	3.15	1.48	1.41
54	2w	46	7MG	C5-N7	-3.13	1.34	1.39
32	2a	527	7MG	C5-N7	-3.13	1.34	1.39
54	1w	39	PSU	C4-C5	3.08	1.48	1.41
1	1A	1939	PSU	C4-C5	3.07	1.48	1.41
54	1y	32	PSU	C5-C1'	-3.05	1.49	1.52
1	2A	2605	PSU	C4-C5	2.93	1.47	1.41
54	2w	55	PSU	C5-C1'	-2.89	1.49	1.52
54	2y	37	MIA	C5-C4	2.81	1.48	1.40
54	2y	37	MIA	C2-N3	2.76	1.36	1.32
54	1y	37	MIA	C5-C4	2.73	1.48	1.40
32	2a	966	M2G	C5-C4	2.68	1.48	1.40
54	1w	46	7MG	C4-N9	-2.67	1.33	1.38
32	2a	1519	MA6	C5-C4	2.64	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	37	MIA	C2-N3	2.64	1.36	1.32
1	1A	2263	OMG	C5-C4	2.62	1.47	1.40
54	2w	37	MIA	C5-C4	2.62	1.47	1.40
32	2a	1518	MA6	C5-C4	2.61	1.47	1.40
54	2w	46	7MG	C4-N9	-2.60	1.33	1.38
55	2x	8	4SU	C2-N3	-2.59	1.33	1.38
54	1w	37	MIA	C5-C4	2.55	1.47	1.40
32	2a	1207	2MG	C5-C4	2.53	1.47	1.40
32	1a	1519	MA6	C5-C4	2.47	1.47	1.40
32	1a	527	7MG	C4-N9	-2.44	1.33	1.38
32	1a	1518	MA6	C5-C4	2.40	1.47	1.40
32	1a	1207	2MG	C5-C4	2.37	1.47	1.40
32	1a	966	M2G	C5-C4	2.36	1.47	1.40
32	1a	1498	UR3	C4-N3	2.34	1.41	1.38
32	2a	527	7MG	C4-N9	-2.34	1.33	1.38
1	2A	2251	OMG	C5-C4	2.33	1.47	1.40
1	2A	2503	2MA	C5-C4	2.33	1.47	1.40
1	1A	1961	5MU	C2-N3	-2.23	1.33	1.38
1	1A	2564	2MU	C2-N3	-2.18	1.33	1.38
54	1y	46	7MG	C4-N3	2.17	1.37	1.34
1	2A	1939	5MU	C2-N3	-2.15	1.33	1.38
54	1w	37	MIA	C6-N1	2.15	1.35	1.32
1	1A	2617	PSU	C2-N1	-2.15	1.33	1.38
1	2A	2605	PSU	C2-N3	-2.14	1.33	1.38
54	1w	39	PSU	O4'-C1'	-2.12	1.41	1.44
32	2a	516	PSU	O4'-C1'	-2.12	1.41	1.44
32	2a	1498	UR3	C4-N3	2.12	1.41	1.38
32	1a	516	PSU	O4'-C1'	-2.12	1.41	1.44
32	1a	516	PSU	C2-N3	-2.11	1.34	1.38
54	2w	37	MIA	C6-N1	2.11	1.35	1.32
54	1y	54	5MU	C2-N3	-2.09	1.34	1.38
1	1A	2515	2MA	C5-C4	2.04	1.46	1.40
1	1A	2617	PSU	O4'-C1'	-2.02	1.41	1.44
55	1x	55	PSU	O4'-C1'	-2.02	1.41	1.44
54	1w	54	5MU	C2-N3	-2.00	1.34	1.38
54	2y	8	4SU	C2-N3	-2.00	1.34	1.38

All (345) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-12.90	76.47	101.85
54	2y	46	7MG	N3-C4-N9	10.14	139.93	126.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	46	7MG	N3-C4-N9	10.10	139.89	126.91
54	2w	39	PSU	N1-C2-N3	-9.51	120.87	128.43
1	1A	1939	PSU	N1-C2-N3	-9.47	120.90	128.43
54	1w	55	PSU	N1-C2-N3	-9.07	121.22	128.43
54	1w	46	7MG	N3-C4-N9	9.02	138.49	126.91
32	2a	516	PSU	N1-C2-N3	-9.00	121.28	128.43
54	2y	32	PSU	N1-C2-N3	-8.94	121.32	128.43
32	1a	527	7MG	N3-C4-N9	8.79	138.20	126.91
32	2a	527	7MG	N3-C4-N9	8.69	138.07	126.91
54	2y	39	PSU	N1-C2-N3	-8.68	121.53	128.43
1	1A	2617	PSU	N1-C2-N3	-8.60	121.59	128.43
54	1w	32	PSU	N1-C2-N3	-8.57	121.62	128.43
32	1a	516	PSU	N1-C2-N3	-8.56	121.62	128.43
54	1y	39	PSU	N1-C2-N3	-8.53	121.64	128.43
54	1y	32	PSU	N1-C2-N3	-8.52	121.66	128.43
55	1x	8	4SU	C2-N3-C4	8.52	127.50	115.15
54	2w	55	PSU	N1-C2-N3	-8.49	121.68	128.43
1	2A	1911	PSU	N1-C2-N3	-8.47	121.69	128.43
1	1A	1933	PSU	N1-C2-N3	-8.46	121.70	128.43
1	2A	2605	PSU	N1-C2-N3	-8.39	121.76	128.43
54	2w	32	PSU	N1-C2-N3	-8.35	121.79	128.43
54	2w	46	7MG	N3-C4-N9	8.31	137.59	126.91
54	1w	37	MIA	C12-C13-C14	-8.27	111.05	127.14
54	2y	55	PSU	N1-C2-N3	-8.26	121.86	128.43
1	2A	1917	PSU	N1-C2-N3	-8.22	121.90	128.43
55	2x	55	PSU	N1-C2-N3	-8.21	121.90	128.43
54	1w	39	PSU	N1-C2-N3	-8.16	121.94	128.43
55	1x	55	PSU	N1-C2-N3	-8.06	122.02	128.43
54	1y	55	PSU	N1-C2-N3	-7.95	122.11	128.43
54	1y	54	5MU	C4-N3-C2	7.88	121.79	115.14
55	2x	8	4SU	C2-N3-C4	7.87	126.56	115.15
54	2w	39	PSU	C4-N3-C2	7.65	121.60	115.14
54	2y	54	5MU	C4-N3-C2	7.46	121.44	115.14
54	2y	32	PSU	C4-N3-C2	7.41	121.40	115.14
54	1w	55	PSU	C4-N3-C2	7.38	121.38	115.14
54	2w	54	5MU	C4-N3-C2	7.37	121.37	115.14
55	1x	54	5MU	C4-N3-C2	7.18	121.20	115.14
32	2a	516	PSU	C4-N3-C2	7.12	121.15	115.14
54	1y	32	PSU	C4-N3-C2	7.10	121.14	115.14
55	1x	55	PSU	C4-N3-C2	7.07	121.11	115.14
54	2w	55	PSU	C4-N3-C2	7.06	121.10	115.14
32	1a	516	PSU	C4-N3-C2	7.02	121.06	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1939	PSU	C4-N3-C2	6.99	121.04	115.14
54	1y	55	PSU	C4-N3-C2	6.99	121.04	115.14
54	1w	32	PSU	C4-N3-C2	6.94	121.00	115.14
1	2A	1917	PSU	C4-N3-C2	6.86	120.93	115.14
1	2A	1911	PSU	C4-N3-C2	6.79	120.88	115.14
55	2x	55	PSU	C4-N3-C2	6.77	120.86	115.14
54	1y	39	PSU	C4-N3-C2	6.74	120.83	115.14
1	1A	1937	5MU	C4-N3-C2	6.69	120.79	115.14
1	1A	2617	PSU	C4-N3-C2	6.67	120.78	115.14
54	1w	54	5MU	C4-N3-C2	6.63	120.74	115.14
54	2y	55	PSU	C4-N3-C2	6.62	120.73	115.14
54	1w	39	PSU	C4-N3-C2	6.56	120.68	115.14
54	2w	32	PSU	C4-N3-C2	6.47	120.61	115.14
54	2y	39	PSU	C4-N3-C2	6.46	120.60	115.14
1	2A	1915	5MU	C4-N3-C2	6.43	120.57	115.14
1	2A	2605	PSU	C4-N3-C2	6.41	120.55	115.14
1	2A	1939	5MU	C4-N3-C2	6.25	120.42	115.14
1	1A	2515	2MA	C2-N3-C4	6.22	120.57	115.52
55	1x	55	PSU	C5-C4-N3	-6.16	117.43	125.36
1	1A	1933	PSU	C4-N3-C2	6.09	120.28	115.14
32	2a	1402	4OC	CM4-N4-C4	-6.03	117.79	122.97
1	2A	2503	2MA	C2-N3-C4	6.00	120.40	115.52
54	1y	55	PSU	C5-C4-N3	-5.92	117.73	125.36
1	1A	1961	5MU	C4-N3-C2	5.85	120.08	115.14
54	1w	46	7MG	C6-N1-C2	5.70	124.99	115.93
1	2A	1917	PSU	C5-C4-N3	-5.69	118.03	125.36
55	2x	55	PSU	C5-C4-N3	-5.66	118.07	125.36
32	2a	527	7MG	N7-C8-N9	-5.63	95.33	103.38
54	2y	46	7MG	C5-C4-N3	-5.62	117.32	126.49
54	1w	32	PSU	C5-C4-N3	-5.60	118.14	125.36
54	2w	46	7MG	N7-C8-N9	-5.52	95.48	103.38
54	2y	32	PSU	C5-C4-N3	-5.49	118.29	125.36
32	2a	516	PSU	C5-C4-N3	-5.45	118.34	125.36
54	1y	46	7MG	C5-C4-N3	-5.45	117.59	126.49
55	2x	54	5MU	C4-N3-C2	5.38	119.69	115.14
1	1A	2617	PSU	C5-C4-N3	-5.38	118.43	125.36
54	2w	55	PSU	C5-C4-N3	-5.36	118.46	125.36
54	1w	39	PSU	C5-C4-N3	-5.35	118.46	125.36
54	1y	32	PSU	C5-C4-N3	-5.35	118.47	125.36
54	2y	55	PSU	C5-C4-N3	-5.35	118.47	125.36
54	2w	55	PSU	C5-C1'-C2'	-5.33	105.81	115.32
1	2A	1911	PSU	C5-C4-N3	-5.33	118.49	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	55	PSU	C5-C4-N3	-5.27	118.58	125.36
54	2w	39	PSU	C5-C4-N3	-5.25	118.59	125.36
32	1a	516	PSU	C5-C4-N3	-5.25	118.59	125.36
54	1w	46	7MG	N7-C8-N9	-5.24	95.89	103.38
54	1y	39	PSU	C5-C4-N3	-5.21	118.65	125.36
54	2w	32	PSU	C5-C4-N3	-5.17	118.71	125.36
54	1y	46	7MG	C6-N1-C2	5.15	124.11	115.93
32	2a	966	M2G	C6-N1-C2	5.14	122.30	116.18
32	1a	966	M2G	C6-N1-C2	5.13	122.29	116.18
54	2y	39	PSU	C5-C4-N3	-5.08	118.82	125.36
32	1a	966	M2G	C2-N3-C4	5.05	121.01	115.28
54	2y	46	7MG	N7-C8-N9	-5.02	96.20	103.38
1	1A	2515	2MA	C5-C6-N1	-4.93	117.89	123.06
32	1a	527	7MG	N7-C8-N9	-4.91	96.35	103.38
1	1A	2263	OMG	C2-N3-C4	4.89	120.94	115.36
32	1a	527	7MG	C5-C4-N3	-4.88	118.52	126.49
54	1y	46	7MG	N7-C8-N9	-4.86	96.42	103.38
32	1a	1402	4OC	CM4-N4-C4	-4.84	118.81	122.97
1	2A	2605	PSU	C5-C4-N3	-4.82	119.14	125.36
54	2y	46	7MG	C6-C5-C4	4.80	120.35	115.20
32	1a	1207	2MG	C6-N1-C2	4.77	123.72	115.18
54	2y	46	7MG	C6-N1-C2	4.77	123.50	115.93
54	2y	8	4SU	C2-N3-C4	4.76	122.06	115.15
32	2a	527	7MG	C5-C4-N3	-4.75	118.73	126.49
54	1y	8	4SU	C2-N3-C4	4.70	121.97	115.15
1	1A	1939	PSU	C5-C4-N3	-4.69	119.32	125.36
1	1A	1933	PSU	C5-C4-N3	-4.68	119.33	125.36
54	2w	46	7MG	C5-C4-N3	-4.66	118.88	126.49
32	1a	1207	2MG	C5-C6-N1	-4.62	117.11	123.43
54	1w	37	MIA	C2-N3-C4	4.60	121.66	115.32
1	2A	2503	2MA	C5-C6-N1	-4.60	118.24	123.06
32	2a	1207	2MG	C2-N3-C4	4.58	120.48	115.28
43	2l	92	0TD	CSB-SB-CB	-4.57	92.87	101.85
54	1w	55	PSU	C5-C1'-C2'	-4.57	107.17	115.32
32	2a	966	M2G	C2-N3-C4	4.53	120.42	115.28
32	1a	1207	2MG	C6-C5-C4	-4.53	116.47	120.80
32	2a	527	7MG	C6-N1-C2	4.50	123.09	115.93
54	2w	46	7MG	C6-N1-C2	4.48	123.04	115.93
1	1A	1942	4OC	C2-N3-C4	4.47	120.87	116.34
32	1a	527	7MG	C6-N1-C2	4.45	123.01	115.93
1	2A	1920	4OC	C2-N3-C4	4.45	120.85	116.34
1	2A	2251	OMG	C2-N3-C4	4.45	120.44	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	8	4SU	C5-C4-N3	-4.44	117.89	123.83
54	1w	46	7MG	C5-C4-N3	-4.43	119.26	126.49
32	1a	1207	2MG	C2-N3-C4	4.41	120.28	115.28
54	1w	39	PSU	C5-C6-N1	-4.38	119.05	124.44
32	1a	966	M2G	C6-C5-C4	-4.36	116.63	120.80
54	1y	46	7MG	C6-C5-C4	4.36	119.88	115.20
55	2x	55	PSU	C5-C6-N1	-4.36	119.08	124.44
1	1A	1939	PSU	C6-N1-C2	4.31	122.47	115.36
54	1w	46	7MG	C5-C6-N1	-4.30	114.30	123.14
54	2y	39	PSU	C6-N1-C2	4.30	122.45	115.36
55	1x	8	4SU	C5-C4-N3	-4.29	118.09	123.83
1	1A	1933	PSU	C6-N1-C2	4.27	122.41	115.36
1	2A	2605	PSU	C5-C6-N1	-4.25	119.21	124.44
32	2a	516	PSU	C6-N1-C2	4.23	122.34	115.36
54	1w	46	7MG	C6-C5-C4	4.23	119.74	115.20
54	2y	55	PSU	C5-C6-N1	-4.21	119.27	124.44
1	1A	2617	PSU	C6-N1-C2	4.19	122.28	115.36
54	2y	39	PSU	C5-C6-N1	-4.19	119.29	124.44
54	2w	32	PSU	C6-N1-C2	4.18	122.25	115.36
1	1A	2263	OMG	C6-N1-C2	4.18	122.57	115.93
54	2w	37	MIA	C2-N3-C4	4.18	121.08	115.32
1	1A	1933	PSU	C5-C6-N1	-4.18	119.31	124.44
54	1y	39	PSU	C6-N1-C2	4.17	122.24	115.36
54	2w	32	PSU	C5-C6-N1	-4.17	119.32	124.44
55	1x	55	PSU	C5-C6-N1	-4.14	119.36	124.44
1	1A	2263	OMG	C5-C6-N1	-4.13	117.78	123.43
54	1w	37	MIA	C15-C14-C13	-4.13	110.72	122.65
32	2a	966	M2G	C5-C6-N1	-4.12	117.79	123.43
1	2A	1917	PSU	C5-C6-N1	-4.12	119.37	124.44
54	2w	39	PSU	C6-N1-C2	4.11	122.15	115.36
54	1w	32	PSU	C6-N1-C2	4.09	122.11	115.36
32	2a	1207	2MG	C5-C6-N1	-4.09	117.84	123.43
1	2A	1917	PSU	C5-C1'-C2'	-4.07	108.05	115.32
55	2x	55	PSU	C6-N1-C2	4.07	122.07	115.36
1	2A	2605	PSU	C6-N1-C2	4.07	122.07	115.36
54	1w	8	4SU	C2-N3-C4	4.06	121.04	115.15
54	2y	32	PSU	C6-N1-C2	4.05	122.04	115.36
54	1w	39	PSU	C6-N1-C2	4.03	122.02	115.36
32	1a	516	PSU	C6-N1-C2	4.02	121.99	115.36
1	2A	1911	PSU	C5-C6-N1	-4.01	119.51	124.44
54	2w	55	PSU	C6-N1-C2	4.01	121.98	115.36
1	2A	1911	PSU	C6-N1-C2	4.01	121.97	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	32	PSU	C5-C6-N1	-4.01	119.52	124.44
32	1a	527	7MG	C6-C5-C4	3.99	119.48	115.20
1	1A	2617	PSU	C5-C6-N1	-3.99	119.54	124.44
1	2A	2251	OMG	C6-N1-C2	3.98	122.26	115.93
54	2y	55	PSU	C6-N1-C2	3.98	121.92	115.36
54	1w	55	PSU	C6-N1-C2	3.98	121.92	115.36
54	1y	32	PSU	C6-N1-C2	3.97	121.91	115.36
32	2a	1207	2MG	C6-N1-C2	3.97	122.28	115.18
54	1y	39	PSU	C5-C6-N1	-3.96	119.57	124.44
1	2A	2605	PSU	C5-C1'-C2'	-3.96	108.26	115.32
1	2A	1917	PSU	C6-N1-C2	3.95	121.88	115.36
32	1a	966	M2G	C5-C6-N1	-3.95	118.03	123.43
32	2a	1207	2MG	C6-C5-C4	-3.95	117.03	120.80
32	2a	516	PSU	C5-C6-N1	-3.92	119.62	124.44
32	2a	1407	5MC	C2-N3-C4	3.86	120.68	116.02
54	2w	39	PSU	C5-C6-N1	-3.86	119.70	124.44
1	2A	2251	OMG	C5-C6-N1	-3.85	118.16	123.43
32	1a	516	PSU	C5-C6-N1	-3.84	119.72	124.44
1	1A	1984	5MC	C2-N3-C4	3.84	120.65	116.02
32	2a	1518	MA6	C4-C5-N7	-3.82	105.42	109.40
32	2a	1518	MA6	C9-N6-C6	-3.82	107.95	119.51
55	1x	55	PSU	C6-N1-C2	3.81	121.65	115.36
54	1w	37	MIA	C16-C14-C13	-3.78	111.71	122.65
1	1A	1964	5MC	C2-N3-C4	3.78	120.58	116.02
54	2y	46	7MG	C5-C6-N1	-3.77	115.39	123.14
32	1a	967	5MC	C2-N3-C4	3.77	120.56	116.02
54	2y	55	PSU	C5-C1'-C2'	-3.75	108.64	115.32
55	2x	32	5MC	C2-N3-C4	3.74	120.53	116.02
54	1y	46	7MG	C5-C6-N1	-3.72	115.50	123.14
54	1y	55	PSU	C5-C6-N1	-3.70	119.89	124.44
54	2y	32	PSU	C5-C6-N1	-3.70	119.89	124.44
32	1a	527	7MG	C5-C6-N1	-3.69	115.55	123.14
1	1A	1939	PSU	C5-C6-N1	-3.69	119.91	124.44
54	1y	32	PSU	C5-C6-N1	-3.69	119.91	124.44
54	1y	55	PSU	C6-N1-C2	3.68	121.44	115.36
1	2A	1962	5MC	C2-N3-C4	3.67	120.44	116.02
32	1a	1407	5MC	C2-N3-C4	3.65	120.43	116.02
54	2w	55	PSU	C5-C6-N1	-3.65	119.95	124.44
32	1a	1207	2MG	CM2-N2-C2	-3.63	119.21	123.59
54	2w	37	MIA	C5-C6-N1	-3.63	117.80	120.81
32	2a	527	7MG	C6-C5-C4	3.62	119.09	115.20
54	2w	46	7MG	C5-C6-N1	-3.62	115.69	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	32	5MC	C2-N3-C4	3.60	120.36	116.02
54	2w	46	7MG	C6-C5-C4	3.59	119.05	115.20
32	2a	527	7MG	C5-C6-N1	-3.59	115.76	123.14
1	2A	2251	OMG	C6-C5-C4	-3.59	117.37	120.80
32	2a	1404	5MC	C2-N3-C4	3.57	120.33	116.02
32	2a	966	M2G	C6-C5-C4	-3.51	117.45	120.80
32	1a	1404	5MC	C2-N3-C4	3.51	120.25	116.02
32	1a	1400	5MC	C2-N3-C4	3.50	120.24	116.02
32	2a	1518	MA6	N3-C2-N1	-3.49	123.23	128.68
32	1a	1207	2MG	C4-C5-N7	-3.48	105.77	109.40
1	1A	2263	OMG	N3-C2-N1	-3.48	122.58	127.22
54	1w	37	MIA	C12-N6-C6	-3.47	117.41	122.55
54	1y	8	4SU	C5-C4-N3	-3.45	119.22	123.83
32	2a	1519	MA6	C9-N6-C6	-3.42	109.15	119.51
54	1w	37	MIA	C5-C6-N1	-3.41	117.97	120.81
1	2A	1942	5MC	C2-N3-C4	3.41	120.13	116.02
32	2a	1519	MA6	C4-C5-N7	-3.41	105.85	109.40
32	1a	1518	MA6	N3-C2-N1	-3.40	123.37	128.68
32	2a	1400	5MC	C2-N3-C4	3.38	120.10	116.02
32	1a	1519	MA6	N3-C2-N1	-3.38	123.40	128.68
54	1y	37	MIA	N3-C2-N1	-3.36	123.42	128.68
54	2y	37	MIA	N3-C2-N1	-3.33	123.47	128.68
54	1w	55	PSU	C5-C6-N1	-3.32	120.36	124.44
32	1a	1519	MA6	C9-N6-C6	-3.31	109.48	119.51
54	2w	37	MIA	C12-N6-C6	-3.28	120.05	122.87
54	1y	55	PSU	C5-C1'-C2'	-3.28	109.48	115.32
32	1a	1518	MA6	C9-N6-C6	-3.27	109.61	119.51
32	1a	1518	MA6	C4-C5-N7	-3.27	105.99	109.40
32	1a	1519	MA6	N1-C6-N6	3.24	120.46	117.06
1	1A	2617	PSU	C5-C1'-C2'	-3.23	109.55	115.32
1	2A	2251	OMG	N3-C2-N1	-3.23	122.91	127.22
54	2y	39	PSU	C5-C1'-C2'	-3.22	109.57	115.32
1	1A	1939	PSU	C5-C1'-C2'	-3.22	109.58	115.32
54	2y	8	4SU	C5-C4-N3	-3.22	119.52	123.83
55	1x	55	PSU	C5-C1'-C2'	-3.21	109.59	115.32
1	1A	1964	5MC	N4-C4-N3	3.19	121.55	117.03
32	2a	967	5MC	C2-N3-C4	3.18	119.86	116.02
1	2A	1962	5MC	N4-C4-N3	3.17	121.51	117.03
1	1A	2263	OMG	C6-C5-C4	-3.16	117.78	120.80
1	2A	1939	5MU	C5-C6-N1	-3.14	118.81	122.19
1	1A	1961	5MU	C5-C6-N1	-3.09	118.87	122.19
32	1a	1207	2MG	N2-C2-N1	3.05	119.89	116.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	8	4SU	C2-N3-C4	3.03	119.54	115.15
32	2a	1407	5MC	N4-C4-N3	3.02	121.30	117.03
1	2A	1911	PSU	C5-C1'-C2'	-3.01	109.95	115.32
54	1w	46	7MG	C5-C4-N9	-3.01	102.23	106.44
54	1y	37	MIA	C4-C5-N7	-3.00	106.27	109.40
54	2w	37	MIA	C4-C5-N7	-2.99	106.28	109.40
32	2a	1207	2MG	C4-C5-N7	-2.99	106.29	109.40
32	2a	1519	MA6	N3-C2-N1	-2.98	124.02	128.68
32	1a	966	M2G	C4-C5-N7	-2.98	106.30	109.40
54	1w	8	4SU	C5-C4-N3	-2.90	119.94	123.83
54	1w	37	MIA	C2-N1-C6	2.89	122.35	117.19
32	2a	967	5MC	C5-C6-N1	-2.87	119.10	122.19
54	1y	46	7MG	C5-C4-N9	-2.81	102.51	106.44
32	2a	527	7MG	C8-N7-C5	2.80	116.23	108.94
55	2x	32	5MC	N4-C4-N3	2.80	121.00	117.03
1	2A	1942	5MC	N4-C4-N3	2.80	120.99	117.03
54	1w	39	PSU	C5-C1'-C2'	-2.77	110.38	115.32
32	2a	1400	5MC	N4-C4-N3	2.77	120.95	117.03
32	1a	1519	MA6	C4-C5-N7	-2.76	106.52	109.40
55	2x	55	PSU	C5-C1'-C2'	-2.75	110.41	115.32
55	2x	54	5MU	C5-C6-N1	-2.70	119.28	122.19
54	2w	46	7MG	C8-N7-C5	2.69	115.94	108.94
32	2a	1207	2MG	CM2-N2-C2	-2.69	120.35	123.59
54	2y	46	7MG	C8-N7-C5	2.68	115.92	108.94
32	1a	1207	2MG	C1'-N9-C4	-2.68	121.93	126.64
1	1A	1942	4OC	N4-C4-N3	2.67	120.71	116.49
54	1w	37	MIA	C4-C5-N7	-2.67	106.62	109.40
54	2w	37	MIA	C2-N1-C6	2.66	121.95	117.19
32	2a	1407	5MC	CM5-C5-C4	-2.65	119.04	121.72
54	2w	8	4SU	C5-C4-N3	-2.65	120.28	123.83
54	2y	37	MIA	C4-C5-N7	-2.65	106.64	109.40
54	2y	46	7MG	C5-C4-N9	-2.64	102.74	106.44
54	1w	37	MIA	N3-C2-N1	-2.63	122.14	126.98
1	2A	2503	2MA	C4-C5-N7	-2.62	106.67	109.40
32	1a	1400	5MC	C5-C6-N1	-2.58	119.41	122.19
55	1x	32	5MC	CM5-C5-C4	-2.58	119.11	121.72
55	1x	32	5MC	N4-C4-N3	2.58	120.67	117.03
54	1y	46	7MG	C8-N7-C5	2.57	115.64	108.94
54	2w	32	PSU	C5-C1'-C2'	-2.57	110.74	115.32
1	2A	1915	5MU	C5-C6-N1	-2.57	119.43	122.19
32	1a	966	M2G	N1-C2-N2	2.56	119.78	117.19
32	2a	1404	5MC	N4-C4-N3	2.53	120.61	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1407	5MC	N4-C4-N3	2.53	120.61	117.03
55	1x	32	5MC	C5-C6-N1	-2.53	119.47	122.19
32	1a	527	7MG	C8-N7-C5	2.51	115.46	108.94
54	1w	32	PSU	C5-C1'-C2'	-2.49	110.88	115.32
1	1A	1933	PSU	C5-C1'-C2'	-2.49	110.89	115.32
32	1a	1400	5MC	N4-C4-N3	2.47	120.52	117.03
1	2A	1942	5MC	C5-C6-N1	-2.44	119.57	122.19
32	1a	1207	2MG	N3-C2-N1	-2.43	122.39	126.23
32	2a	1400	5MC	C5-C6-N1	-2.42	119.58	122.19
32	2a	1407	5MC	C5-C6-N1	-2.41	119.59	122.19
54	1w	46	7MG	C8-N7-C5	2.41	115.21	108.94
1	1A	1984	5MC	N4-C4-N3	2.40	120.43	117.03
32	2a	1518	MA6	C10-N6-C9	-2.39	108.43	116.12
1	1A	2564	2MU	C5-C4-N3	-2.38	118.06	123.31
1	2A	1962	5MC	C5-C6-N1	-2.38	119.63	122.19
32	1a	1404	5MC	C5-C6-N1	-2.37	119.64	122.19
1	1A	2263	OMG	C4-C5-N7	-2.37	106.92	109.40
32	2a	527	7MG	C5-C4-N9	-2.33	103.18	106.44
54	2w	37	MIA	C11-S10-C2	-2.28	100.57	102.27
32	1a	527	7MG	C5-C4-N9	-2.27	103.27	106.44
55	1x	54	5MU	C5-C6-N1	-2.26	119.76	122.19
32	2a	1404	5MC	C5-C6-N1	-2.24	119.78	122.19
54	2w	37	MIA	N3-C2-N1	-2.23	122.88	126.98
32	1a	967	5MC	N4-C4-N3	2.23	120.18	117.03
54	2w	39	PSU	C5-C1'-C2'	-2.22	111.35	115.32
1	2A	1920	4OC	N4-C4-N3	2.22	120.00	116.49
32	2a	966	M2G	C4-C5-N7	-2.22	107.09	109.40
32	1a	1407	5MC	C5-C6-N1	-2.21	119.81	122.19
54	2y	46	7MG	C2-N3-C4	2.21	119.99	113.89
54	1y	46	7MG	C2-N3-C4	2.20	119.99	113.89
1	2A	2251	OMG	C4-C5-N7	-2.19	107.11	109.40
32	2a	516	PSU	O4'-C1'-C2'	2.19	108.21	104.66
32	1a	1404	5MC	N4-C4-N3	2.18	120.12	117.03
54	1w	54	5MU	C5-C6-N1	-2.17	119.85	122.19
32	1a	516	PSU	O4'-C1'-C2'	2.17	108.17	104.66
32	2a	1498	UR3	C3U-N3-C4	2.15	120.97	118.12
32	1a	967	5MC	C5-C6-N1	-2.14	119.89	122.19
1	1A	1984	5MC	C5-C6-N1	-2.12	119.91	122.19
55	2x	32	5MC	C5-C6-N1	-2.10	119.94	122.19
32	2a	966	M2G	CM1-N2-C2	-2.10	119.29	121.29
32	1a	1518	MA6	C10-N6-C6	-2.09	113.17	119.51
32	1a	527	7MG	CM7-N7-C5	2.09	132.05	124.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	46	7MG	C5-C4-N9	-2.09	103.51	106.44
1	1A	2515	2MA	C4-C5-N7	-2.09	107.22	109.40
54	2w	46	7MG	C2-N3-C4	2.09	119.66	113.89
54	1y	46	7MG	N2-C2-N3	2.07	120.48	117.25
1	1A	1964	5MC	C5-C6-N1	-2.04	119.99	122.19
32	2a	527	7MG	C2-N3-C4	2.04	119.53	113.89
32	2a	967	5MC	N4-C4-N3	2.02	119.89	117.03

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	2a	1518	MA6	C5-C6-N6-C9
54	2w	46	7MG	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
54	2w	8	4SU	C2'-C1'-N1-C6
1	1A	1984	5MC	O4'-C1'-N1-C6
1	1A	1984	5MC	C2'-C1'-N1-C6
1	1A	1942	4OC	C2'-C1'-N1-C6
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
54	2y	54	5MU	C2'-C1'-N1-C6
54	2y	54	5MU	C3'-C4'-C5'-O5'
43	2l	92	0TD	O-C-CA-CB
43	2l	92	0TD	CG-CB-SB-CSB
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C2'-C1'-N1-C6
32	2a	1402	4OC	N3-C4-N4-CM4
32	2a	1402	4OC	C5-C4-N4-CM4
54	1y	46	7MG	C4'-C5'-O5'-P
54	2w	37	MIA	N1-C6-N6-C12
54	2y	46	7MG	C4'-C5'-O5'-P
54	1y	54	5MU	C2'-C1'-N1-C6
54	1y	54	5MU	C3'-C4'-C5'-O5'
54	1y	54	5MU	O4'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C16
32	2a	1400	5MC	O4'-C1'-N1-C6
32	2a	1400	5MC	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
54	2w	46	7MG	O4'-C4'-C5'-O5'
54	2y	37	MIA	C3'-C4'-C5'-O5'
54	2y	54	5MU	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
54	2y	8	4SU	C3'-C4'-C5'-O5'
54	2y	8	4SU	O4'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
54	1y	8	4SU	O4'-C4'-C5'-O5'
32	2a	1518	MA6	N1-C6-N6-C9
32	1a	527	7MG	C3'-C4'-C5'-O5'
54	2y	37	MIA	O4'-C4'-C5'-O5'
1	2A	1917	PSU	O4'-C4'-C5'-O5'
32	2a	527	7MG	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	1519	MA6	C5-C6-N6-C9
32	1a	1518	MA6	C5-C6-N6-C10
32	1a	1402	4OC	O4'-C4'-C5'-O5'
55	1x	55	PSU	O4'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
54	2w	37	MIA	C5-C6-N6-C12
54	2w	46	7MG	C2'-C1'-N9-C8
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
32	2a	527	7MG	O4'-C4'-C5'-O5'
54	1y	46	7MG	C2'-C1'-N9-C8
54	1w	46	7MG	C2'-C1'-N9-C8
54	2y	46	7MG	C2'-C1'-N9-C8
32	2a	1518	MA6	C5-C6-N6-C10
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	527	7MG	C4'-C5'-O5'-P
54	1y	37	MIA	C3'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C2'-O2'-CM2
54	2w	46	7MG	C2'-C1'-N9-C4
54	1y	46	7MG	O4'-C1'-N9-C8
1	1A	2515	2MA	C4'-C5'-O5'-P
32	1a	1519	MA6	C4'-C5'-O5'-P
54	1y	32	PSU	C2'-C1'-C5-C6
32	1a	1402	4OC	C3'-C4'-C5'-O5'
1	2A	1917	PSU	C3'-C4'-C5'-O5'
54	2w	46	7MG	O4'-C1'-N9-C8
54	2y	46	7MG	O4'-C1'-N9-C8
32	1a	1400	5MC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
54	1w	46	7MG	C4'-C5'-O5'-P
55	1x	55	PSU	C3'-C4'-C5'-O5'
1	2A	2503	2MA	C3'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
1	1A	2515	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1915	5MU	1	0
1	1A	2564	2MU	1	0
1	2A	2552	2MU	2	0
1	2A	1942	5MC	1	0
1	1A	1939	PSU	1	0
1	2A	2503	2MA	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2867 ligands modelled in this entry, 2863 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	$\# Z  > 2$
57	MT9	1A	4113	-	34,34,34	2.28	4 (11%)	40,50,50	1.57	7 (17%)
60	SF4	1d	501	35	0,12,12	0.00	-	-		
57	MT9	2A	3897	-	34,34,34	2.21	4 (11%)	40,50,50	1.48	6 (15%)
60	SF4	2d	501	35	0,12,12	0.00	-	-		

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
57	MT9	1A	4113	-	-	3/46/62/62	0/1/2/2
60	SF4	1d	501	35	-	-	0/6/5/5
57	MT9	2A	3897	-	-	2/46/62/62	0/1/2/2
60	SF4	2d	501	35	-	-	0/6/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1A	4113	MT9	C4-C5	-9.74	1.39	1.51
57	2A	3897	MT9	C4-C5	-9.65	1.39	1.51
57	1A	4113	MT9	C12-C13	-5.35	1.39	1.51
57	1A	4113	MT9	C8-C7	-5.21	1.42	1.51
57	2A	3897	MT9	C12-C13	-4.83	1.40	1.51
57	2A	3897	MT9	C8-C7	-4.81	1.43	1.51
57	2A	3897	MT9	C6-C5	3.40	1.40	1.32
57	1A	4113	MT9	C6-C5	3.23	1.39	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1A	4113	MT9	C3-O3-C13	-4.14	110.83	118.18
57	1A	4113	MT9	C8-C7-C6	3.45	126.95	118.29
57	2A	3897	MT9	C8-C7-C6	3.44	126.94	118.29
57	2A	3897	MT9	C3-O3-C13	-3.30	112.32	118.18
57	1A	4113	MT9	O3-C3-C2	3.29	113.67	107.40
57	2A	3897	MT9	C18-C17-N1	-3.21	106.60	115.67
57	2A	3897	MT9	C20-C19-C18	-2.77	109.05	113.40
57	1A	4113	MT9	C20-C19-C18	-2.76	109.07	113.40
57	1A	4113	MT9	C5-C6-C7	2.53	127.33	121.93
57	1A	4113	MT9	C18-C17-N1	-2.41	108.88	115.67
57	2A	3897	MT9	C5-C6-C7	2.32	126.88	121.93
57	1A	4113	MT9	C15-O5-C19	-2.15	109.51	112.91
57	2A	3897	MT9	O1-C7-C8	-2.04	117.46	121.25

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	1A	4113	MT9	C18-C17-N1-C21
57	2A	3897	MT9	C18-C17-N1-C21
57	1A	4113	MT9	C25-C4-C5-C6
57	1A	4113	MT9	C12-C13-O3-C3
57	2A	3897	MT9	C1-C2-C3-O3

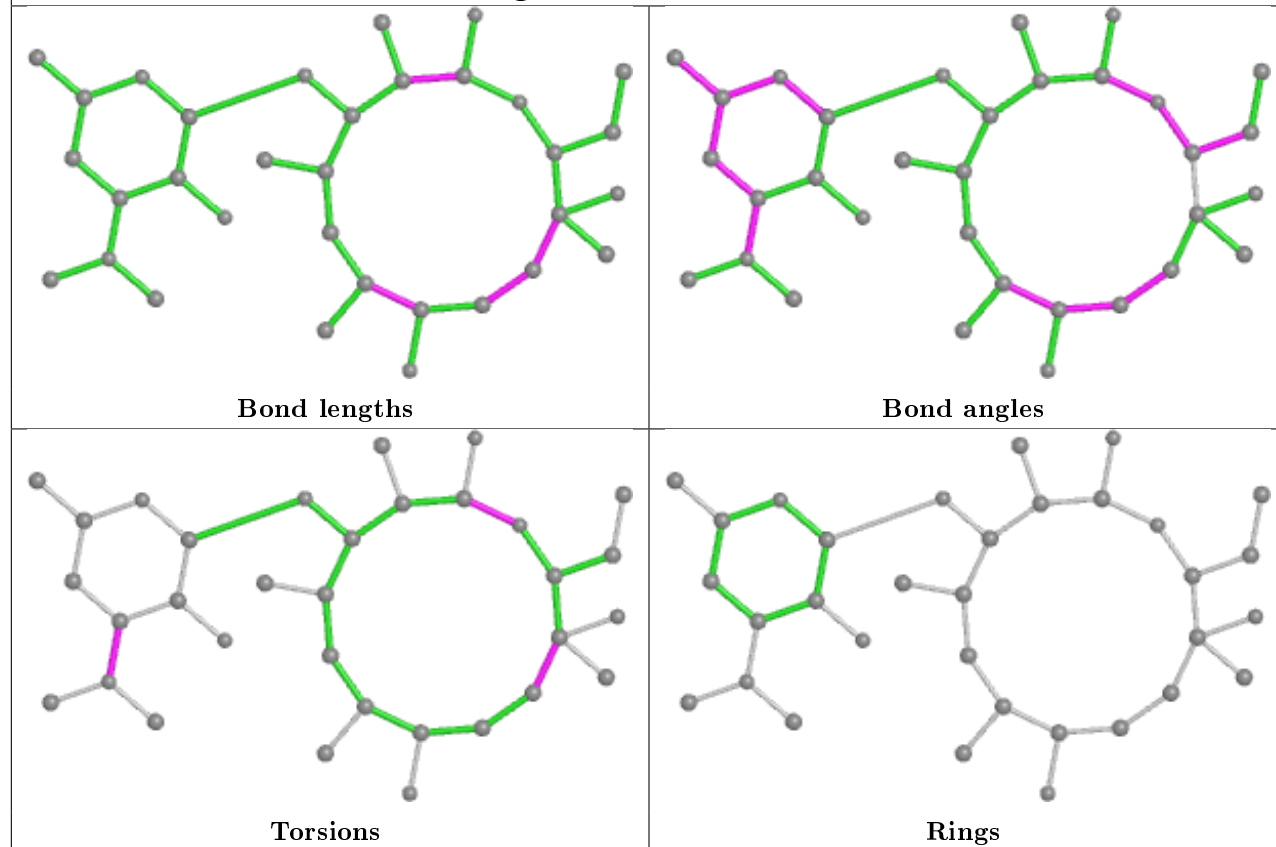
There are no ring outliers.

2 monomers are involved in 2 short contacts:

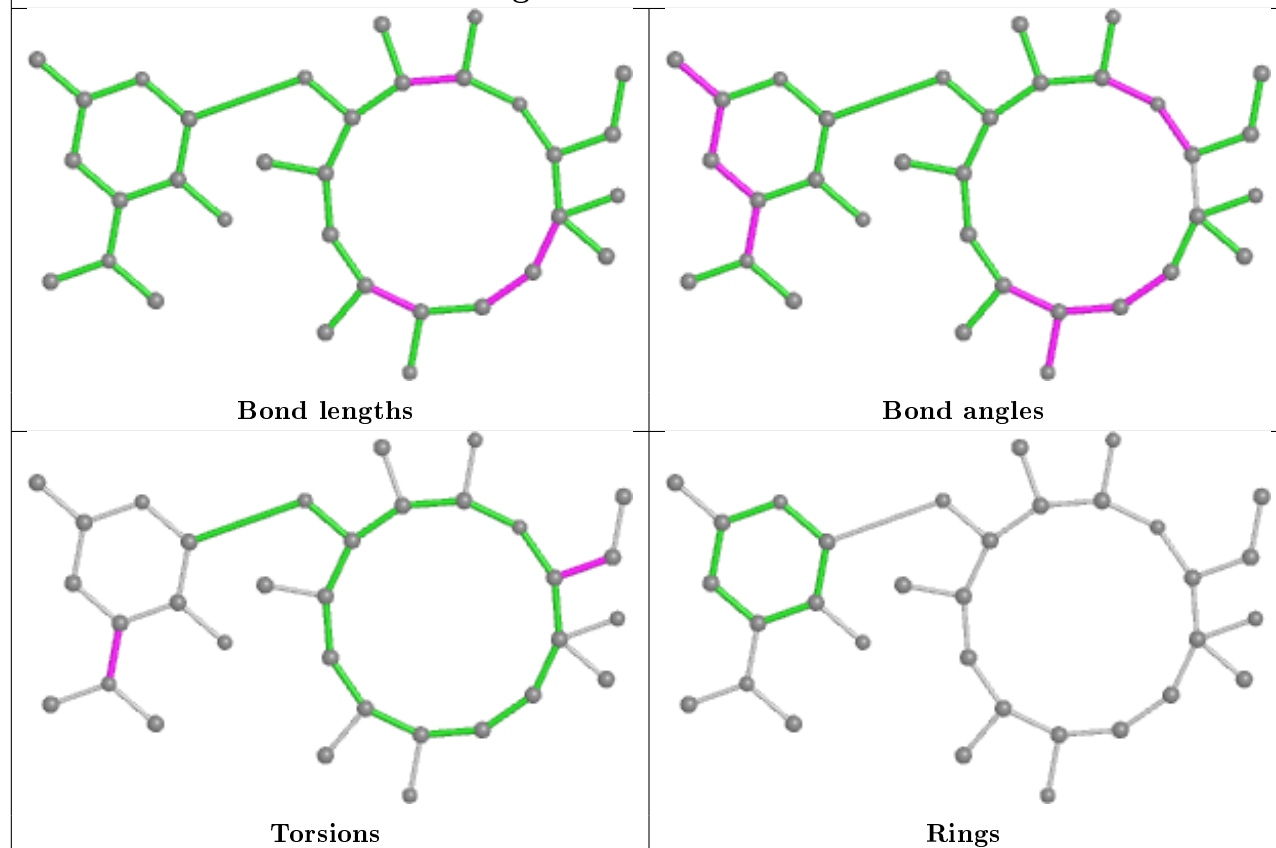
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	1A	4113	MT9	1	0
57	2A	3897	MT9	1	0

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 than 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 MT9 1A 4113



## Ligand MT9 2A 3897





## 5.7 Other polymers

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1A	2860/2915 (98%)	0.33	24 (0%) 86 87	16, 34, 90, 106	0
1	2A	2789/2915 (95%)	0.22	40 (1%) 75 77	32, 57, 91, 107	0
2	1B	120/121 (99%)	0.05	0 100 100	30, 46, 58, 84	0
2	2B	120/121 (99%)	0.16	5 (4%) 36 35	58, 80, 88, 92	0
3	1D	275/276 (99%)	0.59	8 (2%) 51 52	20, 35, 52, 85	0
3	2D	275/276 (99%)	0.93	25 (9%) 9 7	31, 50, 64, 85	0
4	1E	204/206 (99%)	0.42	1 (0%) 91 92	18, 37, 56, 77	0
4	2E	204/206 (99%)	0.63	12 (5%) 22 21	33, 58, 71, 79	0
5	1F	203/210 (96%)	0.36	0 100 100	19, 39, 66, 88	0
5	2F	203/210 (96%)	0.50	9 (4%) 34 33	34, 68, 81, 88	0
6	1G	181/182 (99%)	0.25	1 (0%) 89 91	34, 56, 70, 86	0
6	2G	181/182 (99%)	1.37	56 (30%) 0 0	71, 81, 88, 96	0
7	1H	174/180 (96%)	0.37	1 (0%) 89 91	33, 51, 64, 71	0
7	2H	174/180 (96%)	1.26	45 (25%) 0 0	68, 83, 90, 96	0
8	1I	146/148 (98%)	0.31	4 (2%) 54 55	41, 72, 81, 84	0
8	2I	146/148 (98%)	0.45	8 (5%) 25 24	57, 72, 83, 91	0
9	1N	140/140 (100%)	0.40	1 (0%) 87 89	24, 35, 58, 70	0
9	2N	140/140 (100%)	0.95	26 (18%) 1 1	44, 65, 78, 86	0
10	1O	122/122 (100%)	0.38	0 100 100	24, 37, 56, 62	0
10	2O	122/122 (100%)	0.63	8 (6%) 18 16	45, 58, 69, 72	0
11	1P	149/150 (99%)	0.45	0 100 100	19, 42, 67, 76	0
11	2P	149/150 (99%)	0.96	18 (12%) 4 3	37, 67, 82, 89	0
12	1Q	141/141 (100%)	0.46	0 100 100	26, 38, 54, 78	0
12	2Q	141/141 (100%)	1.28	28 (19%) 1 0	48, 66, 78, 86	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	0.43	0 <span>100</span> <span>100</span>	22, 31, 44, 59	0
13	2R	118/118 (100%)	0.78	11 (9%) <span>8</span> <span>6</span>	39, 52, 63, 67	0
14	1S	110/112 (98%)	0.23	1 (0%) <span>84</span> <span>85</span>	34, 46, 60, 67	0
14	2S	110/112 (98%)	1.05	22 (20%) <span>1</span> <span>0</span>	63, 76, 84, 90	0
15	1T	131/146 (89%)	0.46	3 (2%) <span>60</span> <span>62</span>	30, 42, 63, 77	0
15	2T	131/146 (89%)	0.60	8 (6%) <span>21</span> <span>20</span>	51, 61, 76, 84	0
16	1U	116/118 (98%)	0.47	0 <span>100</span> <span>100</span>	19, 29, 45, 63	0
16	2U	116/118 (98%)	0.86	12 (10%) <span>6</span> <span>5</span>	43, 62, 77, 85	0
17	1V	101/101 (100%)	0.27	0 <span>100</span> <span>100</span>	18, 36, 53, 62	0
17	2V	101/101 (100%)	0.68	10 (9%) <span>7</span> <span>5</span>	43, 70, 79, 84	0
18	1W	112/113 (99%)	0.47	1 (0%) <span>84</span> <span>85</span>	22, 30, 47, 82	0
18	2W	112/113 (99%)	0.63	3 (2%) <span>54</span> <span>55</span>	38, 49, 63, 85	0
19	1X	95/96 (98%)	0.45	2 (2%) <span>63</span> <span>65</span>	26, 36, 54, 72	0
19	2X	95/96 (98%)	0.68	5 (5%) <span>26</span> <span>25</span>	45, 59, 73, 80	0
20	1Y	107/110 (97%)	0.30	0 <span>100</span> <span>100</span>	31, 45, 63, 83	0
20	2Y	107/110 (97%)	1.60	33 (30%) <span>0</span> <span>0</span>	60, 72, 81, 87	0
21	1Z	154/206 (74%)	0.42	2 (1%) <span>77</span> <span>78</span>	39, 59, 81, 89	0
21	2Z	160/206 (77%)	1.22	38 (23%) <span>0</span> <span>0</span>	70, 82, 92, 97	0
22	10	83/85 (97%)	0.69	5 (6%) <span>21</span> <span>20</span>	27, 36, 59, 68	0
22	20	83/85 (97%)	1.08	11 (13%) <span>3</span> <span>2</span>	44, 63, 75, 84	0
23	11	97/98 (98%)	0.62	4 (4%) <span>37</span> <span>36</span>	27, 41, 67, 72	0
23	21	97/98 (98%)	1.23	14 (14%) <span>2</span> <span>1</span>	41, 58, 76, 78	0
24	12	70/72 (97%)	0.40	0 <span>100</span> <span>100</span>	32, 47, 56, 73	0
24	22	70/72 (97%)	0.60	5 (7%) <span>16</span> <span>14</span>	58, 69, 78, 81	0
25	13	59/60 (98%)	0.32	0 <span>100</span> <span>100</span>	21, 33, 56, 76	0
25	23	59/60 (98%)	1.23	12 (20%) <span>1</span> <span>0</span>	56, 65, 80, 90	0
26	14	69/71 (97%)	0.20	2 (2%) <span>51</span> <span>52</span>	47, 72, 86, 92	0
26	24	69/71 (97%)	0.92	13 (18%) <span>1</span> <span>0</span>	78, 88, 94, 95	0
27	15	59/60 (98%)	0.53	2 (3%) <span>45</span> <span>45</span>	18, 29, 48, 62	0
27	25	59/60 (98%)	0.39	0 <span>100</span> <span>100</span>	37, 51, 66, 73	0
28	16	53/54 (98%)	0.21	0 <span>100</span> <span>100</span>	28, 39, 53, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	1.41	14 (26%) 0 0	48, 61, 70, 75	0
29	17	48/49 (97%)	0.88	5 (10%) 6 4	20, 26, 60, 66	0
29	27	48/49 (97%)	1.27	7 (14%) 2 1	32, 41, 65, 76	0
30	18	64/65 (98%)	0.55	1 (1%) 72 74	25, 31, 40, 53	0
30	28	64/65 (98%)	1.44	17 (26%) 0 0	47, 55, 63, 65	0
31	19	37/37 (100%)	0.60	0 100 100	27, 37, 52, 56	0
31	29	37/37 (100%)	1.71	12 (32%) 0 0	62, 69, 75, 78	0
32	1a	1488/1521 (97%)	0.09	19 (1%) 77 78	35, 63, 89, 104	0
32	2a	1491/1521 (98%)	0.26	44 (2%) 50 51	52, 77, 95, 106	0
33	1b	231/256 (90%)	0.50	12 (5%) 27 25	66, 76, 86, 93	0
33	2b	231/256 (90%)	1.73	79 (34%) 0 0	75, 87, 94, 100	0
34	1c	206/239 (86%)	0.43	9 (4%) 34 33	58, 69, 80, 87	0
34	2c	206/239 (86%)	1.54	70 (33%) 0 0	76, 86, 91, 101	0
35	1d	208/209 (99%)	0.71	19 (9%) 9 7	52, 68, 79, 85	0
35	2d	208/209 (99%)	0.89	27 (12%) 3 2	62, 74, 82, 89	0
36	1e	148/162 (91%)	0.38	0 100 100	52, 62, 73, 80	0
36	2e	148/162 (91%)	1.25	39 (26%) 0 0	69, 79, 86, 98	0
37	1f	100/101 (99%)	0.42	2 (2%) 65 67	50, 64, 74, 77	0
37	2f	100/101 (99%)	0.07	1 (1%) 82 83	56, 68, 79, 82	0
38	1g	155/156 (99%)	0.61	13 (8%) 11 9	56, 68, 80, 94	0
38	2g	155/156 (99%)	0.85	20 (12%) 3 2	70, 78, 88, 92	0
39	1h	137/138 (99%)	0.82	15 (10%) 5 4	55, 65, 72, 76	0
39	2h	137/138 (99%)	1.11	23 (16%) 1 1	69, 79, 85, 87	0
40	1i	127/128 (99%)	1.03	16 (12%) 3 3	51, 73, 82, 89	0
40	2i	127/128 (99%)	1.93	58 (45%) 0 0	75, 85, 91, 93	0
41	1j	97/105 (92%)	0.70	12 (12%) 4 3	57, 75, 85, 93	0
41	2j	96/105 (91%)	1.69	34 (35%) 0 0	75, 86, 94, 100	0
42	1k	114/129 (88%)	0.51	4 (3%) 44 44	46, 64, 74, 80	0
42	2k	114/129 (88%)	0.86	12 (10%) 6 4	55, 73, 81, 83	0
43	1l	121/132 (91%)	0.49	2 (1%) 70 72	42, 52, 65, 71	0
43	2l	121/132 (91%)	1.45	40 (33%) 0 0	56, 69, 76, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	123/126 (97%)	0.41	8 (6%) 18 17	52, 67, 77, 81	0
44	2m	122/126 (96%)	1.48	41 (33%) 0 0	71, 84, 90, 95	0
45	1n	60/61 (98%)	0.84	2 (3%) 46 46	55, 64, 71, 74	0
45	2n	60/61 (98%)	3.41	47 (78%) 0 0	77, 85, 91, 94	0
46	1o	88/89 (98%)	0.75	8 (9%) 9 7	49, 62, 73, 78	0
46	2o	88/89 (98%)	0.70	7 (7%) 12 10	60, 73, 82, 87	0
47	1p	82/88 (93%)	1.15	16 (19%) 1 0	53, 68, 76, 78	0
47	2p	82/88 (93%)	1.18	14 (17%) 1 1	62, 68, 78, 85	0
48	1q	99/105 (94%)	0.53	5 (5%) 28 26	52, 65, 74, 79	0
48	2q	99/105 (94%)	1.63	42 (42%) 0 0	63, 72, 80, 83	0
49	1r	68/88 (77%)	0.70	4 (5%) 22 21	53, 63, 76, 80	0
49	2r	68/88 (77%)	0.46	3 (4%) 34 33	63, 71, 79, 88	0
50	1s	83/93 (89%)	0.19	1 (1%) 79 80	57, 68, 78, 84	0
50	2s	83/93 (89%)	1.36	23 (27%) 0 0	78, 86, 91, 94	0
51	1t	96/106 (90%)	0.55	7 (7%) 15 13	56, 68, 75, 84	0
51	2t	96/106 (90%)	1.21	22 (22%) 0 0	59, 70, 84, 87	0
52	1u	23/27 (85%)	1.54	8 (34%) 0 0	57, 65, 70, 74	0
52	2u	23/27 (85%)	3.08	17 (73%) 0 0	78, 80, 84, 85	0
53	1v	13/24 (54%)	1.22	2 (15%) 2 1	45, 58, 78, 95	0
53	2v	13/24 (54%)	2.60	8 (61%) 0 0	67, 82, 96, 98	0
54	1w	67/76 (88%)	0.81	11 (16%) 1 1	47, 86, 97, 105	0
54	1y	67/76 (88%)	0.16	4 (5%) 21 20	37, 90, 98, 101	0
54	2w	65/76 (85%)	2.64	30 (46%) 0 0	67, 94, 102, 105	0
54	2y	66/76 (86%)	0.73	8 (12%) 4 3	56, 97, 101, 103	0
55	1x	72/77 (93%)	0.22	1 (1%) 75 77	34, 65, 81, 87	0
55	2x	72/77 (93%)	0.65	10 (13%) 2 2	55, 80, 90, 92	0
All	All	20875/21748 (95%)	0.56	1514 (7%) 15 13	16, 63, 90, 107	0

All (1514) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
54	2w	71	G	10.5
38	2g	82	GLY	9.4

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Mol	Chain	Res	Type	RSRZ
45	2n	34	TYR	9.2
23	21	2	SER	9.0
38	1g	80	VAL	9.0
6	2G	28	VAL	8.9
54	1w	71	G	8.9
21	2Z	144	LEU	8.7
44	2m	102	ARG	8.3
44	2m	124	PRO	8.3
45	2n	25	VAL	8.2
54	1w	70	G	8.2
44	2m	123	ALA	8.0
54	2w	72	C	8.0
38	2g	80	VAL	7.8
41	2j	55	LYS	7.8
45	2n	39	LEU	7.7
6	2G	29	TRP	7.5
38	1g	82	GLY	7.4
33	2b	165	VAL	7.2
41	2j	47	PHE	7.2
14	2S	32	LEU	7.1
52	2u	14	TRP	7.1
53	2v	14	A	7.1
22	20	5	LYS	7.1
3	2D	276	LYS	7.1
34	2c	33	LEU	7.1
34	2c	198	VAL	7.1
45	2n	38	GLY	7.0
54	2w	73	A	6.8
52	2u	6	ARG	6.8
54	2w	70	G	6.8
45	2n	7	ILE	6.8
40	2i	7	THR	6.7
40	2i	125	TYR	6.7
34	2c	189	ALA	6.6
22	10	6	GLY	6.6
34	2c	190	ARG	6.5
54	2w	4	C	6.5
7	2H	115	VAL	6.4
33	2b	94	ASN	6.4
53	2v	24	A	6.3
21	2Z	170	THR	6.3
1	2A	883	G	6.3

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Mol	Chain	Res	Type	RSRZ
33	2b	214	ILE	6.2
45	2n	6	LEU	6.2
20	2Y	45	VAL	6.2
34	2c	182	ILE	6.2
44	2m	122	LYS	6.1
26	24	56	VAL	6.1
52	2u	11	GLY	6.1
33	2b	187	LEU	6.1
54	2y	36	A	6.0
40	2i	114	TYR	6.0
31	29	37	GLY	6.0
22	20	2	ALA	5.8
1	1A	1555	C	5.8
33	2b	132	LYS	5.8
36	2e	90	VAL	5.7
38	2g	7	ALA	5.7
38	2g	83	ALA	5.7
29	17	48	LYS	5.7
45	2n	36	PHE	5.7
45	2n	2	ALA	5.6
34	2c	188	LEU	5.6
54	2w	76	A	5.6
12	2Q	104	PHE	5.6
33	2b	118	LEU	5.6
3	1D	276	LYS	5.6
32	2a	1030(B)	C	5.6
33	2b	122	PHE	5.5
36	2e	13	ILE	5.5
34	2c	124	ILE	5.5
41	2j	48	THR	5.4
32	1a	1531	A	5.4
26	24	49	PHE	5.4
34	2c	4	LYS	5.4
1	2A	896	A	5.4
26	24	51	ASP	5.4
34	2c	160	ALA	5.4
50	2s	82	GLY	5.4
44	2m	60	VAL	5.4
33	2b	92	TYR	5.4
54	2w	13	C	5.3
6	2G	157	ILE	5.3
33	2b	188	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
54	1w	72	C	5.3
38	2g	81	GLY	5.3
54	2w	69	G	5.2
20	2Y	106	LEU	5.2
33	2b	133	LYS	5.2
7	2H	101	ARG	5.2
19	2X	68	ARG	5.2
54	2w	5	G	5.1
21	2Z	149	SER	5.1
33	2b	201	ILE	5.1
33	2b	197	VAL	5.1
45	2n	37	PHE	5.1
29	27	1	MET	5.1
47	1p	7	ALA	5.1
50	2s	80	TYR	5.1
26	24	50	VAL	5.1
41	2j	56	HIS	5.0
32	2a	1257	U	5.0
42	2k	25	TYR	5.0
45	2n	35	ARG	5.0
6	2G	146	TYR	5.0
54	2w	3	C	5.0
21	2Z	155	LEU	5.0
45	1n	2	ALA	5.0
21	2Z	139	VAL	5.0
33	2b	185	ILE	4.9
41	2j	59	SER	4.9
29	27	47	ARG	4.9
33	2b	97	TRP	4.9
21	2Z	126	VAL	4.9
1	2A	884	C	4.9
41	2j	62	HIS	4.9
54	2w	75	C	4.9
7	2H	107	VAL	4.9
34	2c	197	GLY	4.9
45	2n	42	ILE	4.8
17	2V	73	SER	4.8
33	2b	152	PHE	4.8
32	1a	204	U	4.8
40	2i	109	VAL	4.8
34	2c	185	GLY	4.8
33	2b	123	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
33	2b	186	ALA	4.7
36	2e	21	ALA	4.7
33	2b	70	PHE	4.7
1	2A	2155	G	4.7
3	1D	275	LYS	4.7
40	2i	79	LEU	4.7
40	2i	110	GLU	4.7
50	2s	84	GLY	4.7
12	2Q	66	ILE	4.7
23	2l	28	GLY	4.7
44	2m	5	ALA	4.7
44	2m	4	ILE	4.7
32	1a	1532	U	4.7
54	1w	3	C	4.6
33	2b	163	PHE	4.6
17	2V	72	VAL	4.6
40	2i	115	GLY	4.6
54	2y	34	G	4.6
40	2i	9	ARG	4.6
33	2b	37	ASN	4.6
22	20	7	LEU	4.6
44	2m	6	GLY	4.6
45	2n	12	ARG	4.6
44	2m	104	ARG	4.6
51	2t	9	ASN	4.6
33	2b	232	PRO	4.6
40	2i	14	VAL	4.6
34	2c	39	ILE	4.6
20	2Y	48	ALA	4.6
33	2b	101	MET	4.5
34	2c	158	GLY	4.5
7	2H	159	GLU	4.5
23	1l	2	SER	4.5
45	2n	22	THR	4.5
1	2A	229	A	4.5
41	2j	46	ARG	4.5
43	2l	64	TYR	4.5
50	2s	79	THR	4.5
40	1i	65	VAL	4.5
1	2A	1509	C	4.5
45	2n	10	ALA	4.5
3	2D	38	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
44	2m	66	LEU	4.5
41	2j	63	PHE	4.5
36	2e	31	LEU	4.4
36	2e	29	GLY	4.4
40	2i	17	VAL	4.4
54	2w	6	G	4.4
54	2w	44	G	4.4
7	2H	113	VAL	4.4
1	2A	2154	G	4.4
39	1h	93	VAL	4.4
34	2c	193	TYR	4.4
43	2l	32	PHE	4.4
45	2n	29	ARG	4.4
26	24	40	HIS	4.4
20	2Y	61	ILE	4.4
41	2j	50	ILE	4.4
54	2w	74	C	4.4
33	2b	136	VAL	4.3
29	27	48	LYS	4.3
40	1i	15	ALA	4.3
40	2i	116	LYS	4.3
48	1q	27	PHE	4.3
34	2c	8	ILE	4.3
50	2s	30	LEU	4.3
33	2b	32	ILE	4.3
45	2n	13	THR	4.3
6	2G	34	LEU	4.3
44	2m	90	LEU	4.3
52	2u	10	ARG	4.3
34	2c	10	PHE	4.3
28	26	54	ILE	4.3
42	2k	126	ARG	4.3
33	1b	233	SER	4.3
1	2A	2146	C	4.3
40	2i	127	LYS	4.2
45	2n	61	TRP	4.2
46	2o	60	VAL	4.2
36	2e	12	LEU	4.2
45	2n	31	ARG	4.2
40	1i	106	ALA	4.2
1	2A	2802	G	4.2
53	1v	12	A	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
22	10	7	LEU	4.2
52	2u	23	PRO	4.2
43	2l	39	VAL	4.1
45	2n	49	HIS	4.1
1	1A	1140	U	4.1
38	2g	85	TYR	4.1
53	1v	24	A	4.1
32	2a	89	C	4.1
34	2c	2	GLY	4.1
34	2c	155	GLY	4.1
39	1h	4	ASP	4.1
40	2i	108	VAL	4.1
48	2q	23	VAL	4.1
33	1b	133	LYS	4.1
54	2w	31	A	4.1
51	2t	24	LEU	4.1
38	2g	79	ARG	4.1
45	2n	51	GLY	4.1
41	2j	54	PHE	4.1
44	2m	121	LYS	4.1
42	1k	126	ARG	4.0
35	2d	146	ILE	4.0
21	2Z	156	LYS	4.0
48	2q	32	TYR	4.0
38	1g	79	ARG	4.0
33	2b	71	VAL	4.0
7	2H	94	TYR	4.0
20	2Y	65	ALA	4.0
33	2b	211	ILE	4.0
45	2n	11	LYS	4.0
8	2I	12	LEU	4.0
12	2Q	37	LEU	4.0
34	2c	196	LEU	4.0
40	2i	19	LEU	4.0
29	27	46	VAL	4.0
44	2m	97	PRO	3.9
48	2q	36	ILE	3.9
6	2G	92	VAL	3.9
33	2b	177	ALA	3.9
41	2j	10	GLY	3.9
45	2n	57	ARG	3.9
39	2h	2	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
39	1h	86	ILE	3.9
35	2d	164	ALA	3.9
41	2j	32	ALA	3.9
43	2l	5	PRO	3.9
29	17	47	ARG	3.9
26	24	42	PHE	3.9
33	2b	164	VAL	3.9
54	2w	56	C	3.9
1	2A	1026	U	3.9
45	2n	53	LEU	3.9
40	2i	112	LYS	3.9
47	2p	9	PHE	3.9
23	2l	61	ARG	3.9
53	2v	13	A	3.9
34	2c	21	ARG	3.9
39	2h	131	GLY	3.9
3	2D	217	ARG	3.8
12	2Q	22	LYS	3.8
40	2i	124	GLN	3.8
51	1t	8	ARG	3.8
7	2H	88	LEU	3.8
34	2c	202	ILE	3.8
41	2j	85	LEU	3.8
48	2q	12	SER	3.8
1	1A	1141	A	3.8
51	2t	8	ARG	3.8
44	2m	78	ILE	3.8
45	2n	44	LEU	3.8
48	2q	42	TYR	3.8
54	2w	2	C	3.8
7	2H	145	ALA	3.8
21	2Z	172	ALA	3.8
34	2c	159	GLY	3.8
43	2l	27	LEU	3.8
40	1i	113	LYS	3.8
32	2a	1036	G	3.8
11	2P	45	LEU	3.8
21	2Z	150	LEU	3.8
45	2n	41	ARG	3.7
20	2Y	75	ILE	3.7
34	2c	157	ILE	3.7
39	2h	83	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
8	2l	3	VAL	3.7
48	2q	9	VAL	3.7
53	2v	12	A	3.7
34	2c	154	SER	3.7
38	2g	4	ARG	3.7
44	2m	94	ARG	3.7
36	2e	109	ILE	3.7
41	2j	49	VAL	3.7
34	2c	13	GLY	3.7
54	1y	35	A	3.7
38	1g	156	TRP	3.7
6	2G	159	VAL	3.7
7	2H	114	VAL	3.7
48	2q	11	VAL	3.7
42	2k	117	ASN	3.7
1	2A	2319	G	3.7
52	2u	13	ILE	3.7
6	2G	19	LEU	3.7
21	2Z	125	LEU	3.7
8	1l	117	GLU	3.7
28	26	20	ASN	3.7
44	2m	88	ARG	3.7
18	2W	86	LEU	3.7
32	2a	1532	U	3.7
34	1c	193	TYR	3.7
47	1p	19	ILE	3.7
3	1D	38	LYS	3.7
12	2Q	1	MET	3.7
3	2D	2	ALA	3.7
14	2S	92	TYR	3.7
33	2b	203	GLY	3.7
45	2n	58	LYS	3.7
32	2a	1531	A	3.6
40	2i	5	TYR	3.6
40	2i	36	TYR	3.6
40	2i	64	THR	3.6
52	2u	22	ARG	3.6
18	1W	112	GLY	3.6
50	2s	49	ILE	3.6
32	1a	1030(B)	C	3.6
49	2r	26	LEU	3.6
35	2d	158	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
34	2c	184	TYR	3.6
40	2i	126	SER	3.6
12	2Q	79	LEU	3.6
7	2H	102	ALA	3.6
41	2j	66	ARG	3.6
43	2l	13	LYS	3.6
32	1a	1036	G	3.6
21	2Z	145	GLU	3.6
45	2n	8	GLU	3.6
54	1w	73	A	3.6
38	1g	81	GLY	3.6
6	1G	146	TYR	3.6
1	2A	2132	U	3.6
32	1a	1257	U	3.6
38	2g	16	LEU	3.6
32	1a	1030(A)	G	3.6
34	2c	163	ALA	3.6
44	2m	120	LYS	3.6
48	2q	100	LYS	3.6
51	2t	83	ARG	3.6
54	2w	14	A	3.6
46	1o	87	ILE	3.6
1	2A	885	C	3.6
28	26	11	LEU	3.6
6	2G	39	ILE	3.6
7	2H	45	VAL	3.6
22	10	4	LYS	3.6
11	2P	79	ARG	3.5
20	2Y	5	MET	3.5
39	1h	90	GLY	3.5
41	2j	45	ARG	3.5
14	2S	58	LEU	3.5
38	2g	154	TYR	3.5
25	23	60	GLU	3.5
47	2p	12	LYS	3.5
21	2Z	50	GLN	3.5
1	2A	2897	U	3.5
6	2G	2	PRO	3.5
12	2Q	5	ARG	3.5
39	2h	90	GLY	3.5
43	2l	18	VAL	3.5
20	2Y	35	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
7	2H	165	ALA	3.5
35	2d	160	GLN	3.5
52	1u	16	GLY	3.5
6	2G	48	GLU	3.5
40	1i	59	PHE	3.5
48	2q	91	ARG	3.5
33	2b	95	GLN	3.5
14	2S	3	ARG	3.5
7	2H	166	GLY	3.5
20	2Y	63	LYS	3.5
13	2R	69	ASP	3.5
21	2Z	140	ASP	3.5
52	2u	8	THR	3.5
38	2g	156	TRP	3.5
6	2G	181	ARG	3.5
33	2b	55	PHE	3.5
54	2w	45	U	3.5
11	2P	15	ARG	3.5
35	2d	107	ARG	3.5
1	2A	2131	G	3.4
8	2I	4	ILE	3.4
33	1b	130	ARG	3.4
1	2A	2140	C	3.4
48	2q	7	THR	3.4
33	2b	140	HIS	3.4
21	2Z	173	ALA	3.4
31	29	13	LYS	3.4
45	2n	54	PRO	3.4
7	2H	103	LEU	3.4
21	2Z	53	ILE	3.4
3	2D	15	PHE	3.4
6	2G	15	VAL	3.4
54	1y	20	U	3.4
35	2d	108	LEU	3.4
47	1p	4	ILE	3.4
1	1A	2167	C	3.4
32	2a	1286	A	3.4
43	2l	15	ARG	3.4
34	2c	147	LYS	3.4
29	17	46	VAL	3.4
41	2j	61	GLU	3.4
55	2x	65	C	3.4

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Mol	Chain	Res	Type	RSRZ
34	2c	200	ALA	3.4
1	1A	2176	G	3.4
34	2c	41	GLY	3.4
36	2e	99	GLY	3.4
43	2l	95	GLY	3.4
48	2q	90	ILE	3.4
31	29	16	VAL	3.4
35	2d	49	ARG	3.4
54	2w	7	A	3.4
1	2A	2133	G	3.3
32	2a	1202	G	3.3
34	2c	3	ASN	3.3
36	2e	81	GLU	3.3
11	2P	59	LEU	3.3
28	26	10	LEU	3.3
34	2c	57	ILE	3.3
50	2s	31	ILE	3.3
54	2w	12	U	3.3
50	2s	44	MET	3.3
7	2H	105	LEU	3.3
44	2m	13	LYS	3.3
40	2i	113	LYS	3.3
45	2n	50	LYS	3.3
34	2c	178	LEU	3.3
1	2A	2145	C	3.3
9	2N	113	GLY	3.3
6	2G	35	GLU	3.3
20	2Y	46	LYS	3.3
6	2G	136	ARG	3.3
33	2b	120	ALA	3.3
6	2G	133	LEU	3.3
30	28	61	LEU	3.3
22	10	5	LYS	3.3
33	2b	113	HIS	3.3
34	2c	15	THR	3.3
48	2q	65	ILE	3.3
51	1t	12	ALA	3.3
21	2Z	154	ASP	3.3
35	1d	135	LEU	3.3
4	2E	151	TYR	3.3
40	2i	27	THR	3.3
22	20	4	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
30	28	29	LYS	3.3
38	1g	83	ALA	3.3
44	1m	123	ALA	3.3
52	2u	24	ARG	3.3
1	1A	2160	C	3.2
1	2A	886	C	3.2
33	2b	184	VAL	3.2
14	2S	33	LYS	3.2
31	29	15	LYS	3.2
32	2a	977	A	3.2
35	1d	157	LEU	3.2
19	2X	69	TYR	3.2
44	2m	65	LYS	3.2
7	2H	72	ILE	3.2
46	2o	57	LEU	3.2
48	2q	30	PRO	3.2
36	2e	10	MET	3.2
34	2c	186	PHE	3.2
45	2n	56	VAL	3.2
1	1A	2162	C	3.2
40	2i	61	ALA	3.2
20	2Y	59	GLY	3.2
44	2m	92	HIS	3.2
48	2q	92	ARG	3.2
9	2N	83	LYS	3.2
2	2B	54	G	3.2
45	2n	60	SER	3.2
35	1d	2	GLY	3.2
22	20	3	HIS	3.2
50	2s	41	VAL	3.2
41	2j	89	ASP	3.2
2	2B	58	A	3.2
51	2t	20	LEU	3.2
45	2n	16	PHE	3.2
39	2h	111	ILE	3.2
17	2V	71	LEU	3.2
23	11	98	LEU	3.2
47	2p	74	LEU	3.2
47	1p	48	TRP	3.2
1	2A	2803	C	3.2
54	2w	68	C	3.2
32	2a	1034	G	3.2

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Mol	Chain	Res	Type	RSRZ
6	2G	73	ALA	3.2
39	1h	133	LEU	3.2
45	2n	24	CYS	3.2
33	2b	90	MET	3.1
29	17	45	ALA	3.1
34	1c	12	LEU	3.1
43	2l	10	LEU	3.1
8	2I	85	GLU	3.1
20	2Y	47	LYS	3.1
33	1b	136	VAL	3.1
1	2A	2896	C	3.1
13	2R	68	ARG	3.1
52	2u	12	LYS	3.1
14	2S	5	THR	3.1
20	2Y	12	THR	3.1
12	2Q	6	ARG	3.1
34	2c	162	GLN	3.1
40	2i	120	ARG	3.1
5	2F	64	ILE	3.1
33	2b	210	SER	3.1
11	2P	51	PHE	3.1
23	21	62	VAL	3.1
33	2b	96	ARG	3.1
1	1A	2174	G	3.1
46	2o	86	GLY	3.1
20	2Y	43	ASN	3.1
3	2D	37	LEU	3.1
40	2i	76	ALA	3.1
44	1m	122	LYS	3.1
47	2p	19	ILE	3.1
48	2q	22	LEU	3.1
43	2l	31	PRO	3.1
34	1c	179	ARG	3.1
45	2n	23	ARG	3.1
52	1u	14	TRP	3.1
4	2E	115	GLY	3.1
38	2g	40	ALA	3.1
47	2p	6	LEU	3.1
50	2s	24	ALA	3.1
42	2k	29	ILE	3.1
1	2A	882	G	3.1
25	23	54	VAL	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
32	2a	962	C	3.1
39	2h	19	VAL	3.1
39	2h	95	VAL	3.1
6	2G	140	ILE	3.1
31	29	26	ILE	3.1
20	2Y	50	ARG	3.1
39	2h	93	VAL	3.1
1	2A	2139	C	3.1
43	1l	7	ILE	3.1
33	2b	216	SER	3.0
40	2i	83	ARG	3.0
51	2t	17	ARG	3.0
52	2u	15	ARG	3.0
32	2a	1357	A	3.0
52	2u	2	GLY	3.0
7	2H	49	VAL	3.0
34	2c	201	TYR	3.0
35	2d	168	ARG	3.0
48	2q	73	VAL	3.0
10	2O	81	ASP	3.0
33	2b	221	LEU	3.0
35	2d	78	LEU	3.0
41	2j	65	LEU	3.0
44	1m	124	PRO	3.0
33	2b	223	ILE	3.0
33	2b	139	LYS	3.0
25	23	53	LEU	3.0
47	1p	6	LEU	3.0
49	2r	85	LEU	3.0
15	2T	52	ILE	3.0
14	2S	20	ARG	3.0
45	2n	26	ARG	3.0
7	2H	123	PHE	3.0
11	2P	68	GLN	3.0
1	1A	2163	G	3.0
32	1a	1030	C	3.0
54	1w	4	C	3.0
54	1w	69	G	3.0
55	2x	67	C	3.0
44	2m	101	GLN	3.0
9	2N	104	LYS	3.0
33	2b	147	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
27	15	60	VAL	3.0
45	2n	27	CYS	3.0
25	23	51	ALA	3.0
40	2i	123	PRO	3.0
54	2y	65	G	3.0
1	1A	942	A	3.0
1	1A	1142	A	3.0
40	2i	105	ASP	3.0
10	2O	1	MET	3.0
12	2Q	2	LEU	3.0
33	1b	61	LEU	3.0
12	2Q	114	ALA	3.0
30	28	10	ALA	3.0
39	1h	84	ARG	3.0
7	2H	46	GLU	2.9
52	2u	16	GLY	2.9
31	29	9	ARG	2.9
5	2F	82	ILE	2.9
32	2a	973	G	2.9
6	2G	120	LEU	2.9
34	2c	91	LEU	2.9
41	2j	67	THR	2.9
5	2F	89	VAL	2.9
14	2S	57	LYS	2.9
38	2g	152	ALA	2.9
17	2V	85	LYS	2.9
33	2b	209	ARG	2.9
43	2l	19	ARG	2.9
47	1p	1	MET	2.9
32	1a	1002	G	2.9
17	2V	74	LYS	2.9
30	28	15	LYS	2.9
48	2q	26	GLN	2.9
33	2b	81	VAL	2.9
43	2l	55	VAL	2.9
50	2s	52	TYR	2.9
54	2w	67	C	2.9
9	2N	10	GLU	2.9
1	2A	2156	G	2.9
3	2D	204	ILE	2.9
39	1h	6	ILE	2.9
39	1h	91	ARG	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
39	1h	92	ARG	2.9
55	2x	4	G	2.9
32	2a	983	A	2.9
33	2b	31	TYR	2.9
49	1r	73	ALA	2.9
38	2g	6	ARG	2.9
1	2A	2144	U	2.9
11	2P	78	PRO	2.9
21	2Z	148	ASP	2.9
34	2c	180	ALA	2.9
38	1g	85	TYR	2.9
33	2b	26	PRO	2.9
38	1g	84	ASN	2.9
38	2g	84	ASN	2.9
51	2t	30	LYS	2.9
34	1c	15	THR	2.9
33	2b	217	ARG	2.9
43	2l	94	PRO	2.9
7	2H	31	GLY	2.8
36	2e	8	GLU	2.8
4	2E	77	ILE	2.8
4	2E	134	ILE	2.8
8	1I	79	ILE	2.8
1	1A	932	C	2.8
32	2a	1114	C	2.8
55	1x	67	C	2.8
6	2G	152	LEU	2.8
26	24	58	ARG	2.8
33	2b	173	ALA	2.8
36	2e	148	VAL	2.8
40	2i	26	VAL	2.8
43	2l	48	PRO	2.8
1	1A	2173	G	2.8
32	1a	1030(C)	G	2.8
9	2N	116	LEU	2.8
12	2Q	63	LYS	2.8
44	2m	17	VAL	2.8
28	26	21	TYR	2.8
30	28	41	ILE	2.8
46	1o	65	ARG	2.8
32	2a	1220	G	2.8
48	2q	24	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
11	2P	1	MET	2.8
23	21	26	ARG	2.8
40	2i	128	ARG	2.8
16	2U	17	ILE	2.8
6	2G	3	LEU	2.8
13	2R	65	LEU	2.8
32	2a	1033	G	2.8
53	2v	23	A	2.8
40	2i	117	HIS	2.8
7	2H	124	GLU	2.8
3	2D	61	LEU	2.8
7	2H	148	ILE	2.8
15	2T	48	ILE	2.8
28	26	9	LEU	2.8
12	2Q	15	GLY	2.8
37	1f	58	GLY	2.8
40	2i	122	ALA	2.8
44	2m	91	ARG	2.8
1	2A	1847	A	2.8
14	2S	34	HIS	2.8
32	1a	1030(D)	A	2.8
32	2a	80	G	2.8
10	2O	99	PHE	2.8
21	2Z	147	GLY	2.8
9	2N	44	PRO	2.8
33	2b	131	PRO	2.8
38	2g	32	ARG	2.8
52	2u	21	TYR	2.8
7	2H	71	LEU	2.8
28	26	34	LEU	2.8
32	2a	965	A	2.8
33	2b	200	ILE	2.8
33	2b	215	LEU	2.8
35	2d	188	LEU	2.8
51	2t	13	LEU	2.8
35	2d	184	LYS	2.8
28	26	5	VAL	2.7
33	2b	218	ALA	2.7
40	2i	15	ALA	2.7
43	2l	16	GLU	2.7
43	2l	30	ALA	2.7
48	2q	21	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
22	10	3	HIS	2.7
9	2N	26	LEU	2.7
24	22	60	LEU	2.7
35	2d	135	LEU	2.7
42	2k	90	GLY	2.7
32	2a	1356	G	2.7
40	1i	126	SER	2.7
40	1i	117	HIS	2.7
45	2n	17	LYS	2.7
13	2R	29	LEU	2.7
36	2e	114	GLY	2.7
40	2i	102	LEU	2.7
43	2l	69	TYR	2.7
48	2q	31	LEU	2.7
4	2E	141	ILE	2.7
34	2c	14	ILE	2.7
39	1h	35	ILE	2.7
11	2P	95	VAL	2.7
25	23	47	VAL	2.7
36	2e	115	VAL	2.7
42	2k	115	PRO	2.7
54	1w	44	G	2.7
54	2y	53	G	2.7
20	2Y	31	LEU	2.7
21	2Z	122	ARG	2.7
34	2c	194	GLY	2.7
44	2m	87	TYR	2.7
47	1p	59	TRP	2.7
50	2s	43	GLU	2.7
7	2H	35	VAL	2.7
34	2c	81	GLY	2.7
40	1i	56	LEU	2.7
47	2p	48	TRP	2.7
48	2q	88	TYR	2.7
34	2c	199	LYS	2.7
20	2Y	13	VAL	2.7
34	2c	17	ASP	2.7
34	2c	206	GLU	2.7
44	2m	71	ARG	2.7
47	2p	26	ARG	2.7
50	2s	57	HIS	2.7
51	2t	23	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
6	2G	135	LEU	2.7
20	2Y	34	LYS	2.7
6	2G	11	TYR	2.7
1	1A	1072	U	2.7
51	2t	100	ILE	2.7
11	2P	50	ARG	2.7
21	2Z	51	ALA	2.7
34	2c	174	PRO	2.7
40	1i	51	ARG	2.7
33	2b	228	GLY	2.7
39	1h	119	LEU	2.7
12	2Q	32	TYR	2.7
35	2d	68	TYR	2.7
43	2l	7	ILE	2.7
1	1A	935	C	2.7
20	2Y	107	ASP	2.7
33	2b	129	GLU	2.7
44	2m	103	THR	2.7
52	1u	9	ARG	2.7
53	2v	22	U	2.7
36	2e	55	VAL	2.7
44	2m	74	VAL	2.7
48	2q	85	VAL	2.7
39	1h	2	LEU	2.7
10	2O	7	TYR	2.7
26	24	53	GLU	2.7
21	2Z	124	ILE	2.7
39	2h	94	TYR	2.7
41	2j	6	ILE	2.7
43	2l	100	ILE	2.7
52	2u	5	ASP	2.7
44	1m	105	THR	2.7
32	2a	961	U	2.6
31	29	25	VAL	2.6
19	2X	1	MET	2.6
20	2Y	73	ARG	2.6
41	1j	59	SER	2.6
11	2P	20	GLY	2.6
54	2y	33	U	2.6
44	2m	67	GLU	2.6
5	2F	62	ARG	2.6
38	2g	3	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
9	2N	85	ILE	2.6
33	2b	99	GLY	2.6
35	1d	5	ILE	2.6
55	2x	70	G	2.6
6	2G	43	LEU	2.6
16	2U	52	ARG	2.6
23	2I	46	LEU	2.6
34	2c	43	LEU	2.6
45	2n	45	ARG	2.6
32	2a	1066	C	2.6
13	2R	14	SER	2.6
32	2a	975	A	2.6
45	2n	32	SER	2.6
33	1b	214	ILE	2.6
36	2e	80	ILE	2.6
7	2H	90	LYS	2.6
25	23	12	PRO	2.6
29	27	45	ALA	2.6
30	28	7	HIS	2.6
15	1T	115	ARG	2.6
38	1g	32	ARG	2.6
41	2j	51	ARG	2.6
48	2q	19	VAL	2.6
2	2B	55	U	2.6
9	2N	8	GLN	2.6
33	2b	105	PHE	2.6
7	2H	89	ILE	2.6
28	26	7	ILE	2.6
35	2d	70	ILE	2.6
44	1m	87	TYR	2.6
29	27	23	ARG	2.6
33	2b	130	ARG	2.6
41	2j	60	ARG	2.6
36	2e	33	VAL	2.6
41	2j	44	VAL	2.6
9	2N	23	LEU	2.6
49	1r	31	LEU	2.6
21	2Z	160	GLY	2.6
18	2W	6	ILE	2.6
25	23	29	ARG	2.6
37	1f	46	ARG	2.6
52	1u	13	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
39	2h	58	TYR	2.6
43	2l	24	VAL	2.6
33	2b	69	LEU	2.6
12	2Q	103	MET	2.6
22	20	45	PHE	2.6
26	24	54	GLY	2.6
7	2H	2	SER	2.6
3	1D	263	ARG	2.6
30	28	64	TYR	2.6
9	2N	84	LYS	2.6
34	2c	6	HIS	2.6
41	2j	68	HIS	2.6
47	2p	39	TYR	2.6
6	2G	70	VAL	2.6
45	2n	18	VAL	2.6
5	2F	41	LEU	2.6
20	2Y	29	GLU	2.6
25	23	26	LEU	2.6
50	2s	15	LEU	2.6
35	1d	23	GLY	2.6
52	2u	9	ARG	2.6
54	2w	23	A	2.6
3	2D	202	LYS	2.5
4	2E	126	PRO	2.5
47	2p	33	ILE	2.5
48	2q	95	TYR	2.5
54	2w	15	G	2.5
13	2R	70	LEU	2.5
39	1h	112	LEU	2.5
40	1i	109	VAL	2.5
48	2q	53	LEU	2.5
35	1d	167	GLY	2.5
2	2B	59	A	2.5
23	21	68	PRO	2.5
41	2j	98	ILE	2.5
45	2n	14	PRO	2.5
43	2l	56	ALA	2.5
48	2q	59	ILE	2.5
3	2D	206	LEU	2.5
21	2Z	24	LEU	2.5
30	28	14	VAL	2.5
9	2N	74	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
23	21	76	ARG	2.5
12	2Q	65	PHE	2.5
32	1a	1034	G	2.5
35	1d	73	ARG	2.5
1	2A	888	C	2.5
32	2a	91	C	2.5
3	1D	2	ALA	2.5
17	2V	70	ILE	2.5
21	2Z	57	ILE	2.5
23	21	63	ALA	2.5
31	29	12	ASP	2.5
43	2l	59	ARG	2.5
51	2t	80	ARG	2.5
46	1o	88	ARG	2.5
3	2D	147	LEU	2.5
26	24	63	TYR	2.5
47	1p	21	VAL	2.5
48	2q	98	LEU	2.5
32	1a	1035	A	2.5
42	2k	125	PHE	2.5
5	2F	80	ALA	2.5
7	2H	95	ARG	2.5
21	2Z	69	THR	2.5
41	2j	41	PRO	2.5
43	2l	71	PRO	2.5
51	2t	25	ARG	2.5
32	1a	1001(A)	G	2.5
33	2b	66	GLY	2.5
43	2l	29	GLY	2.5
8	2l	38	LEU	2.5
45	1n	61	TRP	2.5
9	2N	75	TYR	2.5
40	1i	36	TYR	2.5
48	2q	71	PHE	2.5
33	2b	27	LYS	2.5
35	1d	86	LYS	2.5
43	2l	46	LYS	2.5
48	2q	37	LYS	2.5
34	2c	127	ARG	2.5
40	2i	107	ARG	2.5
54	2y	64	A	2.5
17	2V	50	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
52	2u	17	THR	2.5
14	2S	4	LEU	2.5
30	28	60	LEU	2.5
33	1b	215	LEU	2.5
48	2q	43	LEU	2.5
8	1I	142	VAL	2.5
25	23	59	VAL	2.5
42	1k	14	VAL	2.5
6	2G	102	PHE	2.5
36	2e	84	PHE	2.5
51	2t	86	ARG	2.5
7	2H	112	PRO	2.5
1	1A	1144	A	2.5
32	2a	1225	A	2.5
43	2l	85	ILE	2.5
33	1b	213	LEU	2.5
48	2q	89	LEU	2.5
49	1r	78	LEU	2.5
9	2N	46	VAL	2.5
43	2l	104	VAL	2.5
46	1o	60	VAL	2.5
40	2i	92	TYR	2.5
42	1k	25	TYR	2.5
22	20	11	ARG	2.5
1	2A	2127	G	2.5
32	2a	1061	G	2.5
21	2Z	151	HIS	2.4
30	28	34	TRP	2.4
36	2e	45	PHE	2.4
36	2e	133	TYR	2.4
4	2E	158	GLY	2.4
9	2N	108	PRO	2.4
44	1m	2	ALA	2.4
44	1m	107	ALA	2.4
50	2s	47	HIS	2.4
55	2x	53	G	2.4
23	11	97	LEU	2.4
33	2b	162	ILE	2.4
51	1t	72	LEU	2.4
28	26	52	VAL	2.4
35	1d	3	ARG	2.4
36	2e	67	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
43	2l	101	VAL	2.4
6	2G	141	PHE	2.4
44	2m	73	GLU	2.4
7	2H	164	TYR	2.4
47	1p	39	TYR	2.4
8	2I	34	GLY	2.4
32	1a	1503	A	2.4
32	2a	1363(A)	A	2.4
48	2q	33	GLY	2.4
48	2q	80	GLY	2.4
3	2D	273	ARG	2.4
4	2E	136	ARG	2.4
20	2Y	44	ILE	2.4
23	2l	98	LEU	2.4
34	2c	12	LEU	2.4
49	2r	66	LEU	2.4
21	2Z	153	SER	2.4
33	2b	195	ASP	2.4
34	2c	120	VAL	2.4
50	2s	60	VAL	2.4
20	2Y	55	TYR	2.4
37	2f	59	TYR	2.4
9	2N	48	MET	2.4
25	23	16	PRO	2.4
3	1D	176	ARG	2.4
12	2Q	59	ARG	2.4
20	2Y	2	ARG	2.4
52	1u	6	ARG	2.4
53	2v	15	A	2.4
46	1o	66	LEU	2.4
7	1H	2	SER	2.4
32	2a	1223	C	2.4
34	2c	167	TRP	2.4
38	2g	86	GLN	2.4
40	2i	65	VAL	2.4
41	2j	12	ASP	2.4
36	2e	25	ARG	2.4
40	2i	93	ARG	2.4
47	1p	42	ARG	2.4
50	2s	71	LEU	2.4
30	28	16	ILE	2.4
33	2b	78	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
36	2e	5	ASP	2.4
6	2G	37	VAL	2.4
35	2d	161	ASN	2.4
48	1q	33	GLY	2.4
55	2x	66	C	2.4
3	2D	5	LYS	2.4
43	2l	123	LYS	2.4
35	1d	136	PRO	2.4
32	1a	1003	G	2.4
39	2h	120	THR	2.4
41	1j	65	LEU	2.4
48	2q	44	ALA	2.4
6	2G	49	ASP	2.4
33	2b	150	SER	2.4
3	2D	210	GLY	2.4
42	2k	86	GLY	2.4
34	2c	153	VAL	2.4
36	2e	100	VAL	2.4
40	2i	33	PHE	2.4
1	2A	2690	C	2.4
7	2H	97	ARG	2.4
33	2b	114	ARG	2.4
41	1j	46	ARG	2.4
41	2j	29	ARG	2.4
38	1g	154	TYR	2.4
6	2G	165	THR	2.4
7	2H	106	THR	2.4
33	2b	161	ALA	2.4
42	2k	16	SER	2.4
45	2n	47	LEU	2.4
1	1A	2184	G	2.4
6	2G	27	ASN	2.4
32	2a	112	G	2.4
33	2b	58	ILE	2.4
35	1d	204	ILE	2.4
40	2i	81	ILE	2.4
41	1j	50	ILE	2.4
42	2k	49	GLY	2.4
43	2l	28	LYS	2.4
6	2G	33	ARG	2.4
54	1w	2	C	2.3
6	2G	166	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
6	2G	173	LEU	2.3
9	2N	43	THR	2.3
26	24	52	THR	2.3
35	1d	101	LEU	2.3
39	1h	7	ALA	2.3
51	2t	14	LYS	2.3
22	20	12	ASN	2.3
33	1b	222	ILE	2.3
38	1g	42	ILE	2.3
38	2g	78	ARG	2.3
41	1j	47	PHE	2.3
41	2j	34	VAL	2.3
3	2D	241	PRO	2.3
40	2i	88	TYR	2.3
6	2G	90	LEU	2.3
11	2P	123	LEU	2.3
43	2l	22	SER	2.3
32	2a	1287	A	2.3
14	2S	9	ARG	2.3
42	2k	120	ARG	2.3
47	2p	8	ARG	2.3
33	2b	68	ILE	2.3
35	1d	70	ILE	2.3
39	2h	109	ILE	2.3
51	2t	63	ILE	2.3
33	2b	28	PHE	2.3
45	2n	4	LYS	2.3
34	2c	176	HIS	2.3
6	2G	95	ARG	2.3
16	2U	48	ALA	2.3
33	2b	111	ARG	2.3
33	2b	153	ARG	2.3
36	2e	112	LEU	2.3
41	2j	9	ARG	2.3
14	2S	12	PHE	2.3
16	2U	90	VAL	2.3
23	11	49	VAL	2.3
15	1T	109	GLU	2.3
6	2G	51	ARG	2.3
33	1b	187	LEU	2.3
33	2b	196	LEU	2.3
51	2t	72	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
40	2i	82	ALA	2.3
1	2A	2318	G	2.3
51	2t	42	GLN	2.3
36	2e	131	ILE	2.3
47	1p	36	ILE	2.3
4	2E	75	VAL	2.3
20	2Y	42	VAL	2.3
42	2k	14	VAL	2.3
54	2y	35	A	2.3
36	2e	14	ARG	2.3
46	2o	68	ARG	2.3
43	1l	5	PRO	2.3
48	2q	8	GLY	2.3
40	1i	19	LEU	2.3
41	2j	71	LEU	2.3
7	2H	157	TYR	2.3
12	2Q	136	ALA	2.3
16	2U	47	TYR	2.3
39	2h	65	TYR	2.3
34	2c	28	GLN	2.3
51	2t	18	GLN	2.3
3	2D	53	PHE	2.3
10	2O	38	VAL	2.3
23	2l	53	VAL	2.3
44	2m	7	VAL	2.3
48	2q	27	PHE	2.3
32	2a	1224	G	2.3
34	2c	164	ARG	2.3
55	2x	69	C	2.3
3	2D	4	LYS	2.3
48	2q	74	LEU	2.3
50	2s	14	HIS	2.3
50	2s	32	LYS	2.3
15	1T	114	LEU	2.3
35	2d	120	LEU	2.3
36	2e	151	LEU	2.3
41	1j	40	LEU	2.3
50	2s	83	HIS	2.3
32	2a	1503	A	2.3
15	2T	100	TYR	2.3
40	2i	52	ALA	2.3
6	2G	160	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
7	2H	152	ARG	2.3
13	2R	117	VAL	2.3
21	2Z	128	VAL	2.3
30	28	30	ARG	2.3
36	2e	107	ARG	2.3
41	1j	5	ARG	2.3
52	1u	15	ARG	2.3
50	2s	13	ASP	2.3
40	2i	67	GLY	2.3
21	2Z	5	LEU	2.3
44	2m	42	ALA	2.3
17	2V	81	TYR	2.3
47	1p	17	TYR	2.3
52	1u	17	THR	2.3
12	2Q	10	ARG	2.3
35	2d	73	ARG	2.3
39	2h	84	ARG	2.3
40	1i	37	PHE	2.3
40	2i	111	ARG	2.3
6	2G	36	LYS	2.3
20	2Y	30	VAL	2.3
24	22	52	ASP	2.3
34	1c	13	GLY	2.2
6	2G	94	LEU	2.2
7	2H	111	HIS	2.2
14	2S	31	SER	2.2
15	2T	78	LEU	2.2
26	24	41	PRO	2.2
39	2h	76	PRO	2.2
9	2N	68	GLU	2.2
51	2t	66	ALA	2.2
36	2e	98	THR	2.2
1	1A	639	G	2.2
3	2D	54	ARG	2.2
12	2Q	77	LYS	2.2
19	2X	33	LYS	2.2
31	29	33	LYS	2.2
44	2m	23	TYR	2.2
54	1y	56	C	2.2
6	2G	77	ILE	2.2
9	1N	85	ILE	2.2
14	2S	35	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
34	1c	128	PHE	2.2
18	2W	112	GLY	2.2
40	2i	28	VAL	2.2
14	2S	54	LEU	2.2
39	2h	112	LEU	2.2
40	2i	49	PRO	2.2
44	2m	106	ASN	2.2
9	2N	27	ALA	2.2
33	2b	48	MET	2.2
28	26	50	ARG	2.2
45	2n	30	ALA	2.2
40	2i	4	TYR	2.2
15	2T	61	PHE	2.2
33	2b	220	ASP	2.2
26	24	45	GLY	2.2
34	2c	80	GLY	2.2
40	2i	63	ILE	2.2
54	2w	40	C	2.2
32	2a	1030(A)	G	2.2
33	1b	165	VAL	2.2
9	2N	118	LYS	2.2
19	2X	92	LEU	2.2
32	2a	1092	A	2.2
42	1k	123	LYS	2.2
51	1t	24	LEU	2.2
54	1w	14	A	2.2
6	2G	128	ARG	2.2
35	1d	139	ARG	2.2
35	2d	122	ARG	2.2
35	2d	141	ARG	2.2
7	2H	96	ALA	2.2
40	2i	106	ALA	2.2
45	2n	59	ALA	2.2
9	2N	78	TYR	2.2
14	2S	29	PHE	2.2
44	2m	100	GLY	2.2
8	2I	19	VAL	2.2
11	2P	108	LYS	2.2
12	2Q	90	VAL	2.2
21	2Z	96	VAL	2.2
21	2Z	146	ILE	2.2
43	2l	66	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
46	2o	47	LYS	2.2
1	1A	1138	C	2.2
1	2A	614(B)	G	2.2
20	2Y	14	LEU	2.2
21	2Z	121	HIS	2.2
25	23	44	ARG	2.2
40	2i	16	ARG	2.2
43	2l	77	LEU	2.2
1	2A	614(A)	U	2.2
44	2m	105	THR	2.2
17	2V	80	GLN	2.2
23	21	56	GLN	2.2
28	26	35	GLU	2.2
3	2D	275	LYS	2.2
6	2G	75	LYS	2.2
14	2S	7	TYR	2.2
51	2t	21	LYS	2.2
7	2H	162	ILE	2.2
16	2U	8	VAL	2.2
35	2d	126	ILE	2.2
40	1i	14	VAL	2.2
29	17	23	ARG	2.2
39	2h	18	ARG	2.2
44	1m	102	ARG	2.2
48	2q	38	ARG	2.2
9	2N	107	LEU	2.2
21	2Z	159	PRO	2.2
24	22	24	LEU	2.2
27	15	58	LEU	2.2
44	2m	70	LEU	2.2
35	1d	166	LYS	2.2
36	2e	20	GLN	2.2
51	2t	59	ALA	2.2
13	2R	5	LYS	2.2
21	1Z	169	GLU	2.2
32	2a	1150	U	2.2
40	2i	72	GLY	2.2
41	1j	57	LYS	2.2
47	1p	27	LYS	2.2
16	2U	40	PHE	2.2
6	2G	38	VAL	2.2
10	2O	19	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
24	22	57	ILE	2.2
46	1o	68	ARG	2.2
1	1A	2150	C	2.2
4	2E	125	GLY	2.2
14	2S	6	ALA	2.2
29	27	27	GLY	2.2
34	2c	183	ASP	2.2
34	2c	205	GLY	2.2
49	1r	25	THR	2.2
1	1A	2154	U	2.2
6	2G	23	PHE	2.2
21	2Z	4	ARG	2.2
1	1A	2153	G	2.2
31	29	24	TYR	2.2
54	2w	22	G	2.2
54	2w	24	G	2.2
54	2w	29	G	2.2
7	2H	151	ILE	2.2
34	1c	14	ILE	2.2
35	1d	158	ILE	2.2
39	1h	134	ILE	2.2
6	2G	139	LEU	2.2
33	2b	154	LEU	2.2
39	2h	39	LEU	2.2
47	2p	41	PRO	2.2
48	2q	28	PRO	2.2
6	2G	151	ALA	2.2
45	2n	40	CYS	2.2
41	1j	48	THR	2.2
1	1A	2183	C	2.2
55	2x	68	C	2.2
14	2S	36	TYR	2.1
36	2e	88	LYS	2.1
44	2m	12	ASN	2.1
7	2H	121	ILE	2.1
26	14	50	VAL	2.1
48	1q	23	VAL	2.1
32	2a	781	A	2.1
44	2m	119	GLY	2.1
3	1D	259	THR	2.1
28	26	19	ARG	2.1
34	2c	53	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
35	2d	115	ARG	2.1
39	2h	60	ARG	2.1
7	2H	116	GLU	2.1
12	2Q	12	GLN	2.1
33	2b	233	SER	2.1
43	2l	120	TYR	2.1
5	2F	81	PRO	2.1
11	2P	97	PRO	2.1
16	2U	2	PRO	2.1
16	2U	39	LEU	2.1
47	2p	13	HIS	2.1
35	1d	16	GLY	2.1
36	2e	22	GLY	2.1
34	2c	179	ARG	2.1
35	2d	118	ARG	2.1
6	2G	155	MET	2.1
20	2Y	54	LYS	2.1
43	2l	68	ALA	2.1
32	2a	1048	G	2.1
35	1d	181	MET	2.1
30	28	35	GLN	2.1
40	1i	34	ASN	2.1
47	2p	80	PHE	2.1
3	2D	62	TYR	2.1
5	2F	57	VAL	2.1
9	2N	5	VAL	2.1
33	2b	41	ILE	2.1
34	1c	201	TYR	2.1
36	2e	118	ILE	2.1
48	1q	35	VAL	2.1
13	2R	33	ARG	2.1
32	2a	1116	C	2.1
50	1s	71	LEU	2.1
43	2l	41	ARG	2.1
53	2v	21	C	2.1
55	2x	71	C	2.1
21	2Z	21	ALA	2.1
36	2e	17	ALA	2.1
50	2s	50	ALA	2.1
51	1t	9	ASN	2.1
1	2A	1508	A	2.1
32	2a	963	G	2.1

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Mol	Chain	Res	Type	RSRZ
54	2y	52	G	2.1
55	2x	2	G	2.1
3	1D	49	ILE	2.1
6	2G	176	LEU	2.1
7	2H	92	ILE	2.1
10	2O	17	ARG	2.1
34	2c	171	GLY	2.1
36	2e	27	ARG	2.1
38	1g	3	ARG	2.1
38	2g	155	ARG	2.1
44	2m	110	ARG	2.1
45	2n	21	TYR	2.1
52	1u	19	GLY	2.1
34	2c	191	THR	2.1
36	2e	135	THR	2.1
6	2G	84	LYS	2.1
14	2S	11	LYS	2.1
46	1o	8	LYS	2.1
4	2E	167	VAL	2.1
4	2E	195	LEU	2.1
9	2N	9	VAL	2.1
12	2Q	17	LEU	2.1
19	1X	94	GLY	2.1
35	2d	183	GLY	2.1
41	1j	60	ARG	2.1
46	2o	88	ARG	2.1
1	2A	887	A	2.1
1	2A	2147	G	2.1
30	28	2	PRO	2.1
40	1i	125	TYR	2.1
6	2G	163	ALA	2.1
20	2Y	78	ALA	2.1
40	2i	119	ALA	2.1
1	2A	2138	C	2.1
1	2A	2297	C	2.1
6	2G	161	THR	2.1
30	28	5	LYS	2.1
32	2a	1354	C	2.1
44	2m	64	TRP	2.1
48	2q	18	THR	2.1
48	2q	34	LYS	2.1
14	1S	12	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
40	2i	20	ARG	2.1
47	1p	18	ARG	2.1
34	2c	145	GLY	2.1
11	2P	3	LEU	2.1
16	2U	20	LEU	2.1
20	2Y	24	VAL	2.1
20	2Y	67	LEU	2.1
30	28	32	LEU	2.1
4	1E	77	ILE	2.1
14	2S	40	ILE	2.1
34	2c	134	ILE	2.1
43	2l	43	VAL	2.1
47	1p	38	TYR	2.1
48	1q	28	PRO	2.1
20	2Y	105	ALA	2.1
24	22	2	LYS	2.1
32	1a	1033	G	2.1
32	2a	1201	A	2.1
36	2e	94	ALA	2.1
1	1A	1143	U	2.1
8	2I	1	MET	2.1
23	2I	11	ARG	2.1
34	2c	156	ARG	2.1
39	2h	122	ARG	2.1
51	2t	22	ARG	2.1
17	2V	75	PHE	2.1
12	2Q	33	GLY	2.1
20	2Y	10	GLY	2.1
13	2R	4	LEU	2.1
13	2R	20	LEU	2.1
12	2Q	4	PRO	2.1
15	2T	50	ILE	2.1
34	2c	173	VAL	2.1
39	2h	79	VAL	2.1
41	1j	72	VAL	2.1
40	2i	90	PRO	2.1
21	2Z	99	TYR	2.1
35	2d	138	TYR	2.1
51	1t	74	LYS	2.1
11	2P	65	ARG	2.1
33	2b	137	ARG	2.1
43	2l	33	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
22	20	9	SER	2.1
3	2D	55	GLY	2.1
26	14	54	GLY	2.1
54	2w	66	U	2.0
6	2G	41	GLN	2.0
6	2G	182	LYS	2.0
11	2P	39	LYS	2.0
46	1o	57	LEU	2.0
6	2G	142	PRO	2.0
12	2Q	106	VAL	2.0
22	20	38	VAL	2.0
12	2Q	64	ILE	2.0
30	18	2	PRO	2.0
41	2j	74	ILE	2.0
44	2m	10	PRO	2.0
6	2G	12	TYR	2.0
12	2Q	93	TYR	2.0
34	1c	71	ALA	2.0
34	2c	30	ARG	2.0
3	2D	180	GLY	2.0
9	2N	73	THR	2.0
21	1Z	1	MET	2.0
16	2U	19	LYS	2.0
34	2c	26	LYS	2.0
43	2l	23	LYS	2.0
34	2c	87	LEU	2.0
2	2B	56	G	2.0
7	2H	125	VAL	2.0
14	2S	14	VAL	2.0
32	1a	344	A	2.0
32	2a	1285	A	2.0
38	1g	153	HIS	2.0
54	1y	36	A	2.0
3	2D	106	ILE	2.0
9	2N	60	ILE	2.0
23	21	58	ILE	2.0
1	2A	2174	C	2.0
36	2e	60	TYR	2.0
3	2D	156	ALA	2.0
10	2O	41	ALA	2.0
7	2H	122	THR	2.0
40	2i	80	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
15	2T	22	PHE	2.0
21	2Z	48	PHE	2.0
30	28	25	MET	2.0
21	2Z	102	LEU	2.0
22	20	75	LEU	2.0
40	2i	40	LEU	2.0
7	2H	3	ARG	2.0
8	1I	109	ILE	2.0
11	2P	149	GLU	2.0
12	2Q	81	VAL	2.0
32	2a	84	U	2.0
35	1d	118	ARG	2.0
47	1p	2	VAL	2.0
50	2s	78	ARG	2.0
31	29	17	ILE	2.0
1	2A	2158	A	2.0
32	2a	88	A	2.0
1	2A	2137	C	2.0
16	2U	46	ALA	2.0
35	2d	20	TYR	2.0
47	2p	38	TYR	2.0
48	2q	40	LYS	2.0
32	1a	1028	C	2.0
35	2d	180	GLY	2.0
51	1t	69	GLY	2.0
54	1w	15	G	2.0
39	2h	87	SER	2.0
33	1b	163	PHE	2.0
40	2i	37	PHE	2.0
46	2o	15	PHE	2.0
3	2D	252	TRP	2.0
5	2F	56	GLU	2.0
15	2T	108	ARG	2.0
19	1X	66	LEU	2.0
31	29	19	ARG	2.0
39	2h	82	HIS	2.0
41	1j	45	ARG	2.0
41	2j	64	GLU	2.0
7	2H	169	VAL	2.0
25	23	24	LYS	2.0
28	26	8	LYS	2.0
35	2d	148	VAL	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
54	PSU	2y	55	20/21	0.63	0.32	96,103,115,116	0
54	7MG	2y	46	24/25	0.65	0.21	92,100,108,129	0
54	PSU	1y	55	20/21	0.70	0.22	87,94,103,112	0
54	5MU	2y	54	21/22	0.75	0.25	90,96,106,120	0
54	7MG	2w	46	24/25	0.78	0.31	88,94,107,122	0
54	MIA	2y	37	22/30	0.78	0.29	78,90,104,116	0
54	7MG	1w	46	24/25	0.79	0.16	77,87,101,122	0
54	5MU	1y	54	21/22	0.79	0.20	79,91,96,109	0
54	PSU	2y	32	20/21	0.81	0.20	76,88,94,101	0
54	4SU	2w	8	20/21	0.82	0.25	88,96,108,111	0
54	PSU	2w	55	20/21	0.82	0.29	85,91,101,102	0
54	PSU	2y	39	20/21	0.83	0.25	81,87,93,95	0
54	7MG	1y	46	24/25	0.83	0.19	86,94,105,112	0
54	4SU	1y	8	20/21	0.84	0.17	88,94,109,110	0
54	4SU	2y	8	20/21	0.86	0.12	93,100,109,115	0
32	PSU	2a	516	20/21	0.86	0.22	68,76,85,86	0
54	4SU	1w	8	20/21	0.88	0.14	75,83,92,101	0
55	4SU	2x	8	20/21	0.88	0.15	77,83,87,91	0
32	M2G	2a	966	25/26	0.88	0.28	57,73,85,89	0
32	5MC	2a	967	21/22	0.89	0.23	67,72,78,87	0
54	MIA	1y	37	22/30	0.89	0.18	69,81,86,91	0
32	2MG	2a	1207	24/25	0.89	0.19	79,86,93,95	0
43	0TD	2l	92	10/11	0.90	0.23	62,66,69,79	0
54	5MU	2w	54	21/22	0.90	0.19	75,83,91,93	0
54	PSU	1w	55	20/21	0.90	0.17	63,77,81,85	0
55	PSU	2x	55	20/21	0.90	0.22	76,83,88,93	0
54	PSU	1y	32	20/21	0.90	0.20	75,83,94,95	0
54	PSU	1y	39	20/21	0.90	0.18	70,77,86,87	0
43	0TD	1l	92	10/11	0.91	0.19	42,51,56,70	0
54	PSU	1w	32	20/21	0.92	0.21	59,68,77,78	0
54	PSU	2w	39	20/21	0.93	0.31	73,81,88,88	0
54	PSU	2w	32	20/21	0.93	0.28	76,85,94,94	0
32	5MC	2a	1404	21/22	0.93	0.19	52,62,66,67	0
54	MIA	2w	37	25/30	0.93	0.27	74,80,87,95	0
32	7MG	2a	527	24/25	0.93	0.18	63,69,75,81	0
55	5MU	1x	54	21/22	0.93	0.16	61,71,74,78	0
55	5MU	2x	54	21/22	0.93	0.26	80,84,89,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	PSU	2A	1917	20/21	0.94	0.21	62,70,78,83	0
1	5MU	2A	1915	21/22	0.94	0.16	70,75,80,83	0
32	4OC	2a	1402	22/23	0.94	0.19	57,65,69,69	0
1	PSU	2A	1911	20/21	0.94	0.17	61,66,73,74	0
55	5MC	2x	32	21/22	0.94	0.21	68,77,80,81	0
1	5MU	1A	1937	21/22	0.94	0.20	47,53,59,65	0
32	5MC	2a	1407	21/22	0.95	0.20	51,57,62,66	0
55	PSU	1x	55	20/21	0.95	0.15	51,65,73,78	0
32	UR3	2a	1498	21/22	0.95	0.20	50,60,63,68	0
1	4OC	2A	1920	21/23	0.95	0.19	60,66,70,73	0
32	5MC	1a	967	21/22	0.95	0.25	41,54,60,62	0
32	5MC	2a	1400	21/22	0.95	0.24	70,74,79,82	0
55	4SU	1x	8	20/21	0.95	0.18	52,61,78,79	0
1	PSU	1A	1939	20/21	0.95	0.21	34,49,52,57	0
32	5MC	1a	1404	21/22	0.96	0.22	34,40,47,49	0
1	PSU	2A	2605	20/21	0.96	0.22	37,40,46,48	0
32	2MG	1a	1207	24/25	0.96	0.17	52,65,69,73	0
1	5MC	2A	1962	21/22	0.96	0.20	41,50,60,78	0
54	MIA	1w	37	29/30	0.96	0.23	39,54,62,68	0
32	PSU	1a	516	20/21	0.96	0.16	54,58,61,63	0
54	PSU	1w	39	20/21	0.96	0.19	48,61,67,68	0
32	MA6	2a	1519	24/25	0.96	0.24	52,62,69,70	0
55	5MC	1x	32	21/22	0.96	0.23	46,49,55,58	0
32	MA6	2a	1518	24/25	0.96	0.23	56,69,71,72	0
1	4OC	1A	1942	21/23	0.97	0.20	38,42,48,49	0
32	7MG	1a	527	24/25	0.97	0.17	42,48,56,59	0
54	5MU	1w	54	21/22	0.97	0.19	53,66,71,74	0
32	M2G	1a	966	25/26	0.97	0.23	45,51,58,60	0
32	MA6	1a	1518	24/25	0.97	0.23	31,41,46,46	0
1	5MC	2A	1942	21/22	0.97	0.20	49,58,65,68	0
32	5MC	1a	1400	21/22	0.97	0.22	33,48,53,57	0
1	5MU	1A	1961	21/22	0.98	0.21	21,27,32,39	0
1	5MC	1A	1984	21/22	0.98	0.20	28,34,36,43	0
1	5MU	2A	1939	21/22	0.98	0.17	36,42,45,46	0
32	MA6	1a	1519	24/25	0.98	0.23	36,42,47,49	0
1	2MU	2A	2552	21/23	0.98	0.19	36,43,49,57	0
32	4OC	1a	1402	22/23	0.98	0.21	38,46,49,58	0
1	PSU	1A	2617	20/21	0.98	0.20	22,26,30,32	0
1	2MU	1A	2564	21/23	0.98	0.21	22,27,30,32	0
1	5MC	1A	1964	21/22	0.98	0.21	34,41,45,54	0
1	PSU	1A	1933	20/21	0.98	0.18	33,43,49,50	0
1	2MA	2A	2503	23/24	0.98	0.19	30,37,41,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	UR3	1a	1498	21/22	0.98	0.23	32,39,43,44	0
1	OMG	2A	2251	24/25	0.98	0.23	40,45,48,53	0
32	5MC	1a	1407	21/22	0.98	0.20	33,40,45,46	0
1	2MA	1A	2515	23/24	0.99	0.21	16,21,24,25	0
1	OMG	1A	2263	24/25	0.99	0.22	18,23,27,29	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3985	1/1	-0.07	0.22	78,78,78,78	0
56	MG	2a	1745	1/1	0.00	0.09	96,96,96,96	0
56	MG	1A	4066	1/1	0.17	0.16	51,51,51,51	0
56	MG	2y	3005	1/1	0.19	0.18	94,94,94,94	0
56	MG	1a	1758	1/1	0.26	0.14	81,81,81,81	0
56	MG	2B	3019	1/1	0.29	0.30	90,90,90,90	0
56	MG	1A	3966	1/1	0.29	0.18	75,75,75,75	0
56	MG	1A	3905	1/1	0.31	0.29	72,72,72,72	0
56	MG	1v	3001	1/1	0.32	0.31	70,70,70,70	0
56	MG	1A	3997	1/1	0.36	0.09	58,58,58,58	0
56	MG	2Q	3004	1/1	0.36	0.58	58,58,58,58	0
56	MG	1a	1777	1/1	0.37	0.25	65,65,65,65	0
56	MG	1A	4103	1/1	0.38	0.19	60,60,60,60	0
56	MG	2A	3664	1/1	0.38	0.22	82,82,82,82	0
56	MG	2A	3867	1/1	0.38	0.13	75,75,75,75	0
56	MG	2A	3292	1/1	0.42	0.23	65,65,65,65	0
56	MG	2A	3137	1/1	0.43	0.22	61,61,61,61	0
56	MG	1P	203	1/1	0.43	0.34	84,84,84,84	0
56	MG	2A	3579	1/1	0.44	0.14	65,65,65,65	0
56	MG	2a	1826	1/1	0.44	0.21	81,81,81,81	0
56	MG	1A	4112	1/1	0.45	0.19	62,62,62,62	0
56	MG	1a	1668	1/1	0.45	0.30	68,68,68,68	0
56	MG	1A	4015	1/1	0.47	0.14	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1769	1/1	0.47	0.12	81,81,81,81	0
56	MG	2A	3809	1/1	0.48	0.15	78,78,78,78	0
56	MG	2v	103	1/1	0.49	0.18	78,78,78,78	0
56	MG	2A	3795	1/1	0.50	0.36	85,85,85,85	0
56	MG	1A	3495	1/1	0.50	0.35	60,60,60,60	0
56	MG	1A	3507	1/1	0.51	0.25	71,71,71,71	0
56	MG	1x	101	1/1	0.53	0.15	51,51,51,51	0
56	MG	2a	1767	1/1	0.53	0.39	79,79,79,79	0
56	MG	1a	1772	1/1	0.54	0.18	66,66,66,66	0
56	MG	1A	4011	1/1	0.55	0.57	69,69,69,69	0
56	MG	2A	3088	1/1	0.55	0.42	72,72,72,72	0
56	MG	2a	1729	1/1	0.55	0.37	76,76,76,76	0
56	MG	1A	4078	1/1	0.55	0.25	66,66,66,66	0
56	MG	2A	3224	1/1	0.55	0.40	69,69,69,69	0
56	MG	1A	3971	1/1	0.56	0.23	68,68,68,68	0
56	MG	2y	3006	1/1	0.57	0.06	86,86,86,86	0
56	MG	1a	1796	1/1	0.57	0.11	67,67,67,67	0
56	MG	1A	3306	1/1	0.57	0.17	56,56,56,56	0
56	MG	2A	3649	1/1	0.57	0.22	84,84,84,84	0
56	MG	1A	3917	1/1	0.58	0.10	50,50,50,50	0
56	MG	1a	1766	1/1	0.59	0.41	86,86,86,86	0
56	MG	2A	3471	1/1	0.59	0.16	61,61,61,61	0
56	MG	2A	3797	1/1	0.60	0.29	73,73,73,73	0
56	MG	2A	3458	1/1	0.60	0.21	60,60,60,60	0
56	MG	2A	3171	1/1	0.60	0.30	73,73,73,73	0
56	MG	2A	3812	1/1	0.60	0.48	93,93,93,93	0
56	MG	1w	102	1/1	0.61	0.14	73,73,73,73	0
56	MG	2A	3402	1/1	0.61	0.43	80,80,80,80	0
56	MG	2a	1739	1/1	0.61	0.37	84,84,84,84	0
56	MG	2a	1603	1/1	0.61	0.77	71,71,71,71	0
56	MG	2A	3667	1/1	0.61	0.35	62,62,62,62	0
56	MG	2A	3327	1/1	0.62	1.08	60,60,60,60	0
56	MG	1A	3480	1/1	0.62	0.55	46,46,46,46	0
56	MG	2A	3266	1/1	0.62	0.46	67,67,67,67	0
56	MG	2a	1756	1/1	0.62	0.11	88,88,88,88	0
56	MG	10	105	1/1	0.63	0.61	55,55,55,55	0
56	MG	2A	3789	1/1	0.63	0.29	67,67,67,67	0
56	MG	1A	3623	1/1	0.63	0.21	72,72,72,72	0
56	MG	1A	3983	1/1	0.63	0.33	68,68,68,68	0
56	MG	2A	3362	1/1	0.64	0.16	72,72,72,72	0
56	MG	2A	3283	1/1	0.64	0.51	69,69,69,69	0
56	MG	1a	1676	1/1	0.64	0.15	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3101	1/1	0.64	0.20	76,76,76,76	0
56	MG	1A	3826	1/1	0.64	0.13	60,60,60,60	0
56	MG	1A	3394	1/1	0.65	0.35	68,68,68,68	0
56	MG	2A	3285	1/1	0.65	0.32	80,80,80,80	0
56	MG	1A	3347	1/1	0.65	0.20	55,55,55,55	0
56	MG	2a	1613	1/1	0.65	0.24	61,61,61,61	0
56	MG	1A	3707	1/1	0.66	0.18	78,78,78,78	0
56	MG	2A	3032	1/1	0.66	0.29	66,66,66,66	0
56	MG	2A	3293	1/1	0.66	0.46	69,69,69,69	0
56	MG	1A	4034	1/1	0.66	0.43	64,64,64,64	0
56	MG	1A	3942	1/1	0.66	0.21	58,58,58,58	0
56	MG	1A	3437	1/1	0.66	0.21	54,54,54,54	0
56	MG	2A	3790	1/1	0.66	0.16	86,86,86,86	0
56	MG	1a	1693	1/1	0.66	0.23	65,65,65,65	0
56	MG	1a	1773	1/1	0.66	0.21	74,74,74,74	0
56	MG	1y	3002	1/1	0.66	0.21	90,90,90,90	0
56	MG	1A	3783	1/1	0.67	0.10	48,48,48,48	0
56	MG	1A	3968	1/1	0.67	0.42	68,68,68,68	0
56	MG	2A	3493	1/1	0.67	0.73	74,74,74,74	0
56	MG	2A	3835	1/1	0.67	0.13	58,58,58,58	0
56	MG	2A	3642	1/1	0.67	0.18	45,45,45,45	0
56	MG	2A	3380	1/1	0.67	0.34	68,68,68,68	0
56	MG	2j	8001	1/1	0.67	0.16	81,81,81,81	0
56	MG	2A	3860	1/1	0.67	0.23	67,67,67,67	0
56	MG	2A	3100	1/1	0.67	0.19	77,77,77,77	0
56	MG	2A	3787	1/1	0.67	0.17	59,59,59,59	0
56	MG	2A	3733	1/1	0.68	0.16	57,57,57,57	0
56	MG	2a	1730	1/1	0.68	0.25	74,74,74,74	0
56	MG	2A	3871	1/1	0.68	0.33	66,66,66,66	0
56	MG	2a	1829	1/1	0.68	0.15	77,77,77,77	0
56	MG	2A	3876	1/1	0.68	0.12	71,71,71,71	0
56	MG	2A	3691	1/1	0.68	0.35	59,59,59,59	0
56	MG	2A	3486	1/1	0.68	0.18	66,66,66,66	0
56	MG	1A	3989	1/1	0.68	0.15	53,53,53,53	0
56	MG	2A	3610	1/1	0.68	0.12	59,59,59,59	0
56	MG	2A	3237	1/1	0.68	0.21	44,44,44,44	0
56	MG	1a	1656	1/1	0.68	0.17	64,64,64,64	0
56	MG	1A	3469	1/1	0.68	0.22	68,68,68,68	0
56	MG	1A	3998	1/1	0.69	0.09	68,68,68,68	0
56	MG	2a	1768	1/1	0.69	0.21	82,82,82,82	0
56	MG	1A	3980	1/1	0.69	0.07	83,83,83,83	0
56	MG	1A	3501	1/1	0.69	0.17	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3051	1/1	0.69	0.12	69,69,69,69	0
56	MG	1a	1672	1/1	0.69	0.18	69,69,69,69	0
56	MG	2A	3181	1/1	0.69	0.12	76,76,76,76	0
56	MG	2A	3846	1/1	0.69	0.09	61,61,61,61	0
56	MG	2a	1726	1/1	0.69	0.26	71,71,71,71	0
56	MG	2A	3345	1/1	0.69	0.32	59,59,59,59	0
56	MG	2A	3343	1/1	0.69	0.45	74,74,74,74	0
56	MG	2A	3394	1/1	0.69	0.22	72,72,72,72	0
56	MG	1l	202	1/1	0.70	0.14	69,69,69,69	0
56	MG	1B	211	1/1	0.70	0.22	51,51,51,51	0
56	MG	1a	1640	1/1	0.70	0.15	62,62,62,62	0
56	MG	2a	1722	1/1	0.70	0.18	66,66,66,66	0
56	MG	2A	3276	1/1	0.70	0.13	62,62,62,62	0
56	MG	1A	3470	1/1	0.70	0.19	63,63,63,63	0
56	MG	2w	3002	1/1	0.70	0.12	77,77,77,77	0
56	MG	2a	1732	1/1	0.70	0.25	94,94,94,94	0
56	MG	2A	3230	1/1	0.70	0.14	73,73,73,73	0
56	MG	2A	3303	1/1	0.70	0.25	68,68,68,68	0
56	MG	1a	1789	1/1	0.70	0.08	69,69,69,69	0
56	MG	2A	3004	1/1	0.70	0.19	56,56,56,56	0
56	MG	1A	4019	1/1	0.71	0.13	50,50,50,50	0
56	MG	1a	1797	1/1	0.71	0.09	66,66,66,66	0
56	MG	2A	3543	1/1	0.71	0.16	37,37,37,37	0
56	MG	1A	3932	1/1	0.71	0.12	60,60,60,60	0
56	MG	2a	1605	1/1	0.71	0.23	73,73,73,73	0
56	MG	2A	3216	1/1	0.71	0.25	77,77,77,77	0
56	MG	2A	3059	1/1	0.71	0.21	61,61,61,61	0
56	MG	2A	3858	1/1	0.71	0.10	68,68,68,68	0
56	MG	1A	4018	1/1	0.71	0.15	70,70,70,70	0
56	MG	1A	4035	1/1	0.71	0.14	48,48,48,48	0
56	MG	2w	3003	1/1	0.71	0.39	74,74,74,74	0
56	MG	2a	1654	1/1	0.72	0.19	85,85,85,85	0
56	MG	2A	3601	1/1	0.72	0.14	32,32,32,32	0
56	MG	1A	4100	1/1	0.72	0.16	63,63,63,63	0
56	MG	2A	3102	1/1	0.72	0.19	72,72,72,72	0
56	MG	2a	1670	1/1	0.72	0.16	62,62,62,62	0
56	MG	1A	3371	1/1	0.72	0.20	59,59,59,59	0
56	MG	1A	3293	1/1	0.72	0.35	54,54,54,54	0
56	MG	2A	3603	1/1	0.72	0.12	67,67,67,67	0
56	MG	2A	3306	1/1	0.72	0.15	67,67,67,67	0
56	MG	2A	3236	1/1	0.72	0.92	64,64,64,64	0
56	MG	1a	1761	1/1	0.72	0.12	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3440	1/1	0.72	0.50	63,63,63,63	0
56	MG	1A	3360	1/1	0.72	0.20	57,57,57,57	0
56	MG	2A	3357	1/1	0.73	0.14	70,70,70,70	0
56	MG	1A	4044	1/1	0.73	0.12	59,59,59,59	0
56	MG	2a	1627	1/1	0.73	0.17	71,71,71,71	0
56	MG	1A	3428	1/1	0.73	0.21	68,68,68,68	0
56	MG	2a	1831	1/1	0.73	0.11	78,78,78,78	0
56	MG	2A	3422	1/1	0.73	0.17	62,62,62,62	0
56	MG	2a	1751	1/1	0.73	0.09	51,51,51,51	0
56	MG	1A	3266	1/1	0.73	0.31	60,60,60,60	0
56	MG	2A	3782	1/1	0.73	0.24	68,68,68,68	0
56	MG	2A	3097	1/1	0.73	0.17	74,74,74,74	0
56	MG	2A	3713	1/1	0.73	0.14	67,67,67,67	0
56	MG	1A	3974	1/1	0.73	0.22	22,22,22,22	0
56	MG	1A	3991	1/1	0.73	0.20	32,32,32,32	0
56	MG	1A	3573	1/1	0.73	0.18	59,59,59,59	0
56	MG	2l	3003	1/1	0.73	0.19	74,74,74,74	0
56	MG	2A	3766	1/1	0.73	0.54	83,83,83,83	0
56	MG	1A	3984	1/1	0.74	0.49	81,81,81,81	0
56	MG	2a	1784	1/1	0.74	0.12	84,84,84,84	0
56	MG	2A	3395	1/1	0.74	0.67	67,67,67,67	0
56	MG	1A	3730	1/1	0.74	0.18	58,58,58,58	0
56	MG	2a	1766	1/1	0.74	0.28	87,87,87,87	0
56	MG	2a	1781	1/1	0.74	0.12	63,63,63,63	0
56	MG	2A	3054	1/1	0.74	0.18	73,73,73,73	0
56	MG	2A	3428	1/1	0.74	0.20	79,79,79,79	0
56	MG	2a	1644	1/1	0.74	0.25	64,64,64,64	0
56	MG	1Z	303	1/1	0.74	0.15	65,65,65,65	0
56	MG	2W	201	1/1	0.74	0.15	54,54,54,54	0
56	MG	2A	3791	1/1	0.74	0.29	64,64,64,64	0
56	MG	1A	3512	1/1	0.75	0.28	52,52,52,52	0
56	MG	2A	3814	1/1	0.75	0.31	71,71,71,71	0
56	MG	2A	3881	1/1	0.75	0.24	69,69,69,69	0
56	MG	2A	3324	1/1	0.75	0.22	69,69,69,69	0
56	MG	1a	1667	1/1	0.75	0.12	69,69,69,69	0
56	MG	2A	3284	1/1	0.75	0.20	60,60,60,60	0
56	MG	2A	3429	1/1	0.75	0.16	62,62,62,62	0
56	MG	1A	3047	1/1	0.75	0.23	44,44,44,44	0
56	MG	2a	1828	1/1	0.75	0.11	68,68,68,68	0
56	MG	1A	3909	1/1	0.75	0.10	36,36,36,36	0
56	MG	1a	1639	1/1	0.75	0.29	59,59,59,59	0
56	MG	1A	3645	1/1	0.75	0.17	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1715	1/1	0.75	0.16	70,70,70,70	0
56	MG	2x	105	1/1	0.75	0.16	66,66,66,66	0
56	MG	2a	1760	1/1	0.75	0.09	72,72,72,72	0
56	MG	2A	3712	1/1	0.75	0.11	60,60,60,60	0
56	MG	2A	3643	1/1	0.75	0.15	47,47,47,47	0
56	MG	1A	4027	1/1	0.76	0.13	49,49,49,49	0
56	MG	1A	3937	1/1	0.76	0.25	73,73,73,73	0
56	MG	1a	1826	1/1	0.76	0.30	61,61,61,61	0
56	MG	1a	1794	1/1	0.76	0.28	79,79,79,79	0
56	MG	2a	1830	1/1	0.76	0.16	59,59,59,59	0
56	MG	1A	3681	1/1	0.76	0.27	57,57,57,57	0
56	MG	2A	3256	1/1	0.76	0.14	63,63,63,63	0
59	ZN	24	501	1/1	0.76	0.07	119,119,119,119	0
56	MG	2A	3615	1/1	0.76	0.17	49,49,49,49	0
56	MG	2y	3001	1/1	0.76	0.13	76,76,76,76	0
56	MG	2A	3312	1/1	0.76	0.22	67,67,67,67	0
56	MG	1A	3552	1/1	0.76	0.26	49,49,49,49	0
56	MG	1w	101	1/1	0.76	0.13	59,59,59,59	0
56	MG	1A	3526	1/1	0.76	0.13	85,85,85,85	0
56	MG	2a	1702	1/1	0.76	0.11	65,65,65,65	0
56	MG	2A	3646	1/1	0.76	0.12	55,55,55,55	0
56	MG	1A	4017	1/1	0.76	0.19	56,56,56,56	0
56	MG	2A	3360	1/1	0.76	0.18	75,75,75,75	0
56	MG	1A	3369	1/1	0.76	0.26	56,56,56,56	0
56	MG	2A	3693	1/1	0.76	0.16	58,58,58,58	0
56	MG	2A	3423	1/1	0.76	0.13	73,73,73,73	0
56	MG	1A	4030	1/1	0.76	0.10	45,45,45,45	0
56	MG	1A	3366	1/1	0.76	0.82	50,50,50,50	0
56	MG	2A	3683	1/1	0.76	0.13	77,77,77,77	0
56	MG	2A	3342	1/1	0.76	0.32	65,65,65,65	0
56	MG	1a	1661	1/1	0.77	0.16	56,56,56,56	0
56	MG	1A	3562	1/1	0.77	0.26	51,51,51,51	0
56	MG	2a	1824	1/1	0.77	0.16	70,70,70,70	0
56	MG	1A	3941	1/1	0.77	0.13	43,43,43,43	0
56	MG	1A	3221	1/1	0.77	0.14	71,71,71,71	0
56	MG	2A	3830	1/1	0.77	0.23	54,54,54,54	0
56	MG	2A	3466	1/1	0.77	0.13	54,54,54,54	0
56	MG	2A	3243	1/1	0.77	0.55	67,67,67,67	0
56	MG	1A	3210	1/1	0.77	0.32	81,81,81,81	0
56	MG	1A	3999	1/1	0.77	0.12	57,57,57,57	0
56	MG	2x	101	1/1	0.77	0.10	61,61,61,61	0
56	MG	1a	1768	1/1	0.77	0.10	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1U	204	1/1	0.77	1.11	74,74,74,74	0
56	MG	2A	3705	1/1	0.77	0.42	78,78,78,78	0
56	MG	1A	3907	1/1	0.77	0.40	77,77,77,77	0
56	MG	1A	3958	1/1	0.77	0.19	67,67,67,67	0
56	MG	2A	3753	1/1	0.77	0.16	64,64,64,64	0
56	MG	1A	3904	1/1	0.77	0.10	81,81,81,81	0
56	MG	2a	1649	1/1	0.77	0.23	72,72,72,72	0
56	MG	2A	3333	1/1	0.77	0.77	61,61,61,61	0
56	MG	1A	3399	1/1	0.77	0.44	51,51,51,51	0
56	MG	2A	3331	1/1	0.77	0.19	68,68,68,68	0
56	MG	2y	3004	1/1	0.77	0.23	79,79,79,79	0
56	MG	2A	3590	1/1	0.77	0.12	72,72,72,72	0
56	MG	2a	1632	1/1	0.78	0.19	60,60,60,60	0
56	MG	2A	3090	1/1	0.78	0.14	76,76,76,76	0
56	MG	2A	3744	1/1	0.78	0.08	65,65,65,65	0
56	MG	1a	1652	1/1	0.78	0.20	56,56,56,56	0
56	MG	1A	3057	1/1	0.78	0.17	34,34,34,34	0
56	MG	2a	1772	1/1	0.78	0.27	89,89,89,89	0
56	MG	2A	3856	1/1	0.78	0.13	58,58,58,58	0
56	MG	1A	4047	1/1	0.78	0.14	46,46,46,46	0
56	MG	1A	3945	1/1	0.78	0.17	59,59,59,59	0
56	MG	2A	3205	1/1	0.78	0.23	53,53,53,53	0
56	MG	2A	3416	1/1	0.78	0.50	63,63,63,63	0
56	MG	2a	1696	1/1	0.78	0.15	76,76,76,76	0
56	MG	1A	4050	1/1	0.78	0.27	50,50,50,50	0
56	MG	2A	3215	1/1	0.78	0.30	71,71,71,71	0
56	MG	1A	3017	1/1	0.78	0.15	34,34,34,34	0
56	MG	1A	3911	1/1	0.78	0.25	72,72,72,72	0
56	MG	2A	3146	1/1	0.78	0.21	58,58,58,58	0
56	MG	2A	3287	1/1	0.78	0.14	55,55,55,55	0
56	MG	1a	1746	1/1	0.78	0.14	58,58,58,58	0
56	MG	1A	3482	1/1	0.78	0.15	45,45,45,45	0
56	MG	1A	3753	1/1	0.78	0.17	20,20,20,20	0
56	MG	2A	3863	1/1	0.78	0.10	49,49,49,49	0
56	MG	2A	3878	1/1	0.78	0.31	59,59,59,59	0
56	MG	1a	1629	1/1	0.79	0.24	64,64,64,64	0
56	MG	2a	1785	1/1	0.79	0.14	70,70,70,70	0
56	MG	2a	1629	1/1	0.79	1.18	80,80,80,80	0
56	MG	2a	1653	1/1	0.79	0.16	82,82,82,82	0
56	MG	1A	3488	1/1	0.79	0.24	50,50,50,50	0
56	MG	18	101	1/1	0.79	0.39	65,65,65,65	0
56	MG	1A	3355	1/1	0.79	0.30	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3023	1/1	0.79	0.14	73,73,73,73	0
56	MG	1A	3586	1/1	0.79	0.17	51,51,51,51	0
56	MG	2a	1667	1/1	0.79	0.17	59,59,59,59	0
56	MG	1A	3852	1/1	0.79	0.23	39,39,39,39	0
56	MG	2A	3684	1/1	0.79	0.13	51,51,51,51	0
56	MG	2A	3067	1/1	0.79	0.15	58,58,58,58	0
56	MG	2A	3233	1/1	0.79	0.35	52,52,52,52	0
56	MG	2A	3350	1/1	0.79	0.17	63,63,63,63	0
56	MG	2a	1708	1/1	0.79	0.23	75,75,75,75	0
56	MG	2A	3366	1/1	0.79	0.14	61,61,61,61	0
56	MG	2Z	8001	1/1	0.79	0.14	73,73,73,73	0
56	MG	2T	3002	1/1	0.79	0.12	53,53,53,53	0
56	MG	2A	3424	1/1	0.79	0.15	56,56,56,56	0
56	MG	1A	3842	1/1	0.79	0.15	53,53,53,53	0
56	MG	2A	3813	1/1	0.79	0.13	77,77,77,77	0
56	MG	2A	3187	1/1	0.79	0.19	63,63,63,63	0
56	MG	2A	3391	1/1	0.79	0.21	70,70,70,70	0
56	MG	2a	1612	1/1	0.79	0.18	64,64,64,64	0
56	MG	2A	3152	1/1	0.79	0.39	55,55,55,55	0
56	MG	2A	3164	1/1	0.79	0.17	66,66,66,66	0
56	MG	1A	3026	1/1	0.79	0.19	34,34,34,34	0
56	MG	2A	3461	1/1	0.80	0.14	52,52,52,52	0
56	MG	1A	3618	1/1	0.80	0.13	50,50,50,50	0
56	MG	1y	3003	1/1	0.80	0.32	82,82,82,82	0
56	MG	2A	3361	1/1	0.80	0.19	60,60,60,60	0
56	MG	1a	1628	1/1	0.80	0.15	54,54,54,54	0
56	MG	2A	3249	1/1	0.80	0.26	62,62,62,62	0
56	MG	2A	3482	1/1	0.80	0.47	43,43,43,43	0
56	MG	2A	3087	1/1	0.80	0.38	50,50,50,50	0
56	MG	1a	1602	1/1	0.80	0.16	64,64,64,64	0
56	MG	2A	3112	1/1	0.80	0.17	59,59,59,59	0
56	MG	1A	3499	1/1	0.80	0.28	55,55,55,55	0
56	MG	1d	502	1/1	0.80	0.22	52,52,52,52	0
56	MG	2A	3568	1/1	0.80	0.13	34,34,34,34	0
56	MG	2A	3725	1/1	0.80	0.13	65,65,65,65	0
56	MG	2A	3305	1/1	0.80	0.15	67,67,67,67	0
56	MG	2a	1761	1/1	0.80	0.27	95,95,95,95	0
56	MG	1A	3610	1/1	0.80	0.10	30,30,30,30	0
56	MG	2A	3702	1/1	0.80	0.08	75,75,75,75	0
56	MG	2A	3242	1/1	0.80	0.49	67,67,67,67	0
56	MG	2w	3009	1/1	0.80	0.14	73,73,73,73	0
56	MG	1a	1792	1/1	0.80	0.09	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3333	1/1	0.80	0.43	69,69,69,69	0
56	MG	2A	3772	1/1	0.80	0.10	55,55,55,55	0
56	MG	2a	1771	1/1	0.80	0.24	68,68,68,68	0
56	MG	2A	3806	1/1	0.80	0.15	55,55,55,55	0
56	MG	2A	3591	1/1	0.80	0.09	63,63,63,63	0
56	MG	2A	3757	1/1	0.80	0.26	50,50,50,50	0
56	MG	2B	3002	1/1	0.80	0.49	63,63,63,63	0
56	MG	1a	1680	1/1	0.80	0.16	76,76,76,76	0
56	MG	2A	3113	1/1	0.80	0.11	65,65,65,65	0
56	MG	1a	1620	1/1	0.80	0.09	56,56,56,56	0
56	MG	2A	3110	1/1	0.80	0.12	65,65,65,65	0
56	MG	2A	3644	1/1	0.80	0.46	62,62,62,62	0
56	MG	1A	4038	1/1	0.80	0.07	49,49,49,49	0
56	MG	2A	3259	1/1	0.80	0.11	65,65,65,65	0
56	MG	2A	3680	1/1	0.80	0.49	78,78,78,78	0
56	MG	1A	3955	1/1	0.80	0.27	55,55,55,55	0
56	MG	2A	3781	1/1	0.80	0.07	74,74,74,74	0
56	MG	1A	3523	1/1	0.81	0.25	53,53,53,53	0
56	MG	1A	3378	1/1	0.81	0.29	36,36,36,36	0
56	MG	1A	3402	1/1	0.81	0.30	53,53,53,53	0
56	MG	2B	3016	1/1	0.81	0.17	70,70,70,70	0
56	MG	2B	3008	1/1	0.81	0.11	56,56,56,56	0
56	MG	1A	3585	1/1	0.81	0.14	40,40,40,40	0
56	MG	1A	3345	1/1	0.81	0.16	39,39,39,39	0
56	MG	1A	3262	1/1	0.81	0.28	55,55,55,55	0
56	MG	1A	4048	1/1	0.81	0.27	54,54,54,54	0
56	MG	1O	203	1/1	0.81	0.15	53,53,53,53	0
56	MG	1A	3433	1/1	0.81	0.21	53,53,53,53	0
56	MG	2A	3196	1/1	0.81	0.67	69,69,69,69	0
56	MG	2a	1747	1/1	0.81	0.21	80,80,80,80	0
56	MG	2A	3346	1/1	0.81	0.85	69,69,69,69	0
56	MG	2A	3681	1/1	0.81	0.16	56,56,56,56	0
56	MG	1A	4023	1/1	0.81	0.14	68,68,68,68	0
56	MG	1A	3493	1/1	0.81	0.44	52,52,52,52	0
56	MG	2a	1635	1/1	0.81	0.11	71,71,71,71	0
56	MG	1A	4021	1/1	0.81	0.10	60,60,60,60	0
56	MG	2A	3607	1/1	0.81	0.12	53,53,53,53	0
56	MG	1A	4118	1/1	0.81	0.16	27,27,27,27	0
56	MG	1A	3531	1/1	0.81	0.18	60,60,60,60	0
56	MG	2A	3546	1/1	0.81	0.14	42,42,42,42	0
56	MG	1A	3372	1/1	0.81	0.45	41,41,41,41	0
56	MG	2A	3421	1/1	0.81	0.10	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3738	1/1	0.81	0.14	59,59,59,59	0
56	MG	1A	3308	1/1	0.81	0.19	47,47,47,47	0
56	MG	1A	3616	1/1	0.81	0.19	26,26,26,26	0
56	MG	2A	3758	1/1	0.81	0.52	64,64,64,64	0
56	MG	2A	3870	1/1	0.81	0.26	53,53,53,53	0
56	MG	1A	3688	1/1	0.81	0.14	44,44,44,44	0
56	MG	1a	1723	1/1	0.81	0.18	41,41,41,41	0
56	MG	2a	1669	1/1	0.81	0.18	59,59,59,59	0
56	MG	1a	1675	1/1	0.81	0.34	70,70,70,70	0
56	MG	1A	4051	1/1	0.81	0.24	60,60,60,60	0
56	MG	1A	3062	1/1	0.81	0.23	55,55,55,55	0
56	MG	1A	4001	1/1	0.81	0.19	26,26,26,26	0
56	MG	1A	3407	1/1	0.81	0.20	64,64,64,64	0
56	MG	2A	3628	1/1	0.81	0.10	58,58,58,58	0
56	MG	2A	3573	1/1	0.81	0.21	48,48,48,48	0
56	MG	1A	3525	1/1	0.81	0.21	70,70,70,70	0
56	MG	1a	1625	1/1	0.81	0.23	62,62,62,62	0
56	MG	2a	1636	1/1	0.81	0.31	81,81,81,81	0
56	MG	2A	3126	1/1	0.81	0.06	63,63,63,63	0
56	MG	1A	3206	1/1	0.81	0.32	46,46,46,46	0
56	MG	2a	1661	1/1	0.81	0.14	58,58,58,58	0
56	MG	1A	3110	1/1	0.81	0.15	41,41,41,41	0
56	MG	2A	3257	1/1	0.81	0.20	63,63,63,63	0
56	MG	2E	302	1/1	0.81	0.24	55,55,55,55	0
56	MG	1A	3631	1/1	0.81	0.15	52,52,52,52	0
56	MG	2A	3057	1/1	0.81	0.14	66,66,66,66	0
56	MG	2A	3663	1/1	0.81	0.15	84,84,84,84	0
56	MG	2a	1631	1/1	0.81	0.18	61,61,61,61	0
56	MG	1A	3913	1/1	0.81	0.15	25,25,25,25	0
56	MG	2a	1697	1/1	0.81	0.15	70,70,70,70	0
56	MG	2A	3763	1/1	0.81	0.15	66,66,66,66	0
56	MG	2A	3769	1/1	0.81	0.09	56,56,56,56	0
56	MG	2A	3338	1/1	0.81	0.18	64,64,64,64	0
56	MG	1w	110	1/1	0.82	0.12	69,69,69,69	0
56	MG	1A	4059	1/1	0.82	0.52	51,51,51,51	0
56	MG	1A	3051	1/1	0.82	0.22	66,66,66,66	0
56	MG	2A	3248	1/1	0.82	0.54	55,55,55,55	0
56	MG	1A	3556	1/1	0.82	0.15	49,49,49,49	0
56	MG	1A	3414	1/1	0.82	0.18	45,45,45,45	0
56	MG	2a	1748	1/1	0.82	0.15	74,74,74,74	0
56	MG	1A	3420	1/1	0.82	0.35	50,50,50,50	0
56	MG	2A	3794	1/1	0.82	0.23	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3751	1/1	0.82	0.32	77,77,77,77	0
56	MG	1A	3714	1/1	0.82	0.11	62,62,62,62	0
56	MG	2a	1622	1/1	0.82	0.33	65,65,65,65	0
56	MG	1A	3226	1/1	0.82	0.14	52,52,52,52	0
56	MG	1A	3553	1/1	0.82	0.14	58,58,58,58	0
56	MG	2A	3278	1/1	0.82	0.20	42,42,42,42	0
56	MG	2A	3450	1/1	0.82	0.13	53,53,53,53	0
56	MG	1a	1646	1/1	0.82	0.19	78,78,78,78	0
56	MG	1A	3782	1/1	0.82	0.19	60,60,60,60	0
56	MG	1A	3938	1/1	0.82	0.15	41,41,41,41	0
56	MG	2a	1615	1/1	0.82	0.11	69,69,69,69	0
56	MG	2A	3210	1/1	0.82	0.16	62,62,62,62	0
56	MG	2A	3687	1/1	0.82	0.39	69,69,69,69	0
56	MG	2A	3665	1/1	0.82	0.14	69,69,69,69	0
56	MG	2A	3409	1/1	0.82	0.15	69,69,69,69	0
56	MG	2a	1801	1/1	0.82	0.47	72,72,72,72	0
56	MG	1A	4026	1/1	0.82	0.19	52,52,52,52	0
56	MG	1a	1626	1/1	0.82	0.15	58,58,58,58	0
56	MG	1a	1614	1/1	0.82	0.13	48,48,48,48	0
56	MG	1x	102	1/1	0.82	0.27	66,66,66,66	0
56	MG	2a	1640	1/1	0.82	0.15	68,68,68,68	0
56	MG	2A	3839	1/1	0.82	0.08	71,71,71,71	0
56	MG	2a	1671	1/1	0.82	0.11	57,57,57,57	0
56	MG	1A	3970	1/1	0.82	0.13	64,64,64,64	0
56	MG	1A	3479	1/1	0.82	0.40	40,40,40,40	0
56	MG	1A	3835	1/1	0.82	0.07	63,63,63,63	0
56	MG	2A	3523	1/1	0.82	0.10	37,37,37,37	0
56	MG	1A	3723	1/1	0.82	0.19	47,47,47,47	0
56	MG	1a	1619	1/1	0.82	0.23	51,51,51,51	0
56	MG	1a	1767	1/1	0.82	0.17	71,71,71,71	0
56	MG	2A	3208	1/1	0.82	0.26	59,59,59,59	0
56	MG	2a	1630	1/1	0.82	0.47	69,69,69,69	0
56	MG	2A	3006	1/1	0.82	0.18	58,58,58,58	0
56	MG	2a	1839	1/1	0.82	0.12	69,69,69,69	0
56	MG	2a	1789	1/1	0.82	0.12	63,63,63,63	0
56	MG	2A	3465	1/1	0.82	0.10	63,63,63,63	0
56	MG	2A	3505	1/1	0.82	0.27	65,65,65,65	0
56	MG	1a	1660	1/1	0.82	0.28	54,54,54,54	0
56	MG	2A	3556	1/1	0.82	0.20	53,53,53,53	0
56	MG	1A	3549	1/1	0.82	0.27	54,54,54,54	0
56	MG	1A	3551	1/1	0.82	0.24	55,55,55,55	0
56	MG	2A	3204	1/1	0.82	0.16	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3801	1/1	0.82	0.20	47,47,47,47	0
56	MG	1A	3392	1/1	0.82	0.34	48,48,48,48	0
56	MG	2a	1790	1/1	0.83	0.12	66,66,66,66	0
56	MG	1A	3820	1/1	0.83	0.20	47,47,47,47	0
56	MG	2U	202	1/1	0.83	0.93	72,72,72,72	0
56	MG	2A	3238	1/1	0.83	0.47	42,42,42,42	0
56	MG	2a	1736	1/1	0.83	0.08	76,76,76,76	0
56	MG	1A	3940	1/1	0.83	0.07	56,56,56,56	0
56	MG	2A	3430	1/1	0.83	0.44	64,64,64,64	0
56	MG	2A	3612	1/1	0.83	0.12	58,58,58,58	0
56	MG	1w	107	1/1	0.83	0.17	70,70,70,70	0
56	MG	1A	3807	1/1	0.83	0.12	28,28,28,28	0
56	MG	1A	3902	1/1	0.83	0.10	54,54,54,54	0
56	MG	1B	207	1/1	0.83	0.14	69,69,69,69	0
56	MG	1A	3931	1/1	0.83	0.24	36,36,36,36	0
56	MG	2a	1707	1/1	0.83	0.38	76,76,76,76	0
56	MG	2V	202	1/1	0.83	0.11	61,61,61,61	0
56	MG	2a	1656	1/1	0.83	0.39	59,59,59,59	0
56	MG	1A	3246	1/1	0.83	0.14	52,52,52,52	0
56	MG	2A	3107	1/1	0.83	0.36	62,62,62,62	0
56	MG	2A	3541	1/1	0.83	0.13	40,40,40,40	0
56	MG	1A	4072	1/1	0.83	0.22	32,32,32,32	0
56	MG	2A	3390	1/1	0.83	0.19	54,54,54,54	0
56	MG	12	101	1/1	0.83	0.14	50,50,50,50	0
56	MG	1A	3741	1/1	0.83	0.18	17,17,17,17	0
56	MG	2A	3255	1/1	0.83	0.27	71,71,71,71	0
56	MG	2v	102	1/1	0.83	0.16	67,67,67,67	0
56	MG	1x	111	1/1	0.83	0.09	52,52,52,52	0
56	MG	2A	3726	1/1	0.83	0.12	55,55,55,55	0
56	MG	1a	1730	1/1	0.83	0.17	51,51,51,51	0
56	MG	2A	3297	1/1	0.83	0.25	52,52,52,52	0
56	MG	1A	3449	1/1	0.83	0.12	57,57,57,57	0
56	MG	1A	3321	1/1	0.83	0.24	49,49,49,49	0
56	MG	1A	4110	1/1	0.83	0.99	49,49,49,49	0
56	MG	2A	3435	1/1	0.83	0.24	58,58,58,58	0
56	MG	2A	3490	1/1	0.83	0.19	57,57,57,57	0
56	MG	1a	1765	1/1	0.83	0.15	69,69,69,69	0
56	MG	1A	3830	1/1	0.83	0.20	49,49,49,49	0
56	MG	2a	1809	1/1	0.83	0.28	72,72,72,72	0
56	MG	1A	3446	1/1	0.83	0.40	67,67,67,67	0
56	MG	2A	3864	1/1	0.83	0.13	59,59,59,59	0
56	MG	2A	3307	1/1	0.83	0.20	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3298	1/1	0.83	0.14	53,53,53,53	0
56	MG	2A	3453	1/1	0.83	0.27	64,64,64,64	0
56	MG	2A	3058	1/1	0.83	0.24	51,51,51,51	0
56	MG	2a	1650	1/1	0.83	0.47	68,68,68,68	0
56	MG	2a	1727	1/1	0.83	0.11	51,51,51,51	0
56	MG	2A	3387	1/1	0.83	0.45	52,52,52,52	0
56	MG	2A	3406	1/1	0.83	0.10	59,59,59,59	0
56	MG	1a	1784	1/1	0.83	0.14	52,52,52,52	0
56	MG	1A	3259	1/1	0.83	0.20	57,57,57,57	0
56	MG	2A	3274	1/1	0.83	0.16	60,60,60,60	0
56	MG	1A	3661	1/1	0.83	0.20	39,39,39,39	0
56	MG	1A	3772	1/1	0.83	0.20	71,71,71,71	0
56	MG	2a	1795	1/1	0.83	0.15	77,77,77,77	0
56	MG	18	102	1/1	0.83	0.30	40,40,40,40	0
56	MG	2a	1645	1/1	0.83	0.19	70,70,70,70	0
56	MG	2a	1814	1/1	0.83	0.14	62,62,62,62	0
56	MG	1A	3356	1/1	0.83	0.21	55,55,55,55	0
56	MG	1a	1771	1/1	0.83	0.22	73,73,73,73	0
56	MG	1A	3910	1/1	0.83	0.14	71,71,71,71	0
56	MG	1a	1743	1/1	0.83	0.09	58,58,58,58	0
56	MG	1G	3004	1/1	0.83	0.16	67,67,67,67	0
56	MG	1A	3491	1/1	0.83	0.30	60,60,60,60	0
56	MG	1A	3459	1/1	0.83	0.15	53,53,53,53	0
56	MG	2a	1691	1/1	0.83	0.11	63,63,63,63	0
56	MG	2A	3614	1/1	0.83	0.12	32,32,32,32	0
56	MG	2v	101	1/1	0.84	0.13	62,62,62,62	0
56	MG	2A	3477	1/1	0.84	0.15	78,78,78,78	0
56	MG	2A	3700	1/1	0.84	0.26	59,59,59,59	0
56	MG	1A	3829	1/1	0.84	0.09	61,61,61,61	0
56	MG	1A	3666	1/1	0.84	0.23	43,43,43,43	0
56	MG	2A	3618	1/1	0.84	0.13	41,41,41,41	0
56	MG	1A	4016	1/1	0.84	0.14	44,44,44,44	0
56	MG	2A	3432	1/1	0.84	0.14	62,62,62,62	0
56	MG	1A	3489	1/1	0.84	0.25	61,61,61,61	0
56	MG	1t	3001	1/1	0.84	0.18	53,53,53,53	0
56	MG	2A	3222	1/1	0.84	0.09	48,48,48,48	0
56	MG	2A	3899	1/1	0.84	0.14	36,36,36,36	0
56	MG	10	106	1/1	0.84	0.18	58,58,58,58	0
56	MG	1A	3863	1/1	0.84	0.13	50,50,50,50	0
56	MG	2a	1844	1/1	0.84	0.10	66,66,66,66	0
56	MG	2A	3118	1/1	0.84	0.12	53,53,53,53	0
56	MG	1A	3729	1/1	0.84	0.17	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1769	1/1	0.84	0.07	63,63,63,63	0
56	MG	1a	1697	1/1	0.84	0.16	55,55,55,55	0
56	MG	2a	1609	1/1	0.84	0.15	71,71,71,71	0
56	MG	1a	1721	1/1	0.84	0.07	68,68,68,68	0
56	MG	1A	3871	1/1	0.84	0.13	37,37,37,37	0
56	MG	2A	3491	1/1	0.84	0.15	67,67,67,67	0
56	MG	1A	3889	1/1	0.84	0.16	42,42,42,42	0
56	MG	2a	1601	1/1	0.84	0.17	61,61,61,61	0
56	MG	1A	3473	1/1	0.84	0.13	62,62,62,62	0
56	MG	2A	3197	1/1	0.84	0.97	72,72,72,72	0
56	MG	1a	1604	1/1	0.84	0.09	55,55,55,55	0
56	MG	2a	1621	1/1	0.84	0.19	67,67,67,67	0
56	MG	1A	3668	1/1	0.84	0.15	56,56,56,56	0
56	MG	2B	3017	1/1	0.84	0.12	50,50,50,50	0
56	MG	2B	3006	1/1	0.84	0.12	72,72,72,72	0
56	MG	2E	304	1/1	0.84	0.39	70,70,70,70	0
56	MG	1A	3315	1/1	0.84	0.19	52,52,52,52	0
56	MG	2B	3021	1/1	0.84	0.10	79,79,79,79	0
56	MG	1a	1611	1/1	0.84	0.16	55,55,55,55	0
56	MG	1E	312	1/1	0.84	0.07	34,34,34,34	0
56	MG	2A	3089	1/1	0.84	0.51	50,50,50,50	0
56	MG	1A	3899	1/1	0.84	0.23	37,37,37,37	0
56	MG	2A	3500	1/1	0.84	0.13	69,69,69,69	0
56	MG	2A	3822	1/1	0.84	0.20	82,82,82,82	0
56	MG	1A	3296	1/1	0.84	0.43	66,66,66,66	0
56	MG	1A	3256	1/1	0.84	0.18	65,65,65,65	0
56	MG	2A	3452	1/1	0.84	0.12	68,68,68,68	0
56	MG	2A	3200	1/1	0.84	0.34	66,66,66,66	0
56	MG	2A	3609	1/1	0.84	0.12	42,42,42,42	0
56	MG	2x	102	1/1	0.84	0.24	58,58,58,58	0
56	MG	1A	3528	1/1	0.84	0.22	52,52,52,52	0
56	MG	1a	1738	1/1	0.84	0.15	54,54,54,54	0
56	MG	1A	3317	1/1	0.84	0.28	33,33,33,33	0
56	MG	1A	3211	1/1	0.84	0.16	46,46,46,46	0
56	MG	1x	104	1/1	0.84	0.19	64,64,64,64	0
56	MG	2A	3547	1/1	0.84	0.07	52,52,52,52	0
56	MG	1A	3758	1/1	0.84	0.14	67,67,67,67	0
56	MG	2A	3804	1/1	0.84	0.17	61,61,61,61	0
56	MG	1A	3498	1/1	0.84	0.34	30,30,30,30	0
56	MG	1A	3454	1/1	0.84	0.17	61,61,61,61	0
56	MG	1a	1637	1/1	0.84	0.24	68,68,68,68	0
56	MG	1A	3220	1/1	0.84	0.21	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3718	1/1	0.84	0.19	57,57,57,57	0
56	MG	2A	3826	1/1	0.84	0.08	50,50,50,50	0
56	MG	1A	3535	1/1	0.84	0.18	57,57,57,57	0
56	MG	2A	3721	1/1	0.84	0.17	67,67,67,67	0
56	MG	1a	1722	1/1	0.84	0.09	53,53,53,53	0
56	MG	2a	1672	1/1	0.84	0.10	68,68,68,68	0
56	MG	1A	3988	1/1	0.84	0.12	41,41,41,41	0
56	MG	1A	3962	1/1	0.84	0.12	63,63,63,63	0
56	MG	2A	3464	1/1	0.84	0.14	60,60,60,60	0
56	MG	1A	3239	1/1	0.84	0.24	48,48,48,48	0
56	MG	2A	3506	1/1	0.84	0.12	47,47,47,47	0
56	MG	1A	3471	1/1	0.84	0.17	51,51,51,51	0
56	MG	1a	1818	1/1	0.84	0.08	69,69,69,69	0
56	MG	1B	209	1/1	0.84	0.21	48,48,48,48	0
56	MG	1A	3930	1/1	0.84	0.17	23,23,23,23	0
56	MG	2a	1704	1/1	0.85	0.14	65,65,65,65	0
56	MG	1A	3139	1/1	0.85	0.20	43,43,43,43	0
56	MG	2B	3011	1/1	0.85	0.17	72,72,72,72	0
56	MG	2B	3014	1/1	0.85	0.11	78,78,78,78	0
56	MG	23	101	1/1	0.85	0.59	62,62,62,62	0
56	MG	2A	3417	1/1	0.85	0.76	64,64,64,64	0
56	MG	1a	1664	1/1	0.85	0.16	74,74,74,74	0
56	MG	1a	1828	1/1	0.85	0.13	57,57,57,57	0
56	MG	2A	3281	1/1	0.85	0.35	81,81,81,81	0
56	MG	2A	3175	1/1	0.85	0.09	84,84,84,84	0
56	MG	1A	3780	1/1	0.85	0.14	36,36,36,36	0
56	MG	1A	3518	1/1	0.85	0.42	46,46,46,46	0
56	MG	1A	3635	1/1	0.85	0.08	50,50,50,50	0
56	MG	2A	3898	1/1	0.85	0.58	52,52,52,52	0
56	MG	1A	3963	1/1	0.85	0.14	49,49,49,49	0
56	MG	1A	3819	1/1	0.85	0.17	52,52,52,52	0
56	MG	2a	1810	1/1	0.85	0.08	78,78,78,78	0
56	MG	1A	4056	1/1	0.85	0.34	54,54,54,54	0
56	MG	2A	3866	1/1	0.85	0.11	34,34,34,34	0
56	MG	2A	3567	1/1	0.85	0.09	52,52,52,52	0
56	MG	1D	305	1/1	0.85	0.32	52,52,52,52	0
56	MG	2A	3498	1/1	0.85	0.11	62,62,62,62	0
56	MG	1A	3249	1/1	0.85	0.18	70,70,70,70	0
56	MG	2A	3678	1/1	0.85	0.07	59,59,59,59	0
56	MG	1A	3584	1/1	0.85	0.14	22,22,22,22	0
56	MG	1A	3722	1/1	0.85	0.10	53,53,53,53	0
56	MG	2B	3018	1/1	0.85	0.08	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1x	108	1/1	0.85	0.23	59,59,59,59	0
56	MG	2a	1733	1/1	0.85	0.14	61,61,61,61	0
56	MG	1A	3762	1/1	0.85	0.11	41,41,41,41	0
56	MG	2a	1734	1/1	0.85	0.21	62,62,62,62	0
56	MG	2A	3438	1/1	0.85	0.23	53,53,53,53	0
56	MG	2a	1813	1/1	0.85	0.13	62,62,62,62	0
56	MG	2A	3666	1/1	0.85	0.16	34,34,34,34	0
56	MG	1A	3232	1/1	0.85	0.15	51,51,51,51	0
56	MG	1A	3494	1/1	0.85	0.16	51,51,51,51	0
56	MG	1a	1685	1/1	0.85	0.20	59,59,59,59	0
56	MG	2A	3586	1/1	0.85	0.16	49,49,49,49	0
56	MG	1A	3214	1/1	0.85	0.32	46,46,46,46	0
56	MG	2a	1742	1/1	0.85	0.14	74,74,74,74	0
56	MG	1A	3923	1/1	0.85	0.12	23,23,23,23	0
56	MG	2a	1607	1/1	0.85	0.12	73,73,73,73	0
56	MG	2A	3315	1/1	0.85	0.12	65,65,65,65	0
56	MG	1a	1745	1/1	0.85	0.21	80,80,80,80	0
56	MG	2A	3883	1/1	0.85	0.15	42,42,42,42	0
56	MG	2a	1658	1/1	0.85	0.10	73,73,73,73	0
56	MG	2A	3734	1/1	0.85	0.12	70,70,70,70	0
56	MG	1w	104	1/1	0.85	0.20	52,52,52,52	0
56	MG	2A	3433	1/1	0.85	0.21	64,64,64,64	0
56	MG	2A	3415	1/1	0.85	0.15	70,70,70,70	0
56	MG	2A	3288	1/1	0.85	0.19	63,63,63,63	0
56	MG	2a	1832	1/1	0.85	0.11	75,75,75,75	0
56	MG	1A	3779	1/1	0.85	0.17	23,23,23,23	0
56	MG	2A	3656	1/1	0.85	0.16	80,80,80,80	0
56	MG	1a	1819	1/1	0.85	0.15	49,49,49,49	0
56	MG	2a	1737	1/1	0.85	0.25	86,86,86,86	0
56	MG	1A	3950	1/1	0.85	0.34	57,57,57,57	0
56	MG	2A	3062	1/1	0.85	0.27	67,67,67,67	0
56	MG	2a	1657	1/1	0.85	0.33	65,65,65,65	0
56	MG	2A	3080	1/1	0.85	0.12	52,52,52,52	0
56	MG	1A	3853	1/1	0.85	0.13	28,28,28,28	0
56	MG	2A	3824	1/1	0.85	0.35	80,80,80,80	0
56	MG	2A	3074	1/1	0.85	0.41	66,66,66,66	0
56	MG	1I	3001	1/1	0.85	0.14	61,61,61,61	0
56	MG	2A	3263	1/1	0.85	0.37	66,66,66,66	0
56	MG	1A	3875	1/1	0.85	0.18	25,25,25,25	0
56	MG	1a	1798	1/1	0.85	0.13	69,69,69,69	0
56	MG	2A	3818	1/1	0.85	0.24	70,70,70,70	0
56	MG	1B	201	1/1	0.85	0.43	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3189	1/1	0.85	0.22	65,65,65,65	0
56	MG	1A	3576	1/1	0.85	0.26	41,41,41,41	0
56	MG	1A	3238	1/1	0.85	0.24	41,41,41,41	0
56	MG	1A	3502	1/1	0.85	0.18	40,40,40,40	0
56	MG	1a	1804	1/1	0.86	0.10	62,62,62,62	0
56	MG	2A	3688	1/1	0.86	0.09	48,48,48,48	0
56	MG	1A	3986	1/1	0.86	0.10	59,59,59,59	0
56	MG	2A	3457	1/1	0.86	0.32	59,59,59,59	0
56	MG	2A	3630	1/1	0.86	0.11	61,61,61,61	0
56	MG	2a	1787	1/1	0.86	0.15	77,77,77,77	0
56	MG	2A	3220	1/1	0.86	0.42	47,47,47,47	0
56	MG	1A	3981	1/1	0.86	0.07	71,71,71,71	0
56	MG	1A	3674	1/1	0.86	0.14	22,22,22,22	0
56	MG	1a	1657	1/1	0.86	0.17	54,54,54,54	0
56	MG	2A	3513	1/1	0.86	0.15	43,43,43,43	0
56	MG	1A	4071	1/1	0.86	0.22	40,40,40,40	0
56	MG	1A	3648	1/1	0.86	0.19	25,25,25,25	0
56	MG	1A	3506	1/1	0.86	0.23	43,43,43,43	0
56	MG	2A	3195	1/1	0.86	0.23	65,65,65,65	0
56	MG	1A	3405	1/1	0.86	0.51	45,45,45,45	0
56	MG	1A	3466	1/1	0.86	0.15	48,48,48,48	0
56	MG	1A	3822	1/1	0.86	0.11	41,41,41,41	0
56	MG	1A	3747	1/1	0.86	0.24	38,38,38,38	0
56	MG	2A	3254	1/1	0.86	0.11	61,61,61,61	0
56	MG	1A	3334	1/1	0.86	0.22	43,43,43,43	0
56	MG	1a	1801	1/1	0.86	0.09	63,63,63,63	0
56	MG	2A	3484	1/1	0.86	0.21	67,67,67,67	0
56	MG	2a	1776	1/1	0.86	0.10	77,77,77,77	0
56	MG	1A	3248	1/1	0.86	0.15	56,56,56,56	0
56	MG	2A	3025	1/1	0.86	0.48	65,65,65,65	0
56	MG	2A	3508	1/1	0.86	0.13	61,61,61,61	0
56	MG	1s	3001	1/1	0.86	0.19	63,63,63,63	0
56	MG	2A	3253	1/1	0.86	0.28	60,60,60,60	0
56	MG	1A	3415	1/1	0.86	0.64	61,61,61,61	0
56	MG	2A	3892	1/1	0.86	0.40	64,64,64,64	0
56	MG	1A	3209	1/1	0.86	0.31	51,51,51,51	0
56	MG	2A	3096	1/1	0.86	0.14	60,60,60,60	0
56	MG	1B	226	1/1	0.86	0.19	69,69,69,69	0
56	MG	1A	3331	1/1	0.86	0.24	50,50,50,50	0
56	MG	2A	3653	1/1	0.86	0.18	66,66,66,66	0
56	MG	2A	3295	1/1	0.86	0.68	55,55,55,55	0
56	MG	10	109	1/1	0.86	0.19	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3082	1/1	0.86	0.11	54,54,54,54	0
56	MG	1A	3927	1/1	0.86	0.08	50,50,50,50	0
56	MG	2r	101	1/1	0.86	0.24	70,70,70,70	0
56	MG	1A	3638	1/1	0.86	0.14	48,48,48,48	0
56	MG	2A	3304	1/1	0.86	0.15	55,55,55,55	0
56	MG	1E	307	1/1	0.86	0.30	50,50,50,50	0
56	MG	2A	3536	1/1	0.86	0.15	73,73,73,73	0
56	MG	2A	3223	1/1	0.86	0.13	54,54,54,54	0
56	MG	1A	3280	1/1	0.86	0.19	42,42,42,42	0
56	MG	1a	1781	1/1	0.86	0.11	53,53,53,53	0
56	MG	1A	3056	1/1	0.86	0.22	47,47,47,47	0
56	MG	2A	3349	1/1	0.86	0.22	63,63,63,63	0
56	MG	2A	3754	1/1	0.86	0.14	48,48,48,48	0
56	MG	1A	4014	1/1	0.86	0.20	54,54,54,54	0
56	MG	2A	3808	1/1	0.86	0.14	42,42,42,42	0
56	MG	1A	3561	1/1	0.86	0.18	41,41,41,41	0
56	MG	2a	1682	1/1	0.86	0.20	62,62,62,62	0
56	MG	2A	3286	1/1	0.86	0.14	67,67,67,67	0
56	MG	1A	3543	1/1	0.86	0.28	62,62,62,62	0
56	MG	1A	4054	1/1	0.86	0.13	54,54,54,54	0
56	MG	1a	1733	1/1	0.86	0.13	55,55,55,55	0
56	MG	2A	3309	1/1	0.86	0.38	72,72,72,72	0
56	MG	2a	1608	1/1	0.86	0.19	63,63,63,63	0
56	MG	1A	3846	1/1	0.86	0.18	58,58,58,58	0
56	MG	1A	3858	1/1	0.86	0.44	47,47,47,47	0
56	MG	1A	3690	1/1	0.86	0.15	43,43,43,43	0
56	MG	1a	1752	1/1	0.86	0.15	66,66,66,66	0
56	MG	1A	3436	1/1	0.86	0.44	61,61,61,61	0
56	MG	2A	3853	1/1	0.86	0.13	48,48,48,48	0
56	MG	2A	3755	1/1	0.86	0.14	71,71,71,71	0
56	MG	2w	3004	1/1	0.86	0.26	77,77,77,77	0
56	MG	2Q	3003	1/1	0.86	0.40	57,57,57,57	0
56	MG	1x	109	1/1	0.86	0.14	68,68,68,68	0
56	MG	1a	1634	1/1	0.86	0.07	72,72,72,72	0
56	MG	2A	3540	1/1	0.86	0.13	60,60,60,60	0
56	MG	1A	3555	1/1	0.86	0.13	68,68,68,68	0
56	MG	2A	3330	1/1	0.86	0.14	53,53,53,53	0
56	MG	1A	3592	1/1	0.86	0.21	51,51,51,51	0
56	MG	1a	1735	1/1	0.86	0.13	60,60,60,60	0
56	MG	1A	3353	1/1	0.86	0.40	65,65,65,65	0
56	MG	2a	1677	1/1	0.86	0.14	55,55,55,55	0
56	MG	2A	3252	1/1	0.86	0.99	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3002	1/1	0.86	0.21	55,55,55,55	0
56	MG	2a	1662	1/1	0.86	0.09	81,81,81,81	0
56	MG	1A	3105	1/1	0.86	0.58	33,33,33,33	0
56	MG	1A	3581	1/1	0.86	0.15	42,42,42,42	0
56	MG	2A	3322	1/1	0.87	0.15	60,60,60,60	0
56	MG	1a	1803	1/1	0.87	0.19	63,63,63,63	0
56	MG	2a	1709	1/1	0.87	0.50	69,69,69,69	0
56	MG	1a	1605	1/1	0.87	0.11	57,57,57,57	0
56	MG	2a	1685	1/1	0.87	0.17	65,65,65,65	0
56	MG	2A	3496	1/1	0.87	0.08	53,53,53,53	0
56	MG	1w	106	1/1	0.87	0.14	66,66,66,66	0
56	MG	1A	3330	1/1	0.87	0.11	67,67,67,67	0
56	MG	1A	3792	1/1	0.87	0.12	32,32,32,32	0
56	MG	1w	109	1/1	0.87	0.18	76,76,76,76	0
56	MG	1A	3052	1/1	0.87	0.23	48,48,48,48	0
56	MG	2A	3675	1/1	0.87	0.45	62,62,62,62	0
56	MG	1A	3203	1/1	0.87	0.19	45,45,45,45	0
56	MG	1A	3391	1/1	0.87	0.26	32,32,32,32	0
56	MG	1A	3158	1/1	0.87	0.23	47,47,47,47	0
56	MG	2A	3501	1/1	0.87	0.15	62,62,62,62	0
56	MG	2a	1821	1/1	0.87	0.15	75,75,75,75	0
56	MG	2a	1843	1/1	0.87	0.12	66,66,66,66	0
56	MG	2A	3260	1/1	0.87	0.14	69,69,69,69	0
56	MG	2A	3030	1/1	0.87	0.14	54,54,54,54	0
56	MG	2A	3840	1/1	0.87	0.12	45,45,45,45	0
56	MG	2A	3833	1/1	0.87	0.13	47,47,47,47	0
56	MG	2x	104	1/1	0.87	0.11	68,68,68,68	0
56	MG	2a	1794	1/1	0.87	0.17	75,75,75,75	0
56	MG	2A	3109	1/1	0.87	0.12	68,68,68,68	0
56	MG	2A	3320	1/1	0.87	0.22	57,57,57,57	0
56	MG	1A	3257	1/1	0.87	0.21	61,61,61,61	0
56	MG	1A	3872	1/1	0.87	0.20	28,28,28,28	0
56	MG	2A	3825	1/1	0.87	0.15	55,55,55,55	0
56	MG	2a	1817	1/1	0.87	0.22	59,59,59,59	0
56	MG	1A	3298	1/1	0.87	0.21	44,44,44,44	0
56	MG	2a	1808	1/1	0.87	0.18	75,75,75,75	0
56	MG	1A	3694	1/1	0.87	0.13	55,55,55,55	0
56	MG	2A	3065	1/1	0.87	0.20	65,65,65,65	0
56	MG	2A	3426	1/1	0.87	0.18	60,60,60,60	0
56	MG	2A	3079	1/1	0.87	0.31	51,51,51,51	0
56	MG	2A	3214	1/1	0.87	0.22	64,64,64,64	0
56	MG	2a	1720	1/1	0.87	0.09	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3872	1/1	0.87	0.12	47,47,47,47	0
56	MG	2A	3117	1/1	0.87	0.19	57,57,57,57	0
56	MG	1a	1695	1/1	0.87	0.25	49,49,49,49	0
56	MG	2A	3015	1/1	0.87	0.49	48,48,48,48	0
56	MG	2A	3269	1/1	0.87	0.23	63,63,63,63	0
56	MG	2A	3267	1/1	0.87	0.12	62,62,62,62	0
56	MG	1W	207	1/1	0.87	0.23	35,35,35,35	0
56	MG	2A	3212	1/1	0.87	0.30	52,52,52,52	0
56	MG	2a	1687	1/1	0.87	0.17	65,65,65,65	0
56	MG	2A	3180	1/1	0.87	0.09	47,47,47,47	0
56	MG	1A	3920	1/1	0.87	0.16	65,65,65,65	0
56	MG	1A	3401	1/1	0.87	0.12	43,43,43,43	0
56	MG	2D	301	1/1	0.87	0.18	58,58,58,58	0
56	MG	1A	3699	1/1	0.87	0.14	53,53,53,53	0
56	MG	2a	1604	1/1	0.87	0.12	67,67,67,67	0
56	MG	1A	3327	1/1	0.87	0.18	34,34,34,34	0
56	MG	1A	3563	1/1	0.87	0.14	64,64,64,64	0
56	MG	2A	3334	1/1	0.87	0.46	61,61,61,61	0
56	MG	1A	3906	1/1	0.87	0.26	68,68,68,68	0
56	MG	2A	3695	1/1	0.87	0.12	45,45,45,45	0
56	MG	1A	3483	1/1	0.87	0.34	60,60,60,60	0
56	MG	1A	3236	1/1	0.87	0.29	31,31,31,31	0
56	MG	1A	3886	1/1	0.87	0.17	38,38,38,38	0
56	MG	2A	3201	1/1	0.87	0.14	71,71,71,71	0
56	MG	1B	227	1/1	0.87	0.32	54,54,54,54	0
56	MG	2a	1820	1/1	0.87	0.08	58,58,58,58	0
56	MG	2a	1690	1/1	0.87	0.13	61,61,61,61	0
56	MG	2A	3661	1/1	0.87	0.23	63,63,63,63	0
56	MG	1A	4062	1/1	0.87	0.10	21,21,21,21	0
56	MG	2a	1652	1/1	0.87	0.14	71,71,71,71	0
56	MG	1A	3217	1/1	0.87	0.31	33,33,33,33	0
56	MG	2A	3497	1/1	0.87	0.09	67,67,67,67	0
56	MG	1A	3050	1/1	0.87	0.44	48,48,48,48	0
56	MG	2a	1735	1/1	0.87	0.23	75,75,75,75	0
56	MG	2A	3105	1/1	0.87	0.14	69,69,69,69	0
56	MG	2A	3273	1/1	0.87	0.47	59,59,59,59	0
56	MG	2A	3018	1/1	0.87	0.14	44,44,44,44	0
56	MG	1A	3634	1/1	0.87	0.18	34,34,34,34	0
56	MG	1A	3024	1/1	0.87	0.32	47,47,47,47	0
56	MG	1a	1712	1/1	0.87	0.28	56,56,56,56	0
56	MG	2A	3098	1/1	0.87	0.11	51,51,51,51	0
56	MG	1A	3174	1/1	0.87	0.20	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3232	1/1	0.87	0.71	65,65,65,65	0
56	MG	2a	1655	1/1	0.88	0.74	75,75,75,75	0
56	MG	2A	3810	1/1	0.88	0.20	63,63,63,63	0
56	MG	2a	1681	1/1	0.88	0.10	57,57,57,57	0
56	MG	1a	1615	1/1	0.88	0.19	60,60,60,60	0
56	MG	1A	3444	1/1	0.88	0.59	36,36,36,36	0
56	MG	2F	301	1/1	0.88	0.42	48,48,48,48	0
56	MG	1A	3336	1/1	0.88	0.15	39,39,39,39	0
56	MG	1A	4064	1/1	0.88	0.19	45,45,45,45	0
56	MG	2A	3358	1/1	0.88	0.13	57,57,57,57	0
56	MG	2A	3852	1/1	0.88	0.26	46,46,46,46	0
56	MG	2A	3885	1/1	0.88	0.16	49,49,49,49	0
56	MG	13	101	1/1	0.88	0.13	55,55,55,55	0
56	MG	1A	3967	1/1	0.88	0.19	59,59,59,59	0
56	MG	2A	3027	1/1	0.88	1.10	53,53,53,53	0
56	MG	2a	1807	1/1	0.88	0.06	89,89,89,89	0
56	MG	1A	3164	1/1	0.88	0.22	55,55,55,55	0
56	MG	1A	3329	1/1	0.88	0.10	42,42,42,42	0
56	MG	2a	1740	1/1	0.88	0.27	71,71,71,71	0
56	MG	1A	4043	1/1	0.88	0.39	54,54,54,54	0
56	MG	2A	3042	1/1	0.88	0.16	49,49,49,49	0
56	MG	1a	1786	1/1	0.88	0.10	67,67,67,67	0
56	MG	1A	3659	1/1	0.88	0.17	21,21,21,21	0
56	MG	1A	3776	1/1	0.88	0.18	23,23,23,23	0
56	MG	1A	3995	1/1	0.88	0.15	21,21,21,21	0
56	MG	2A	3158	1/1	0.88	0.13	46,46,46,46	0
56	MG	28	101	1/1	0.88	0.23	52,52,52,52	0
56	MG	2A	3379	1/1	0.88	0.17	61,61,61,61	0
56	MG	1A	4069	1/1	0.88	0.07	55,55,55,55	0
56	MG	1A	3485	1/1	0.88	0.18	38,38,38,38	0
56	MG	1a	1728	1/1	0.88	0.16	53,53,53,53	0
56	MG	2A	3321	1/1	0.88	0.43	68,68,68,68	0
56	MG	2A	3441	1/1	0.88	0.20	39,39,39,39	0
56	MG	1A	3460	1/1	0.88	0.21	53,53,53,53	0
56	MG	2A	3784	1/1	0.88	0.19	72,72,72,72	0
56	MG	1A	3936	1/1	0.88	0.06	50,50,50,50	0
56	MG	2a	1651	1/1	0.88	0.12	60,60,60,60	0
56	MG	2A	3077	1/1	0.88	0.29	53,53,53,53	0
56	MG	2a	1836	1/1	0.88	0.11	65,65,65,65	0
56	MG	2A	3745	1/1	0.88	0.12	41,41,41,41	0
56	MG	1A	3948	1/1	0.88	0.09	54,54,54,54	0
56	MG	2A	3483	1/1	0.88	0.23	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1793	1/1	0.88	0.11	71,71,71,71	0
56	MG	2a	1680	1/1	0.88	0.48	64,64,64,64	0
56	MG	1x	110	1/1	0.88	0.11	53,53,53,53	0
56	MG	2A	3468	1/1	0.88	0.14	49,49,49,49	0
56	MG	1A	3733	1/1	0.88	0.17	49,49,49,49	0
56	MG	1A	3947	1/1	0.88	0.08	34,34,34,34	0
56	MG	1B	212	1/1	0.88	0.13	50,50,50,50	0
56	MG	1A	4036	1/1	0.88	0.17	34,34,34,34	0
56	MG	1a	1825	1/1	0.88	0.35	56,56,56,56	0
56	MG	2A	3412	1/1	0.88	0.11	60,60,60,60	0
56	MG	2a	1678	1/1	0.88	0.76	72,72,72,72	0
56	MG	2A	3418	1/1	0.88	0.65	60,60,60,60	0
56	MG	2A	3528	1/1	0.88	0.18	55,55,55,55	0
56	MG	1a	1734	1/1	0.88	0.20	56,56,56,56	0
56	MG	2a	1619	1/1	0.88	0.09	48,48,48,48	0
56	MG	2A	3124	1/1	0.88	0.20	68,68,68,68	0
56	MG	2A	3499	1/1	0.88	0.08	49,49,49,49	0
56	MG	2A	3022	1/1	0.88	0.41	45,45,45,45	0
56	MG	1A	3144	1/1	0.88	0.50	31,31,31,31	0
56	MG	1A	4033	1/1	0.88	0.09	56,56,56,56	0
56	MG	2a	1706	1/1	0.88	0.10	64,64,64,64	0
56	MG	1a	1669	1/1	0.88	0.11	56,56,56,56	0
56	MG	2A	3905	1/1	0.88	0.18	56,56,56,56	0
56	MG	1A	3511	1/1	0.88	0.14	43,43,43,43	0
56	MG	2A	3341	1/1	0.88	0.21	50,50,50,50	0
56	MG	2A	3344	1/1	0.88	0.88	55,55,55,55	0
56	MG	2w	3005	1/1	0.88	0.18	76,76,76,76	0
56	MG	2a	1634	1/1	0.88	0.10	85,85,85,85	0
56	MG	1A	4022	1/1	0.88	0.08	55,55,55,55	0
56	MG	1A	3370	1/1	0.88	0.80	56,56,56,56	0
56	MG	2A	3831	1/1	0.88	0.10	52,52,52,52	0
56	MG	1A	4077	1/1	0.88	0.08	63,63,63,63	0
56	MG	2A	3566	1/1	0.88	0.12	34,34,34,34	0
56	MG	2Q	3002	1/1	0.88	0.17	54,54,54,54	0
56	MG	1A	3090	1/1	0.88	0.20	47,47,47,47	0
56	MG	1A	3186	1/1	0.88	0.14	45,45,45,45	0
56	MG	2A	3370	1/1	0.88	0.28	57,57,57,57	0
56	MG	2A	3008	1/1	0.88	0.17	56,56,56,56	0
56	MG	1A	3547	1/1	0.88	0.14	56,56,56,56	0
56	MG	2q	3001	1/1	0.88	0.14	47,47,47,47	0
56	MG	1A	3862	1/1	0.88	0.10	35,35,35,35	0
56	MG	2a	1818	1/1	0.88	0.23	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3596	1/1	0.88	0.29	57,57,57,57	0
56	MG	2A	3091	1/1	0.88	0.16	69,69,69,69	0
56	MG	1A	3153	1/1	0.88	0.26	50,50,50,50	0
56	MG	2a	1811	1/1	0.88	0.10	68,68,68,68	0
56	MG	2A	3339	1/1	0.88	0.35	62,62,62,62	0
56	MG	2A	3262	1/1	0.88	0.24	69,69,69,69	0
56	MG	2A	3177	1/1	0.88	0.91	55,55,55,55	0
56	MG	1A	3160	1/1	0.88	0.34	32,32,32,32	0
56	MG	1A	3877	1/1	0.88	0.11	67,67,67,67	0
56	MG	2A	3891	1/1	0.88	0.12	49,49,49,49	0
56	MG	1A	4085	1/1	0.88	0.17	46,46,46,46	0
56	MG	1A	4092	1/1	0.88	0.36	55,55,55,55	0
56	MG	1e	201	1/1	0.88	0.17	51,51,51,51	0
56	MG	2A	3801	1/1	0.88	0.16	65,65,65,65	0
56	MG	1A	3142	1/1	0.88	0.24	47,47,47,47	0
56	MG	1A	3119	1/1	0.88	0.31	39,39,39,39	0
56	MG	1A	3869	1/1	0.88	0.15	32,32,32,32	0
56	MG	1A	3368	1/1	0.88	0.13	36,36,36,36	0
56	MG	1D	301	1/1	0.88	0.16	43,43,43,43	0
56	MG	1A	3683	1/1	0.88	0.16	21,21,21,21	0
56	MG	1a	1822	1/1	0.88	0.23	58,58,58,58	0
56	MG	1A	3960	1/1	0.88	0.13	67,67,67,67	0
56	MG	1A	3619	1/1	0.88	0.14	35,35,35,35	0
56	MG	1A	3421	1/1	0.88	0.28	62,62,62,62	0
56	MG	2A	3815	1/1	0.88	0.30	67,67,67,67	0
56	MG	1x	106	1/1	0.88	0.20	68,68,68,68	0
56	MG	2A	3510	1/1	0.88	0.17	53,53,53,53	0
56	MG	2A	3455	1/1	0.88	0.18	68,68,68,68	0
56	MG	1a	1658	1/1	0.88	0.11	61,61,61,61	0
56	MG	2A	3776	1/1	0.88	0.22	68,68,68,68	0
56	MG	1a	1662	1/1	0.88	0.33	67,67,67,67	0
56	MG	1A	3903	1/1	0.89	0.12	30,30,30,30	0
56	MG	2a	1660	1/1	0.89	0.10	82,82,82,82	0
56	MG	1A	3359	1/1	0.89	0.17	49,49,49,49	0
56	MG	2A	3385	1/1	0.89	0.17	59,59,59,59	0
56	MG	2A	3194	1/1	0.89	0.29	65,65,65,65	0
56	MG	2A	3645	1/1	0.89	0.16	56,56,56,56	0
56	MG	1a	1698	1/1	0.89	0.22	68,68,68,68	0
56	MG	2A	3397	1/1	0.89	0.14	53,53,53,53	0
56	MG	2A	3217	1/1	0.89	0.13	63,63,63,63	0
56	MG	1A	3582	1/1	0.89	0.13	49,49,49,49	0
56	MG	2A	3228	1/1	0.89	0.21	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1757	1/1	0.89	0.15	66,66,66,66	0
56	MG	2A	3479	1/1	0.89	0.14	56,56,56,56	0
56	MG	2A	3043	1/1	0.89	0.19	53,53,53,53	0
56	MG	2A	3682	1/1	0.89	0.09	71,71,71,71	0
56	MG	2a	1683	1/1	0.89	0.12	66,66,66,66	0
56	MG	1A	3120	1/1	0.89	0.19	28,28,28,28	0
56	MG	2A	3619	1/1	0.89	0.21	50,50,50,50	0
56	MG	2a	1799	1/1	0.89	0.24	67,67,67,67	0
56	MG	2A	3562	1/1	0.89	0.12	41,41,41,41	0
56	MG	1a	1603	1/1	0.89	0.14	57,57,57,57	0
56	MG	1A	3497	1/1	0.89	0.33	32,32,32,32	0
56	MG	2A	3135	1/1	0.89	0.26	39,39,39,39	0
56	MG	1A	3796	1/1	0.89	0.13	64,64,64,64	0
56	MG	1a	1763	1/1	0.89	0.14	75,75,75,75	0
56	MG	1A	4020	1/1	0.89	0.17	50,50,50,50	0
56	MG	1a	1700	1/1	0.89	0.18	56,56,56,56	0
56	MG	2A	3577	1/1	0.89	0.19	53,53,53,53	0
56	MG	1A	3933	1/1	0.89	0.17	52,52,52,52	0
56	MG	1w	108	1/1	0.89	0.15	36,36,36,36	0
56	MG	2A	3767	1/1	0.89	0.13	54,54,54,54	0
56	MG	1A	3319	1/1	0.89	0.39	36,36,36,36	0
56	MG	2a	1705	1/1	0.89	0.45	86,86,86,86	0
56	MG	1a	1650	1/1	0.89	0.20	46,46,46,46	0
56	MG	2A	3033	1/1	0.89	0.21	48,48,48,48	0
56	MG	17	101	1/1	0.89	0.29	52,52,52,52	0
56	MG	2A	3901	1/1	0.89	0.11	67,67,67,67	0
56	MG	1a	1651	1/1	0.89	0.19	75,75,75,75	0
56	MG	1A	3254	1/1	0.89	0.20	52,52,52,52	0
56	MG	2A	3188	1/1	0.89	0.17	53,53,53,53	0
56	MG	1A	3227	1/1	0.89	0.19	49,49,49,49	0
56	MG	2A	3844	1/1	0.89	0.13	39,39,39,39	0
56	MG	2A	3832	1/1	0.89	0.19	79,79,79,79	0
56	MG	2g	8001	1/1	0.89	0.12	69,69,69,69	0
56	MG	1A	3672	1/1	0.89	0.17	24,24,24,24	0
56	MG	2A	3779	1/1	0.89	0.12	60,60,60,60	0
56	MG	1Y	203	1/1	0.89	0.14	66,66,66,66	0
56	MG	1A	3476	1/1	0.89	0.16	56,56,56,56	0
56	MG	2A	3026	1/1	0.89	0.77	48,48,48,48	0
56	MG	1A	4032	1/1	0.89	0.09	37,37,37,37	0
56	MG	1N	205	1/1	0.89	0.26	46,46,46,46	0
56	MG	2A	3553	1/1	0.89	0.10	56,56,56,56	0
56	MG	1A	3956	1/1	0.89	0.39	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3492	1/1	0.89	0.40	59,59,59,59	0
56	MG	2a	1835	1/1	0.89	0.15	72,72,72,72	0
56	MG	2A	3447	1/1	0.89	0.22	49,49,49,49	0
56	MG	2a	1764	1/1	0.89	0.16	72,72,72,72	0
56	MG	1A	3309	1/1	0.89	0.17	53,53,53,53	0
56	MG	1A	3332	1/1	0.89	0.16	39,39,39,39	0
56	MG	2a	1701	1/1	0.89	0.09	55,55,55,55	0
56	MG	2A	3710	1/1	0.89	0.13	69,69,69,69	0
56	MG	2A	3329	1/1	0.89	0.26	59,59,59,59	0
56	MG	2A	3323	1/1	0.89	0.20	68,68,68,68	0
56	MG	1A	3795	1/1	0.89	0.19	39,39,39,39	0
56	MG	2a	1770	1/1	0.89	0.09	77,77,77,77	0
56	MG	1A	3724	1/1	0.89	0.21	13,13,13,13	0
56	MG	1a	1729	1/1	0.89	0.10	79,79,79,79	0
56	MG	1A	3191	1/1	0.89	0.10	50,50,50,50	0
56	MG	1a	1621	1/1	0.89	0.26	56,56,56,56	0
56	MG	1A	3735	1/1	0.89	0.16	34,34,34,34	0
56	MG	1a	1610	1/1	0.89	0.17	57,57,57,57	0
56	MG	1A	3463	1/1	0.89	0.25	62,62,62,62	0
56	MG	1r	101	1/1	0.89	0.28	69,69,69,69	0
56	MG	2X	101	1/1	0.89	0.13	46,46,46,46	0
56	MG	1A	3921	1/1	0.89	0.08	53,53,53,53	0
56	MG	2A	3382	1/1	0.89	0.20	75,75,75,75	0
56	MG	1a	1754	1/1	0.89	0.13	65,65,65,65	0
56	MG	2A	3162	1/1	0.89	0.41	55,55,55,55	0
56	MG	2a	1837	1/1	0.89	1.04	89,89,89,89	0
56	MG	1A	3567	1/1	0.89	0.21	36,36,36,36	0
56	MG	1a	1788	1/1	0.89	0.15	65,65,65,65	0
56	MG	2A	3123	1/1	0.89	0.22	47,47,47,47	0
56	MG	2F	303	1/1	0.89	0.20	46,46,46,46	0
56	MG	2a	1804	1/1	0.89	0.08	61,61,61,61	0
56	MG	1A	3770	1/1	0.89	0.12	40,40,40,40	0
56	MG	2A	3150	1/1	0.89	0.13	41,41,41,41	0
56	MG	1A	4012	1/1	0.89	0.08	71,71,71,71	0
56	MG	2A	3218	1/1	0.89	0.42	63,63,63,63	0
56	MG	2a	1648	1/1	0.89	0.22	76,76,76,76	0
56	MG	2A	3847	1/1	0.89	0.07	46,46,46,46	0
56	MG	2A	3803	1/1	0.89	0.07	70,70,70,70	0
56	MG	1A	3165	1/1	0.89	0.13	41,41,41,41	0
56	MG	2a	1749	1/1	0.89	0.06	64,64,64,64	0
56	MG	1A	3085	1/1	0.89	0.21	35,35,35,35	0
56	MG	1a	1688	1/1	0.89	0.15	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1624	1/1	0.89	0.12	59,59,59,59	0
56	MG	1A	3088	1/1	0.89	0.17	50,50,50,50	0
56	MG	2A	3698	1/1	0.89	0.10	69,69,69,69	0
56	MG	2A	3128	1/1	0.89	0.14	47,47,47,47	0
56	MG	1A	3646	1/1	0.89	0.25	46,46,46,46	0
56	MG	20	102	1/1	0.89	0.24	62,62,62,62	0
56	MG	2A	3819	1/1	0.89	0.09	57,57,57,57	0
56	MG	2A	3674	1/1	0.89	0.09	50,50,50,50	0
56	MG	1A	3851	1/1	0.89	0.15	28,28,28,28	0
56	MG	1A	3800	1/1	0.89	0.13	52,52,52,52	0
56	MG	2A	3133	1/1	0.89	0.28	69,69,69,69	0
56	MG	2A	3352	1/1	0.89	0.13	49,49,49,49	0
56	MG	1A	3292	1/1	0.89	0.11	60,60,60,60	0
56	MG	1A	3388	1/1	0.89	0.22	29,29,29,29	0
56	MG	2A	3052	1/1	0.89	0.12	48,48,48,48	0
56	MG	2B	3007	1/1	0.89	0.17	63,63,63,63	0
56	MG	2A	3723	1/1	0.89	0.07	47,47,47,47	0
56	MG	2A	3834	1/1	0.89	0.12	42,42,42,42	0
56	MG	2A	3071	1/1	0.89	0.11	56,56,56,56	0
56	MG	1A	3748	1/1	0.89	0.16	24,24,24,24	0
56	MG	2A	3799	1/1	0.89	0.11	54,54,54,54	0
56	MG	13	103	1/1	0.89	0.22	45,45,45,45	0
56	MG	2A	3879	1/1	0.89	0.32	52,52,52,52	0
56	MG	2a	1774	1/1	0.89	0.08	67,67,67,67	0
56	MG	1A	3406	1/1	0.89	0.14	68,68,68,68	0
56	MG	2a	1659	1/1	0.89	0.08	75,75,75,75	0
56	MG	1a	1704	1/1	0.89	0.09	50,50,50,50	0
56	MG	2A	3246	1/1	0.89	0.32	35,35,35,35	0
56	MG	2A	3595	1/1	0.89	0.10	58,58,58,58	0
56	MG	1A	3060	1/1	0.89	0.14	42,42,42,42	0
56	MG	1A	3976	1/1	0.89	0.17	32,32,32,32	0
56	MG	2A	3277	1/1	0.89	0.33	51,51,51,51	0
56	MG	2A	3743	1/1	0.89	0.18	58,58,58,58	0
56	MG	2A	3798	1/1	0.90	0.23	75,75,75,75	0
56	MG	2A	3777	1/1	0.90	0.10	76,76,76,76	0
57	MT9	2A	3897	33/33	0.90	0.53	37,55,61,64	0
56	MG	2A	3444	1/1	0.90	0.19	49,49,49,49	0
56	MG	2A	3145	1/1	0.90	0.12	52,52,52,52	0
56	MG	1a	1677	1/1	0.90	0.18	68,68,68,68	0
56	MG	2A	3120	1/1	0.90	0.13	35,35,35,35	0
56	MG	1R	202	1/1	0.90	0.26	38,38,38,38	0
56	MG	1a	1644	1/1	0.90	0.17	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1716	1/1	0.90	0.18	63,63,63,63	0
56	MG	1A	3510	1/1	0.90	0.17	48,48,48,48	0
56	MG	1A	3253	1/1	0.90	0.12	52,52,52,52	0
56	MG	1A	3882	1/1	0.90	0.10	57,57,57,57	0
56	MG	1A	3219	1/1	0.90	0.37	45,45,45,45	0
56	MG	1A	3566	1/1	0.90	0.33	38,38,38,38	0
56	MG	1a	1793	1/1	0.90	0.06	71,71,71,71	0
56	MG	2Q	3001	1/1	0.90	0.08	53,53,53,53	0
56	MG	2A	3066	1/1	0.90	0.15	53,53,53,53	0
56	MG	2w	3008	1/1	0.90	0.12	75,75,75,75	0
56	MG	2B	3005	1/1	0.90	0.11	57,57,57,57	0
56	MG	2a	1616	1/1	0.90	0.09	54,54,54,54	0
56	MG	2A	3388	1/1	0.90	0.44	58,58,58,58	0
56	MG	2A	3209	1/1	0.90	0.56	68,68,68,68	0
56	MG	2A	3532	1/1	0.90	0.08	61,61,61,61	0
59	ZN	14	501	1/1	0.90	0.11	95,95,95,95	0
56	MG	2a	1754	1/1	0.90	0.15	82,82,82,82	0
56	MG	2A	3005	1/1	0.90	0.20	58,58,58,58	0
56	MG	1A	4025	1/1	0.90	0.13	45,45,45,45	0
56	MG	2a	1759	1/1	0.90	0.14	83,83,83,83	0
56	MG	2A	3704	1/1	0.90	0.11	75,75,75,75	0
56	MG	1a	1823	1/1	0.90	0.09	55,55,55,55	0
56	MG	2A	3165	1/1	0.90	0.17	52,52,52,52	0
56	MG	2A	3529	1/1	0.90	0.16	64,64,64,64	0
56	MG	2A	3598	1/1	0.90	0.27	57,57,57,57	0
56	MG	1A	3621	1/1	0.90	0.14	23,23,23,23	0
56	MG	2A	3002	1/1	0.90	0.24	55,55,55,55	0
56	MG	1A	3934	1/1	0.90	0.13	41,41,41,41	0
56	MG	1G	3003	1/1	0.90	0.18	64,64,64,64	0
56	MG	1A	3461	1/1	0.90	0.13	50,50,50,50	0
56	MG	2A	3176	1/1	0.90	0.10	41,41,41,41	0
56	MG	2A	3655	1/1	0.90	0.15	67,67,67,67	0
56	MG	2A	3251	1/1	0.90	0.59	58,58,58,58	0
56	MG	1a	1736	1/1	0.90	0.13	51,51,51,51	0
56	MG	1A	3379	1/1	0.90	0.27	26,26,26,26	0
56	MG	2A	3821	1/1	0.90	0.26	61,61,61,61	0
56	MG	2A	3861	1/1	0.90	0.19	65,65,65,65	0
56	MG	1a	1633	1/1	0.90	0.26	56,56,56,56	0
56	MG	2a	1642	1/1	0.90	0.14	63,63,63,63	0
56	MG	1A	3268	1/1	0.90	0.33	44,44,44,44	0
56	MG	1A	3825	1/1	0.90	0.10	54,54,54,54	0
56	MG	1a	1689	1/1	0.90	0.18	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3624	1/1	0.90	0.18	63,63,63,63	0
56	MG	1A	3357	1/1	0.90	0.17	46,46,46,46	0
56	MG	1a	1707	1/1	0.90	0.22	62,62,62,62	0
56	MG	1A	3704	1/1	0.90	0.09	46,46,46,46	0
56	MG	2A	3363	1/1	0.90	0.19	65,65,65,65	0
56	MG	1A	4037	1/1	0.90	0.35	48,48,48,48	0
56	MG	1A	3386	1/1	0.90	0.41	38,38,38,38	0
56	MG	2A	3716	1/1	0.90	0.16	48,48,48,48	0
56	MG	1A	3111	1/1	0.90	0.12	34,34,34,34	0
56	MG	1A	3541	1/1	0.90	0.20	47,47,47,47	0
56	MG	2a	1777	1/1	0.90	0.16	64,64,64,64	0
56	MG	2A	3047	1/1	0.90	0.10	54,54,54,54	0
56	MG	2A	3185	1/1	0.90	0.49	55,55,55,55	0
56	MG	2A	3169	1/1	0.90	0.10	52,52,52,52	0
56	MG	2A	3302	1/1	0.90	0.09	69,69,69,69	0
56	MG	2A	3788	1/1	0.90	0.11	54,54,54,54	0
56	MG	1a	1691	1/1	0.90	0.24	64,64,64,64	0
56	MG	1A	3827	1/1	0.90	0.10	47,47,47,47	0
56	MG	2A	3894	1/1	0.90	0.11	62,62,62,62	0
56	MG	1A	3928	1/1	0.90	0.23	51,51,51,51	0
56	MG	2A	3449	1/1	0.90	0.26	55,55,55,55	0
56	MG	1B	235	1/1	0.90	0.17	31,31,31,31	0
56	MG	1A	3258	1/1	0.90	0.19	47,47,47,47	0
56	MG	1A	3400	1/1	0.90	0.14	36,36,36,36	0
56	MG	1U	205	1/1	0.90	0.17	40,40,40,40	0
56	MG	2A	3862	1/1	0.90	0.52	84,84,84,84	0
56	MG	1A	3451	1/1	0.90	0.16	49,49,49,49	0
56	MG	2A	3720	1/1	0.90	0.28	52,52,52,52	0
56	MG	2a	1714	1/1	0.90	0.11	79,79,79,79	0
56	MG	1a	1659	1/1	0.90	0.19	64,64,64,64	0
56	MG	1A	3817	1/1	0.90	0.16	23,23,23,23	0
56	MG	2A	3469	1/1	0.90	0.31	54,54,54,54	0
56	MG	2A	3796	1/1	0.90	0.18	70,70,70,70	0
56	MG	2A	3724	1/1	0.90	0.10	67,67,67,67	0
56	MG	1A	3745	1/1	0.90	0.18	34,34,34,34	0
56	MG	2A	3140	1/1	0.90	0.07	71,71,71,71	0
56	MG	2A	3820	1/1	0.90	0.19	74,74,74,74	0
56	MG	1A	3749	1/1	0.90	0.24	19,19,19,19	0
56	MG	1A	3973	1/1	0.90	0.09	51,51,51,51	0
56	MG	1a	1756	1/1	0.90	0.11	87,87,87,87	0
56	MG	1x	107	1/1	0.90	0.11	66,66,66,66	0
56	MG	2A	3639	1/1	0.90	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3993	1/1	0.90	0.19	42,42,42,42	0
56	MG	2w	3006	1/1	0.90	0.89	77,77,77,77	0
56	MG	2A	3425	1/1	0.90	0.13	58,58,58,58	0
56	MG	1A	4094	1/1	0.90	0.38	39,39,39,39	0
56	MG	1E	301	1/1	0.90	0.18	49,49,49,49	0
56	MG	1a	1622	1/1	0.90	0.19	41,41,41,41	0
56	MG	1U	201	1/1	0.90	0.25	33,33,33,33	0
56	MG	1w	105	1/1	0.90	0.17	67,67,67,67	0
56	MG	1A	4057	1/1	0.90	0.17	59,59,59,59	0
56	MG	1A	3267	1/1	0.90	0.23	30,30,30,30	0
56	MG	2A	3203	1/1	0.90	0.16	47,47,47,47	0
56	MG	1a	1612	1/1	0.90	0.15	51,51,51,51	0
56	MG	2A	3829	1/1	0.90	0.10	60,60,60,60	0
56	MG	1l	203	1/1	0.90	0.21	52,52,52,52	0
56	MG	2A	3554	1/1	0.90	0.07	45,45,45,45	0
56	MG	2A	3836	1/1	0.90	0.15	44,44,44,44	0
56	MG	2A	3040	1/1	0.90	0.14	50,50,50,50	0
56	MG	2A	3375	1/1	0.90	0.37	61,61,61,61	0
56	MG	1U	203	1/1	0.90	0.71	40,40,40,40	0
56	MG	2a	1750	1/1	0.90	0.07	70,70,70,70	0
56	MG	1A	3023	1/1	0.90	0.13	37,37,37,37	0
56	MG	1P	204	1/1	0.90	0.38	32,32,32,32	0
56	MG	1a	1648	1/1	0.90	0.20	57,57,57,57	0
56	MG	2A	3880	1/1	0.90	0.23	65,65,65,65	0
56	MG	2A	3419	1/1	0.90	0.18	59,59,59,59	0
56	MG	1A	3914	1/1	0.90	0.14	39,39,39,39	0
56	MG	2A	3178	1/1	0.90	0.27	55,55,55,55	0
56	MG	1A	4070	1/1	0.90	0.24	45,45,45,45	0
56	MG	1E	310	1/1	0.90	0.20	35,35,35,35	0
56	MG	1A	3159	1/1	0.90	0.21	56,56,56,56	0
56	MG	2A	3184	1/1	0.90	0.23	49,49,49,49	0
56	MG	1A	3287	1/1	0.90	0.59	52,52,52,52	0
56	MG	2e	3001	1/1	0.90	0.08	76,76,76,76	0
56	MG	2a	1746	1/1	0.90	0.21	70,70,70,70	0
56	MG	1A	3798	1/1	0.90	0.15	56,56,56,56	0
56	MG	2A	3377	1/1	0.90	0.21	57,57,57,57	0
56	MG	19	101	1/1	0.90	0.18	44,44,44,44	0
56	MG	1A	3361	1/1	0.90	0.16	47,47,47,47	0
56	MG	1x	115	1/1	0.90	0.08	68,68,68,68	0
56	MG	2A	3182	1/1	0.90	0.26	53,53,53,53	0
56	MG	2a	1791	1/1	0.90	0.13	71,71,71,71	0
56	MG	1B	220	1/1	0.90	0.20	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2l	3001	1/1	0.90	0.13	60,60,60,60	0
56	MG	2A	3355	1/1	0.90	0.13	79,79,79,79	0
56	MG	2t	3001	1/1	0.90	0.11	62,62,62,62	0
56	MG	2a	1625	1/1	0.90	0.10	80,80,80,80	0
56	MG	1A	3866	1/1	0.90	0.16	26,26,26,26	0
56	MG	2A	3106	1/1	0.90	0.13	49,49,49,49	0
56	MG	1A	3978	1/1	0.90	0.15	26,26,26,26	0
56	MG	2A	3347	1/1	0.90	0.49	68,68,68,68	0
56	MG	1A	3134	1/1	0.90	0.35	35,35,35,35	0
56	MG	2O	8001	1/1	0.90	0.17	48,48,48,48	0
56	MG	1w	103	1/1	0.90	0.10	51,51,51,51	0
56	MG	2A	3671	1/1	0.90	0.10	63,63,63,63	0
56	MG	1A	3452	1/1	0.90	0.25	49,49,49,49	0
56	MG	2w	3007	1/1	0.90	0.33	71,71,71,71	0
56	MG	2A	3354	1/1	0.90	0.20	50,50,50,50	0
56	MG	2A	3122	1/1	0.90	0.51	67,67,67,67	0
56	MG	2a	1633	1/1	0.90	0.16	57,57,57,57	0
56	MG	2A	3053	1/1	0.90	0.15	64,64,64,64	0
56	MG	1l	103	1/1	0.90	0.12	45,45,45,45	0
56	MG	2A	3183	1/1	0.90	0.21	53,53,53,53	0
56	MG	1A	3283	1/1	0.90	0.13	51,51,51,51	0
56	MG	2A	3048	1/1	0.90	0.15	55,55,55,55	0
56	MG	2A	3001	1/1	0.90	0.13	56,56,56,56	0
56	MG	1A	4111	1/1	0.91	0.19	41,41,41,41	0
56	MG	1A	3467	1/1	0.91	0.34	41,41,41,41	0
56	MG	1A	3373	1/1	0.91	0.29	40,40,40,40	0
56	MG	1A	3112	1/1	0.91	0.34	42,42,42,42	0
56	MG	2A	3752	1/1	0.91	0.24	59,59,59,59	0
56	MG	1A	3201	1/1	0.91	0.12	61,61,61,61	0
56	MG	1A	3204	1/1	0.91	0.18	68,68,68,68	0
56	MG	1a	1692	1/1	0.91	0.18	63,63,63,63	0
56	MG	2A	3731	1/1	0.91	0.15	62,62,62,62	0
56	MG	1A	4133	1/1	0.91	0.15	30,30,30,30	0
56	MG	2l	3002	1/1	0.91	0.31	62,62,62,62	0
56	MG	1a	1617	1/1	0.91	0.10	65,65,65,65	0
56	MG	2A	3476	1/1	0.91	0.47	57,57,57,57	0
56	MG	1A	3691	1/1	0.91	0.12	60,60,60,60	0
56	MG	2A	3807	1/1	0.91	0.09	65,65,65,65	0
56	MG	2A	3373	1/1	0.91	0.47	57,57,57,57	0
56	MG	1A	3548	1/1	0.91	0.28	56,56,56,56	0
56	MG	2A	3371	1/1	0.91	0.31	61,61,61,61	0
56	MG	1A	3809	1/1	0.91	0.11	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1w	111	1/1	0.91	0.11	61,61,61,61	0
56	MG	2A	3234	1/1	0.91	0.22	62,62,62,62	0
56	MG	1A	3856	1/1	0.91	0.20	33,33,33,33	0
56	MG	2A	3318	1/1	0.91	0.20	44,44,44,44	0
56	MG	1a	1601	1/1	0.91	0.22	54,54,54,54	0
56	MG	2A	3574	1/1	0.91	0.14	57,57,57,57	0
56	MG	2A	3549	1/1	0.91	0.18	56,56,56,56	0
56	MG	1A	3708	1/1	0.91	0.07	51,51,51,51	0
56	MG	2A	3368	1/1	0.91	0.78	47,47,47,47	0
56	MG	2A	3151	1/1	0.91	0.11	59,59,59,59	0
56	MG	2A	3587	1/1	0.91	0.13	44,44,44,44	0
56	MG	1A	3565	1/1	0.91	0.24	47,47,47,47	0
56	MG	1A	3384	1/1	0.91	0.16	48,48,48,48	0
56	MG	1A	3430	1/1	0.91	0.17	41,41,41,41	0
56	MG	1A	3879	1/1	0.91	0.33	30,30,30,30	0
56	MG	1Q	204	1/1	0.91	0.15	38,38,38,38	0
56	MG	1A	3285	1/1	0.91	0.19	43,43,43,43	0
56	MG	1A	3338	1/1	0.91	0.29	45,45,45,45	0
56	MG	2A	3647	1/1	0.91	0.52	51,51,51,51	0
56	MG	2U	204	1/1	0.91	0.44	62,62,62,62	0
56	MG	1A	4042	1/1	0.91	0.17	24,24,24,24	0
56	MG	1F	306	1/1	0.91	0.13	47,47,47,47	0
56	MG	2A	3396	1/1	0.91	0.13	60,60,60,60	0
56	MG	2A	3174	1/1	0.91	0.27	51,51,51,51	0
56	MG	2a	1647	1/1	0.91	0.33	55,55,55,55	0
56	MG	2A	3760	1/1	0.91	0.16	60,60,60,60	0
56	MG	1A	3477	1/1	0.91	0.14	44,44,44,44	0
56	MG	2A	3359	1/1	0.91	0.36	63,63,63,63	0
56	MG	23	102	1/1	0.91	0.22	52,52,52,52	0
56	MG	2A	3094	1/1	0.91	0.37	47,47,47,47	0
56	MG	1A	3987	1/1	0.91	0.09	40,40,40,40	0
56	MG	2A	3889	1/1	0.91	0.60	39,39,39,39	0
56	MG	2A	3633	1/1	0.91	0.13	58,58,58,58	0
56	MG	1A	3125	1/1	0.91	0.19	45,45,45,45	0
56	MG	2a	1614	1/1	0.91	0.10	59,59,59,59	0
56	MG	1A	4129	1/1	0.91	0.23	33,33,33,33	0
56	MG	2a	1797	1/1	0.91	0.14	65,65,65,65	0
56	MG	2a	1842	1/1	0.91	0.13	49,49,49,49	0
56	MG	1A	3403	1/1	0.91	0.23	46,46,46,46	0
56	MG	2A	3392	1/1	0.91	0.12	52,52,52,52	0
56	MG	2A	3198	1/1	0.91	0.20	49,49,49,49	0
56	MG	2A	3410	1/1	0.91	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3823	1/1	0.91	0.13	48,48,48,48	0
56	MG	1B	216	1/1	0.91	0.18	34,34,34,34	0
56	MG	1A	3328	1/1	0.91	0.20	48,48,48,48	0
56	MG	2A	3086	1/1	0.91	0.09	41,41,41,41	0
56	MG	2A	3849	1/1	0.91	0.12	51,51,51,51	0
56	MG	1A	3087	1/1	0.91	0.16	43,43,43,43	0
56	MG	1A	3750	1/1	0.91	0.19	41,41,41,41	0
56	MG	2A	3694	1/1	0.91	0.10	64,64,64,64	0
56	MG	1A	3109	1/1	0.91	0.25	31,31,31,31	0
56	MG	1A	3812	1/1	0.91	0.23	54,54,54,54	0
56	MG	1A	3949	1/1	0.91	0.09	19,19,19,19	0
56	MG	1A	3663	1/1	0.91	0.13	30,30,30,30	0
56	MG	2A	3011	1/1	0.91	0.11	49,49,49,49	0
56	MG	1A	3234	1/1	0.91	0.13	34,34,34,34	0
56	MG	17	102	1/1	0.91	0.36	38,38,38,38	0
56	MG	1A	3705	1/1	0.91	0.18	44,44,44,44	0
56	MG	2A	3308	1/1	0.91	0.08	63,63,63,63	0
56	MG	2A	3046	1/1	0.91	0.14	65,65,65,65	0
56	MG	2a	1703	1/1	0.91	0.13	64,64,64,64	0
56	MG	1a	1655	1/1	0.91	0.09	63,63,63,63	0
56	MG	1A	3915	1/1	0.91	0.12	41,41,41,41	0
56	MG	1A	3083	1/1	0.91	0.24	34,34,34,34	0
56	MG	2a	1617	1/1	0.91	0.16	59,59,59,59	0
56	MG	1A	3143	1/1	0.91	0.72	46,46,46,46	0
56	MG	1a	1782	1/1	0.91	0.13	66,66,66,66	0
56	MG	1A	3569	1/1	0.91	0.31	52,52,52,52	0
56	MG	2a	1639	1/1	0.91	0.24	68,68,68,68	0
56	MG	2a	1806	1/1	0.91	0.11	67,67,67,67	0
56	MG	1A	3059	1/1	0.91	0.19	53,53,53,53	0
56	MG	1A	3252	1/1	0.91	0.14	34,34,34,34	0
56	MG	2A	3480	1/1	0.91	0.55	65,65,65,65	0
56	MG	1A	3597	1/1	0.91	0.13	32,32,32,32	0
56	MG	2A	3800	1/1	0.91	0.20	70,70,70,70	0
56	MG	2a	1840	1/1	0.91	0.14	78,78,78,78	0
56	MG	2A	3081	1/1	0.91	0.32	44,44,44,44	0
56	MG	2A	3472	1/1	0.91	0.13	58,58,58,58	0
56	MG	2x	103	1/1	0.91	0.12	77,77,77,77	0
56	MG	2A	3728	1/1	0.91	0.09	69,69,69,69	0
56	MG	1A	3559	1/1	0.91	0.55	36,36,36,36	0
56	MG	2A	3589	1/1	0.91	0.09	51,51,51,51	0
56	MG	1a	1616	1/1	0.91	0.15	51,51,51,51	0
56	MG	25	105	1/1	0.91	0.11	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1759	1/1	0.91	0.05	81,81,81,81	0
56	MG	1A	3387	1/1	0.91	0.34	37,37,37,37	0
56	MG	10	107	1/1	0.91	0.15	53,53,53,53	0
56	MG	2a	1792	1/1	0.91	0.20	74,74,74,74	0
56	MG	1A	3700	1/1	0.91	0.22	44,44,44,44	0
56	MG	1A	3255	1/1	0.91	0.20	63,63,63,63	0
56	MG	1A	3572	1/1	0.91	0.22	15,15,15,15	0
56	MG	2A	3037	1/1	0.91	0.17	42,42,42,42	0
56	MG	1A	3721	1/1	0.91	0.10	60,60,60,60	0
56	MG	1A	3348	1/1	0.91	0.14	41,41,41,41	0
56	MG	2A	3039	1/1	0.91	0.10	33,33,33,33	0
56	MG	1a	1671	1/1	0.91	0.19	48,48,48,48	0
56	MG	2A	3559	1/1	0.91	0.14	47,47,47,47	0
56	MG	2A	3545	1/1	0.91	0.35	58,58,58,58	0
56	MG	2a	1724	1/1	0.91	0.26	53,53,53,53	0
56	MG	2A	3519	1/1	0.91	0.14	46,46,46,46	0
56	MG	1B	221	1/1	0.91	0.13	55,55,55,55	0
56	MG	1A	4107	1/1	0.91	0.17	37,37,37,37	0
56	MG	2a	1741	1/1	0.91	0.18	77,77,77,77	0
56	MG	1a	1670	1/1	0.91	0.09	43,43,43,43	0
56	MG	2a	1637	1/1	0.91	0.27	63,63,63,63	0
56	MG	2A	3903	1/1	0.91	0.45	45,45,45,45	0
56	MG	1A	3685	1/1	0.91	0.14	38,38,38,38	0
56	MG	2A	3314	1/1	0.91	0.19	60,60,60,60	0
56	MG	1A	3977	1/1	0.91	0.16	22,22,22,22	0
56	MG	1b	3001	1/1	0.91	0.17	82,82,82,82	0
56	MG	2a	1606	1/1	0.91	0.17	58,58,58,58	0
56	MG	1A	3924	1/1	0.91	0.18	39,39,39,39	0
56	MG	1a	1809	1/1	0.91	0.16	47,47,47,47	0
56	MG	2A	3473	1/1	0.91	0.19	59,59,59,59	0
56	MG	2A	3431	1/1	0.91	0.12	55,55,55,55	0
56	MG	2A	3742	1/1	0.91	0.12	53,53,53,53	0
56	MG	11	104	1/1	0.91	0.30	69,69,69,69	0
56	MG	1A	3012	1/1	0.91	0.26	29,29,29,29	0
56	MG	1A	3487	1/1	0.91	0.24	55,55,55,55	0
56	MG	1A	3564	1/1	0.91	0.35	43,43,43,43	0
56	MG	1A	3350	1/1	0.91	0.13	53,53,53,53	0
56	MG	2y	3003	1/1	0.91	0.07	63,63,63,63	0
56	MG	2A	3613	1/1	0.91	0.13	24,24,24,24	0
56	MG	1A	3580	1/1	0.91	0.66	33,33,33,33	0
56	MG	2a	1719	1/1	0.91	0.24	67,67,67,67	0
56	MG	2A	3376	1/1	0.91	0.13	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3768	1/1	0.91	0.10	24,24,24,24	0
56	MG	2A	3353	1/1	0.91	0.52	56,56,56,56	0
56	MG	2A	3565	1/1	0.91	0.11	45,45,45,45	0
56	MG	2A	3685	1/1	0.91	0.11	55,55,55,55	0
56	MG	1A	3766	1/1	0.91	0.07	66,66,66,66	0
56	MG	2A	3888	1/1	0.91	0.33	71,71,71,71	0
56	MG	2A	3648	1/1	0.91	0.08	47,47,47,47	0
56	MG	1A	3382	1/1	0.91	0.16	35,35,35,35	0
56	MG	1A	3727	1/1	0.91	0.13	14,14,14,14	0
56	MG	1A	3409	1/1	0.92	0.17	52,52,52,52	0
56	MG	1A	3957	1/1	0.92	0.10	37,37,37,37	0
56	MG	1A	3416	1/1	0.92	0.17	51,51,51,51	0
56	MG	1A	3324	1/1	0.92	0.15	54,54,54,54	0
56	MG	2x	106	1/1	0.92	0.15	62,62,62,62	0
56	MG	1A	3990	1/1	0.92	0.16	39,39,39,39	0
56	MG	1A	4053	1/1	0.92	0.11	43,43,43,43	0
56	MG	1A	3198	1/1	0.92	0.18	39,39,39,39	0
56	MG	1A	3086	1/1	0.92	0.15	53,53,53,53	0
56	MG	2a	1674	1/1	0.92	0.08	58,58,58,58	0
56	MG	2A	3467	1/1	0.92	0.14	40,40,40,40	0
59	ZN	29	501	1/1	0.92	0.10	74,74,74,74	0
56	MG	2a	1802	1/1	0.92	0.15	60,60,60,60	0
56	MG	1A	3037	1/1	0.92	0.25	54,54,54,54	0
56	MG	2a	1819	1/1	0.92	0.10	61,61,61,61	0
56	MG	1q	201	1/1	0.92	0.09	59,59,59,59	0
56	MG	1W	202	1/1	0.92	0.11	50,50,50,50	0
56	MG	1a	1665	1/1	0.92	0.28	61,61,61,61	0
56	MG	2A	3144	1/1	0.92	0.17	38,38,38,38	0
56	MG	2A	3485	1/1	0.92	0.10	47,47,47,47	0
56	MG	2A	3481	1/1	0.92	0.40	48,48,48,48	0
56	MG	1A	3096	1/1	0.92	0.15	56,56,56,56	0
56	MG	1A	3687	1/1	0.92	0.15	29,29,29,29	0
56	MG	1A	3358	1/1	0.92	0.15	42,42,42,42	0
56	MG	1F	307	1/1	0.92	0.13	44,44,44,44	0
56	MG	1A	3777	1/1	0.92	0.20	20,20,20,20	0
56	MG	2A	3624	1/1	0.92	0.12	33,33,33,33	0
56	MG	2E	305	1/1	0.92	0.08	53,53,53,53	0
56	MG	1A	3429	1/1	0.92	0.30	45,45,45,45	0
56	MG	2a	1626	1/1	0.92	0.37	68,68,68,68	0
56	MG	1a	1702	1/1	0.92	0.15	54,54,54,54	0
56	MG	10	102	1/1	0.92	0.10	40,40,40,40	0
56	MG	1Y	201	1/1	0.92	0.20	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3713	1/1	0.92	0.16	15,15,15,15	0
56	MG	2A	3319	1/1	0.92	0.08	52,52,52,52	0
56	MG	2A	3389	1/1	0.92	0.85	51,51,51,51	0
56	MG	2A	3337	1/1	0.92	0.46	68,68,68,68	0
56	MG	2A	3226	1/1	0.92	0.33	54,54,54,54	0
56	MG	2A	3525	1/1	0.92	0.11	41,41,41,41	0
56	MG	1H	3001	1/1	0.92	0.30	37,37,37,37	0
56	MG	1A	3032	1/1	0.92	0.12	38,38,38,38	0
56	MG	1A	3438	1/1	0.92	0.32	41,41,41,41	0
56	MG	2a	1665	1/1	0.92	0.14	64,64,64,64	0
56	MG	1A	3064	1/1	0.92	0.16	49,49,49,49	0
56	MG	2a	1723	1/1	0.92	0.11	47,47,47,47	0
56	MG	2A	3588	1/1	0.92	0.11	71,71,71,71	0
56	MG	2a	1773	1/1	0.92	0.17	76,76,76,76	0
56	MG	2a	1664	1/1	0.92	0.08	57,57,57,57	0
56	MG	1A	3146	1/1	0.92	0.35	32,32,32,32	0
56	MG	1A	3804	1/1	0.92	0.13	28,28,28,28	0
56	MG	1Z	304	1/1	0.92	0.24	53,53,53,53	0
56	MG	1x	116	1/1	0.92	0.14	62,62,62,62	0
56	MG	2A	3564	1/1	0.92	0.13	36,36,36,36	0
56	MG	1F	301	1/1	0.92	0.17	62,62,62,62	0
56	MG	2A	3560	1/1	0.92	0.14	71,71,71,71	0
56	MG	2A	3770	1/1	0.92	0.17	55,55,55,55	0
56	MG	1A	3098	1/1	0.92	0.16	66,66,66,66	0
56	MG	2a	1743	1/1	0.92	0.10	78,78,78,78	0
56	MG	1B	203	1/1	0.92	0.24	55,55,55,55	0
56	MG	2a	1827	1/1	0.92	0.12	71,71,71,71	0
56	MG	1A	3049	1/1	0.92	0.20	36,36,36,36	0
56	MG	1A	3408	1/1	0.92	0.19	48,48,48,48	0
56	MG	2a	1684	1/1	0.92	0.09	63,63,63,63	0
56	MG	1B	205	1/1	0.92	0.29	60,60,60,60	0
56	MG	1a	1623	1/1	0.92	0.13	48,48,48,48	0
56	MG	26	502	1/1	0.92	0.80	69,69,69,69	0
56	MG	2R	3001	1/1	0.92	0.34	65,65,65,65	0
56	MG	2A	3786	1/1	0.92	0.18	64,64,64,64	0
56	MG	1A	4117	1/1	0.92	0.36	38,38,38,38	0
56	MG	1A	3001	1/1	0.92	0.17	38,38,38,38	0
56	MG	1A	3492	1/1	0.92	0.12	45,45,45,45	0
56	MG	2A	3365	1/1	0.92	0.60	71,71,71,71	0
56	MG	1A	3522	1/1	0.92	0.30	58,58,58,58	0
56	MG	1A	3244	1/1	0.92	0.12	61,61,61,61	0
56	MG	1a	1779	1/1	0.92	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3381	1/1	0.92	0.17	48,48,48,48	0
56	MG	25	103	1/1	0.92	0.14	54,54,54,54	0
56	MG	2A	3637	1/1	0.92	0.08	39,39,39,39	0
56	MG	1X	102	1/1	0.92	0.28	29,29,29,29	0
56	MG	2A	3488	1/1	0.92	0.41	71,71,71,71	0
56	MG	2a	1700	1/1	0.92	0.51	59,59,59,59	0
56	MG	1A	3939	1/1	0.92	0.16	48,48,48,48	0
56	MG	1A	3018	1/1	0.92	0.23	37,37,37,37	0
56	MG	1A	3322	1/1	0.92	0.24	40,40,40,40	0
56	MG	1A	3952	1/1	0.92	0.15	40,40,40,40	0
56	MG	2A	3475	1/1	0.92	0.14	46,46,46,46	0
56	MG	1A	3247	1/1	0.92	0.21	41,41,41,41	0
56	MG	2A	3802	1/1	0.92	0.07	60,60,60,60	0
56	MG	2A	3459	1/1	0.92	0.10	60,60,60,60	0
56	MG	2A	3244	1/1	0.92	0.08	74,74,74,74	0
56	MG	2A	3351	1/1	0.92	0.14	64,64,64,64	0
56	MG	1A	4084	1/1	0.92	0.30	31,31,31,31	0
56	MG	2a	1666	1/1	0.92	0.11	64,64,64,64	0
56	MG	2E	301	1/1	0.92	0.09	49,49,49,49	0
56	MG	2A	3765	1/1	0.92	0.09	56,56,56,56	0
56	MG	1A	4065	1/1	0.92	0.06	37,37,37,37	0
56	MG	1A	3664	1/1	0.92	0.16	66,66,66,66	0
56	MG	1a	1783	1/1	0.92	0.09	58,58,58,58	0
56	MG	1A	3757	1/1	0.92	0.10	30,30,30,30	0
56	MG	1A	3147	1/1	0.92	0.23	33,33,33,33	0
56	MG	1S	3002	1/1	0.92	0.35	49,49,49,49	0
56	MG	2a	1646	1/1	0.92	0.12	53,53,53,53	0
56	MG	1A	3442	1/1	0.92	0.51	48,48,48,48	0
56	MG	1x	105	1/1	0.92	0.22	53,53,53,53	0
56	MG	2A	3582	1/1	0.92	0.17	61,61,61,61	0
56	MG	1A	3652	1/1	0.92	0.09	37,37,37,37	0
56	MG	2A	3213	1/1	0.92	0.24	48,48,48,48	0
56	MG	1a	1741	1/1	0.92	0.12	52,52,52,52	0
56	MG	1A	3265	1/1	0.92	0.15	46,46,46,46	0
56	MG	1A	3213	1/1	0.92	0.21	44,44,44,44	0
56	MG	2A	3828	1/1	0.92	0.08	59,59,59,59	0
56	MG	1B	232	1/1	0.92	0.16	52,52,52,52	0
56	MG	1A	3996	1/1	0.92	0.27	60,60,60,60	0
56	MG	1A	3880	1/1	0.92	0.09	38,38,38,38	0
56	MG	1A	3975	1/1	0.92	0.15	36,36,36,36	0
56	MG	2y	3002	1/1	0.92	0.10	63,63,63,63	0
56	MG	2a	1610	1/1	0.92	0.14	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3637	1/1	0.92	0.15	44,44,44,44	0
56	MG	1A	3084	1/1	0.92	0.20	44,44,44,44	0
56	MG	2A	3010	1/1	0.92	0.17	57,57,57,57	0
56	MG	1F	305	1/1	0.92	0.20	45,45,45,45	0
56	MG	1A	3418	1/1	0.92	0.26	47,47,47,47	0
56	MG	1A	3769	1/1	0.92	0.12	42,42,42,42	0
56	MG	1A	3300	1/1	0.92	0.14	29,29,29,29	0
56	MG	1a	1716	1/1	0.92	0.26	58,58,58,58	0
56	MG	1A	3264	1/1	0.92	0.12	50,50,50,50	0
56	MG	1B	206	1/1	0.92	0.11	34,34,34,34	0
56	MG	1a	1708	1/1	0.92	0.29	49,49,49,49	0
56	MG	2A	3272	1/1	0.92	0.19	47,47,47,47	0
56	MG	2B	3003	1/1	0.92	0.08	60,60,60,60	0
56	MG	2a	1676	1/1	0.92	0.10	63,63,63,63	0
56	MG	1A	4058	1/1	0.92	0.19	36,36,36,36	0
56	MG	1A	3063	1/1	0.92	0.17	30,30,30,30	0
56	MG	1A	3411	1/1	0.92	0.12	58,58,58,58	0
56	MG	1A	3901	1/1	0.92	0.42	48,48,48,48	0
56	MG	1a	1757	1/1	0.92	0.08	61,61,61,61	0
56	MG	1a	1785	1/1	0.92	0.27	69,69,69,69	0
56	MG	1A	3362	1/1	0.92	0.66	50,50,50,50	0
56	MG	2A	3622	1/1	0.92	0.28	67,67,67,67	0
56	MG	1A	3849	1/1	0.92	0.15	38,38,38,38	0
56	MG	2A	3199	1/1	0.92	0.09	54,54,54,54	0
56	MG	2A	3635	1/1	0.92	0.14	39,39,39,39	0
56	MG	1A	3873	1/1	0.92	0.12	25,25,25,25	0
56	MG	1O	202	1/1	0.92	0.16	58,58,58,58	0
56	MG	1A	3857	1/1	0.92	0.28	30,30,30,30	0
56	MG	2A	3850	1/1	0.92	0.19	77,77,77,77	0
56	MG	2A	3746	1/1	0.92	0.12	76,76,76,76	0
56	MG	2A	3764	1/1	0.92	0.15	66,66,66,66	0
56	MG	1A	3726	1/1	0.92	0.16	42,42,42,42	0
56	MG	1a	1829	1/1	0.92	0.36	57,57,57,57	0
56	MG	2A	3247	1/1	0.92	0.31	47,47,47,47	0
56	MG	1A	3891	1/1	0.92	0.16	53,53,53,53	0
56	MG	2N	8001	1/1	0.92	0.13	52,52,52,52	0
56	MG	2A	3136	1/1	0.92	0.16	46,46,46,46	0
56	MG	1A	3218	1/1	0.92	0.21	47,47,47,47	0
56	MG	2a	1624	1/1	0.92	0.17	48,48,48,48	0
56	MG	2A	3877	1/1	0.92	0.16	47,47,47,47	0
56	MG	1A	3273	1/1	0.92	0.36	41,41,41,41	0
56	MG	1D	307	1/1	0.92	0.41	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3413	1/1	0.92	0.21	51,51,51,51	0
56	MG	2A	3369	1/1	0.92	0.20	68,68,68,68	0
56	MG	2A	3445	1/1	0.92	0.28	57,57,57,57	0
56	MG	2B	3001	1/1	0.92	0.11	57,57,57,57	0
56	MG	1A	3022	1/1	0.92	0.18	44,44,44,44	0
56	MG	1A	3458	1/1	0.92	0.22	46,46,46,46	0
56	MG	1A	3133	1/1	0.92	0.31	26,26,26,26	0
56	MG	25	101	1/1	0.92	0.72	56,56,56,56	0
56	MG	1A	3376	1/1	0.92	0.21	44,44,44,44	0
56	MG	2A	3393	1/1	0.92	0.46	55,55,55,55	0
56	MG	1A	3840	1/1	0.92	0.16	47,47,47,47	0
56	MG	1A	4088	1/1	0.92	0.14	36,36,36,36	0
56	MG	2A	3014	1/1	0.92	0.37	51,51,51,51	0
56	MG	2a	1713	1/1	0.92	0.17	76,76,76,76	0
56	MG	1A	4101	1/1	0.92	0.14	43,43,43,43	0
56	MG	1A	3070	1/1	0.92	0.13	27,27,27,27	0
56	MG	1A	3746	1/1	0.92	0.18	22,22,22,22	0
56	MG	1A	3441	1/1	0.92	0.44	42,42,42,42	0
56	MG	1A	3282	1/1	0.92	0.27	45,45,45,45	0
56	MG	1a	1696	1/1	0.92	0.17	50,50,50,50	0
56	MG	2A	3869	1/1	0.92	0.15	46,46,46,46	0
56	MG	2a	1725	1/1	0.92	0.14	66,66,66,66	0
56	MG	2T	3001	1/1	0.92	0.18	52,52,52,52	0
56	MG	1y	3004	1/1	0.92	0.21	83,83,83,83	0
56	MG	2A	3404	1/1	0.92	0.26	52,52,52,52	0
56	MG	1a	1703	1/1	0.92	0.18	49,49,49,49	0
56	MG	2a	1755	1/1	0.92	0.13	70,70,70,70	0
56	MG	2A	3115	1/1	0.92	0.23	58,58,58,58	0
56	MG	2A	3542	1/1	0.92	0.12	43,43,43,43	0
56	MG	2A	3427	1/1	0.92	0.31	60,60,60,60	0
56	MG	2a	1699	1/1	0.92	0.15	62,62,62,62	0
56	MG	1a	1666	1/1	0.92	0.52	64,64,64,64	0
56	MG	1A	3737	1/1	0.93	0.10	34,34,34,34	0
56	MG	2X	102	1/1	0.93	0.18	66,66,66,66	0
56	MG	2a	1765	1/1	0.93	0.08	80,80,80,80	0
56	MG	2B	3010	1/1	0.93	0.07	68,68,68,68	0
56	MG	1A	3728	1/1	0.93	0.19	62,62,62,62	0
56	MG	1A	3390	1/1	0.93	0.38	43,43,43,43	0
56	MG	1A	3303	1/1	0.93	0.27	51,51,51,51	0
56	MG	2A	3736	1/1	0.93	0.21	69,69,69,69	0
56	MG	2A	3531	1/1	0.93	0.12	57,57,57,57	0
56	MG	2A	3890	1/1	0.93	0.59	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3341	1/1	0.93	0.14	50,50,50,50	0
56	MG	1O	208	1/1	0.93	0.18	75,75,75,75	0
56	MG	10	103	1/1	0.93	0.19	35,35,35,35	0
56	MG	1A	3307	1/1	0.93	0.23	44,44,44,44	0
56	MG	2A	3759	1/1	0.93	0.54	39,39,39,39	0
56	MG	1A	3354	1/1	0.93	0.19	50,50,50,50	0
56	MG	1A	4003	1/1	0.93	0.20	27,27,27,27	0
56	MG	2a	1796	1/1	0.93	0.21	69,69,69,69	0
56	MG	1A	3593	1/1	0.93	0.12	33,33,33,33	0
56	MG	1a	1791	1/1	0.93	0.15	53,53,53,53	0
56	MG	1A	3982	1/1	0.93	0.26	40,40,40,40	0
56	MG	1A	4024	1/1	0.93	0.14	46,46,46,46	0
56	MG	1A	3365	1/1	0.93	0.30	39,39,39,39	0
56	MG	1A	4135	1/1	0.93	0.18	36,36,36,36	0
56	MG	1A	3834	1/1	0.93	0.15	40,40,40,40	0
56	MG	1a	1750	1/1	0.93	0.13	63,63,63,63	0
56	MG	1A	3431	1/1	0.93	0.16	46,46,46,46	0
56	MG	1a	1694	1/1	0.93	0.16	58,58,58,58	0
56	MG	1a	1627	1/1	0.93	0.18	23,23,23,23	0
56	MG	1A	4031	1/1	0.93	0.23	52,52,52,52	0
56	MG	2A	3153	1/1	0.93	0.14	69,69,69,69	0
56	MG	2A	3413	1/1	0.93	0.55	55,55,55,55	0
56	MG	1a	1780	1/1	0.93	0.12	51,51,51,51	0
56	MG	1O	205	1/1	0.93	0.41	45,45,45,45	0
56	MG	2A	3552	1/1	0.93	0.14	51,51,51,51	0
56	MG	1A	3457	1/1	0.93	0.28	42,42,42,42	0
56	MG	1a	1705	1/1	0.93	0.25	50,50,50,50	0
56	MG	1a	1642	1/1	0.93	0.10	48,48,48,48	0
56	MG	1A	3383	1/1	0.93	0.23	37,37,37,37	0
56	MG	2A	3159	1/1	0.93	0.49	37,37,37,37	0
56	MG	1x	113	1/1	0.93	0.22	69,69,69,69	0
56	MG	2A	3114	1/1	0.93	0.14	49,49,49,49	0
56	MG	1A	3128	1/1	0.93	0.39	37,37,37,37	0
56	MG	2A	3783	1/1	0.93	0.07	60,60,60,60	0
56	MG	1W	201	1/1	0.93	0.34	50,50,50,50	0
56	MG	1G	3002	1/1	0.93	0.11	46,46,46,46	0
56	MG	1A	4006	1/1	0.93	0.13	25,25,25,25	0
56	MG	2A	3229	1/1	0.93	0.11	58,58,58,58	0
56	MG	1A	4146	1/1	0.93	0.37	38,38,38,38	0
56	MG	2A	3517	1/1	0.93	0.11	51,51,51,51	0
56	MG	1A	3130	1/1	0.93	0.19	37,37,37,37	0
56	MG	2A	3258	1/1	0.93	0.24	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3689	1/1	0.93	0.14	62,62,62,62	0
56	MG	2A	3495	1/1	0.93	0.73	73,73,73,73	0
56	MG	1A	4083	1/1	0.93	0.25	51,51,51,51	0
56	MG	2A	3084	1/1	0.93	0.24	54,54,54,54	0
56	MG	1A	3484	1/1	0.93	0.10	46,46,46,46	0
56	MG	2A	3638	1/1	0.93	0.14	34,34,34,34	0
56	MG	1A	3587	1/1	0.93	0.17	27,27,27,27	0
56	MG	2A	3148	1/1	0.93	0.10	58,58,58,58	0
56	MG	1A	3554	1/1	0.93	0.10	51,51,51,51	0
56	MG	2A	3225	1/1	0.93	0.15	51,51,51,51	0
56	MG	2A	3793	1/1	0.93	0.28	60,60,60,60	0
56	MG	1A	3509	1/1	0.93	0.26	38,38,38,38	0
56	MG	1A	3530	1/1	0.93	0.12	45,45,45,45	0
56	MG	1A	3695	1/1	0.93	0.29	58,58,58,58	0
56	MG	1A	4010	1/1	0.93	0.14	47,47,47,47	0
56	MG	1A	3398	1/1	0.93	0.37	38,38,38,38	0
56	MG	2a	1731	1/1	0.93	0.12	55,55,55,55	0
56	MG	1l	102	1/1	0.93	0.36	39,39,39,39	0
56	MG	2A	3202	1/1	0.93	0.12	46,46,46,46	0
56	MG	2a	1753	1/1	0.93	0.06	48,48,48,48	0
56	MG	1A	3448	1/1	0.93	0.18	50,50,50,50	0
56	MG	1A	3393	1/1	0.93	0.22	48,48,48,48	0
58	K	1A	4148	1/1	0.93	0.13	56,56,56,56	0
56	MG	2a	1788	1/1	0.93	0.09	71,71,71,71	0
56	MG	2a	1717	1/1	0.93	0.12	58,58,58,58	0
56	MG	1Q	201	1/1	0.93	0.21	26,26,26,26	0
56	MG	1A	3500	1/1	0.93	0.26	33,33,33,33	0
56	MG	2A	3049	1/1	0.93	0.14	57,57,57,57	0
56	MG	1A	3720	1/1	0.93	0.15	52,52,52,52	0
56	MG	2A	3792	1/1	0.93	0.11	55,55,55,55	0
56	MG	2A	3436	1/1	0.93	0.17	43,43,43,43	0
56	MG	2A	3811	1/1	0.93	0.21	59,59,59,59	0
56	MG	1A	3048	1/1	0.93	0.26	22,22,22,22	0
56	MG	1A	4109	1/1	0.93	0.30	30,30,30,30	0
56	MG	1E	309	1/1	0.93	0.13	51,51,51,51	0
56	MG	1A	3380	1/1	0.93	0.25	38,38,38,38	0
56	MG	1A	3601	1/1	0.93	0.08	61,61,61,61	0
56	MG	1A	4039	1/1	0.93	0.10	48,48,48,48	0
56	MG	1a	1824	1/1	0.93	0.18	36,36,36,36	0
56	MG	16	103	1/1	0.93	0.23	53,53,53,53	0
56	MG	2A	3227	1/1	0.93	0.09	57,57,57,57	0
56	MG	1Z	301	1/1	0.93	0.18	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3464	1/1	0.93	0.27	34,34,34,34	0
56	MG	2A	3604	1/1	0.93	0.21	55,55,55,55	0
56	MG	2A	3268	1/1	0.93	0.33	60,60,60,60	0
56	MG	2A	3875	1/1	0.93	0.12	60,60,60,60	0
56	MG	1a	1764	1/1	0.93	0.16	63,63,63,63	0
56	MG	1A	3053	1/1	0.93	0.16	33,33,33,33	0
56	MG	1A	3716	1/1	0.93	0.13	65,65,65,65	0
56	MG	1A	3465	1/1	0.93	0.19	46,46,46,46	0
56	MG	1A	3657	1/1	0.93	0.16	29,29,29,29	0
56	MG	15	103	1/1	0.93	0.12	45,45,45,45	0
56	MG	1A	3588	1/1	0.93	0.13	48,48,48,48	0
56	MG	2A	3372	1/1	0.93	0.51	50,50,50,50	0
56	MG	2A	3749	1/1	0.93	0.09	52,52,52,52	0
56	MG	1A	3892	1/1	0.93	0.18	38,38,38,38	0
56	MG	2A	3756	1/1	0.93	0.21	55,55,55,55	0
56	MG	1A	3148	1/1	0.93	0.13	33,33,33,33	0
56	MG	2A	3235	1/1	0.93	0.34	42,42,42,42	0
56	MG	2A	3405	1/1	0.93	0.13	48,48,48,48	0
56	MG	2A	3511	1/1	0.93	0.12	24,24,24,24	0
56	MG	1A	3781	1/1	0.93	0.13	36,36,36,36	0
56	MG	2A	3509	1/1	0.93	0.10	36,36,36,36	0
56	MG	1A	4091	1/1	0.93	0.34	46,46,46,46	0
56	MG	1A	3916	1/1	0.93	0.16	39,39,39,39	0
56	MG	2A	3031	1/1	0.93	0.12	45,45,45,45	0
56	MG	2A	3116	1/1	0.93	0.17	56,56,56,56	0
56	MG	1A	3229	1/1	0.93	0.20	54,54,54,54	0
56	MG	10	104	1/1	0.93	0.44	41,41,41,41	0
56	MG	1A	3126	1/1	0.93	0.16	28,28,28,28	0
56	MG	1A	3340	1/1	0.93	0.27	38,38,38,38	0
56	MG	2A	3282	1/1	0.93	0.21	58,58,58,58	0
56	MG	2a	1786	1/1	0.93	0.15	66,66,66,66	0
56	MG	2A	3557	1/1	0.93	0.07	47,47,47,47	0
56	MG	2A	3316	1/1	0.93	0.13	52,52,52,52	0
56	MG	1A	3943	1/1	0.93	0.17	53,53,53,53	0
56	MG	1Z	302	1/1	0.93	0.16	40,40,40,40	0
56	MG	1A	4055	1/1	0.93	0.12	47,47,47,47	0
56	MG	1A	3079	1/1	0.93	0.12	36,36,36,36	0
56	MG	2A	3192	1/1	0.93	0.12	55,55,55,55	0
56	MG	1A	4105	1/1	0.93	0.19	41,41,41,41	0
56	MG	1A	3320	1/1	0.93	0.15	57,57,57,57	0
56	MG	1A	3926	1/1	0.93	0.14	31,31,31,31	0
56	MG	1A	3845	1/1	0.93	0.10	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3762	1/1	0.93	0.08	58,58,58,58	0
59	ZN	2Y	501	1/1	0.93	0.14	87,87,87,87	0
56	MG	1A	3676	1/1	0.93	0.18	31,31,31,31	0
56	MG	1a	1747	1/1	0.93	0.11	51,51,51,51	0
56	MG	1A	3591	1/1	0.93	0.19	29,29,29,29	0
56	MG	1A	3577	1/1	0.93	0.19	29,29,29,29	0
56	MG	1a	1643	1/1	0.93	0.14	47,47,47,47	0
56	MG	2A	3606	1/1	0.93	0.15	65,65,65,65	0
56	MG	1A	3233	1/1	0.93	0.29	26,26,26,26	0
56	MG	2A	3838	1/1	0.93	0.07	53,53,53,53	0
56	MG	1A	3108	1/1	0.93	0.23	32,32,32,32	0
56	MG	1W	206	1/1	0.93	0.24	19,19,19,19	0
56	MG	1A	3560	1/1	0.93	0.28	43,43,43,43	0
56	MG	2A	3374	1/1	0.93	0.33	48,48,48,48	0
56	MG	1A	3533	1/1	0.93	0.36	43,43,43,43	0
56	MG	2A	3044	1/1	0.93	0.19	56,56,56,56	0
56	MG	2A	3660	1/1	0.93	0.11	57,57,57,57	0
56	MG	2A	3778	1/1	0.93	0.14	71,71,71,71	0
56	MG	1A	3396	1/1	0.93	0.19	36,36,36,36	0
56	MG	1a	1608	1/1	0.93	0.09	56,56,56,56	0
56	MG	2A	3865	1/1	0.93	0.07	40,40,40,40	0
56	MG	2A	3325	1/1	0.93	0.07	53,53,53,53	0
56	MG	2a	1834	1/1	0.93	0.20	81,81,81,81	0
56	MG	1B	204	1/1	0.93	0.19	42,42,42,42	0
56	MG	2A	3085	1/1	0.93	0.16	41,41,41,41	0
56	MG	2A	3290	1/1	0.93	0.73	64,64,64,64	0
56	MG	1A	3272	1/1	0.93	0.17	42,42,42,42	0
56	MG	2a	1833	1/1	0.93	0.06	52,52,52,52	0
56	MG	2A	3735	1/1	0.93	0.08	69,69,69,69	0
56	MG	1A	3113	1/1	0.93	0.19	25,25,25,25	0
56	MG	1A	4115	1/1	0.93	0.10	33,33,33,33	0
56	MG	1A	3310	1/1	0.93	0.23	52,52,52,52	0
56	MG	2a	1780	1/1	0.93	0.09	57,57,57,57	0
56	MG	2A	3518	1/1	0.93	0.11	67,67,67,67	0
56	MG	1A	3594	1/1	0.93	0.18	45,45,45,45	0
56	MG	2A	3463	1/1	0.93	0.15	47,47,47,47	0
56	MG	2A	3019	1/1	0.93	0.26	37,37,37,37	0
56	MG	2a	1744	1/1	0.93	0.13	81,81,81,81	0
56	MG	2B	3013	1/1	0.93	0.21	68,68,68,68	0
56	MG	2a	1800	1/1	0.93	0.16	60,60,60,60	0
56	MG	1A	3269	1/1	0.93	0.21	36,36,36,36	0
56	MG	2A	3460	1/1	0.93	0.13	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3788	1/1	0.93	0.10	30,30,30,30	0
56	MG	1A	3790	1/1	0.93	0.12	45,45,45,45	0
56	MG	2a	1641	1/1	0.93	0.12	71,71,71,71	0
56	MG	1A	3599	1/1	0.93	0.20	25,25,25,25	0
56	MG	1A	4081	1/1	0.93	0.16	39,39,39,39	0
56	MG	2A	3558	1/1	0.93	0.13	30,30,30,30	0
56	MG	1A	3335	1/1	0.93	0.21	43,43,43,43	0
56	MG	1O	201	1/1	0.93	0.17	54,54,54,54	0
56	MG	2A	3544	1/1	0.93	0.17	45,45,45,45	0
56	MG	1a	1776	1/1	0.93	0.21	46,46,46,46	0
56	MG	2a	1693	1/1	0.93	0.11	40,40,40,40	0
56	MG	2A	3348	1/1	0.93	0.09	44,44,44,44	0
56	MG	25	104	1/1	0.93	0.16	52,52,52,52	0
56	MG	1A	3763	1/1	0.93	0.16	48,48,48,48	0
56	MG	1A	3122	1/1	0.93	0.66	40,40,40,40	0
56	MG	2A	3571	1/1	0.94	0.11	36,36,36,36	0
56	MG	1A	3279	1/1	0.94	0.48	25,25,25,25	0
56	MG	1A	3190	1/1	0.94	0.35	30,30,30,30	0
56	MG	1O	207	1/1	0.94	0.30	67,67,67,67	0
56	MG	1A	3425	1/1	0.94	0.22	46,46,46,46	0
56	MG	1E	311	1/1	0.94	0.14	49,49,49,49	0
56	MG	2a	1838	1/1	0.94	0.12	64,64,64,64	0
56	MG	2A	3172	1/1	0.94	0.07	66,66,66,66	0
56	MG	1A	3640	1/1	0.94	0.17	28,28,28,28	0
56	MG	1A	3082	1/1	0.94	0.26	29,29,29,29	0
56	MG	1A	3718	1/1	0.94	0.14	38,38,38,38	0
56	MG	1A	3456	1/1	0.94	0.14	33,33,33,33	0
56	MG	1A	3375	1/1	0.94	0.43	39,39,39,39	0
56	MG	1A	3422	1/1	0.94	0.50	46,46,46,46	0
56	MG	1a	1724	1/1	0.94	0.14	43,43,43,43	0
56	MG	2A	3056	1/1	0.94	0.31	45,45,45,45	0
56	MG	1A	3791	1/1	0.94	0.20	47,47,47,47	0
56	MG	2A	3717	1/1	0.94	0.09	40,40,40,40	0
56	MG	2A	3692	1/1	0.94	0.10	65,65,65,65	0
56	MG	1A	3629	1/1	0.94	0.11	32,32,32,32	0
56	MG	1A	4125	1/1	0.94	0.21	38,38,38,38	0
56	MG	2A	3584	1/1	0.94	0.22	62,62,62,62	0
56	MG	2A	3173	1/1	0.94	0.09	77,77,77,77	0
56	MG	1a	1753	1/1	0.94	0.12	56,56,56,56	0
56	MG	1Y	204	1/1	0.94	0.53	48,48,48,48	0
56	MG	1A	3885	1/1	0.94	0.11	40,40,40,40	0
56	MG	2A	3160	1/1	0.94	0.35	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3241	1/1	0.94	0.44	58,58,58,58	0
56	MG	1S	3003	1/1	0.94	0.08	64,64,64,64	0
56	MG	2A	3706	1/1	0.94	0.06	68,68,68,68	0
56	MG	2q	3002	1/1	0.94	0.13	74,74,74,74	0
56	MG	2A	3024	1/1	0.94	0.46	47,47,47,47	0
56	MG	1A	3069	1/1	0.94	0.38	55,55,55,55	0
56	MG	2A	3007	1/1	0.94	0.11	53,53,53,53	0
56	MG	2A	3386	1/1	0.94	0.18	67,67,67,67	0
56	MG	1A	3579	1/1	0.94	0.17	43,43,43,43	0
56	MG	1A	3639	1/1	0.94	0.13	51,51,51,51	0
56	MG	1A	3260	1/1	0.94	0.18	47,47,47,47	0
56	MG	1A	3604	1/1	0.94	0.17	25,25,25,25	0
56	MG	2A	3470	1/1	0.94	0.11	51,51,51,51	0
56	MG	1A	3093	1/1	0.94	0.11	29,29,29,29	0
56	MG	1A	3132	1/1	0.94	0.12	44,44,44,44	0
56	MG	2A	3563	1/1	0.94	0.10	65,65,65,65	0
56	MG	1y	3001	1/1	0.94	0.12	62,62,62,62	0
56	MG	2A	3817	1/1	0.94	0.06	84,84,84,84	0
56	MG	2A	3895	1/1	0.94	0.16	62,62,62,62	0
56	MG	2a	1628	1/1	0.94	0.77	56,56,56,56	0
56	MG	1a	1714	1/1	0.94	0.14	48,48,48,48	0
56	MG	1A	3878	1/1	0.94	0.10	39,39,39,39	0
56	MG	1A	3025	1/1	0.94	0.22	73,73,73,73	0
56	MG	1a	1727	1/1	0.94	0.22	65,65,65,65	0
56	MG	1Q	203	1/1	0.94	0.21	51,51,51,51	0
56	MG	2A	3696	1/1	0.94	0.29	79,79,79,79	0
56	MG	2A	3474	1/1	0.94	0.14	46,46,46,46	0
56	MG	1A	3742	1/1	0.94	0.16	49,49,49,49	0
56	MG	2A	3504	1/1	0.94	0.07	51,51,51,51	0
56	MG	1A	3339	1/1	0.94	0.58	47,47,47,47	0
56	MG	2A	3328	1/1	0.94	0.14	55,55,55,55	0
56	MG	2A	3206	1/1	0.94	0.10	59,59,59,59	0
56	MG	1V	203	1/1	0.94	0.11	49,49,49,49	0
56	MG	1x	112	1/1	0.94	0.10	64,64,64,64	0
56	MG	2A	3017	1/1	0.94	0.14	46,46,46,46	0
56	MG	1A	3823	1/1	0.94	0.20	47,47,47,47	0
56	MG	1A	3571	1/1	0.94	0.22	35,35,35,35	0
56	MG	2A	3069	1/1	0.94	0.11	29,29,29,29	0
56	MG	1a	1647	1/1	0.94	0.12	56,56,56,56	0
56	MG	2A	3336	1/1	0.94	0.28	67,67,67,67	0
56	MG	1A	3424	1/1	0.94	0.14	38,38,38,38	0
56	MG	1A	3242	1/1	0.94	0.17	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1663	1/1	0.94	0.12	66,66,66,66	0
56	MG	1N	206	1/1	0.94	0.25	31,31,31,31	0
56	MG	1A	3692	1/1	0.94	0.20	56,56,56,56	0
56	MG	2A	3670	1/1	0.94	0.21	55,55,55,55	0
56	MG	1A	3847	1/1	0.94	0.16	54,54,54,54	0
56	MG	1A	3170	1/1	0.94	0.26	33,33,33,33	0
56	MG	2A	3383	1/1	0.94	0.10	51,51,51,51	0
56	MG	2a	1822	1/1	0.94	0.07	65,65,65,65	0
56	MG	2A	3138	1/1	0.94	0.49	43,43,43,43	0
56	MG	1A	3447	1/1	0.94	0.32	42,42,42,42	0
56	MG	2E	306	1/1	0.94	0.13	40,40,40,40	0
56	MG	1A	3900	1/1	0.94	0.20	41,41,41,41	0
56	MG	1A	4063	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3265	1/1	0.94	0.16	56,56,56,56	0
56	MG	2A	3535	1/1	0.94	0.22	53,53,53,53	0
56	MG	1A	3194	1/1	0.94	0.12	38,38,38,38	0
56	MG	20	101	1/1	0.94	0.14	48,48,48,48	0
56	MG	2A	3658	1/1	0.94	0.09	54,54,54,54	0
56	MG	1P	202	1/1	0.94	0.50	28,28,28,28	0
56	MG	2a	1718	1/1	0.94	0.71	69,69,69,69	0
56	MG	2A	3132	1/1	0.94	0.10	55,55,55,55	0
56	MG	2A	3837	1/1	0.94	0.12	33,33,33,33	0
56	MG	1A	3953	1/1	0.94	0.13	46,46,46,46	0
56	MG	1A	3656	1/1	0.94	0.20	19,19,19,19	0
56	MG	2A	3750	1/1	0.94	0.12	49,49,49,49	0
56	MG	1a	1673	1/1	0.94	0.19	55,55,55,55	0
56	MG	2A	3843	1/1	0.94	0.15	52,52,52,52	0
56	MG	2A	3625	1/1	0.94	0.29	63,63,63,63	0
56	MG	2A	3859	1/1	0.94	0.06	52,52,52,52	0
56	MG	1A	3961	1/1	0.94	0.05	60,60,60,60	0
56	MG	1A	3439	1/1	0.94	0.26	29,29,29,29	0
56	MG	2A	3719	1/1	0.94	0.26	61,61,61,61	0
56	MG	1a	1653	1/1	0.94	0.14	70,70,70,70	0
56	MG	1A	4138	1/1	0.94	0.13	35,35,35,35	0
56	MG	1N	203	1/1	0.94	0.18	42,42,42,42	0
56	MG	2A	3576	1/1	0.94	0.13	41,41,41,41	0
56	MG	2A	3727	1/1	0.94	0.15	42,42,42,42	0
56	MG	1A	3614	1/1	0.94	0.14	22,22,22,22	0
56	MG	1A	3009	1/1	0.94	0.17	30,30,30,30	0
56	MG	2a	1798	1/1	0.94	0.22	53,53,53,53	0
56	MG	1A	4028	1/1	0.94	0.14	55,55,55,55	0
56	MG	1A	3521	1/1	0.94	0.31	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1695	1/1	0.94	0.11	51,51,51,51	0
56	MG	1A	4060	1/1	0.94	0.13	37,37,37,37	0
56	MG	1A	3706	1/1	0.94	0.10	51,51,51,51	0
56	MG	27	101	1/1	0.94	0.16	48,48,48,48	0
56	MG	1A	3270	1/1	0.94	0.16	53,53,53,53	0
56	MG	1A	3709	1/1	0.94	0.17	55,55,55,55	0
56	MG	1A	4000	1/1	0.94	0.16	29,29,29,29	0
56	MG	2A	3451	1/1	0.94	0.25	61,61,61,61	0
56	MG	1A	3570	1/1	0.94	0.23	27,27,27,27	0
56	MG	1a	1811	1/1	0.94	0.11	63,63,63,63	0
56	MG	1A	3178	1/1	0.94	0.15	61,61,61,61	0
56	MG	1A	3529	1/1	0.94	0.36	45,45,45,45	0
56	MG	2A	3061	1/1	0.94	0.16	58,58,58,58	0
56	MG	1A	3536	1/1	0.94	0.19	39,39,39,39	0
56	MG	1A	3893	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3152	1/1	0.94	0.25	30,30,30,30	0
56	MG	1A	3633	1/1	0.94	0.09	45,45,45,45	0
56	MG	1A	3101	1/1	0.94	0.24	45,45,45,45	0
56	MG	2d	502	1/1	0.94	0.15	74,74,74,74	0
56	MG	1A	4139	1/1	0.94	0.16	33,33,33,33	0
56	MG	1A	3887	1/1	0.94	0.31	20,20,20,20	0
56	MG	1V	202	1/1	0.94	0.24	35,35,35,35	0
56	MG	1a	1645	1/1	0.94	0.17	50,50,50,50	0
56	MG	1A	3224	1/1	0.94	0.21	39,39,39,39	0
56	MG	1a	1760	1/1	0.94	0.10	61,61,61,61	0
56	MG	1A	3006	1/1	0.94	0.08	24,24,24,24	0
56	MG	1A	3081	1/1	0.94	0.39	29,29,29,29	0
56	MG	1O	204	1/1	0.94	0.55	62,62,62,62	0
56	MG	2A	3239	1/1	0.94	0.53	39,39,39,39	0
56	MG	1A	3678	1/1	0.94	0.16	14,14,14,14	0
56	MG	1a	1701	1/1	0.94	0.08	59,59,59,59	0
56	MG	2A	3072	1/1	0.94	0.12	53,53,53,53	0
56	MG	2A	3420	1/1	0.94	0.10	72,72,72,72	0
56	MG	1A	3043	1/1	0.94	0.10	26,26,26,26	0
56	MG	2A	3036	1/1	0.94	0.16	35,35,35,35	0
56	MG	1A	3188	1/1	0.94	0.39	32,32,32,32	0
56	MG	2A	3294	1/1	0.94	0.44	47,47,47,47	0
56	MG	2A	3207	1/1	0.94	0.23	55,55,55,55	0
56	MG	1A	3514	1/1	0.94	0.26	24,24,24,24	0
56	MG	2A	3608	1/1	0.94	0.08	63,63,63,63	0
56	MG	1F	302	1/1	0.94	0.10	31,31,31,31	0
56	MG	2A	3515	1/1	0.94	0.17	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3884	1/1	0.94	0.15	45,45,45,45	0
56	MG	2A	3093	1/1	0.94	0.65	53,53,53,53	0
56	MG	2A	3629	1/1	0.94	0.17	44,44,44,44	0
56	MG	1A	3175	1/1	0.94	0.16	41,41,41,41	0
56	MG	1A	3711	1/1	0.94	0.11	37,37,37,37	0
56	MG	1A	4130	1/1	0.94	0.40	36,36,36,36	0
56	MG	1A	3474	1/1	0.94	0.32	48,48,48,48	0
56	MG	1A	3754	1/1	0.94	0.10	53,53,53,53	0
56	MG	2A	3275	1/1	0.94	0.14	56,56,56,56	0
56	MG	1A	3177	1/1	0.94	0.22	55,55,55,55	0
56	MG	1a	1802	1/1	0.94	0.09	54,54,54,54	0
56	MG	2R	3002	1/1	0.94	0.14	52,52,52,52	0
56	MG	1a	1690	1/1	0.94	0.11	56,56,56,56	0
56	MG	1A	3472	1/1	0.94	0.11	48,48,48,48	0
56	MG	1a	1638	1/1	0.94	0.20	53,53,53,53	0
56	MG	2A	3221	1/1	0.94	0.09	42,42,42,42	0
56	MG	1D	311	1/1	0.94	0.26	43,43,43,43	0
56	MG	1A	3972	1/1	0.94	0.26	63,63,63,63	0
56	MG	2A	3572	1/1	0.94	0.11	58,58,58,58	0
56	MG	1A	3545	1/1	0.94	0.22	22,22,22,22	0
56	MG	1A	3237	1/1	0.94	0.57	51,51,51,51	0
56	MG	1A	3091	1/1	0.94	0.23	43,43,43,43	0
56	MG	1A	3814	1/1	0.94	0.12	48,48,48,48	0
56	MG	1A	3513	1/1	0.94	0.20	56,56,56,56	0
56	MG	2A	3581	1/1	0.94	0.14	30,30,30,30	0
56	MG	1A	4104	1/1	0.94	0.20	37,37,37,37	0
56	MG	2a	1692	1/1	0.94	0.08	52,52,52,52	0
56	MG	1A	3150	1/1	0.94	0.12	45,45,45,45	0
56	MG	2A	3378	1/1	0.94	0.28	57,57,57,57	0
56	MG	1a	1613	1/1	0.94	0.08	47,47,47,47	0
56	MG	1A	3608	1/1	0.94	0.14	17,17,17,17	0
56	MG	2A	3134	1/1	0.94	0.12	38,38,38,38	0
56	MG	1A	3216	1/1	0.94	0.17	40,40,40,40	0
56	MG	1A	3503	1/1	0.94	0.13	54,54,54,54	0
56	MG	2A	3739	1/1	0.94	0.07	52,52,52,52	0
56	MG	1A	3815	1/1	0.94	0.07	53,53,53,53	0
56	MG	1A	3182	1/1	0.94	0.20	41,41,41,41	0
56	MG	1a	1699	1/1	0.94	0.09	74,74,74,74	0
56	MG	2G	3001	1/1	0.94	0.09	62,62,62,62	0
56	MG	2A	3627	1/1	0.94	0.08	37,37,37,37	0
56	MG	1A	3290	1/1	0.94	0.17	38,38,38,38	0
56	MG	1A	3679	1/1	0.94	0.14	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3659	1/1	0.94	0.08	67,67,67,67	0
56	MG	1A	3179	1/1	0.94	0.21	36,36,36,36	0
56	MG	2A	3271	1/1	0.94	0.14	68,68,68,68	0
56	MG	1a	1739	1/1	0.94	0.10	64,64,64,64	0
56	MG	2A	3193	1/1	0.94	0.21	62,62,62,62	0
56	MG	1A	3041	1/1	0.94	0.23	35,35,35,35	0
56	MG	2A	3191	1/1	0.94	0.26	71,71,71,71	0
56	MG	1h	3001	1/1	0.94	0.24	64,64,64,64	0
56	MG	1A	3419	1/1	0.94	0.16	39,39,39,39	0
56	MG	2A	3580	1/1	0.94	0.17	67,67,67,67	0
56	MG	1A	3071	1/1	0.94	0.09	31,31,31,31	0
56	MG	1A	3515	1/1	0.94	0.20	28,28,28,28	0
56	MG	1a	1631	1/1	0.94	0.30	59,59,59,59	0
56	MG	1A	3075	1/1	0.94	0.23	47,47,47,47	0
56	MG	2A	3884	1/1	0.94	1.20	66,66,66,66	0
56	MG	1A	3395	1/1	0.94	0.30	43,43,43,43	0
56	MG	2A	3147	1/1	0.94	0.11	56,56,56,56	0
56	MG	2B	3015	1/1	0.94	0.19	59,59,59,59	0
56	MG	2A	3887	1/1	0.94	0.11	51,51,51,51	0
56	MG	1a	1770	1/1	0.94	0.10	62,62,62,62	0
56	MG	1A	4099	1/1	0.94	0.31	51,51,51,51	0
56	MG	2A	3873	1/1	0.94	0.15	46,46,46,46	0
56	MG	1A	3918	1/1	0.94	0.09	44,44,44,44	0
56	MG	2A	3632	1/1	0.94	0.09	47,47,47,47	0
56	MG	1A	3865	1/1	0.94	0.15	25,25,25,25	0
56	MG	2A	3041	1/1	0.94	0.35	52,52,52,52	0
56	MG	1A	3630	1/1	0.94	0.09	56,56,56,56	0
56	MG	2A	3886	1/1	0.94	0.94	54,54,54,54	0
56	MG	1E	306	1/1	0.94	0.13	32,32,32,32	0
56	MG	1A	3602	1/1	0.94	0.18	29,29,29,29	0
56	MG	1A	3675	1/1	0.94	0.14	51,51,51,51	0
56	MG	2A	3855	1/1	0.94	0.08	49,49,49,49	0
56	MG	2A	3900	1/1	0.94	0.52	44,44,44,44	0
56	MG	1A	3636	1/1	0.94	0.20	28,28,28,28	0
56	MG	1A	3450	1/1	0.94	0.41	46,46,46,46	0
56	MG	1A	3739	1/1	0.94	0.16	44,44,44,44	0
56	MG	1A	3326	1/1	0.94	0.15	46,46,46,46	0
56	MG	1a	1663	1/1	0.94	0.09	64,64,64,64	0
56	MG	1B	218	1/1	0.94	0.18	58,58,58,58	0
56	MG	1A	3154	1/1	0.94	0.34	31,31,31,31	0
56	MG	1A	3654	1/1	0.94	0.17	20,20,20,20	0
56	MG	2A	3676	1/1	0.94	0.17	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3275	1/1	0.94	0.24	27,27,27,27	0
56	MG	1A	3774	1/1	0.94	0.16	49,49,49,49	0
56	MG	2A	3161	1/1	0.94	0.12	71,71,71,71	0
56	MG	2a	1698	1/1	0.94	0.14	51,51,51,51	0
56	MG	2A	3569	1/1	0.94	0.17	61,61,61,61	0
56	MG	1A	3145	1/1	0.94	0.57	37,37,37,37	0
56	MG	1A	4137	1/1	0.94	0.75	39,39,39,39	0
56	MG	2A	3780	1/1	0.94	0.15	53,53,53,53	0
56	MG	1A	3738	1/1	0.94	0.19	45,45,45,45	0
56	MG	1A	3313	1/1	0.94	0.11	38,38,38,38	0
56	MG	2U	201	1/1	0.94	0.13	47,47,47,47	0
56	MG	1N	201	1/1	0.94	0.34	43,43,43,43	0
56	MG	1A	3868	1/1	0.94	0.19	30,30,30,30	0
56	MG	1A	3208	1/1	0.94	0.10	35,35,35,35	0
56	MG	1A	3837	1/1	0.94	0.16	25,25,25,25	0
56	MG	2a	1694	1/1	0.94	0.16	67,67,67,67	0
56	MG	2A	3827	1/1	0.94	0.12	44,44,44,44	0
56	MG	2A	3512	1/1	0.94	0.07	66,66,66,66	0
56	MG	17	103	1/1	0.94	0.08	60,60,60,60	0
56	MG	2j	8002	1/1	0.94	0.14	82,82,82,82	0
56	MG	1A	3925	1/1	0.95	0.09	59,59,59,59	0
56	MG	1a	1679	1/1	0.95	0.14	56,56,56,56	0
56	MG	1B	213	1/1	0.95	0.09	49,49,49,49	0
56	MG	2A	3747	1/1	0.95	0.12	55,55,55,55	0
56	MG	1a	1681	1/1	0.95	0.07	51,51,51,51	0
56	MG	1A	3183	1/1	0.95	0.28	35,35,35,35	0
56	MG	2A	3602	1/1	0.95	0.16	55,55,55,55	0
56	MG	1A	3168	1/1	0.95	0.45	32,32,32,32	0
56	MG	1A	3628	1/1	0.95	0.18	32,32,32,32	0
56	MG	1o	3001	1/1	0.95	0.12	64,64,64,64	0
56	MG	1A	4080	1/1	0.95	0.18	19,19,19,19	0
56	MG	2A	3291	1/1	0.95	0.21	58,58,58,58	0
56	MG	2A	3520	1/1	0.95	0.09	69,69,69,69	0
56	MG	2A	3585	1/1	0.95	0.11	62,62,62,62	0
56	MG	1A	4007	1/1	0.95	0.08	29,29,29,29	0
56	MG	2a	1763	1/1	0.95	0.07	75,75,75,75	0
56	MG	1A	4052	1/1	0.95	0.15	18,18,18,18	0
56	MG	10	101	1/1	0.95	0.10	44,44,44,44	0
56	MG	2B	3004	1/1	0.95	0.12	66,66,66,66	0
56	MG	1A	3412	1/1	0.95	0.22	36,36,36,36	0
56	MG	1A	4097	1/1	0.95	0.21	39,39,39,39	0
56	MG	2A	3516	1/1	0.95	0.11	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3698	1/1	0.95	0.10	33,33,33,33	0
56	MG	1a	1737	1/1	0.95	0.14	39,39,39,39	0
56	MG	1A	3040	1/1	0.95	0.48	33,33,33,33	0
56	MG	1a	1807	1/1	0.95	0.25	54,54,54,54	0
56	MG	2a	1825	1/1	0.95	0.30	74,74,74,74	0
56	MG	2A	3437	1/1	0.95	0.11	51,51,51,51	0
56	MG	2A	3168	1/1	0.95	0.12	53,53,53,53	0
56	MG	1A	3305	1/1	0.95	0.18	51,51,51,51	0
56	MG	1N	202	1/1	0.95	0.12	35,35,35,35	0
56	MG	1A	3524	1/1	0.95	0.08	59,59,59,59	0
56	MG	1A	3325	1/1	0.95	0.25	45,45,45,45	0
56	MG	2A	3654	1/1	0.95	0.15	52,52,52,52	0
56	MG	1A	3859	1/1	0.95	0.24	29,29,29,29	0
56	MG	1a	1744	1/1	0.95	0.13	60,60,60,60	0
56	MG	2a	1620	1/1	0.95	0.35	63,63,63,63	0
56	MG	2A	3407	1/1	0.95	0.12	61,61,61,61	0
56	MG	1A	3558	1/1	0.95	0.23	23,23,23,23	0
56	MG	2A	3732	1/1	0.95	0.09	40,40,40,40	0
56	MG	1A	3671	1/1	0.95	0.17	30,30,30,30	0
56	MG	1A	4123	1/1	0.95	0.22	31,31,31,31	0
56	MG	1A	3841	1/1	0.95	0.42	36,36,36,36	0
56	MG	2a	1775	1/1	0.95	0.08	62,62,62,62	0
56	MG	1A	3864	1/1	0.95	0.08	49,49,49,49	0
56	MG	2A	3555	1/1	0.95	0.12	34,34,34,34	0
56	MG	2A	3657	1/1	0.95	0.43	55,55,55,55	0
56	MG	1A	3848	1/1	0.95	0.11	33,33,33,33	0
56	MG	2A	3279	1/1	0.95	0.16	64,64,64,64	0
56	MG	1B	231	1/1	0.95	0.11	42,42,42,42	0
56	MG	1A	3894	1/1	0.95	0.64	37,37,37,37	0
56	MG	1A	4090	1/1	0.95	0.13	48,48,48,48	0
56	MG	1a	1810	1/1	0.95	0.21	61,61,61,61	0
56	MG	1l	201	1/1	0.95	0.16	38,38,38,38	0
56	MG	1a	1636	1/1	0.95	0.10	58,58,58,58	0
56	MG	1A	3251	1/1	0.95	0.14	40,40,40,40	0
56	MG	1A	3595	1/1	0.95	0.13	51,51,51,51	0
56	MG	2A	3679	1/1	0.95	0.08	43,43,43,43	0
56	MG	2A	3414	1/1	0.95	0.23	52,52,52,52	0
56	MG	1A	3486	1/1	0.95	0.20	51,51,51,51	0
56	MG	1A	3058	1/1	0.95	0.14	69,69,69,69	0
56	MG	2A	3443	1/1	0.95	0.23	44,44,44,44	0
56	MG	2A	3551	1/1	0.95	0.10	33,33,33,33	0
56	MG	2A	3121	1/1	0.95	0.27	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3179	1/1	0.95	0.17	35,35,35,35	0
56	MG	1A	3377	1/1	0.95	0.10	49,49,49,49	0
56	MG	1a	1778	1/1	0.95	0.10	59,59,59,59	0
56	MG	1A	3181	1/1	0.95	0.31	33,33,33,33	0
56	MG	1A	3016	1/1	0.95	0.13	62,62,62,62	0
56	MG	2a	1611	1/1	0.95	0.06	75,75,75,75	0
56	MG	1A	3426	1/1	0.95	0.63	50,50,50,50	0
56	MG	2a	1841	1/1	0.95	0.13	89,89,89,89	0
56	MG	1A	3443	1/1	0.95	0.29	35,35,35,35	0
56	MG	1A	3240	1/1	0.95	0.39	54,54,54,54	0
56	MG	2A	3768	1/1	0.95	0.10	54,54,54,54	0
56	MG	1A	4045	1/1	0.95	0.13	32,32,32,32	0
56	MG	1A	3288	1/1	0.95	0.22	20,20,20,20	0
56	MG	1a	1682	1/1	0.95	0.23	43,43,43,43	0
56	MG	1A	3613	1/1	0.95	0.18	29,29,29,29	0
56	MG	1B	217	1/1	0.95	0.16	56,56,56,56	0
56	MG	2U	205	1/1	0.95	0.31	53,53,53,53	0
56	MG	1a	1687	1/1	0.95	0.16	55,55,55,55	0
56	MG	2A	3521	1/1	0.95	0.30	52,52,52,52	0
56	MG	1A	3346	1/1	0.95	0.19	38,38,38,38	0
56	MG	1A	3099	1/1	0.95	0.16	30,30,30,30	0
56	MG	1U	202	1/1	0.95	0.41	32,32,32,32	0
56	MG	1A	4141	1/1	0.95	0.25	30,30,30,30	0
56	MG	2A	3690	1/1	0.95	0.15	66,66,66,66	0
56	MG	1A	3481	1/1	0.95	0.18	46,46,46,46	0
56	MG	1e	202	1/1	0.95	0.13	69,69,69,69	0
56	MG	1D	309	1/1	0.95	0.17	48,48,48,48	0
56	MG	2A	3446	1/1	0.95	0.17	41,41,41,41	0
56	MG	1A	3427	1/1	0.95	0.19	50,50,50,50	0
56	MG	2A	3104	1/1	0.95	0.16	52,52,52,52	0
56	MG	1A	3874	1/1	0.95	0.14	19,19,19,19	0
56	MG	1A	4074	1/1	0.95	0.12	47,47,47,47	0
56	MG	2A	3142	1/1	0.95	0.08	59,59,59,59	0
56	MG	1A	3534	1/1	0.95	0.24	40,40,40,40	0
56	MG	1A	3771	1/1	0.95	0.19	18,18,18,18	0
56	MG	2A	3108	1/1	0.95	0.16	42,42,42,42	0
56	MG	1A	3799	1/1	0.95	0.57	33,33,33,33	0
56	MG	1A	3689	1/1	0.95	0.19	28,28,28,28	0
56	MG	2A	3594	1/1	0.95	0.09	37,37,37,37	0
56	MG	1A	3751	1/1	0.95	0.23	25,25,25,25	0
56	MG	1a	1808	1/1	0.95	0.22	58,58,58,58	0
56	MG	2A	3125	1/1	0.95	0.12	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1B	214	1/1	0.95	0.16	44,44,44,44	0
56	MG	2A	3502	1/1	0.95	0.12	43,43,43,43	0
56	MG	1A	3222	1/1	0.95	0.25	31,31,31,31	0
56	MG	1A	3281	1/1	0.95	0.17	46,46,46,46	0
56	MG	1A	3276	1/1	0.95	0.42	35,35,35,35	0
56	MG	2a	1643	1/1	0.95	0.11	63,63,63,63	0
56	MG	2A	3076	1/1	0.95	0.41	48,48,48,48	0
56	MG	1A	3323	1/1	0.95	0.15	43,43,43,43	0
56	MG	1a	1775	1/1	0.95	0.23	68,68,68,68	0
56	MG	1A	3897	1/1	0.95	0.13	29,29,29,29	0
56	MG	1x	114	1/1	0.95	0.13	65,65,65,65	0
56	MG	2A	3400	1/1	0.95	0.22	48,48,48,48	0
56	MG	1B	230	1/1	0.95	0.13	53,53,53,53	0
56	MG	2a	1721	1/1	0.95	0.13	76,76,76,76	0
56	MG	1a	1814	1/1	0.95	0.09	55,55,55,55	0
56	MG	2A	3709	1/1	0.95	0.14	26,26,26,26	0
56	MG	1A	3397	1/1	0.95	0.12	30,30,30,30	0
56	MG	2A	3020	1/1	0.95	0.21	63,63,63,63	0
56	MG	1A	4041	1/1	0.95	0.16	33,33,33,33	0
56	MG	2a	1602	1/1	0.95	0.10	53,53,53,53	0
56	MG	2A	3641	1/1	0.95	0.07	60,60,60,60	0
56	MG	1A	3828	1/1	0.95	0.10	43,43,43,43	0
56	MG	1A	3620	1/1	0.95	0.11	38,38,38,38	0
56	MG	2A	3034	1/1	0.95	0.13	46,46,46,46	0
56	MG	1A	3245	1/1	0.95	0.14	37,37,37,37	0
56	MG	1A	3813	1/1	0.95	0.16	50,50,50,50	0
56	MG	1a	1720	1/1	0.95	0.08	54,54,54,54	0
56	MG	1A	3575	1/1	0.95	0.17	34,34,34,34	0
56	MG	2A	3550	1/1	0.95	0.13	35,35,35,35	0
56	MG	2A	3620	1/1	0.95	0.18	67,67,67,67	0
56	MG	1B	223	1/1	0.95	0.21	62,62,62,62	0
56	MG	2A	3882	1/1	0.95	0.20	49,49,49,49	0
56	MG	2D	304	1/1	0.95	0.76	53,53,53,53	0
56	MG	1A	3644	1/1	0.95	0.21	17,17,17,17	0
56	MG	1A	3606	1/1	0.95	0.15	45,45,45,45	0
56	MG	2a	1752	1/1	0.95	0.14	57,57,57,57	0
56	MG	1A	3935	1/1	0.95	0.17	39,39,39,39	0
56	MG	1A	3015	1/1	0.95	0.27	47,47,47,47	0
56	MG	2A	3167	1/1	0.95	0.25	57,57,57,57	0
56	MG	2A	3711	1/1	0.95	0.13	52,52,52,52	0
56	MG	1A	4075	1/1	0.95	0.12	47,47,47,47	0
56	MG	2f	3002	1/1	0.95	0.27	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3013	1/1	0.95	0.44	56,56,56,56	0
56	MG	1A	3404	1/1	0.95	0.31	49,49,49,49	0
56	MG	2a	1803	1/1	0.95	0.27	65,65,65,65	0
56	MG	1A	3385	1/1	0.95	0.41	37,37,37,37	0
56	MG	1A	3596	1/1	0.95	0.13	19,19,19,19	0
56	MG	2A	3055	1/1	0.95	0.08	56,56,56,56	0
56	MG	2A	3737	1/1	0.95	0.15	52,52,52,52	0
56	MG	1A	3367	1/1	0.95	0.36	43,43,43,43	0
56	MG	1a	1799	1/1	0.95	0.13	64,64,64,64	0
56	MG	1A	3478	1/1	0.95	0.31	43,43,43,43	0
56	MG	1A	3114	1/1	0.95	0.20	25,25,25,25	0
56	MG	2A	3583	1/1	0.95	0.16	68,68,68,68	0
56	MG	2A	3028	1/1	0.95	0.11	39,39,39,39	0
56	MG	1A	3189	1/1	0.95	0.41	34,34,34,34	0
56	MG	1A	3455	1/1	0.95	0.24	59,59,59,59	0
56	MG	1A	4095	1/1	0.95	0.18	31,31,31,31	0
56	MG	1A	3677	1/1	0.95	0.09	31,31,31,31	0
56	MG	1A	4147	1/1	0.95	0.63	40,40,40,40	0
56	MG	2A	3578	1/1	0.95	0.12	51,51,51,51	0
56	MG	1F	308	1/1	0.95	0.27	54,54,54,54	0
56	MG	2B	3020	1/1	0.95	0.16	78,78,78,78	0
56	MG	1A	3035	1/1	0.95	0.31	32,32,32,32	0
56	MG	2A	3068	1/1	0.95	0.18	59,59,59,59	0
56	MG	2A	3289	1/1	0.95	0.14	46,46,46,46	0
56	MG	1a	1710	1/1	0.95	0.31	62,62,62,62	0
56	MG	2A	3708	1/1	0.95	0.13	63,63,63,63	0
56	MG	2A	3131	1/1	0.95	0.44	48,48,48,48	0
56	MG	1A	3682	1/1	0.95	0.19	25,25,25,25	0
56	MG	1x	103	1/1	0.95	0.17	56,56,56,56	0
56	MG	2A	3621	1/1	0.95	0.15	50,50,50,50	0
57	MT9	1A	4113	33/33	0.95	0.28	25,34,43,56	0
56	MG	1A	3516	1/1	0.95	0.45	34,34,34,34	0
56	MG	1A	3734	1/1	0.95	0.13	38,38,38,38	0
56	MG	1A	3816	1/1	0.95	0.12	36,36,36,36	0
56	MG	1A	3116	1/1	0.95	0.37	47,47,47,47	0
56	MG	1a	1683	1/1	0.95	0.20	42,42,42,42	0
56	MG	1a	1709	1/1	0.95	0.24	48,48,48,48	0
56	MG	1A	3964	1/1	0.95	0.14	26,26,26,26	0
56	MG	2a	1823	1/1	0.95	0.21	72,72,72,72	0
56	MG	1a	1806	1/1	0.95	0.12	49,49,49,49	0
56	MG	1a	1715	1/1	0.95	0.13	40,40,40,40	0
56	MG	1A	3590	1/1	0.95	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3192	1/1	0.95	0.18	48,48,48,48	0
56	MG	2A	3597	1/1	0.95	0.11	54,54,54,54	0
56	MG	1A	3951	1/1	0.95	0.11	50,50,50,50	0
56	MG	1A	3632	1/1	0.95	0.14	33,33,33,33	0
56	MG	1a	1805	1/1	0.95	0.11	59,59,59,59	0
56	MG	1A	3117	1/1	0.95	0.16	35,35,35,35	0
56	MG	1A	3207	1/1	0.95	0.47	35,35,35,35	0
56	MG	1A	4067	1/1	0.95	0.14	58,58,58,58	0
56	MG	20	103	1/1	0.95	0.11	55,55,55,55	0
56	MG	1A	3123	1/1	0.95	0.31	39,39,39,39	0
56	MG	1a	1816	1/1	0.95	0.18	56,56,56,56	0
56	MG	2A	3848	1/1	0.95	0.05	46,46,46,46	0
56	MG	2B	3009	1/1	0.95	0.15	66,66,66,66	0
56	MG	1A	3162	1/1	0.95	0.20	28,28,28,28	0
56	MG	2A	3156	1/1	0.95	0.09	58,58,58,58	0
56	MG	1F	303	1/1	0.95	0.26	24,24,24,24	0
56	MG	1A	3230	1/1	0.95	0.40	32,32,32,32	0
56	MG	1a	1827	1/1	0.95	0.20	49,49,49,49	0
56	MG	1S	3001	1/1	0.95	0.38	42,42,42,42	0
56	MG	1A	3417	1/1	0.95	0.35	52,52,52,52	0
56	MG	1A	4073	1/1	0.95	0.17	40,40,40,40	0
56	MG	2A	3231	1/1	0.95	1.19	49,49,49,49	0
56	MG	1f	3001	1/1	0.95	0.24	40,40,40,40	0
56	MG	2A	3075	1/1	0.95	0.47	44,44,44,44	0
56	MG	2a	1779	1/1	0.95	0.07	60,60,60,60	0
56	MG	2a	1805	1/1	0.95	0.09	51,51,51,51	0
56	MG	2A	3310	1/1	0.95	0.32	58,58,58,58	0
56	MG	2A	3514	1/1	0.95	0.11	39,39,39,39	0
56	MG	1A	4009	1/1	0.95	0.15	35,35,35,35	0
56	MG	2a	1689	1/1	0.95	0.15	54,54,54,54	0
56	MG	1A	3311	1/1	0.95	0.24	53,53,53,53	0
56	MG	1A	3228	1/1	0.95	0.68	44,44,44,44	0
56	MG	18	103	1/1	0.95	0.23	29,29,29,29	0
56	MG	1A	3870	1/1	0.95	0.14	46,46,46,46	0
56	MG	1a	1731	1/1	0.95	0.11	34,34,34,34	0
56	MG	1A	3944	1/1	0.95	0.07	40,40,40,40	0
56	MG	2A	3139	1/1	0.95	0.57	46,46,46,46	0
56	MG	2a	1675	1/1	0.95	0.23	63,63,63,63	0
56	MG	1A	3077	1/1	0.95	0.15	30,30,30,30	0
56	MG	2q	3003	1/1	0.95	0.14	68,68,68,68	0
56	MG	2A	3904	1/1	0.95	0.11	40,40,40,40	0
56	MG	2y	3007	1/1	0.95	0.08	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3301	1/1	0.95	0.32	68,68,68,68	0
56	MG	2A	3701	1/1	0.95	0.22	48,48,48,48	0
56	MG	2E	307	1/1	0.95	0.11	36,36,36,36	0
56	MG	2A	3605	1/1	0.95	0.20	56,56,56,56	0
56	MG	1A	3732	1/1	0.95	0.15	26,26,26,26	0
56	MG	1A	3537	1/1	0.95	0.22	38,38,38,38	0
56	MG	1A	3773	1/1	0.95	0.12	44,44,44,44	0
56	MG	1A	3658	1/1	0.96	0.12	27,27,27,27	0
56	MG	2a	1738	1/1	0.96	0.25	69,69,69,69	0
56	MG	1A	4121	1/1	0.96	0.31	29,29,29,29	0
56	MG	1A	4002	1/1	0.96	0.11	29,29,29,29	0
56	MG	1A	3744	1/1	0.96	0.18	19,19,19,19	0
56	MG	1A	3605	1/1	0.96	0.11	37,37,37,37	0
56	MG	2A	3045	1/1	0.96	0.10	42,42,42,42	0
56	MG	1A	3490	1/1	0.96	0.24	44,44,44,44	0
56	MG	1A	3389	1/1	0.96	0.20	43,43,43,43	0
56	MG	1A	3789	1/1	0.96	0.61	36,36,36,36	0
56	MG	2A	3677	1/1	0.96	0.41	48,48,48,48	0
56	MG	2A	3434	1/1	0.96	0.17	40,40,40,40	0
56	MG	16	101	1/1	0.96	0.14	42,42,42,42	0
56	MG	1A	3994	1/1	0.96	0.17	17,17,17,17	0
56	MG	1A	3519	1/1	0.96	0.36	29,29,29,29	0
56	MG	1D	302	1/1	0.96	0.25	51,51,51,51	0
56	MG	2E	308	1/1	0.96	0.14	53,53,53,53	0
56	MG	2A	3166	1/1	0.96	0.11	47,47,47,47	0
56	MG	1A	3277	1/1	0.96	0.47	31,31,31,31	0
56	MG	1A	3193	1/1	0.96	0.43	38,38,38,38	0
56	MG	1A	3137	1/1	0.96	0.20	15,15,15,15	0
56	MG	1A	3103	1/1	0.96	0.10	23,23,23,23	0
56	MG	2A	3335	1/1	0.96	0.20	55,55,55,55	0
56	MG	2W	202	1/1	0.96	0.60	40,40,40,40	0
56	MG	1a	1641	1/1	0.96	0.14	47,47,47,47	0
56	MG	1A	3725	1/1	0.96	0.21	25,25,25,25	0
56	MG	1a	1762	1/1	0.96	0.10	52,52,52,52	0
56	MG	1A	3312	1/1	0.96	0.19	45,45,45,45	0
56	MG	1a	1751	1/1	0.96	0.08	44,44,44,44	0
56	MG	2A	3640	1/1	0.96	0.27	52,52,52,52	0
56	MG	2A	3874	1/1	0.96	0.21	38,38,38,38	0
56	MG	16	104	1/1	0.96	0.15	39,39,39,39	0
56	MG	1E	303	1/1	0.96	0.23	30,30,30,30	0
56	MG	2A	3522	1/1	0.96	0.10	60,60,60,60	0
56	MG	2A	3103	1/1	0.96	0.13	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3839	1/1	0.96	0.16	28,28,28,28	0
56	MG	1A	3187	1/1	0.96	0.29	25,25,25,25	0
56	MG	1D	308	1/1	0.96	0.21	40,40,40,40	0
56	MG	1A	3263	1/1	0.96	0.26	34,34,34,34	0
56	MG	1G	3001	1/1	0.96	0.19	33,33,33,33	0
56	MG	2A	3570	1/1	0.96	0.11	53,53,53,53	0
56	MG	2A	3029	1/1	0.96	0.62	56,56,56,56	0
56	MG	1A	4131	1/1	0.96	0.35	31,31,31,31	0
56	MG	2A	3599	1/1	0.96	0.15	57,57,57,57	0
56	MG	1a	1774	1/1	0.96	0.13	61,61,61,61	0
56	MG	1A	3046	1/1	0.96	0.11	15,15,15,15	0
56	MG	1A	3702	1/1	0.96	0.14	42,42,42,42	0
56	MG	2A	3893	1/1	0.96	0.08	49,49,49,49	0
56	MG	1A	3097	1/1	0.96	0.19	33,33,33,33	0
56	MG	1A	3838	1/1	0.96	0.20	26,26,26,26	0
56	MG	1A	3314	1/1	0.96	0.16	39,39,39,39	0
56	MG	1a	1674	1/1	0.96	0.11	56,56,56,56	0
56	MG	2A	3623	1/1	0.96	0.09	44,44,44,44	0
56	MG	1A	3546	1/1	0.96	0.31	42,42,42,42	0
56	MG	2A	3439	1/1	0.96	0.25	55,55,55,55	0
56	MG	1A	3655	1/1	0.96	0.21	18,18,18,18	0
56	MG	1A	3806	1/1	0.96	0.13	35,35,35,35	0
56	MG	1A	3764	1/1	0.96	0.12	50,50,50,50	0
56	MG	1A	3136	1/1	0.96	0.15	33,33,33,33	0
56	MG	1E	305	1/1	0.96	0.29	54,54,54,54	0
56	MG	1b	3002	1/1	0.96	0.16	68,68,68,68	0
56	MG	1n	502	1/1	0.96	0.11	55,55,55,55	0
56	MG	1A	3693	1/1	0.96	0.13	47,47,47,47	0
56	MG	2A	3857	1/1	0.96	0.10	32,32,32,32	0
56	MG	1A	3197	1/1	0.96	0.25	31,31,31,31	0
56	MG	1A	3818	1/1	0.96	0.09	51,51,51,51	0
56	MG	1A	3151	1/1	0.96	0.47	37,37,37,37	0
56	MG	2A	3313	1/1	0.96	0.23	70,70,70,70	0
56	MG	1a	1678	1/1	0.96	0.17	54,54,54,54	0
56	MG	1B	222	1/1	0.96	0.06	56,56,56,56	0
56	MG	2A	3741	1/1	0.96	0.32	71,71,71,71	0
56	MG	2A	3448	1/1	0.96	0.44	52,52,52,52	0
56	MG	1A	3919	1/1	0.96	0.15	8,8,8,8	0
56	MG	2A	3119	1/1	0.96	0.09	62,62,62,62	0
56	MG	1B	224	1/1	0.96	0.19	34,34,34,34	0
56	MG	1D	303	1/1	0.96	0.25	34,34,34,34	0
56	MG	2A	3130	1/1	0.96	0.11	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1618	1/1	0.96	0.09	63,63,63,63	0
56	MG	2a	1673	1/1	0.96	0.19	51,51,51,51	0
56	MG	1A	3301	1/1	0.96	0.18	40,40,40,40	0
56	MG	2A	3785	1/1	0.96	0.06	56,56,56,56	0
56	MG	1a	1821	1/1	0.96	0.16	51,51,51,51	0
56	MG	1A	3005	1/1	0.96	0.22	58,58,58,58	0
56	MG	1A	3095	1/1	0.96	0.19	42,42,42,42	0
56	MG	1B	210	1/1	0.96	0.52	42,42,42,42	0
56	MG	1a	1630	1/1	0.96	0.14	44,44,44,44	0
56	MG	2A	3816	1/1	0.96	0.17	59,59,59,59	0
56	MG	1A	3908	1/1	0.96	0.19	37,37,37,37	0
56	MG	1A	3343	1/1	0.96	0.23	37,37,37,37	0
56	MG	1A	3855	1/1	0.96	0.17	40,40,40,40	0
56	MG	1A	3797	1/1	0.96	0.11	28,28,28,28	0
56	MG	1A	3832	1/1	0.96	0.33	49,49,49,49	0
56	MG	1A	3342	1/1	0.96	0.31	44,44,44,44	0
56	MG	1A	3076	1/1	0.96	0.16	34,34,34,34	0
56	MG	1a	1725	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3140	1/1	0.96	0.28	34,34,34,34	0
56	MG	1A	4096	1/1	0.96	0.23	40,40,40,40	0
56	MG	1a	1795	1/1	0.96	0.11	61,61,61,61	0
56	MG	1a	1607	1/1	0.96	0.17	41,41,41,41	0
56	MG	1A	3199	1/1	0.96	0.17	15,15,15,15	0
56	MG	1B	236	1/1	0.96	0.20	23,23,23,23	0
56	MG	1a	1820	1/1	0.96	0.26	41,41,41,41	0
56	MG	2W	203	1/1	0.96	0.17	54,54,54,54	0
56	MG	2A	3356	1/1	0.96	0.09	55,55,55,55	0
56	MG	2A	3539	1/1	0.96	0.12	60,60,60,60	0
56	MG	1A	3761	1/1	0.96	0.17	22,22,22,22	0
56	MG	2A	3155	1/1	0.96	0.21	63,63,63,63	0
56	MG	1A	3922	1/1	0.96	0.11	19,19,19,19	0
56	MG	2A	3003	1/1	0.96	0.18	40,40,40,40	0
56	MG	2A	3527	1/1	0.96	0.11	35,35,35,35	0
56	MG	2A	3651	1/1	0.96	0.13	41,41,41,41	0
56	MG	2A	3534	1/1	0.96	0.12	39,39,39,39	0
56	MG	2A	3740	1/1	0.96	0.08	45,45,45,45	0
56	MG	1A	3092	1/1	0.96	0.25	35,35,35,35	0
56	MG	1A	3611	1/1	0.96	0.12	31,31,31,31	0
56	MG	1a	1713	1/1	0.96	0.15	60,60,60,60	0
56	MG	2A	3868	1/1	0.96	0.07	62,62,62,62	0
56	MG	1A	4082	1/1	0.96	0.24	27,27,27,27	0
56	MG	1A	3432	1/1	0.96	0.16	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3074	1/1	0.96	0.21	25,25,25,25	0
56	MG	2a	1783	1/1	0.96	0.13	65,65,65,65	0
56	MG	1A	3860	1/1	0.96	0.23	38,38,38,38	0
56	MG	2A	3401	1/1	0.96	0.14	48,48,48,48	0
56	MG	1A	3642	1/1	0.96	0.15	20,20,20,20	0
56	MG	1A	3004	1/1	0.96	0.14	47,47,47,47	0
56	MG	1B	208	1/1	0.96	0.14	57,57,57,57	0
56	MG	1A	3717	1/1	0.96	0.13	44,44,44,44	0
56	MG	1A	3615	1/1	0.96	0.15	58,58,58,58	0
56	MG	2D	303	1/1	0.96	0.66	40,40,40,40	0
56	MG	1A	3673	1/1	0.96	0.17	16,16,16,16	0
56	MG	1A	3505	1/1	0.96	0.15	39,39,39,39	0
59	ZN	2n	501	1/1	0.96	0.08	104,104,104,104	0
56	MG	2A	3240	1/1	0.96	0.36	54,54,54,54	0
56	MG	1A	3715	1/1	0.96	0.14	45,45,45,45	0
56	MG	2A	3592	1/1	0.96	0.20	56,56,56,56	0
56	MG	1N	204	1/1	0.96	0.65	43,43,43,43	0
56	MG	1A	3504	1/1	0.96	0.14	50,50,50,50	0
56	MG	1A	3106	1/1	0.96	0.20	25,25,25,25	0
56	MG	1a	1706	1/1	0.96	0.37	52,52,52,52	0
56	MG	1A	3701	1/1	0.96	0.13	48,48,48,48	0
56	MG	2A	3845	1/1	0.96	0.12	40,40,40,40	0
56	MG	1A	3316	1/1	0.96	0.37	34,34,34,34	0
56	MG	1A	4040	1/1	0.96	0.15	25,25,25,25	0
56	MG	2A	3686	1/1	0.96	0.16	71,71,71,71	0
56	MG	1A	3410	1/1	0.96	0.17	37,37,37,37	0
56	MG	1A	3184	1/1	0.96	0.14	25,25,25,25	0
56	MG	1a	1711	1/1	0.96	0.12	60,60,60,60	0
56	MG	1A	3019	1/1	0.96	0.38	32,32,32,32	0
56	MG	1A	3843	1/1	0.96	0.13	35,35,35,35	0
56	MG	1A	3102	1/1	0.96	0.22	33,33,33,33	0
56	MG	1a	1749	1/1	0.96	0.16	57,57,57,57	0
56	MG	1A	4108	1/1	0.96	0.13	40,40,40,40	0
56	MG	1a	1632	1/1	0.96	0.15	40,40,40,40	0
56	MG	2A	3261	1/1	0.96	0.14	71,71,71,71	0
56	MG	1A	3883	1/1	0.96	0.19	47,47,47,47	0
56	MG	2A	3170	1/1	0.96	0.11	54,54,54,54	0
56	MG	1A	3805	1/1	0.96	0.42	34,34,34,34	0
56	MG	1A	3241	1/1	0.96	0.18	54,54,54,54	0
56	MG	1A	3929	1/1	0.96	0.12	42,42,42,42	0
56	MG	2A	3384	1/1	0.96	0.22	69,69,69,69	0
56	MG	1a	1742	1/1	0.96	0.18	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3651	1/1	0.96	0.14	24,24,24,24	0
56	MG	1A	3583	1/1	0.96	0.19	47,47,47,47	0
56	MG	1A	3622	1/1	0.96	0.14	14,14,14,14	0
56	MG	1A	3979	1/1	0.96	0.15	21,21,21,21	0
56	MG	2A	3035	1/1	0.96	0.11	44,44,44,44	0
56	MG	2A	3730	1/1	0.96	0.15	35,35,35,35	0
56	MG	1A	3212	1/1	0.96	0.34	32,32,32,32	0
56	MG	1A	3072	1/1	0.96	0.23	40,40,40,40	0
56	MG	2A	3157	1/1	0.96	0.15	51,51,51,51	0
56	MG	1a	1654	1/1	0.96	0.17	61,61,61,61	0
56	MG	2a	1816	1/1	0.96	0.10	53,53,53,53	0
56	MG	2A	3403	1/1	0.96	0.17	55,55,55,55	0
56	MG	2A	3099	1/1	0.96	0.23	49,49,49,49	0
56	MG	1A	3740	1/1	0.96	0.22	44,44,44,44	0
56	MG	1A	3496	1/1	0.96	0.17	40,40,40,40	0
56	MG	2A	3064	1/1	0.96	0.10	76,76,76,76	0
56	MG	1A	3294	1/1	0.96	0.17	23,23,23,23	0
56	MG	2A	3902	1/1	0.96	0.52	51,51,51,51	0
56	MG	1A	3155	1/1	0.96	0.24	26,26,26,26	0
56	MG	2A	3773	1/1	0.96	0.07	38,38,38,38	0
56	MG	1A	3344	1/1	0.96	0.62	36,36,36,36	0
56	MG	1A	3284	1/1	0.96	0.20	33,33,33,33	0
56	MG	1A	3231	1/1	0.96	0.27	26,26,26,26	0
56	MG	2A	3774	1/1	0.96	0.11	36,36,36,36	0
56	MG	1A	3954	1/1	0.96	0.45	36,36,36,36	0
56	MG	1A	3030	1/1	0.96	0.44	26,26,26,26	0
56	MG	1A	3854	1/1	0.96	0.17	25,25,25,25	0
56	MG	1A	3778	1/1	0.96	0.20	21,21,21,21	0
56	MG	1A	4114	1/1	0.96	0.42	28,28,28,28	0
56	MG	1A	3271	1/1	0.96	0.23	38,38,38,38	0
56	MG	2A	3668	1/1	0.96	0.17	50,50,50,50	0
56	MG	2A	3652	1/1	0.96	0.36	53,53,53,53	0
56	MG	1A	3044	1/1	0.96	0.14	31,31,31,31	0
56	MG	1A	3297	1/1	0.96	0.30	39,39,39,39	0
56	MG	1a	1609	1/1	0.96	0.16	27,27,27,27	0
56	MG	2a	1679	1/1	0.96	0.10	71,71,71,71	0
56	MG	1A	3304	1/1	0.96	0.13	29,29,29,29	0
56	MG	1A	3540	1/1	0.96	0.19	37,37,37,37	0
56	MG	1A	3653	1/1	0.96	0.11	25,25,25,25	0
56	MG	1A	3898	1/1	0.96	0.18	19,19,19,19	0
56	MG	2A	3083	1/1	0.96	0.42	53,53,53,53	0
56	MG	1B	229	1/1	0.96	0.08	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4140	1/1	0.96	0.39	37,37,37,37	0
56	MG	1a	1732	1/1	0.96	0.15	32,32,32,32	0
56	MG	2A	3300	1/1	0.96	0.25	66,66,66,66	0
56	MG	1A	3736	1/1	0.96	0.17	20,20,20,20	0
56	MG	1A	3104	1/1	0.96	0.28	29,29,29,29	0
56	MG	2A	3600	1/1	0.96	0.17	61,61,61,61	0
56	MG	1A	3289	1/1	0.96	0.12	27,27,27,27	0
56	MG	1P	201	1/1	0.96	0.40	26,26,26,26	0
56	MG	1A	3568	1/1	0.96	0.31	44,44,44,44	0
56	MG	2f	3001	1/1	0.96	0.13	47,47,47,47	0
56	MG	2A	3715	1/1	0.96	0.11	26,26,26,26	0
56	MG	1A	3302	1/1	0.96	0.23	41,41,41,41	0
56	MG	1A	3895	1/1	0.96	0.43	32,32,32,32	0
56	MG	1a	1606	1/1	0.96	0.18	62,62,62,62	0
56	MG	2A	3186	1/1	0.96	0.11	40,40,40,40	0
56	MG	2A	3299	1/1	0.96	0.26	65,65,65,65	0
56	MG	1A	3649	1/1	0.96	0.19	20,20,20,20	0
56	MG	1A	3135	1/1	0.96	0.18	36,36,36,36	0
56	MG	2A	3714	1/1	0.96	0.18	48,48,48,48	0
56	MG	2A	3050	1/1	0.96	0.14	22,22,22,22	0
56	MG	1X	103	1/1	0.96	0.18	34,34,34,34	0
56	MG	1A	3719	1/1	0.96	0.11	42,42,42,42	0
56	MG	1B	233	1/1	0.96	0.11	64,64,64,64	0
56	MG	2A	3245	1/1	0.96	0.27	57,57,57,57	0
56	MG	1A	3802	1/1	0.96	0.09	15,15,15,15	0
56	MG	1a	1790	1/1	0.96	0.11	38,38,38,38	0
56	MG	2A	3364	1/1	0.96	0.27	56,56,56,56	0
56	MG	1A	3215	1/1	0.96	0.17	38,38,38,38	0
56	MG	1a	1635	1/1	0.96	0.19	49,49,49,49	0
56	MG	1W	205	1/1	0.97	0.18	30,30,30,30	0
56	MG	2A	3340	1/1	0.97	0.32	74,74,74,74	0
56	MG	1A	3731	1/1	0.97	0.14	30,30,30,30	0
56	MG	1A	3031	1/1	0.97	0.51	32,32,32,32	0
56	MG	2a	1711	1/1	0.97	0.15	64,64,64,64	0
56	MG	1A	3129	1/1	0.97	0.23	35,35,35,35	0
56	MG	1A	3867	1/1	0.97	0.13	26,26,26,26	0
56	MG	1A	3172	1/1	0.97	0.19	15,15,15,15	0
56	MG	2A	3697	1/1	0.97	0.13	36,36,36,36	0
56	MG	1a	1755	1/1	0.97	0.12	51,51,51,51	0
56	MG	1A	3149	1/1	0.97	0.46	44,44,44,44	0
56	MG	1A	3888	1/1	0.97	0.11	59,59,59,59	0
56	MG	1B	225	1/1	0.97	0.12	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4126	1/1	0.97	0.41	30,30,30,30	0
56	MG	1a	1726	1/1	0.97	0.13	46,46,46,46	0
56	MG	1A	3028	1/1	0.97	0.21	24,24,24,24	0
56	MG	2A	3250	1/1	0.97	0.34	58,58,58,58	0
56	MG	2A	3070	1/1	0.97	0.35	60,60,60,60	0
56	MG	1Q	202	1/1	0.97	0.10	39,39,39,39	0
56	MG	2A	3722	1/1	0.97	0.10	62,62,62,62	0
56	MG	1a	1686	1/1	0.97	0.17	48,48,48,48	0
56	MG	2A	3503	1/1	0.97	0.12	56,56,56,56	0
56	MG	2A	3399	1/1	0.97	0.10	36,36,36,36	0
56	MG	1A	4127	1/1	0.97	0.25	29,29,29,29	0
56	MG	1a	1719	1/1	0.97	0.15	42,42,42,42	0
56	MG	1a	1684	1/1	0.97	0.32	49,49,49,49	0
56	MG	1D	312	1/1	0.97	0.36	34,34,34,34	0
56	MG	15	101	1/1	0.97	0.23	36,36,36,36	0
56	MG	2A	3631	1/1	0.97	0.10	36,36,36,36	0
56	MG	2A	3311	1/1	0.97	0.14	56,56,56,56	0
56	MG	2A	3296	1/1	0.97	0.20	42,42,42,42	0
56	MG	1A	3243	1/1	0.97	0.32	35,35,35,35	0
56	MG	1X	105	1/1	0.97	0.16	48,48,48,48	0
56	MG	1A	4029	1/1	0.97	0.12	20,20,20,20	0
56	MG	2A	3073	1/1	0.97	0.06	53,53,53,53	0
56	MG	1A	3684	1/1	0.97	0.14	14,14,14,14	0
56	MG	2A	3092	1/1	0.97	0.19	39,39,39,39	0
56	MG	12	102	1/1	0.97	0.23	37,37,37,37	0
56	MG	1A	3755	1/1	0.97	0.20	20,20,20,20	0
56	MG	1B	228	1/1	0.97	0.16	53,53,53,53	0
56	MG	1A	3844	1/1	0.97	0.12	38,38,38,38	0
56	MG	1A	3364	1/1	0.97	0.47	42,42,42,42	0
56	MG	2A	3494	1/1	0.97	0.45	59,59,59,59	0
56	MG	2a	1812	1/1	0.97	0.14	62,62,62,62	0
56	MG	1R	201	1/1	0.97	0.41	27,27,27,27	0
56	MG	1A	3107	1/1	0.97	0.12	31,31,31,31	0
56	MG	1A	4145	1/1	0.97	0.18	25,25,25,25	0
56	MG	2A	3141	1/1	0.97	0.13	47,47,47,47	0
56	MG	2E	303	1/1	0.97	0.09	38,38,38,38	0
56	MG	1a	1817	1/1	0.97	0.15	59,59,59,59	0
56	MG	2A	3063	1/1	0.97	0.09	68,68,68,68	0
56	MG	1a	1812	1/1	0.97	0.05	54,54,54,54	0
56	MG	2A	3538	1/1	0.97	0.12	47,47,47,47	0
56	MG	2a	1758	1/1	0.97	0.18	56,56,56,56	0
56	MG	1A	3786	1/1	0.97	0.16	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3544	1/1	0.97	0.32	40,40,40,40	0
56	MG	2Y	502	1/1	0.97	0.16	49,49,49,49	0
56	MG	1A	3250	1/1	0.97	0.29	21,21,21,21	0
56	MG	1A	3435	1/1	0.97	0.25	41,41,41,41	0
56	MG	1A	3156	1/1	0.97	0.20	33,33,33,33	0
56	MG	1A	3067	1/1	0.97	0.45	30,30,30,30	0
56	MG	1E	302	1/1	0.97	0.29	36,36,36,36	0
56	MG	1D	306	1/1	0.97	0.21	22,22,22,22	0
56	MG	2A	3761	1/1	0.97	0.12	50,50,50,50	0
56	MG	1A	4061	1/1	0.97	0.12	33,33,33,33	0
56	MG	2A	3060	1/1	0.97	0.16	41,41,41,41	0
56	MG	2A	3507	1/1	0.97	0.15	57,57,57,57	0
56	MG	2a	1710	1/1	0.97	0.09	70,70,70,70	0
56	MG	1a	1740	1/1	0.97	0.15	33,33,33,33	0
56	MG	2A	3317	1/1	0.97	0.34	69,69,69,69	0
56	MG	1A	3033	1/1	0.97	0.24	34,34,34,34	0
56	MG	1m	201	1/1	0.97	0.23	40,40,40,40	0
56	MG	2A	3616	1/1	0.97	0.16	34,34,34,34	0
56	MG	2A	3440	1/1	0.97	0.24	40,40,40,40	0
56	MG	1A	3065	1/1	0.97	0.22	24,24,24,24	0
56	MG	1A	3318	1/1	0.97	0.21	54,54,54,54	0
56	MG	2V	201	1/1	0.97	0.34	42,42,42,42	0
56	MG	1A	3850	1/1	0.97	0.14	38,38,38,38	0
56	MG	1A	3363	1/1	0.97	0.14	32,32,32,32	0
56	MG	1A	3176	1/1	0.97	0.09	46,46,46,46	0
56	MG	1A	3127	1/1	0.97	0.14	61,61,61,61	0
56	MG	2A	3703	1/1	0.97	0.11	61,61,61,61	0
56	MG	1A	3014	1/1	0.97	0.26	32,32,32,32	0
56	MG	1A	3643	1/1	0.97	0.17	21,21,21,21	0
56	MG	1X	104	1/1	0.97	0.50	39,39,39,39	0
56	MG	2A	3367	1/1	0.97	0.15	50,50,50,50	0
56	MG	2A	3851	1/1	0.97	0.11	66,66,66,66	0
56	MG	1A	3710	1/1	0.97	0.18	29,29,29,29	0
56	MG	1E	308	1/1	0.97	0.17	21,21,21,21	0
56	MG	1A	3785	1/1	0.97	0.08	23,23,23,23	0
56	MG	2A	3398	1/1	0.97	0.04	59,59,59,59	0
56	MG	1A	3121	1/1	0.97	0.39	28,28,28,28	0
56	MG	1A	3508	1/1	0.97	0.08	56,56,56,56	0
56	MG	1A	3589	1/1	0.97	0.15	20,20,20,20	0
56	MG	11	101	1/1	0.97	0.19	31,31,31,31	0
56	MG	1A	3992	1/1	0.97	0.11	22,22,22,22	0
56	MG	2a	1712	1/1	0.97	0.14	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2w	3001	1/1	0.97	0.14	48,48,48,48	0
56	MG	1A	3861	1/1	0.97	0.08	53,53,53,53	0
56	MG	1A	3205	1/1	0.97	0.18	33,33,33,33	0
59	ZN	1Y	202	1/1	0.97	0.19	66,66,66,66	0
56	MG	2A	3143	1/1	0.97	0.14	41,41,41,41	0
56	MG	1A	4119	1/1	0.97	0.26	34,34,34,34	0
56	MG	2A	3841	1/1	0.97	0.13	27,27,27,27	0
56	MG	1A	3696	1/1	0.97	0.14	16,16,16,16	0
56	MG	1A	3539	1/1	0.97	0.26	33,33,33,33	0
56	MG	2F	304	1/1	0.97	0.68	51,51,51,51	0
56	MG	1A	3578	1/1	0.97	0.43	27,27,27,27	0
56	MG	1A	4128	1/1	0.97	0.26	32,32,32,32	0
56	MG	1a	1717	1/1	0.97	0.14	54,54,54,54	0
56	MG	1A	3520	1/1	0.97	0.41	47,47,47,47	0
56	MG	1A	3665	1/1	0.97	0.18	19,19,19,19	0
56	MG	1a	1618	1/1	0.97	0.08	42,42,42,42	0
56	MG	1A	4116	1/1	0.97	0.22	30,30,30,30	0
56	MG	1A	3202	1/1	0.97	0.11	28,28,28,28	0
56	MG	1A	3462	1/1	0.97	0.14	34,34,34,34	0
56	MG	1A	3468	1/1	0.97	0.25	45,45,45,45	0
56	MG	1A	3712	1/1	0.97	0.12	21,21,21,21	0
56	MG	2A	3190	1/1	0.97	0.14	49,49,49,49	0
56	MG	2A	3021	1/1	0.97	0.09	28,28,28,28	0
56	MG	1A	3080	1/1	0.97	0.30	33,33,33,33	0
56	MG	1B	215	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3527	1/1	0.97	0.10	40,40,40,40	0
56	MG	2A	3332	1/1	0.97	0.09	52,52,52,52	0
56	MG	1A	3890	1/1	0.97	0.17	35,35,35,35	0
56	MG	2a	1782	1/1	0.97	0.07	54,54,54,54	0
56	MG	2A	3462	1/1	0.97	0.16	47,47,47,47	0
56	MG	2A	3673	1/1	0.97	0.16	65,65,65,65	0
56	MG	1A	3042	1/1	0.97	0.16	29,29,29,29	0
56	MG	1A	3423	1/1	0.97	0.31	39,39,39,39	0
56	MG	1D	304	1/1	0.97	0.14	15,15,15,15	0
56	MG	1A	3794	1/1	0.97	0.14	46,46,46,46	0
56	MG	1A	3538	1/1	0.97	0.27	49,49,49,49	0
56	MG	1A	3811	1/1	0.97	0.19	47,47,47,47	0
56	MG	1A	3100	1/1	0.97	0.35	32,32,32,32	0
56	MG	1A	3196	1/1	0.97	0.20	36,36,36,36	0
56	MG	1A	3810	1/1	0.97	0.14	55,55,55,55	0
56	MG	1a	1813	1/1	0.97	0.17	50,50,50,50	0
56	MG	2A	3672	1/1	0.97	0.13	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3699	1/1	0.97	0.09	59,59,59,59	0
56	MG	2A	3411	1/1	0.97	0.31	54,54,54,54	0
56	MG	1A	3286	1/1	0.97	0.33	52,52,52,52	0
56	MG	2A	3626	1/1	0.97	0.15	50,50,50,50	0
56	MG	1A	3557	1/1	0.97	0.55	33,33,33,33	0
56	MG	2A	3478	1/1	0.97	0.23	49,49,49,49	0
56	MG	1A	3434	1/1	0.97	0.57	39,39,39,39	0
56	MG	1A	3607	1/1	0.97	0.15	45,45,45,45	0
56	MG	13	102	1/1	0.97	0.20	38,38,38,38	0
56	MG	2A	3617	1/1	0.97	0.08	44,44,44,44	0
56	MG	2A	3408	1/1	0.97	0.09	47,47,47,47	0
56	MG	2A	3095	1/1	0.97	0.19	40,40,40,40	0
56	MG	2B	3012	1/1	0.97	0.23	69,69,69,69	0
56	MG	1A	3138	1/1	0.97	0.07	37,37,37,37	0
56	MG	2A	3669	1/1	0.97	0.17	47,47,47,47	0
56	MG	1A	3532	1/1	0.97	0.15	29,29,29,29	0
56	MG	2A	3016	1/1	0.97	0.13	66,66,66,66	0
56	MG	1A	3089	1/1	0.97	0.17	14,14,14,14	0
56	MG	1A	3349	1/1	0.97	0.20	35,35,35,35	0
56	MG	1A	3038	1/1	0.97	0.17	25,25,25,25	0
56	MG	1A	3787	1/1	0.97	0.09	34,34,34,34	0
56	MG	10	108	1/1	0.97	0.13	44,44,44,44	0
56	MG	1A	3115	1/1	0.97	0.27	31,31,31,31	0
56	MG	1A	4106	1/1	0.97	0.15	47,47,47,47	0
56	MG	1A	4013	1/1	0.97	0.11	54,54,54,54	0
56	MG	1A	3475	1/1	0.97	0.16	41,41,41,41	0
56	MG	1G	3005	1/1	0.97	0.11	58,58,58,58	0
56	MG	2a	1638	1/1	0.97	0.14	78,78,78,78	0
56	MG	1A	3759	1/1	0.97	0.10	40,40,40,40	0
56	MG	1A	3274	1/1	0.97	0.17	20,20,20,20	0
56	MG	1D	310	1/1	0.97	0.22	15,15,15,15	0
56	MG	1A	3225	1/1	0.97	0.28	57,57,57,57	0
56	MG	1A	3185	1/1	0.97	0.32	34,34,34,34	0
56	MG	1A	4076	1/1	0.97	0.12	29,29,29,29	0
56	MG	1A	3352	1/1	0.97	0.10	29,29,29,29	0
56	MG	1A	3517	1/1	0.97	0.30	29,29,29,29	0
56	MG	2A	3127	1/1	0.97	0.09	60,60,60,60	0
56	MG	1A	3163	1/1	0.97	0.37	41,41,41,41	0
56	MG	1A	3765	1/1	0.97	0.15	16,16,16,16	0
56	MG	1A	3166	1/1	0.97	0.61	40,40,40,40	0
56	MG	1A	3752	1/1	0.97	0.13	25,25,25,25	0
56	MG	1a	1815	1/1	0.97	0.09	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3061	1/1	0.98	0.15	34,34,34,34	0
56	MG	1A	3660	1/1	0.98	0.12	23,23,23,23	0
56	MG	1A	4005	1/1	0.98	0.10	28,28,28,28	0
56	MG	1A	3235	1/1	0.98	0.28	27,27,27,27	0
56	MG	2A	3533	1/1	0.98	0.10	48,48,48,48	0
56	MG	1A	3157	1/1	0.98	0.69	33,33,33,33	0
56	MG	1B	202	1/1	0.98	0.29	38,38,38,38	0
56	MG	1A	4086	1/1	0.98	0.20	19,19,19,19	0
56	MG	1A	4004	1/1	0.98	0.10	20,20,20,20	0
56	MG	1A	3010	1/1	0.98	0.16	33,33,33,33	0
56	MG	1A	3775	1/1	0.98	0.10	45,45,45,45	0
56	MG	2A	3456	1/1	0.98	0.13	47,47,47,47	0
56	MG	2A	3537	1/1	0.98	0.13	51,51,51,51	0
56	MG	1A	3073	1/1	0.98	0.17	33,33,33,33	0
56	MG	1A	3261	1/1	0.98	0.46	40,40,40,40	0
56	MG	2A	3524	1/1	0.98	0.11	46,46,46,46	0
56	MG	1A	3141	1/1	0.98	0.30	27,27,27,27	0
56	MG	2A	3326	1/1	0.98	0.41	46,46,46,46	0
56	MG	1A	3598	1/1	0.98	0.17	12,12,12,12	0
56	MG	1A	3223	1/1	0.98	0.45	27,27,27,27	0
56	MG	1A	3641	1/1	0.98	0.17	29,29,29,29	0
60	SF4	1d	501	8/8	0.98	0.16	58,66,74,76	0
56	MG	2A	3526	1/1	0.98	0.10	45,45,45,45	0
56	MG	2A	3381	1/1	0.98	0.15	58,58,58,58	0
56	MG	1A	3078	1/1	0.98	0.18	42,42,42,42	0
56	MG	1O	206	1/1	0.98	0.23	54,54,54,54	0
56	MG	1A	3617	1/1	0.98	0.12	18,18,18,18	0
56	MG	1A	3896	1/1	0.98	0.13	21,21,21,21	0
56	MG	1A	4093	1/1	0.98	0.22	27,27,27,27	0
56	MG	1A	4098	1/1	0.98	0.14	29,29,29,29	0
56	MG	2a	1623	1/1	0.98	0.15	69,69,69,69	0
56	MG	1A	3374	1/1	0.98	0.14	32,32,32,32	0
56	MG	2U	203	1/1	0.98	0.84	63,63,63,63	0
56	MG	2A	3280	1/1	0.98	0.18	62,62,62,62	0
56	MG	2A	3154	1/1	0.98	0.13	72,72,72,72	0
56	MG	1A	3881	1/1	0.98	0.18	26,26,26,26	0
56	MG	1W	203	1/1	0.98	0.18	30,30,30,30	0
56	MG	1A	3195	1/1	0.98	0.18	16,16,16,16	0
56	MG	2a	1815	1/1	0.98	0.06	49,49,49,49	0
56	MG	1Q	205	1/1	0.98	0.14	28,28,28,28	0
56	MG	1A	3036	1/1	0.98	0.24	25,25,25,25	0
56	MG	1V	201	1/1	0.98	0.28	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1762	1/1	0.98	0.09	51,51,51,51	0
56	MG	2A	3489	1/1	0.98	0.09	73,73,73,73	0
56	MG	1A	4087	1/1	0.98	0.16	46,46,46,46	0
56	MG	1A	3703	1/1	0.98	0.17	20,20,20,20	0
56	MG	1A	3808	1/1	0.98	0.14	39,39,39,39	0
56	MG	1A	3626	1/1	0.98	0.16	28,28,28,28	0
56	MG	1A	3337	1/1	0.98	0.17	38,38,38,38	0
56	MG	23	103	1/1	0.98	0.23	56,56,56,56	0
56	MG	1A	4046	1/1	0.98	0.11	40,40,40,40	0
56	MG	1f	3002	1/1	0.98	0.16	45,45,45,45	0
60	SF4	2d	501	8/8	0.98	0.15	67,71,80,97	0
56	MG	1E	304	1/1	0.98	0.19	24,24,24,24	0
56	MG	2a	1688	1/1	0.98	0.10	71,71,71,71	0
56	MG	2A	3748	1/1	0.98	0.32	40,40,40,40	0
56	MG	1F	304	1/1	0.98	0.39	29,29,29,29	0
56	MG	1A	3068	1/1	0.98	0.14	15,15,15,15	0
56	MG	2A	3611	1/1	0.98	0.18	62,62,62,62	0
56	MG	1A	3180	1/1	0.98	0.21	36,36,36,36	0
56	MG	2A	3650	1/1	0.98	0.37	42,42,42,42	0
56	MG	1A	3756	1/1	0.98	0.20	17,17,17,17	0
56	MG	2A	3129	1/1	0.98	0.21	62,62,62,62	0
56	MG	1A	3351	1/1	0.98	0.16	47,47,47,47	0
56	MG	1A	3836	1/1	0.98	0.17	54,54,54,54	0
56	MG	1A	3278	1/1	0.98	0.55	33,33,33,33	0
56	MG	1A	4120	1/1	0.98	0.25	27,27,27,27	0
56	MG	1A	3094	1/1	0.98	0.23	21,21,21,21	0
56	MG	1A	3969	1/1	0.98	0.10	59,59,59,59	0
56	MG	1A	4068	1/1	0.98	0.11	22,22,22,22	0
56	MG	1A	3627	1/1	0.98	0.15	30,30,30,30	0
56	MG	2A	3442	1/1	0.98	0.23	45,45,45,45	0
56	MG	1A	4079	1/1	0.98	0.16	10,10,10,10	0
56	MG	2A	3270	1/1	0.98	0.22	63,63,63,63	0
56	MG	2a	1728	1/1	0.98	0.10	73,73,73,73	0
56	MG	1A	3600	1/1	0.98	0.20	28,28,28,28	0
56	MG	1A	3161	1/1	0.98	0.28	33,33,33,33	0
56	MG	1A	3680	1/1	0.98	0.20	24,24,24,24	0
56	MG	1A	3008	1/1	0.98	0.10	15,15,15,15	0
56	MG	1A	3295	1/1	0.98	0.26	43,43,43,43	0
56	MG	1A	3833	1/1	0.98	0.17	14,14,14,14	0
56	MG	1a	1787	1/1	0.98	0.10	33,33,33,33	0
56	MG	1A	3821	1/1	0.98	0.20	44,44,44,44	0
56	MG	1U	206	1/1	0.98	0.27	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3805	1/1	0.98	0.10	70,70,70,70	0
56	MG	1A	4142	1/1	0.98	0.28	29,29,29,29	0
56	MG	2A	3729	1/1	0.98	0.23	36,36,36,36	0
56	MG	2A	3487	1/1	0.98	0.13	23,23,23,23	0
56	MG	2D	302	1/1	0.98	0.08	33,33,33,33	0
56	MG	2A	3530	1/1	0.98	0.13	33,33,33,33	0
56	MG	1A	3650	1/1	0.98	0.13	18,18,18,18	0
56	MG	1A	3965	1/1	0.98	0.08	55,55,55,55	0
56	MG	2A	3854	1/1	0.98	0.13	37,37,37,37	0
56	MG	1A	3445	1/1	0.98	0.10	24,24,24,24	0
56	MG	2A	3662	1/1	0.98	0.14	54,54,54,54	0
56	MG	1A	4136	1/1	0.98	0.54	39,39,39,39	0
56	MG	2A	3454	1/1	0.98	0.16	45,45,45,45	0
56	MG	1A	3667	1/1	0.98	0.16	21,21,21,21	0
56	MG	2A	3575	1/1	0.98	0.09	38,38,38,38	0
56	MG	1B	234	1/1	0.98	0.12	42,42,42,42	0
56	MG	1A	3054	1/1	0.98	0.16	37,37,37,37	0
56	MG	1A	4089	1/1	0.98	0.16	30,30,30,30	0
56	MG	1A	3831	1/1	0.98	0.12	54,54,54,54	0
56	MG	1T	8001	1/1	0.98	0.17	41,41,41,41	0
56	MG	1A	3876	1/1	0.98	0.19	22,22,22,22	0
56	MG	2A	3149	1/1	0.98	0.24	34,34,34,34	0
56	MG	2A	3771	1/1	0.98	0.08	65,65,65,65	0
56	MG	1X	101	1/1	0.98	0.16	26,26,26,26	0
56	MG	2A	3038	1/1	0.98	0.12	35,35,35,35	0
56	MG	1A	3612	1/1	0.98	0.10	18,18,18,18	0
56	MG	1A	3647	1/1	0.98	0.17	29,29,29,29	0
56	MG	2a	1686	1/1	0.98	0.14	62,62,62,62	0
56	MG	1A	3029	1/1	0.98	0.39	30,30,30,30	0
56	MG	1A	3550	1/1	0.98	0.13	54,54,54,54	0
56	MG	1A	4124	1/1	0.98	0.45	39,39,39,39	0
56	MG	1A	3007	1/1	0.98	0.13	18,18,18,18	0
56	MG	1A	4122	1/1	0.98	0.09	37,37,37,37	0
56	MG	2A	3561	1/1	0.98	0.11	52,52,52,52	0
56	MG	1A	3020	1/1	0.98	0.12	40,40,40,40	0
56	MG	2A	3078	1/1	0.98	0.15	31,31,31,31	0
56	MG	2A	3775	1/1	0.98	0.09	53,53,53,53	0
56	MG	2A	3163	1/1	0.98	0.47	55,55,55,55	0
56	MG	1A	3784	1/1	0.98	0.10	43,43,43,43	0
56	MG	2A	3634	1/1	0.98	0.12	33,33,33,33	0
56	MG	1A	3912	1/1	0.98	0.16	48,48,48,48	0
56	MG	1A	3760	1/1	0.98	0.14	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3803	1/1	0.98	0.11	25,25,25,25	0
56	MG	2A	3111	1/1	0.98	0.21	40,40,40,40	0
56	MG	2A	3219	1/1	0.98	0.13	65,65,65,65	0
58	K	2A	3896	1/1	0.98	0.13	56,56,56,56	0
56	MG	1A	3662	1/1	0.98	0.10	38,38,38,38	0
56	MG	1A	3066	1/1	0.98	0.19	16,16,16,16	0
56	MG	2A	3548	1/1	0.98	0.12	32,32,32,32	0
56	MG	1A	3021	1/1	0.98	0.12	15,15,15,15	0
56	MG	1A	3131	1/1	0.98	0.18	28,28,28,28	0
56	MG	1A	4049	1/1	0.98	0.14	26,26,26,26	0
56	MG	1A	3793	1/1	0.98	0.17	40,40,40,40	0
56	MG	2A	3636	1/1	0.98	0.16	54,54,54,54	0
56	MG	2A	3211	1/1	0.98	0.10	37,37,37,37	0
56	MG	1A	3045	1/1	0.98	0.23	31,31,31,31	0
56	MG	1A	3167	1/1	0.98	0.34	33,33,33,33	0
56	MG	1A	3124	1/1	0.98	0.19	24,24,24,24	0
56	MG	1W	204	1/1	0.98	0.24	30,30,30,30	0
56	MG	1A	4143	1/1	0.98	0.57	28,28,28,28	0
56	MG	2a	1778	1/1	0.98	0.14	62,62,62,62	0
56	MG	1a	1649	1/1	0.98	0.07	62,62,62,62	0
59	ZN	1n	501	1/1	0.98	0.18	59,59,59,59	0
56	MG	1a	1748	1/1	0.98	0.14	37,37,37,37	0
56	MG	1A	3453	1/1	0.98	0.26	39,39,39,39	0
56	MG	2A	3842	1/1	0.98	0.05	45,45,45,45	0
56	MG	1A	3055	1/1	0.98	0.16	23,23,23,23	0
56	MG	2A	3707	1/1	0.98	0.06	62,62,62,62	0
56	MG	1A	3946	1/1	0.98	0.09	35,35,35,35	0
56	MG	1a	1800	1/1	0.98	0.06	57,57,57,57	0
56	MG	1a	1718	1/1	0.99	0.13	48,48,48,48	0
56	MG	2A	3012	1/1	0.99	0.12	41,41,41,41	0
56	MG	1A	3034	1/1	0.99	0.17	24,24,24,24	0
56	MG	1A	3027	1/1	0.99	0.17	32,32,32,32	0
56	MG	1A	3118	1/1	0.99	0.26	27,27,27,27	0
56	MG	1A	3039	1/1	0.99	0.22	27,27,27,27	0
56	MG	1A	3743	1/1	0.99	0.19	38,38,38,38	0
56	MG	1A	3574	1/1	0.99	0.43	35,35,35,35	0
56	MG	1A	4102	1/1	0.99	0.21	32,32,32,32	0
56	MG	1A	3200	1/1	0.99	0.14	27,27,27,27	0
56	MG	1A	3013	1/1	0.99	0.24	27,27,27,27	0
56	MG	1A	3697	1/1	0.99	0.11	51,51,51,51	0
56	MG	1A	3959	1/1	0.99	0.10	43,43,43,43	0
56	MG	1A	3767	1/1	0.99	0.14	43,43,43,43	0

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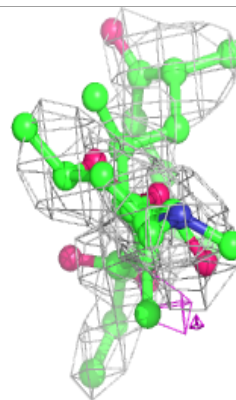
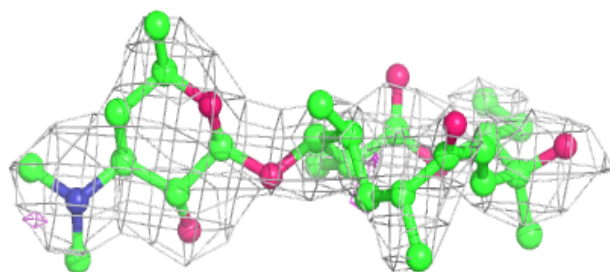
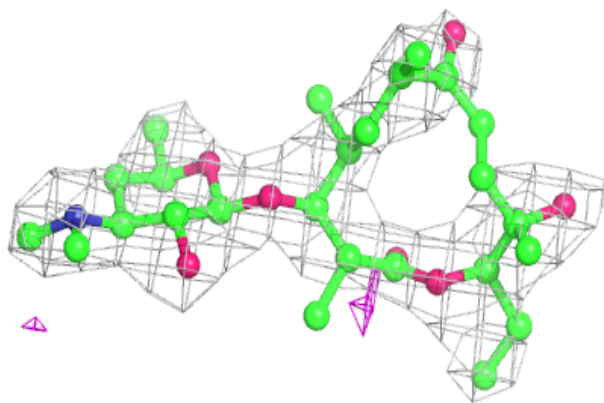
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4008	1/1	0.99	0.17	30,30,30,30	0
56	MG	2A	3593	1/1	0.99	0.12	36,36,36,36	0
56	MG	1A	3603	1/1	0.99	0.15	23,23,23,23	0
56	MG	1A	3011	1/1	0.99	0.13	22,22,22,22	0
56	MG	1A	3670	1/1	0.99	0.16	23,23,23,23	0
59	ZN	19	102	1/1	0.99	0.21	41,41,41,41	0
56	MG	1A	3609	1/1	0.99	0.10	35,35,35,35	0
56	MG	2a	1668	1/1	0.99	0.09	46,46,46,46	0
56	MG	1A	3003	1/1	0.99	0.15	22,22,22,22	0
59	ZN	25	102	1/1	0.99	0.18	55,55,55,55	0
56	MG	1A	3169	1/1	0.99	0.37	34,34,34,34	0
56	MG	1A	3625	1/1	0.99	0.24	22,22,22,22	0
56	MG	2F	302	1/1	0.99	0.09	57,57,57,57	0
56	MG	2A	3264	1/1	0.99	0.19	64,64,64,64	0
56	MG	1A	3542	1/1	0.99	0.25	22,22,22,22	0
56	MG	1A	3824	1/1	0.99	0.12	37,37,37,37	0
56	MG	1A	3686	1/1	0.99	0.16	27,27,27,27	0
56	MG	1A	4144	1/1	0.99	0.18	30,30,30,30	0
56	MG	1A	3669	1/1	0.99	0.14	21,21,21,21	0
56	MG	1A	3171	1/1	0.99	0.11	34,34,34,34	0
56	MG	1A	4132	1/1	0.99	0.36	22,22,22,22	0
59	ZN	26	501	1/1	0.99	0.18	56,56,56,56	0
56	MG	1A	3299	1/1	0.99	0.20	23,23,23,23	0
56	MG	1A	4134	1/1	0.99	0.19	27,27,27,27	0
56	MG	1A	3291	1/1	0.99	0.16	41,41,41,41	0
56	MG	1A	3173	1/1	0.99	0.13	24,24,24,24	0
56	MG	2A	3009	1/1	0.99	0.17	43,43,43,43	0
59	ZN	15	102	1/1	1.00	0.22	41,41,41,41	0
59	ZN	16	102	1/1	1.00	0.22	38,38,38,38	0
56	MG	1B	219	1/1	1.00	0.17	52,52,52,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

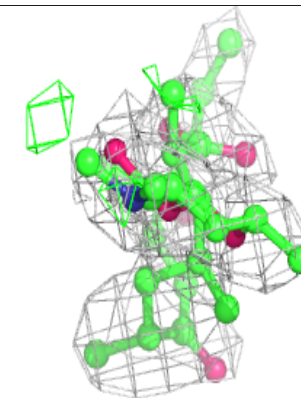
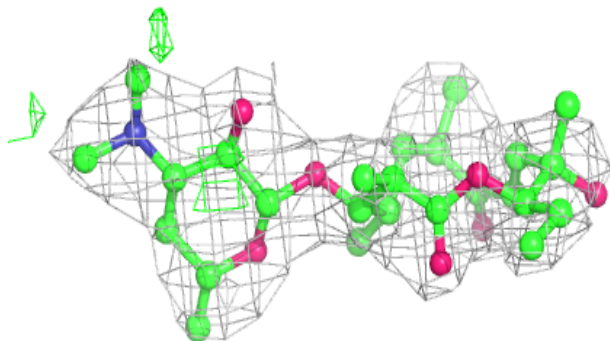
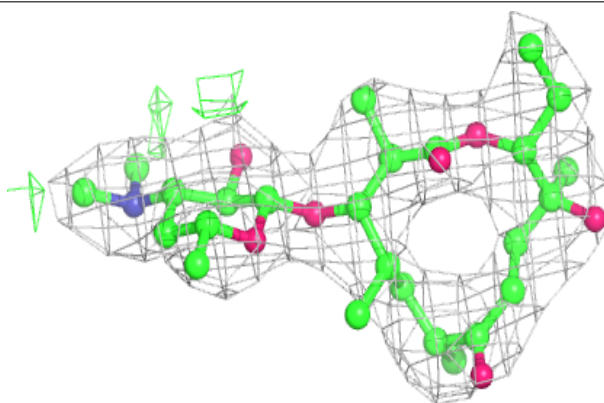


**Electron density around MT9 2A 3897:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around MT9 1A 4113:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.