



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 05:22 AM EDT

PDB ID : 8UD8 / pdb_00008ud8
Title : Crystal structure of the A2503-C2,C8-dimethylated *Thermus thermophilus* 70S ribosome in complex with cresomycin, mRNA, deacylated A-site tRNA^{phe}, aminoacylated P-site fMet-tRNA^{met}, and deacylated E-site tRNA^{phe} at 2.70Å resolution
Authors : Aleksandrova, E.V.; Syroegin, E.A.; Wu, K.J.Y.; Tresco, B.I.C.; Ramkissoon, A.; See, D.N.Y.; Liow, P.; Dittamore, G.A.; Yu, M.; Testolin, G.; Mitcheltree, M.J.; Liu, R.Y.; Svetlov, M.S.; Myers, A.G.; Polikanov, Y.S.
Deposited on : 2023-09-28
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	: 4-5-2 with Phenix2.0
Mogul	: 2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	: 2.0
EDS	: 3.0
Buster-report	: wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	: 9.0.015 (Gargrove)
Density-Fitness	: 1.0.12

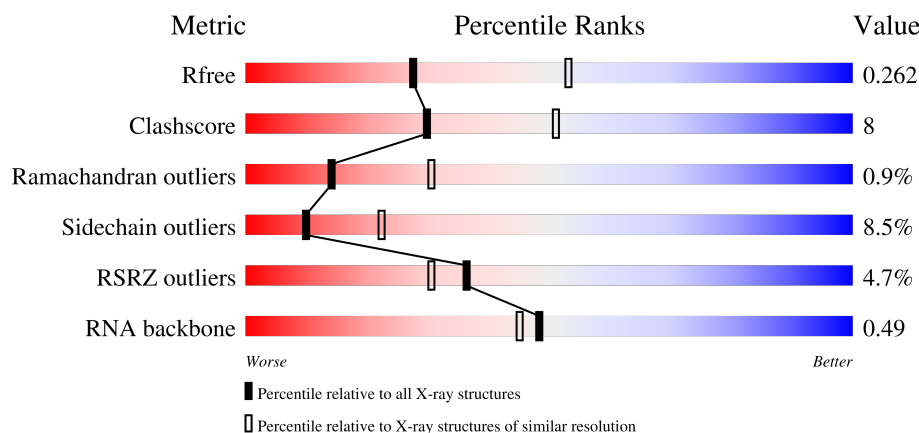
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
1	2A	2915	
2	1B	121	
2	2B	121	
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	

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

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Mol	Chain	Length	Quality of chain
26	24	71	
27	15	60	
27	25	60	
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	

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

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Mol	Chain	Length	Quality of chain
51	2t	106	
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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

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

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 299649 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2871	Total	C	N	O	P	0	0	0
			61853	27532	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60323	26849	11284	19390	2800			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	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 MF-mRNA.

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

- Molecule 54 is a RNA chain called A- and E-site Deacylated tRNA^{phe}.

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

- Molecule 55 is a RNA chain called P-site Aminoacyl-tRNA fMet-tRNA^{met}.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1096	Total	Mg	0	0
			1096	1096		
56	1B	36	Total	Mg	0	0
			36	36		
56	1D	14	Total	Mg	0	0
			14	14		
56	1E	15	Total	Mg	0	0
			15	15		
56	1F	15	Total	Mg	0	0
			15	15		
56	1G	5	Total	Mg	0	0
			5	5		
56	1H	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1I	1	Total Mg 1 1	0	0
56	1N	6	Total Mg 6 6	0	0
56	1O	5	Total Mg 5 5	0	0
56	1P	5	Total Mg 5 5	0	0
56	1Q	6	Total Mg 6 6	0	0
56	1R	6	Total Mg 6 6	0	0
56	1S	3	Total Mg 3 3	0	0
56	1T	2	Total Mg 2 2	0	0
56	1U	9	Total Mg 9 9	0	0
56	1V	6	Total Mg 6 6	0	0
56	1W	7	Total Mg 7 7	0	0
56	1X	7	Total Mg 7 7	0	0
56	1Y	5	Total Mg 5 5	0	0
56	1Z	4	Total Mg 4 4	0	0
56	10	8	Total Mg 8 8	0	0
56	11	6	Total Mg 6 6	0	0
56	12	2	Total Mg 2 2	0	0
56	13	3	Total Mg 3 3	0	0
56	14	1	Total Mg 1 1	0	0
56	15	10	Total Mg 10 10	0	0
56	16	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	17	6	Total Mg 6 6	0	0
56	18	6	Total Mg 6 6	0	0
56	19	1	Total Mg 1 1	0	0
56	1a	210	Total Mg 210 210	0	0
56	1b	1	Total Mg 1 1	0	0
56	1d	1	Total Mg 1 1	0	0
56	1e	2	Total Mg 2 2	0	0
56	1f	2	Total Mg 2 2	0	0
56	1k	1	Total Mg 1 1	0	0
56	1l	2	Total Mg 2 2	0	0
56	1m	1	Total Mg 1 1	0	0
56	1n	2	Total Mg 2 2	0	0
56	1p	1	Total Mg 1 1	0	0
56	1t	1	Total Mg 1 1	0	0
56	1w	8	Total Mg 8 8	0	0
56	1x	15	Total Mg 15 15	0	0
56	1y	1	Total Mg 1 1	0	0
56	2A	844	Total Mg 844 844	0	0
56	2B	19	Total Mg 19 19	0	0
56	2D	8	Total Mg 8 8	0	0
56	2E	9	Total Mg 9 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2F	8	Total 8	Mg 8	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2N	1	Total 1	Mg 1	0	0
56	2O	1	Total 1	Mg 1	0	0
56	2P	2	Total 2	Mg 2	0	0
56	2Q	4	Total 4	Mg 4	0	0
56	2R	4	Total 4	Mg 4	0	0
56	2T	3	Total 3	Mg 3	0	0
56	2U	2	Total 2	Mg 2	0	0
56	2V	2	Total 2	Mg 2	0	0
56	2W	3	Total 3	Mg 3	0	0
56	2X	2	Total 2	Mg 2	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	4	Total 4	Mg 4	0	0
56	21	1	Total 1	Mg 1	0	0
56	23	2	Total 2	Mg 2	0	0
56	25	6	Total 6	Mg 6	0	0
56	26	1	Total 1	Mg 1	0	0
56	27	3	Total 3	Mg 3	0	0
56	28	3	Total 3	Mg 3	0	0
56	2a	225	Total 225	Mg 225	0	0

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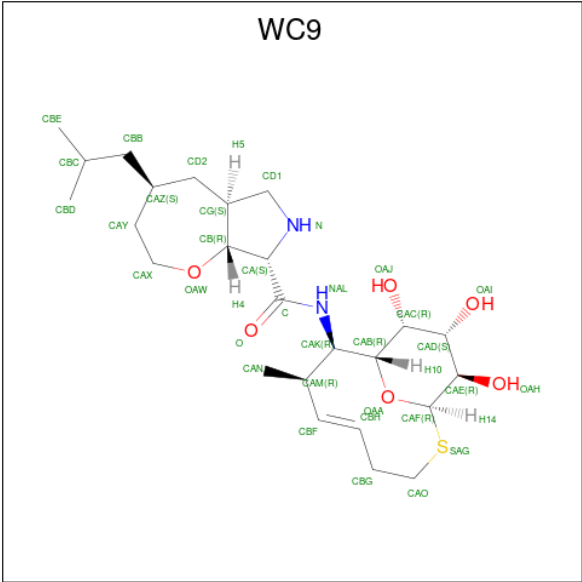
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2d	2	Total Mg 2 2	0	0
56	2e	1	Total Mg 1 1	0	0
56	2f	2	Total Mg 2 2	0	0
56	2g	1	Total Mg 1 1	0	0
56	2j	1	Total Mg 1 1	0	0
56	2l	5	Total Mg 5 5	0	0
56	2m	1	Total Mg 1 1	0	0
56	2q	3	Total Mg 3 3	0	0
56	2t	1	Total Mg 1 1	0	0
56	2v	3	Total Mg 3 3	0	0
56	2w	6	Total Mg 6 6	0	0
56	2x	7	Total Mg 7 7	0	0
56	2y	7	Total Mg 7 7	0	0

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

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

- Molecule 58 is (4S,5aS,8S,8aR)-4-(2-methylpropyl)-N-[(1R,5Z,7R,8R,9R,10R,11S,12R)-10,11,12-trihydroxy-7-methyl-13-oxa-2-thiabicyclo[7.3.1]tridec-5-en-8-yl]octahydro-2H-oxepino[2,3-c]pyrrole-8-carboxamide (non-preferred name) (CCD ID: WC9) (formula: C₂₅H₄₂N₂O₆S) (labeled as "Ligand of Interest" by depositor).



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

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

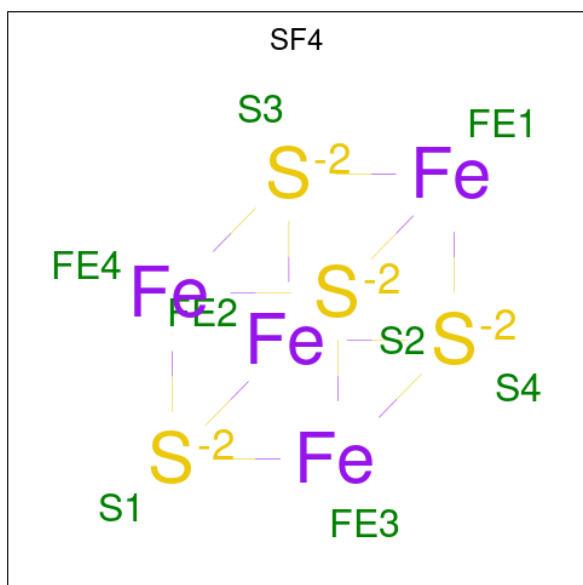
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0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

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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	1d	1	Total	Fe	S	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	1907	Total	O	0	0
			1907	1907		
61	1B	59	Total	O	0	0
			59	59		
61	1D	26	Total	O	0	0
			26	26		
61	1E	28	Total	O	0	0
			28	28		
61	1F	17	Total	O	0	0
			17	17		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1G	2	Total	O	0	0
			2	2		
61	1H	2	Total	O	0	0
			2	2		
61	1N	4	Total	O	0	0
			4	4		
61	1O	4	Total	O	0	0
			4	4		
61	1P	23	Total	O	0	0
			23	23		
61	1Q	5	Total	O	0	0
			5	5		
61	1R	10	Total	O	0	0
			10	10		
61	1S	3	Total	O	0	0
			3	3		
61	1T	8	Total	O	0	0
			8	8		
61	1U	14	Total	O	0	0
			14	14		
61	1V	7	Total	O	0	0
			7	7		
61	1W	7	Total	O	0	0
			7	7		
61	1X	6	Total	O	0	0
			6	6		
61	1Y	2	Total	O	0	0
			2	2		
61	1Z	1	Total	O	0	0
			1	1		
61	10	11	Total	O	0	0
			11	11		
61	11	9	Total	O	0	0
			9	9		
61	12	3	Total	O	0	0
			3	3		
61	13	5	Total	O	0	0
			5	5		
61	14	1	Total	O	0	0
			1	1		
61	15	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	16	3	Total 3	O 3	0	0
61	17	8	Total 8	O 8	0	0
61	18	7	Total 7	O 7	0	0
61	1a	267	Total 267	O 267	0	0
61	1b	1	Total 1	O 1	0	0
61	1e	1	Total 1	O 1	0	0
61	1j	1	Total 1	O 1	0	0
61	1l	3	Total 3	O 3	0	0
61	1n	1	Total 1	O 1	0	0
61	1q	2	Total 2	O 2	0	0
61	1v	4	Total 4	O 4	0	0
61	1w	15	Total 15	O 15	0	0
61	1x	10	Total 10	O 10	0	0
61	1y	2	Total 2	O 2	0	0
61	2A	1000	Total 1000	O 1000	0	0
61	2B	18	Total 18	O 18	0	0
61	2D	17	Total 17	O 17	0	0
61	2E	10	Total 10	O 10	0	0
61	2F	12	Total 12	O 12	0	0
61	2O	2	Total 2	O 2	0	0
61	2P	8	Total 8	O 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2Q	2	Total 2	O 2	0	0
61	2R	2	Total 2	O 2	0	0
61	2T	4	Total 4	O 4	0	0
61	2U	2	Total 2	O 2	0	0
61	2V	1	Total 1	O 1	0	0
61	2W	3	Total 3	O 3	0	0
61	2X	1	Total 1	O 1	0	0
61	2Y	2	Total 2	O 2	0	0
61	20	3	Total 3	O 3	0	0
61	21	8	Total 8	O 8	0	0
61	23	1	Total 1	O 1	0	0
61	27	4	Total 4	O 4	0	0
61	28	3	Total 3	O 3	0	0
61	29	1	Total 1	O 1	0	0
61	2a	172	Total 172	O 172	0	0
61	2d	2	Total 2	O 2	0	0
61	2e	1	Total 1	O 1	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	2	Total 2	O 2	0	0
61	2l	4	Total 4	O 4	0	0
61	2p	1	Total 1	O 1	0	0

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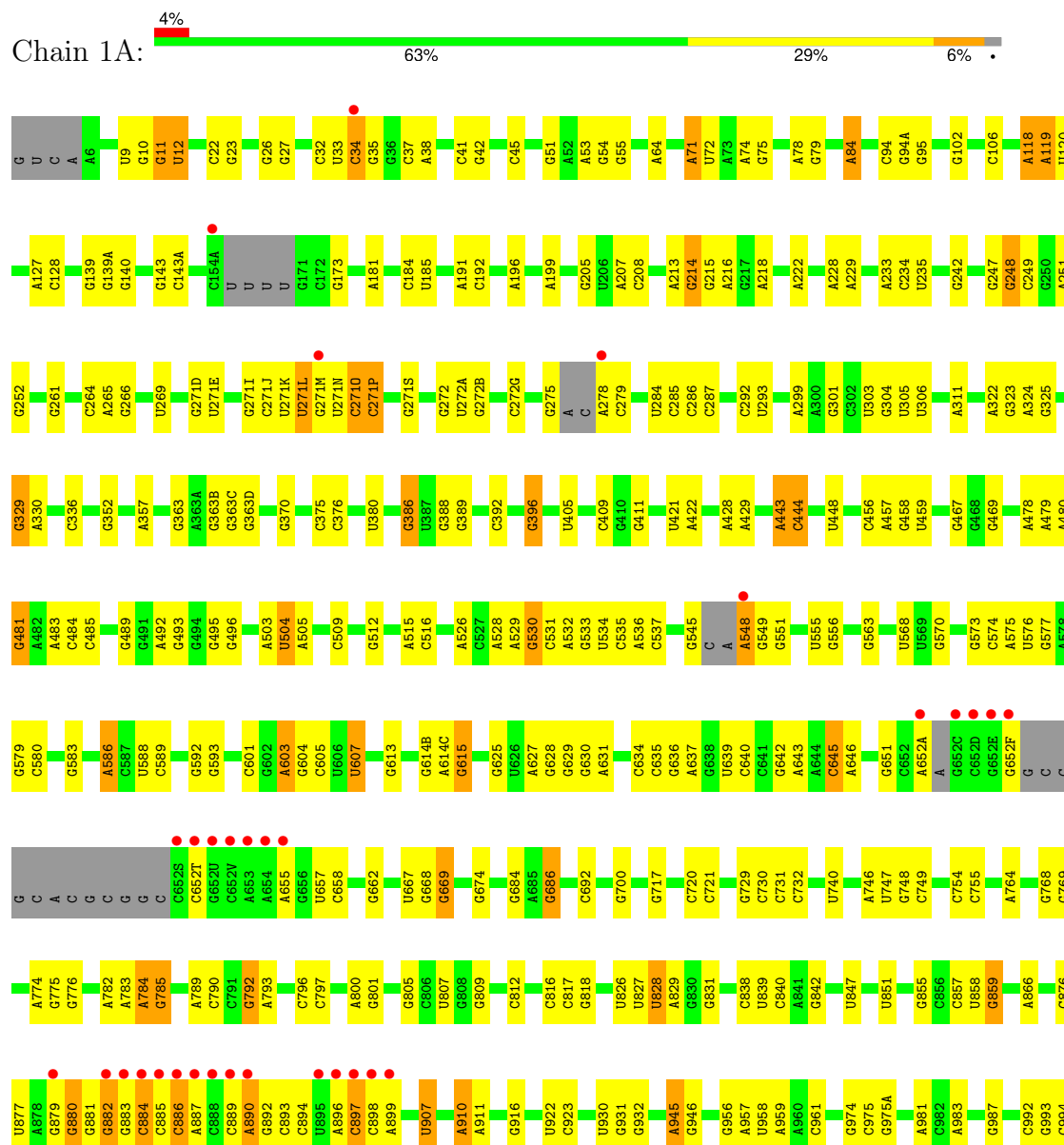
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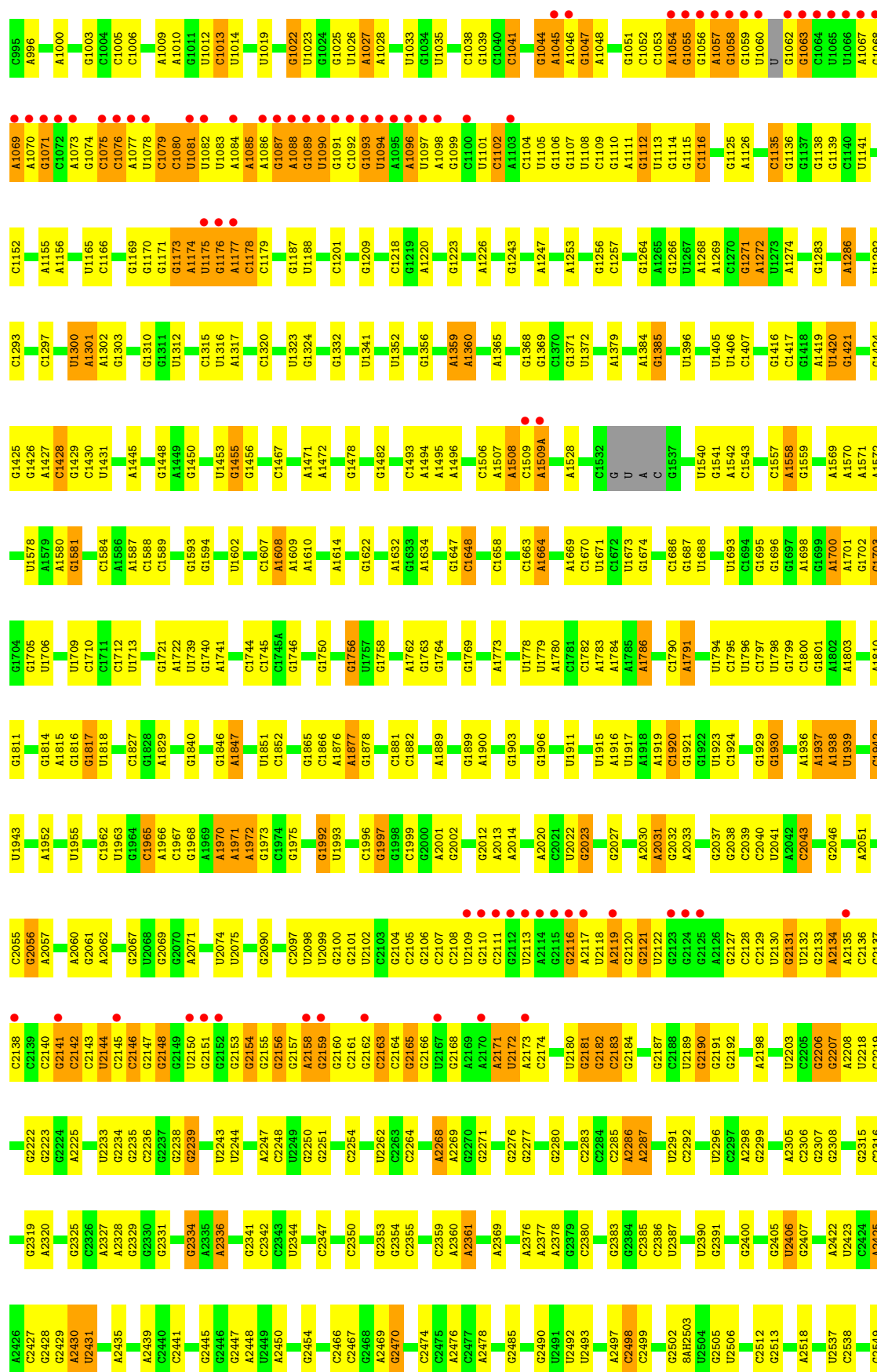
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2q	1	Total	O	0	0
			1	1		
61	2r	1	Total	O	0	0
			1	1		
61	2t	2	Total	O	0	0
			2	2		
61	2v	3	Total	O	0	0
			3	3		
61	2w	3	Total	O	0	0
			3	3		
61	2x	4	Total	O	0	0
			4	4		
61	2y	4	Total	O	0	0
			4	4		

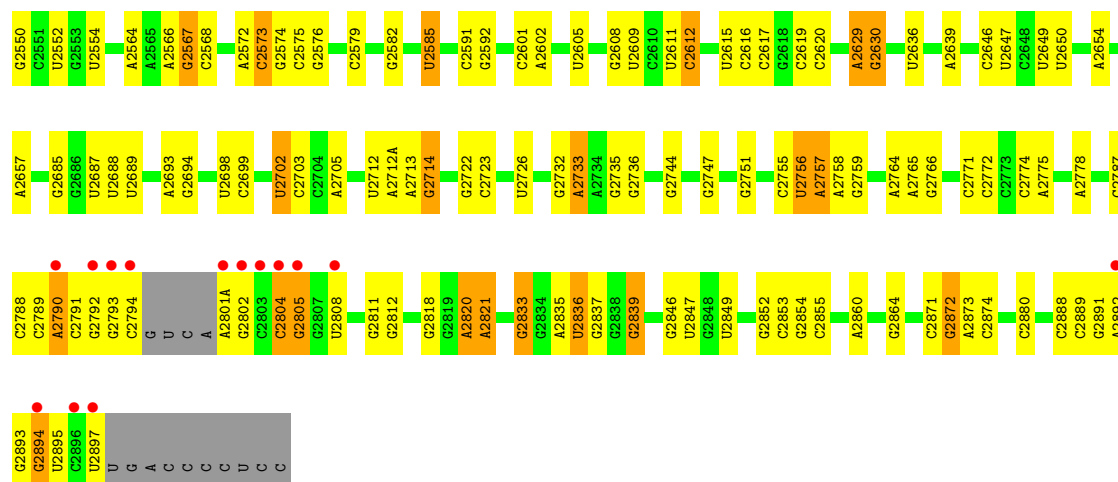
3 Residue-property plots

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

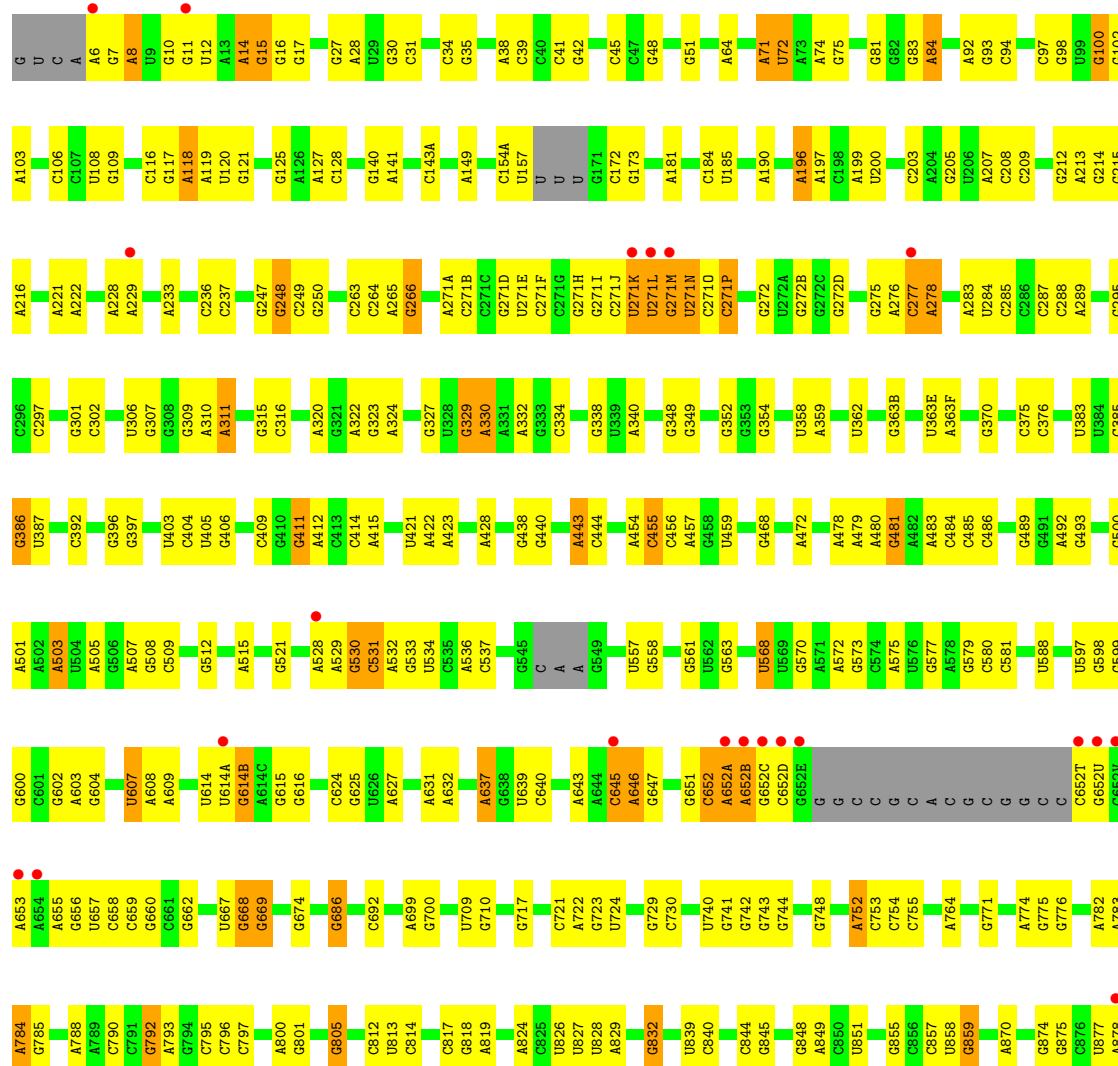
• Molecule 1: 23S Ribosomal RNA



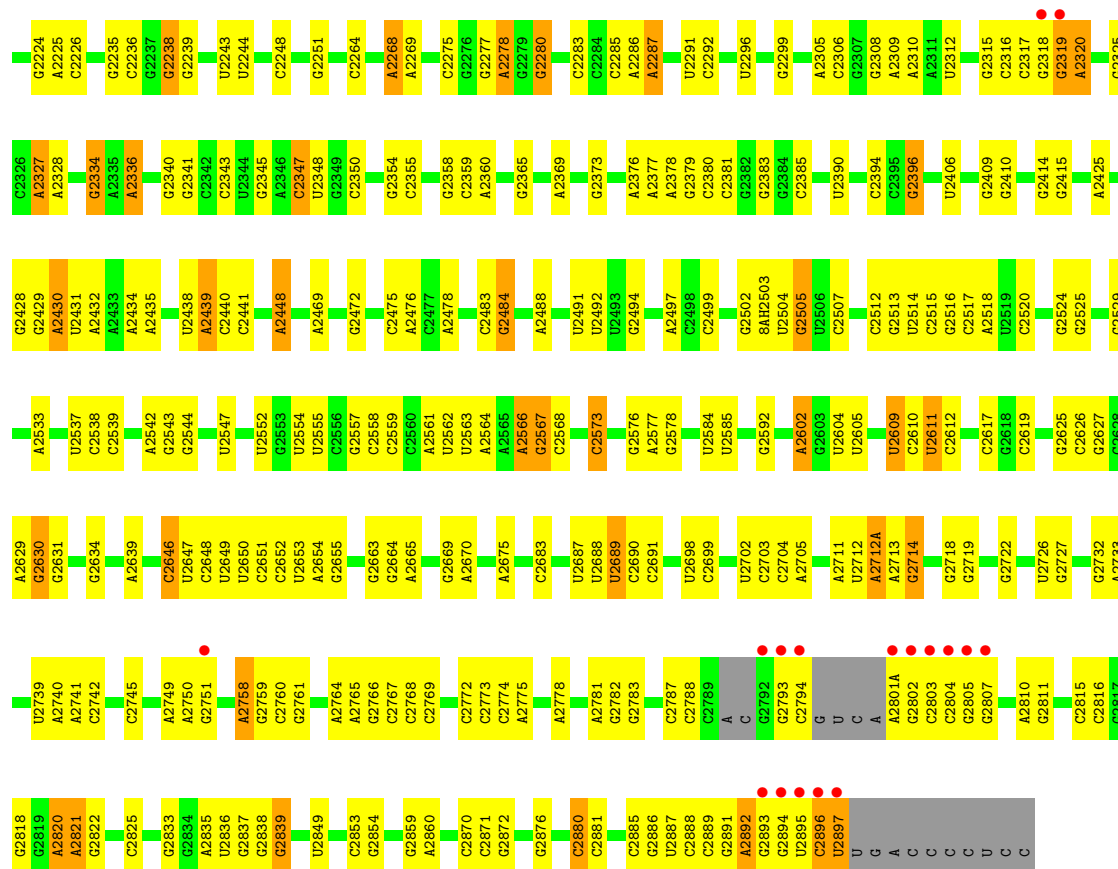




● Molecule 1: 23S Ribosomal RNA

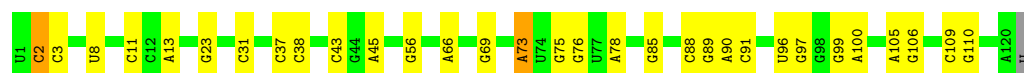


C2139	C2140	C2141	C2142	C2143	C2144	C2145	C2064	C2065	C2069	C2070	C2071	C2079	C2151	C2152	C2153	C2154	C2155	C2156	C2157	C2158	C2159	C2160	C2161	C2162	C2163	C2166	C2167	C2168	C2169	C2170	C2108	C2109	C2110	C2111	C2112	C2113	C2114	C2115	C2176	C2177	C2178	C2179	C2180	C2181	C2182	C2183	C2184	C2185	C2186	C2187	C2188	C2189	C2192	C2193	C2198	C2206	C2207	C2208	C2209	C2210	C2219																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
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- Molecule 2: 5S Ribosomal RNA

Chain 1B: 74% 24% ..



- Molecule 2: 5S Ribosomal RNA

Chain 2B: 52% 38% 9% .



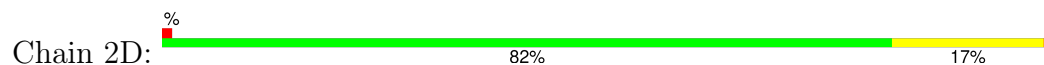
- Molecule 3: 50S ribosomal protein L2

Chain 1D: 77% 21% .

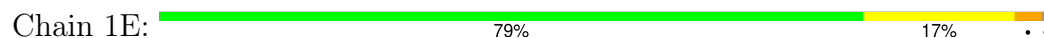




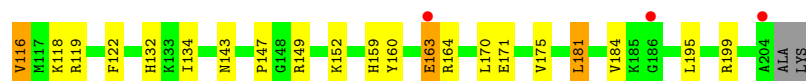
- Molecule 3: 50S ribosomal protein L2



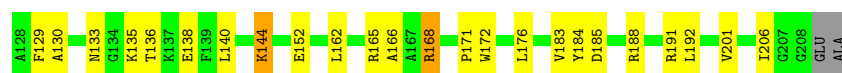
- Molecule 4: 50S ribosomal protein L3



- Molecule 4: 50S ribosomal protein L3

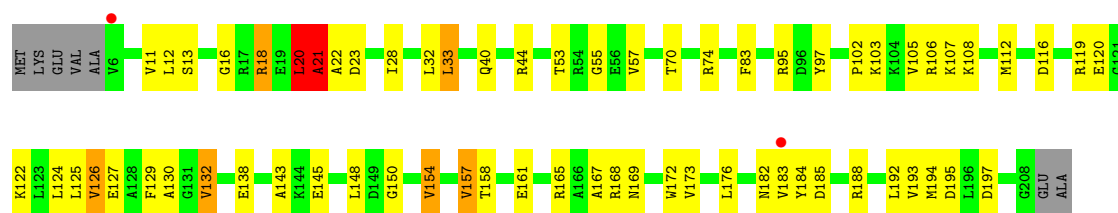


- Molecule 5: 50S ribosomal protein L4

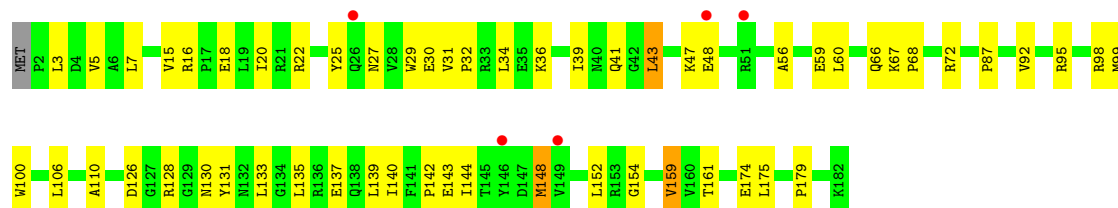


- Molecule 5: 50S ribosomal protein L4

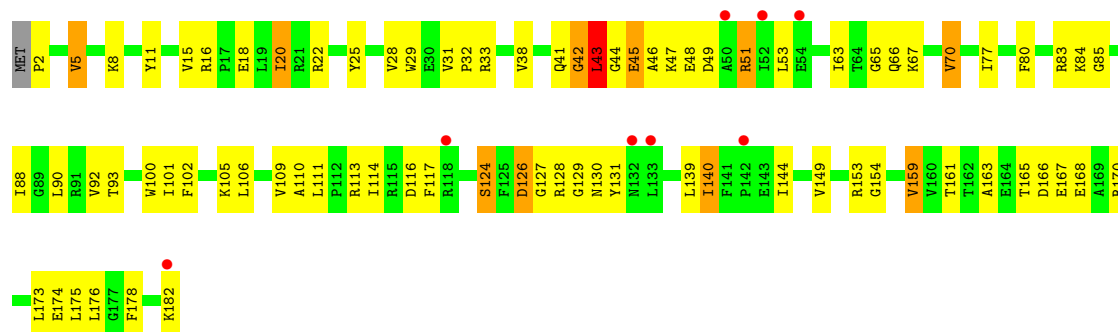




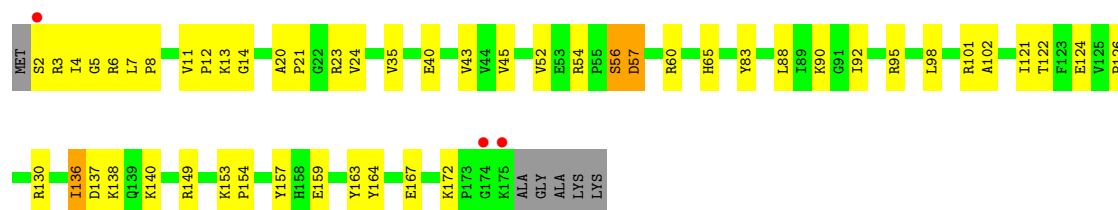
• Molecule 6: 50S ribosomal protein L5



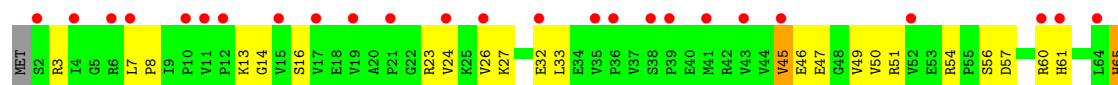
• Molecule 6: 50S ribosomal protein L5

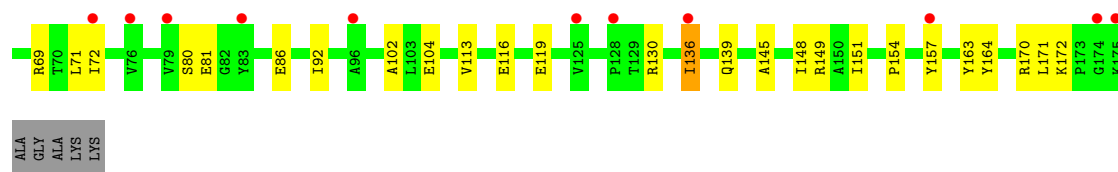


• Molecule 7: 50S ribosomal protein L6

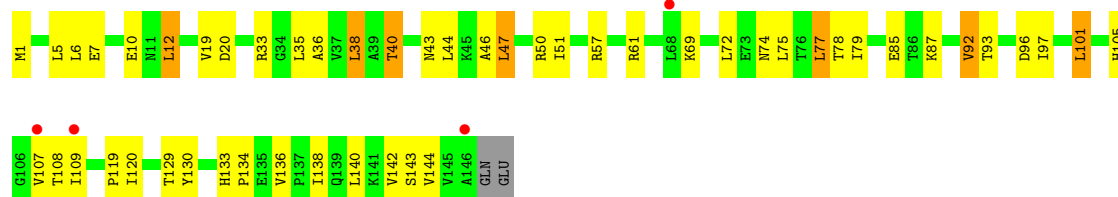


• Molecule 7: 50S ribosomal protein L6

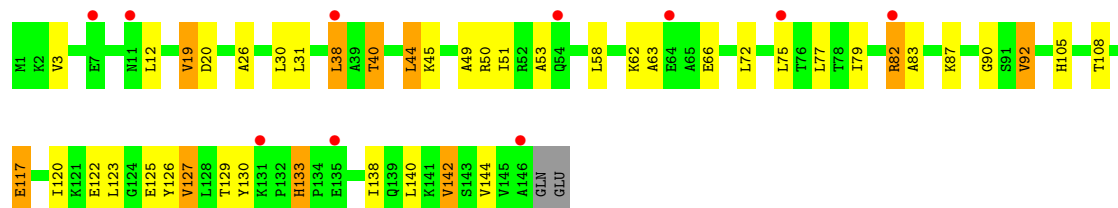




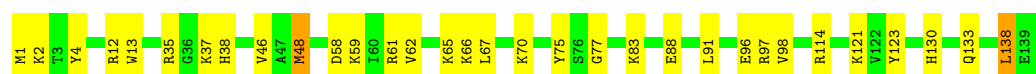
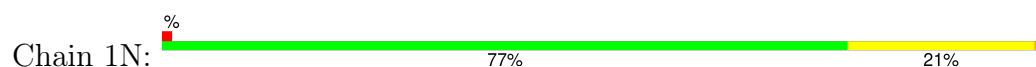
- Molecule 8: 50S ribosomal protein L9



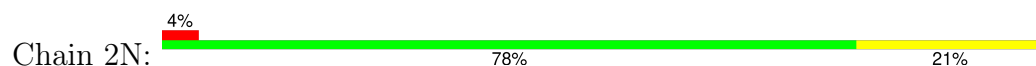
- Molecule 8: 50S ribosomal protein L9



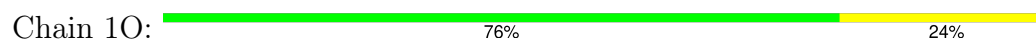
- Molecule 9: 50S ribosomal protein L13



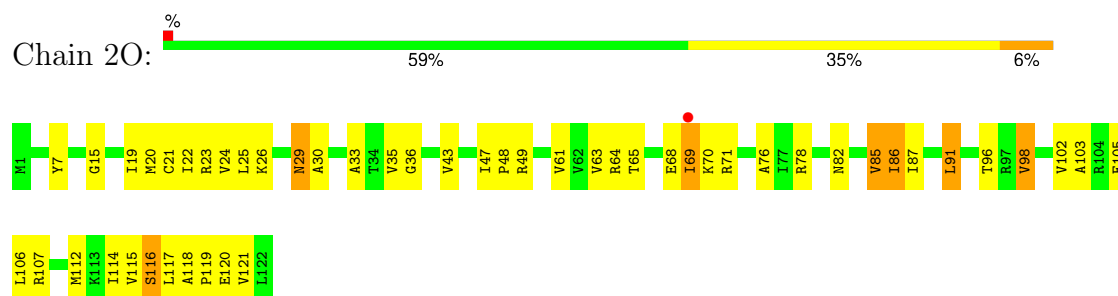
- Molecule 9: 50S ribosomal protein L13



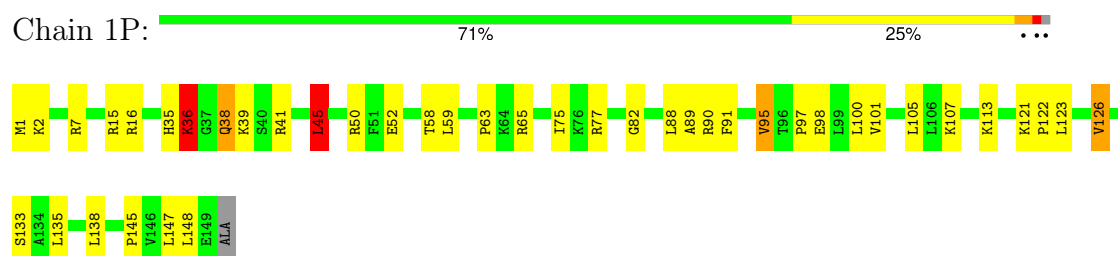
- Molecule 10: 50S ribosomal protein L14



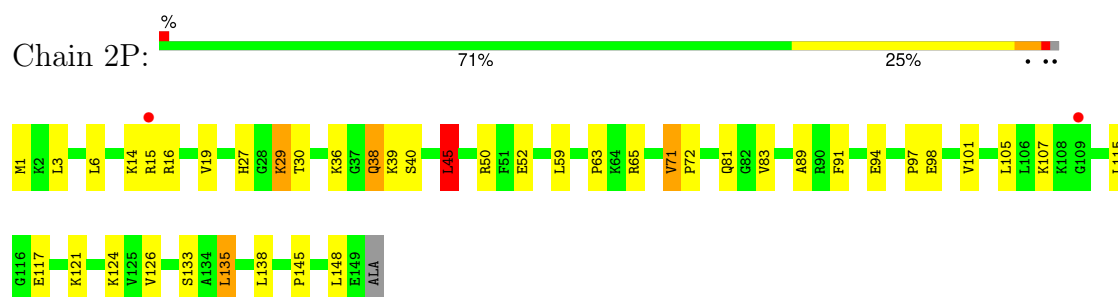
- Molecule 10: 50S ribosomal protein L14



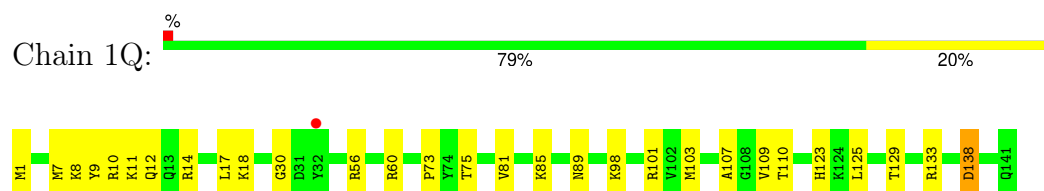
- Molecule 11: 50S ribosomal protein L15



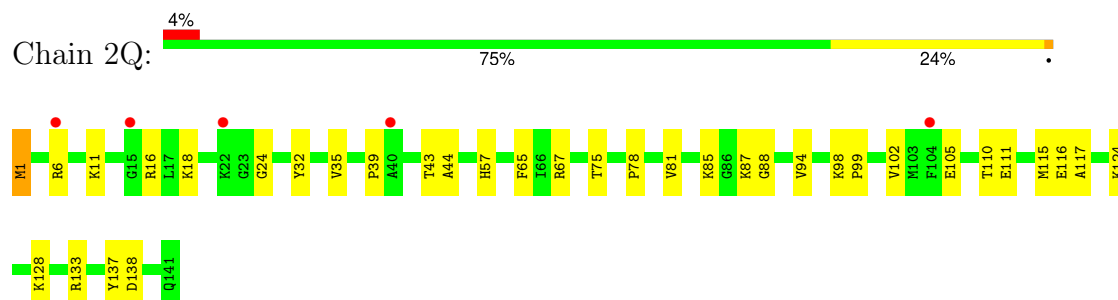
- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17

Chain 1R:  78% 20% .



- Molecule 13: 50S ribosomal protein L17

Chain 2R:  76% 19% .



- Molecule 14: 50S ribosomal protein L18

Chain 1S:  73% 23% . .



- Molecule 14: 50S ribosomal protein L18

Chain 2S:  63% 28% 7% .



- Molecule 15: 50S ribosomal protein L19

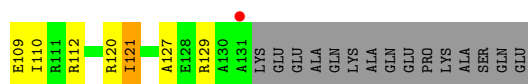
Chain 1T:  71% 18% 10%



- Molecule 15: 50S ribosomal protein L19

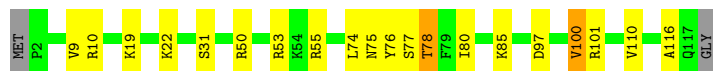
Chain 2T:  62% 25% 10%





- Molecule 16: 50S ribosomal protein L20

Chain 1U: 81% 15% ..



- Molecule 16: 50S ribosomal protein L20

Chain 2U: 3% 76% 21% ..



- Molecule 17: 50S ribosomal protein L21

Chain 1V: 82% 16% ..



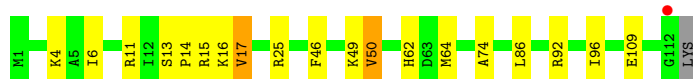
- Molecule 17: 50S ribosomal protein L21

Chain 2V: 76% 22% ..



- Molecule 18: 50S ribosomal protein L22

Chain 1W: 82% 15% ..



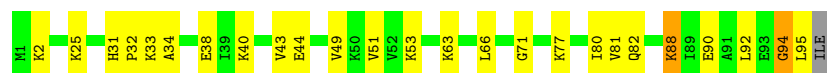
- Molecule 18: 50S ribosomal protein L22

Chain 2W: 76% 21% ..



- Molecule 19: 50S ribosomal protein L23

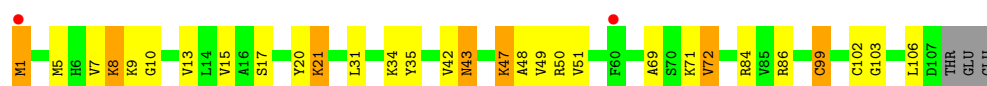
Chain 1X: 73% 24% ..



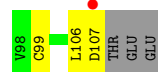
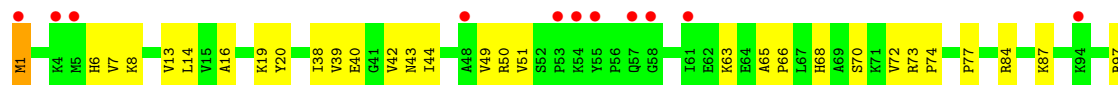
- Molecule 19: 50S ribosomal protein L23



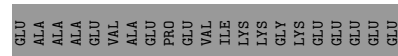
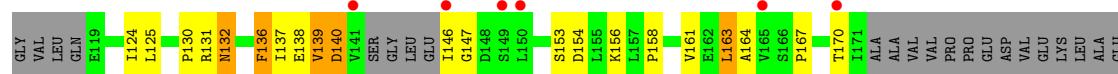
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

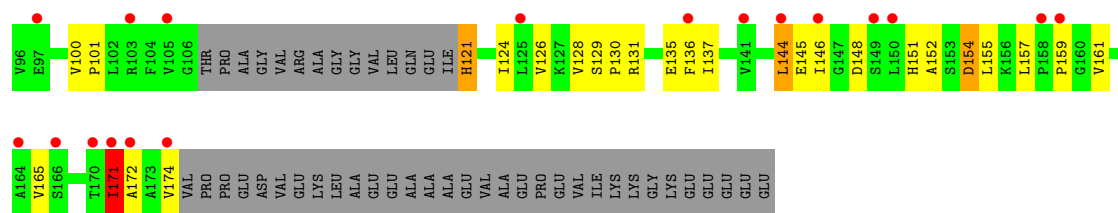


- Molecule 21: 50S ribosomal protein L25

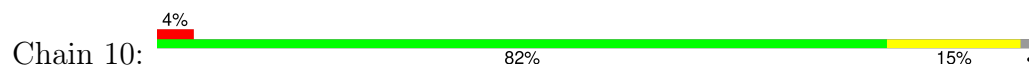


- Molecule 21: 50S ribosomal protein L25

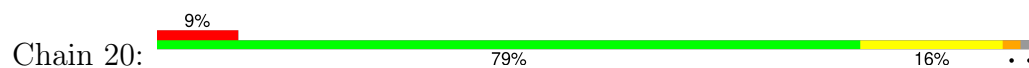




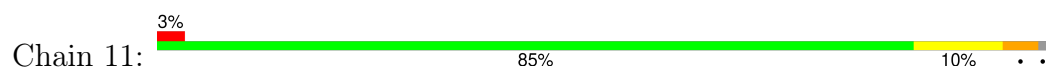
- Molecule 22: 50S ribosomal protein L27



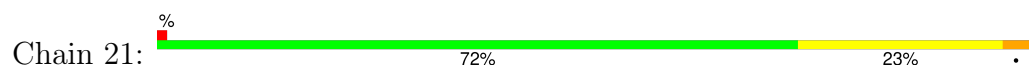
- Molecule 22: 50S ribosomal protein L27



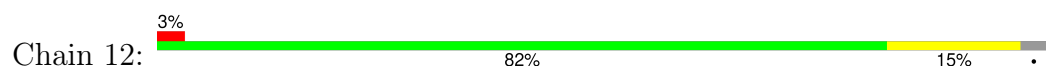
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28

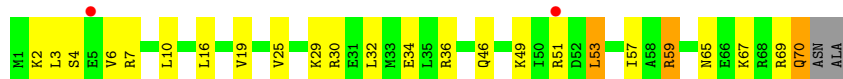


- Molecule 24: 50S ribosomal protein L29

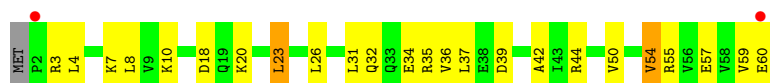


- Molecule 24: 50S ribosomal protein L29





- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



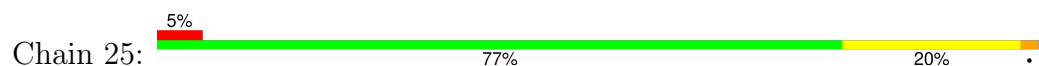
- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32

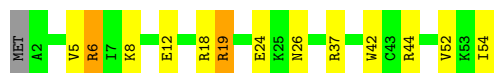


- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33

Chain 16:  74% 20% . .



- Molecule 28: 50S ribosomal protein L33

Chain 26:  85% 13% .



- Molecule 29: 50S ribosomal protein L34

Chain 17:  6% 73% 20% . .



- Molecule 29: 50S ribosomal protein L34

Chain 27:  6% 69% 24% . .



- Molecule 30: 50S ribosomal protein L35

Chain 18:  68% 31% .



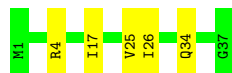
- Molecule 30: 50S ribosomal protein L35

Chain 28:  2% 75% 23% .

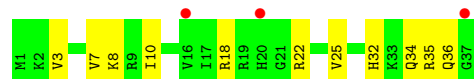


- Molecule 31: 50S ribosomal protein L36

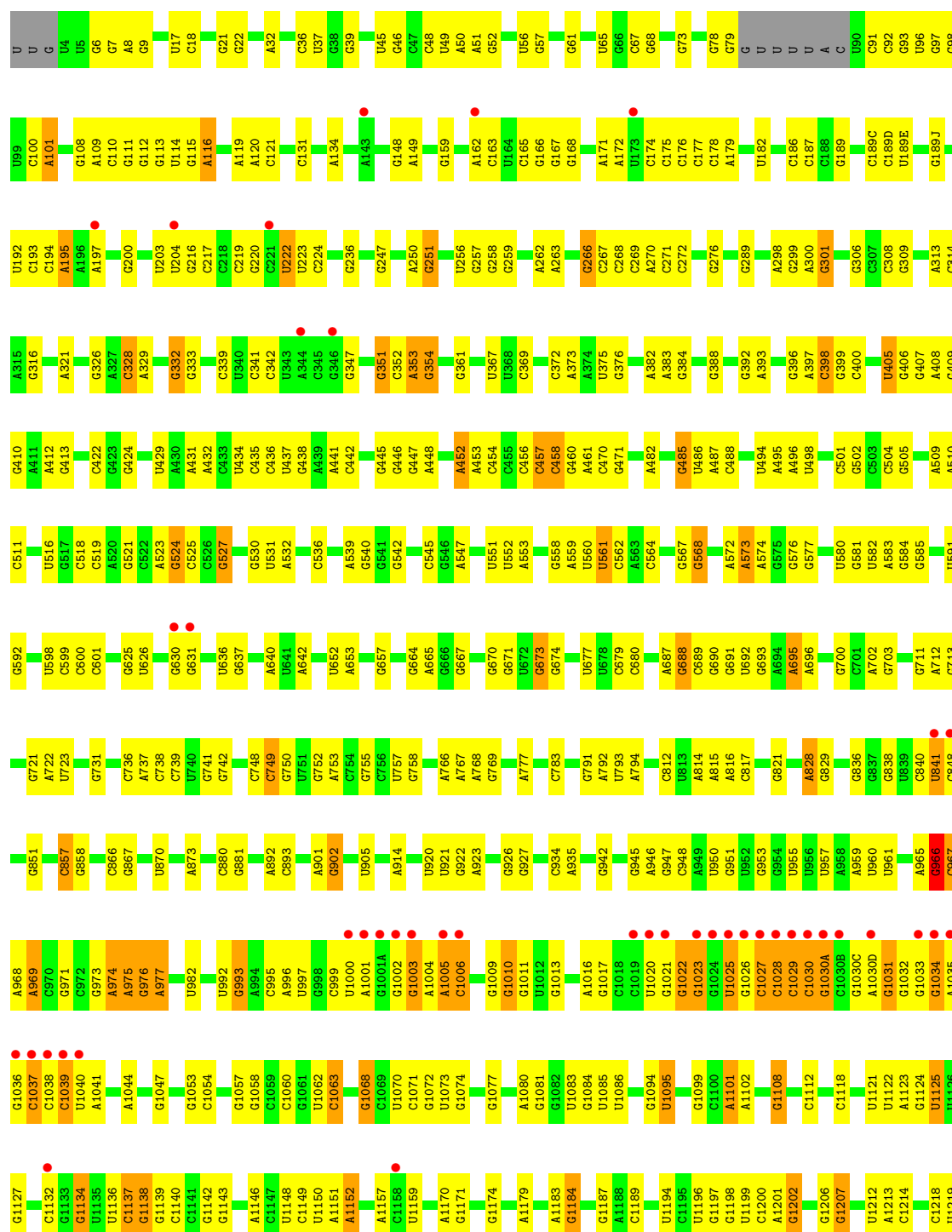
Chain 19:  86% 14%

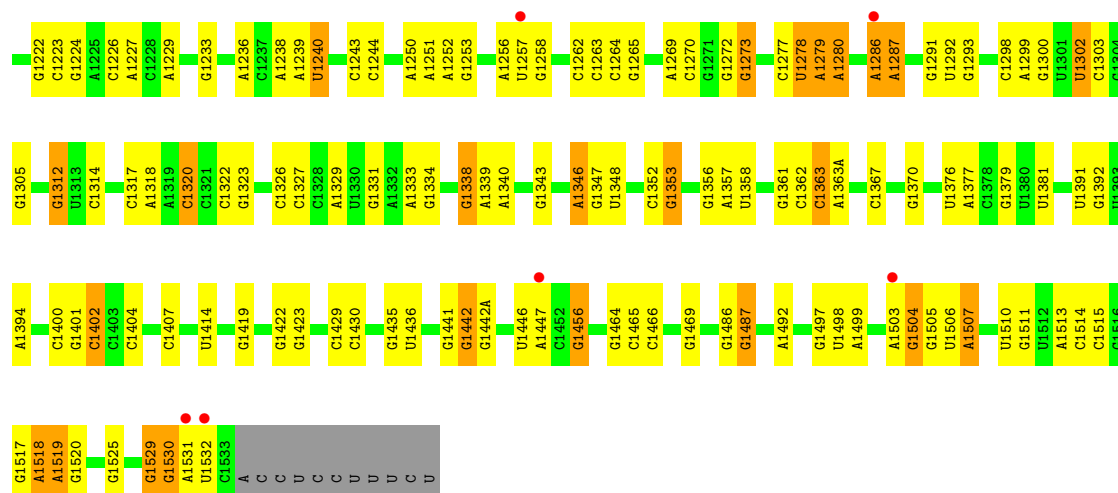


- Molecule 31: 50S ribosomal protein L36

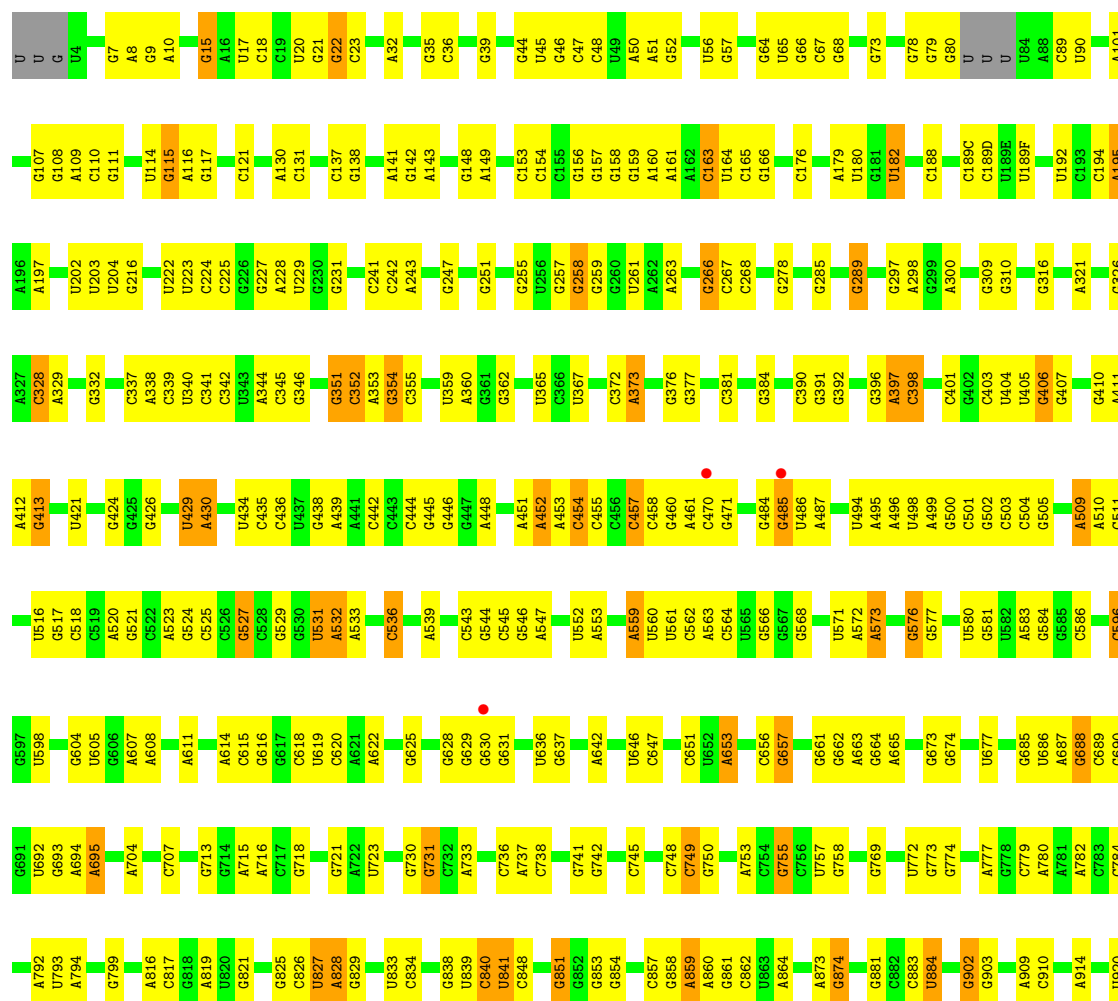


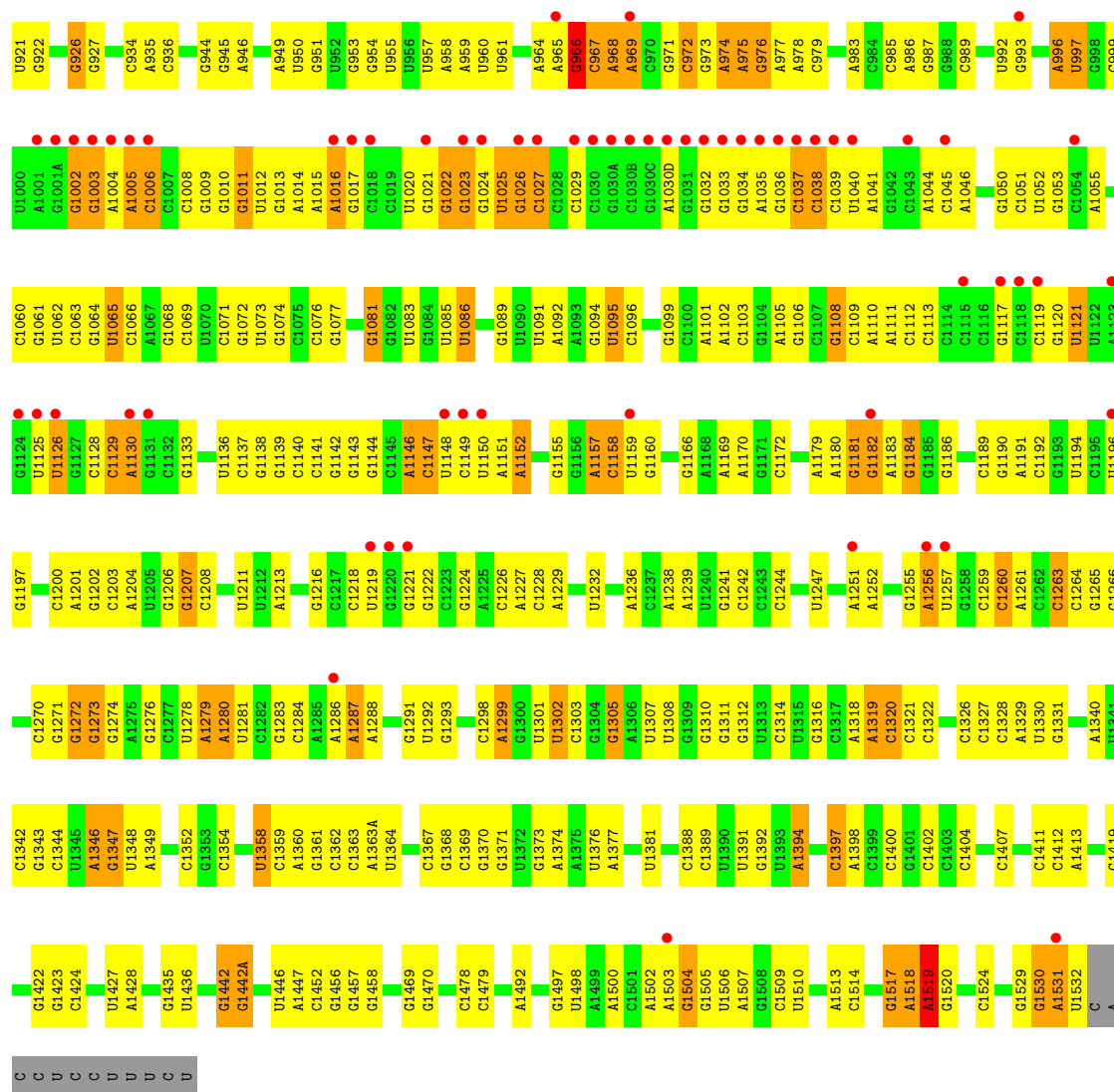
• Molecule 32: 16S Ribosomal RNA



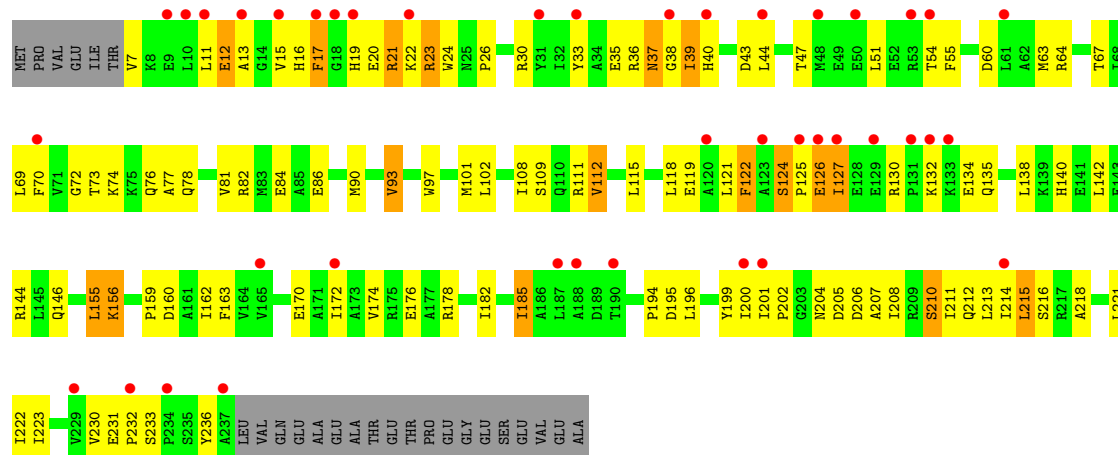


• Molecule 32: 16S Ribosomal RNA

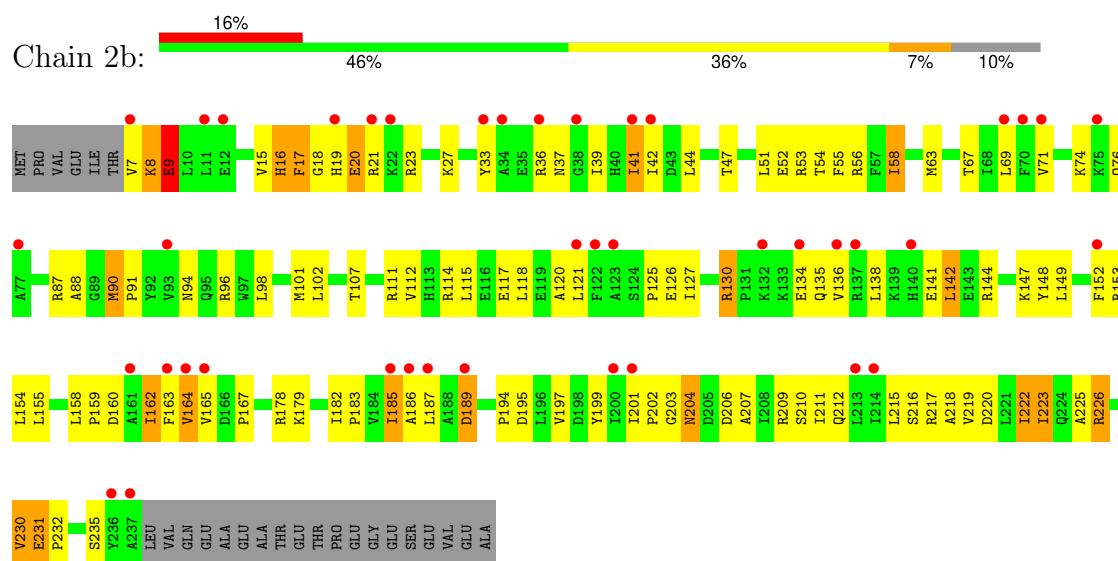




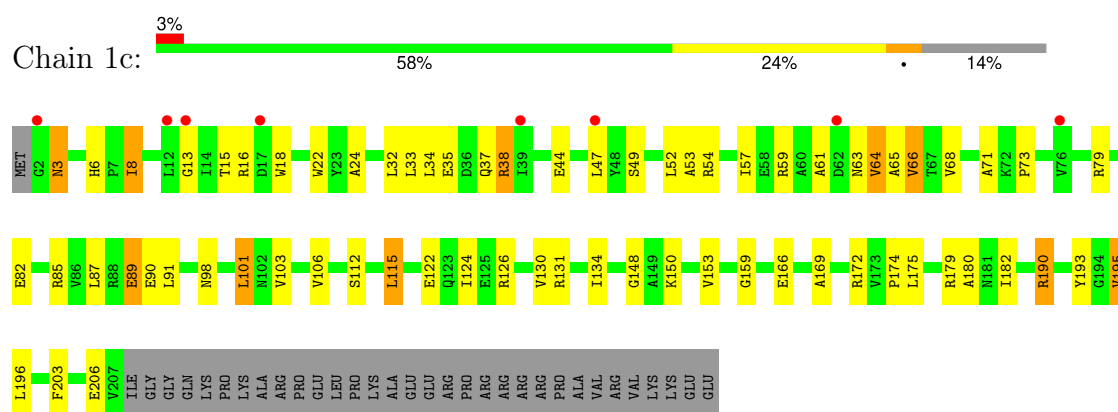
• Molecule 33: 30S ribosomal protein S2



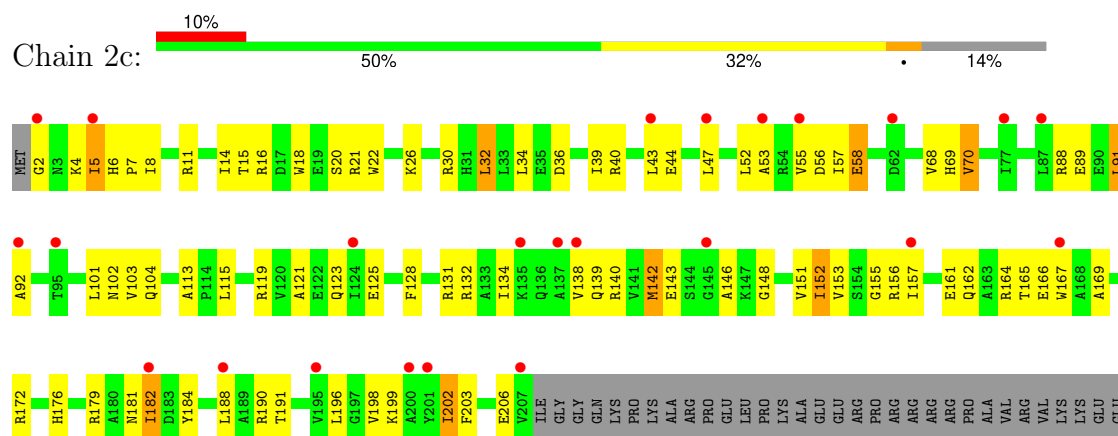
• Molecule 33: 30S ribosomal protein S2



• Molecule 34: 30S ribosomal protein S3

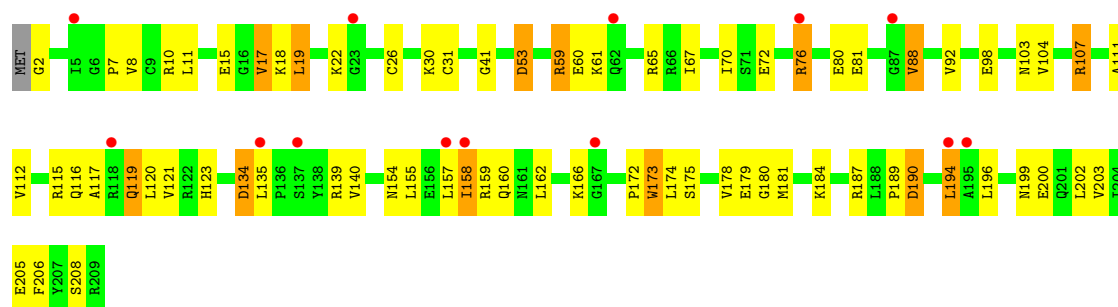


• Molecule 34: 30S ribosomal protein S3

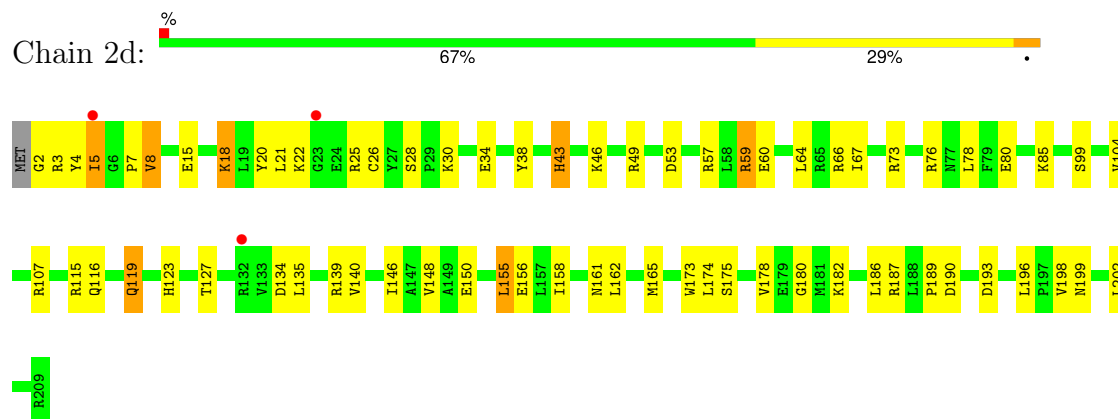


• Molecule 35: 30S ribosomal protein S4

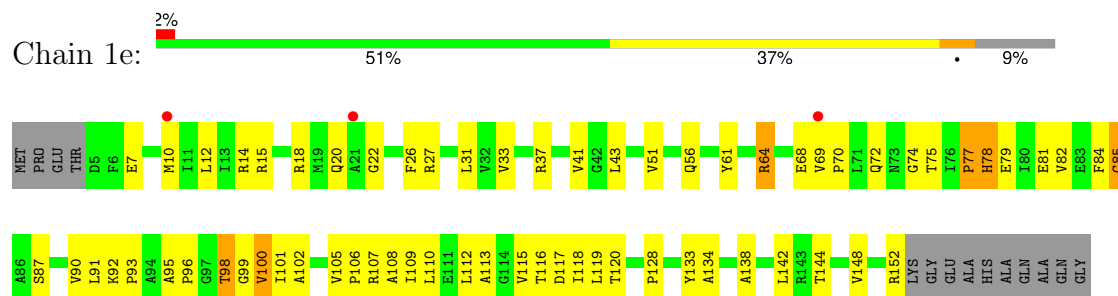




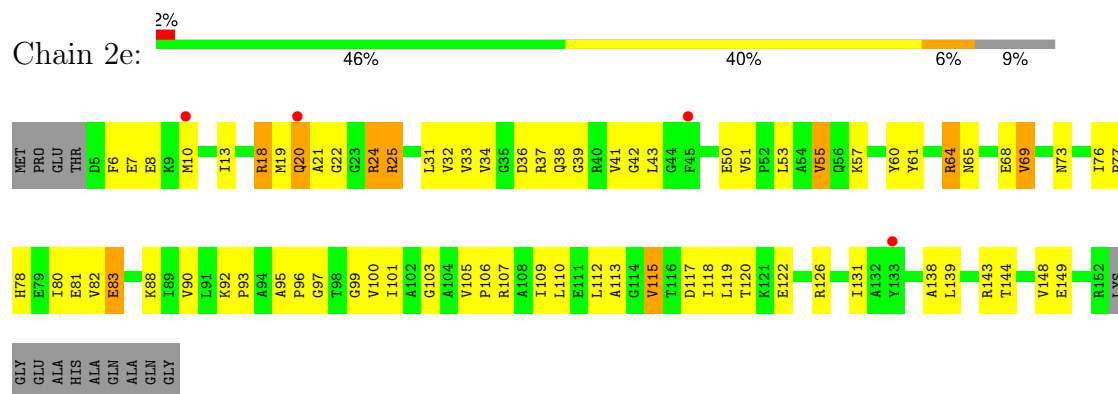
- Molecule 35: 30S ribosomal protein S4



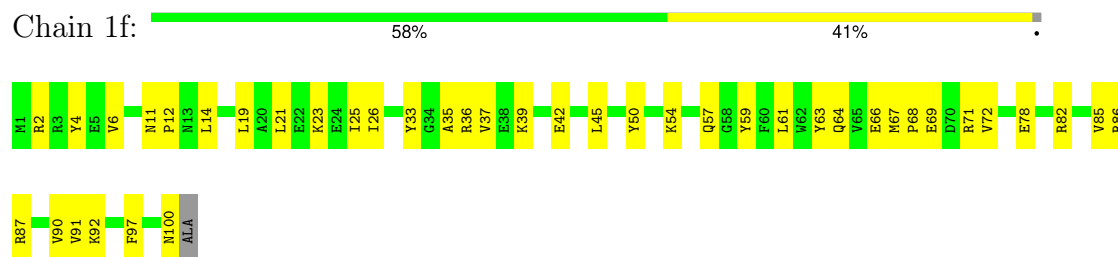
- Molecule 36: 30S ribosomal protein S5



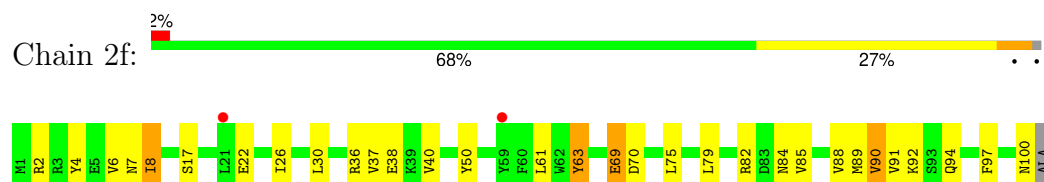
- Molecule 36: 30S ribosomal protein S5



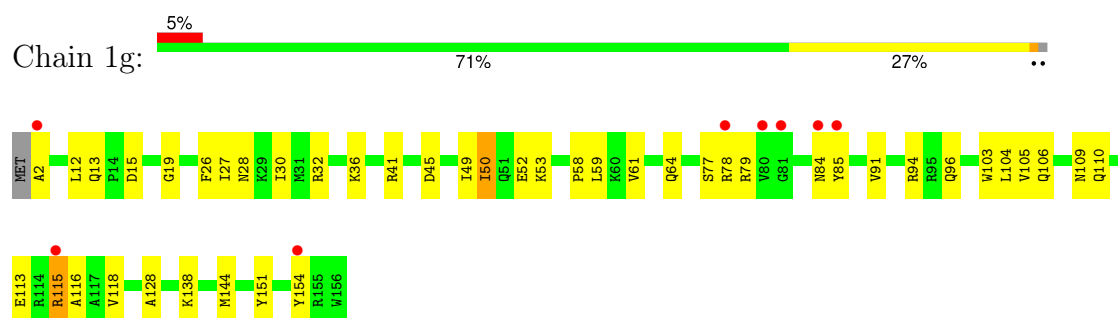
- Molecule 37: 30S ribosomal protein S6



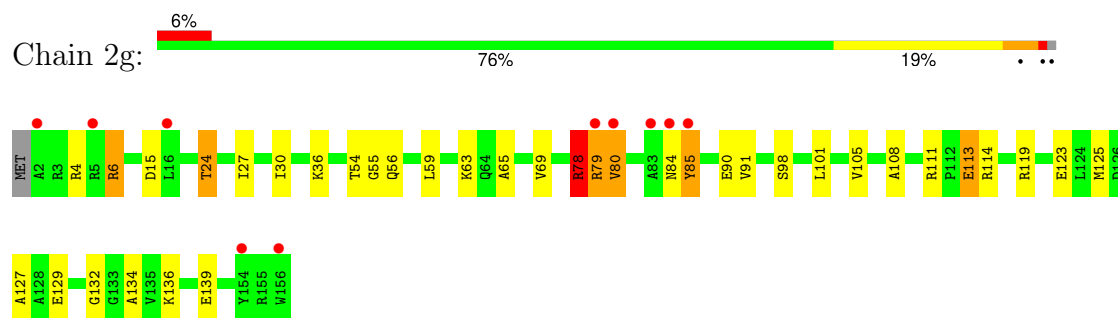
- Molecule 37: 30S ribosomal protein S6



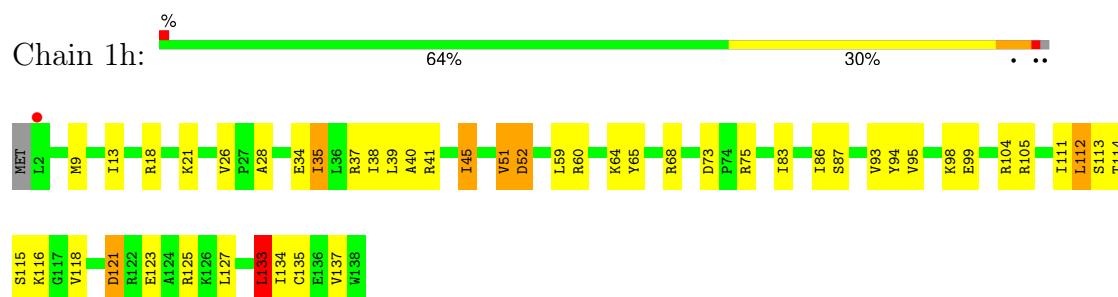
- Molecule 38: 30S ribosomal protein S7



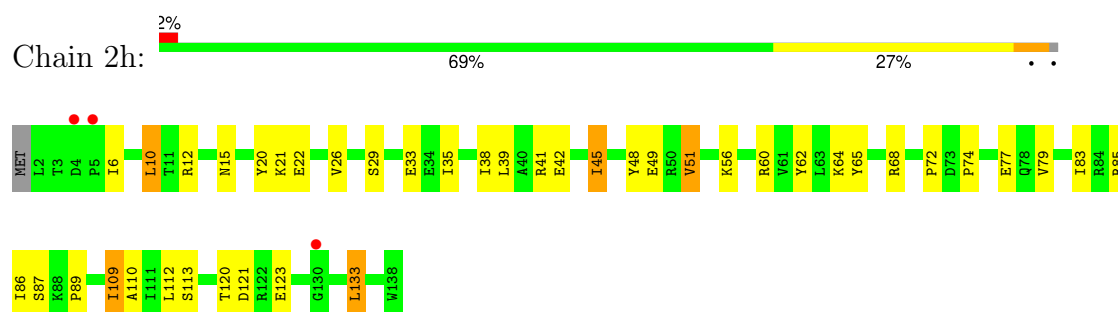
- Molecule 38: 30S ribosomal protein S7



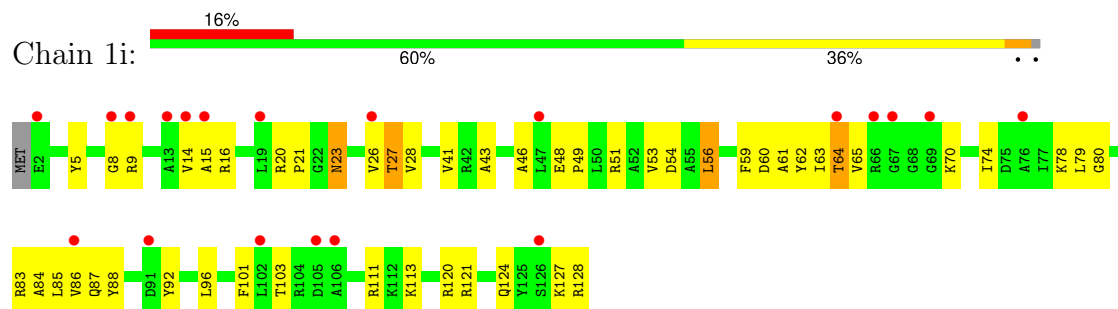
- Molecule 39: 30S ribosomal protein S8



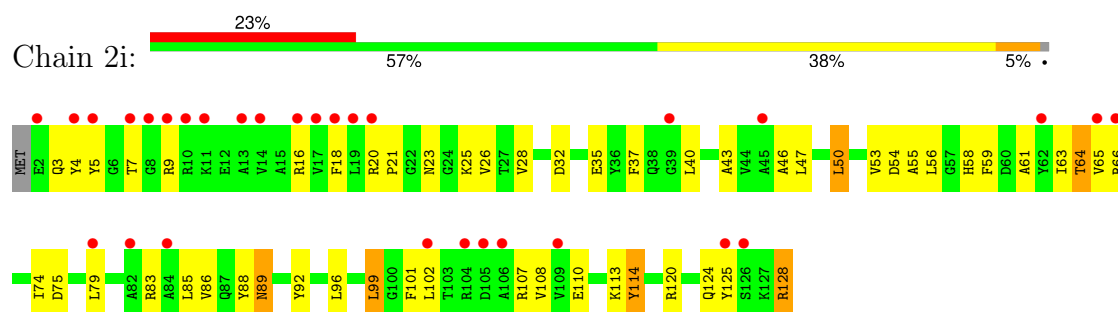
- Molecule 39: 30S ribosomal protein S8



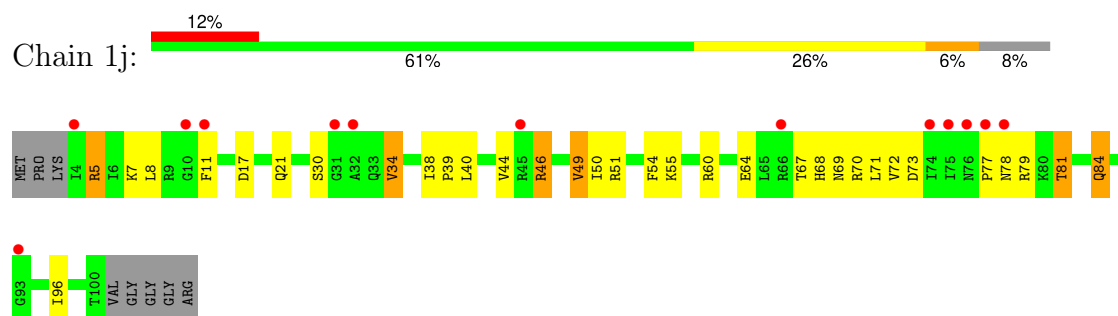
- Molecule 40: 30S ribosomal protein S9



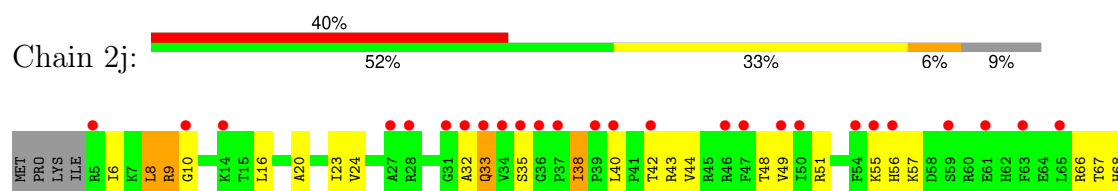
- Molecule 40: 30S ribosomal protein S9



- Molecule 41: 30S ribosomal protein S10



- Molecule 41: 30S ribosomal protein S10

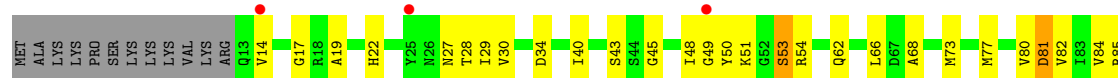




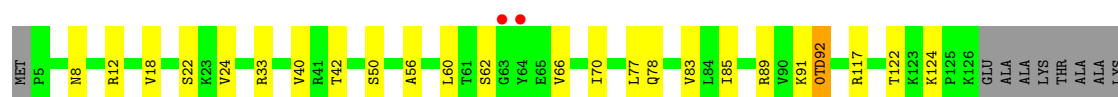
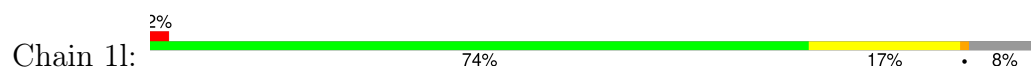
- Molecule 42: 30S ribosomal protein S11



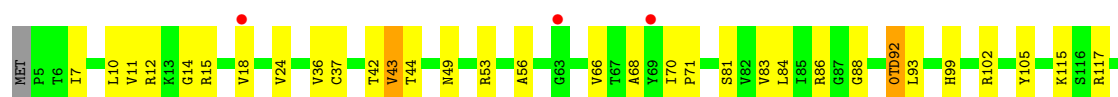
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12

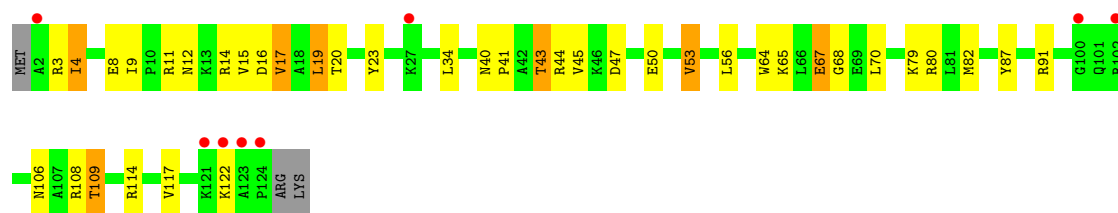


- Molecule 43: 30S ribosomal protein S12

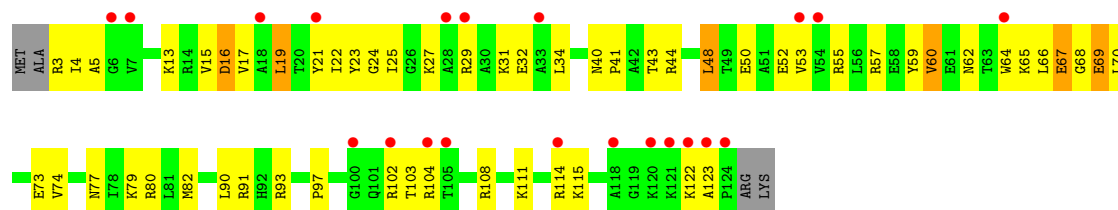


- Molecule 44: 30S ribosomal protein S13





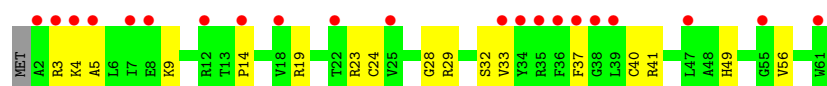
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



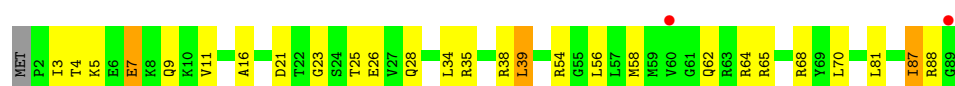
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15



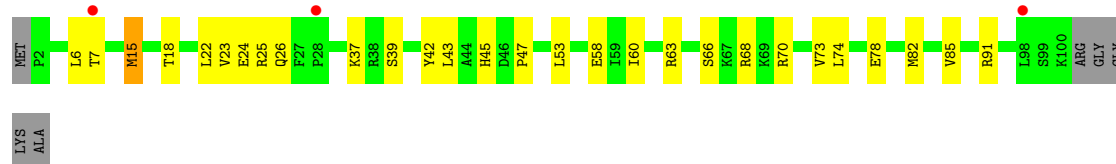
- Molecule 47: 30S ribosomal protein S16



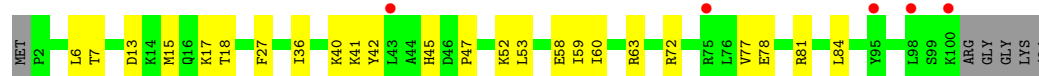
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



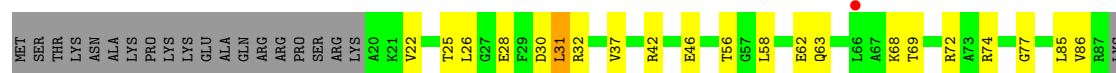
- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18

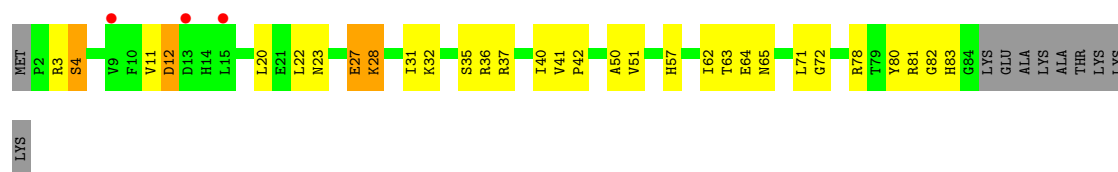


- Molecule 49: 30S ribosomal protein S18

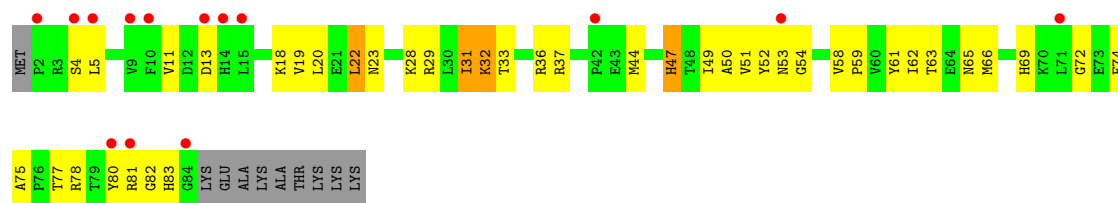


- Molecule 50: 30S ribosomal protein S19

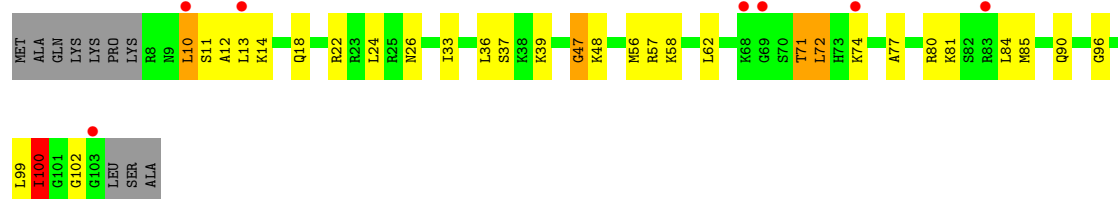




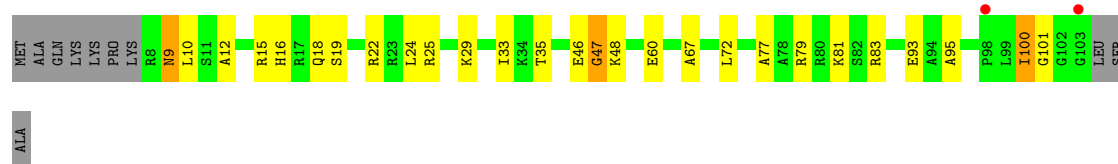
- Molecule 50: 30S ribosomal protein S19



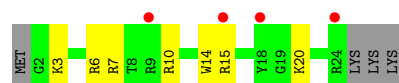
- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20

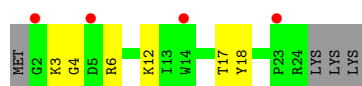


- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx





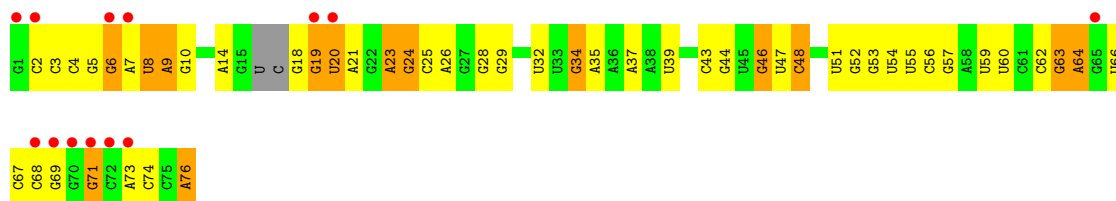
• Molecule 53: MF-mRNA



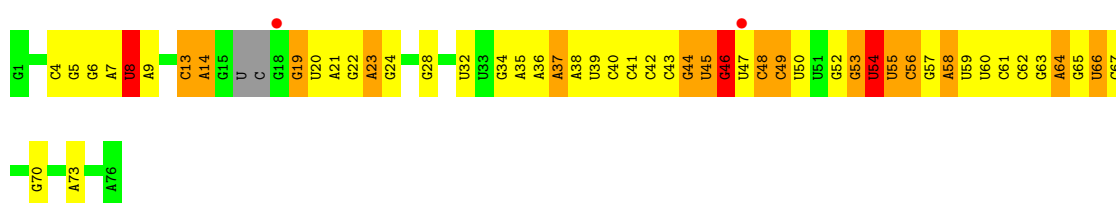
• Molecule 53: MF-mRNA



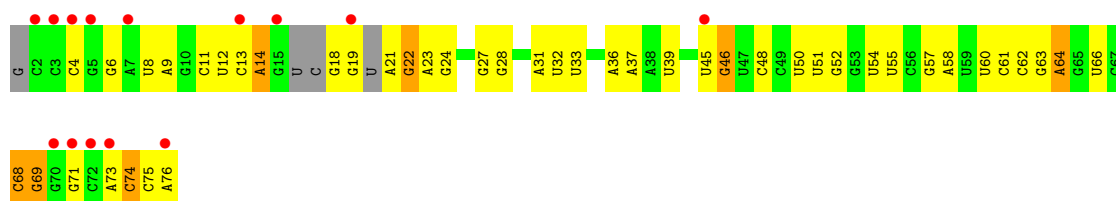
• Molecule 54: A- and E-site Deacylated tRNAphe



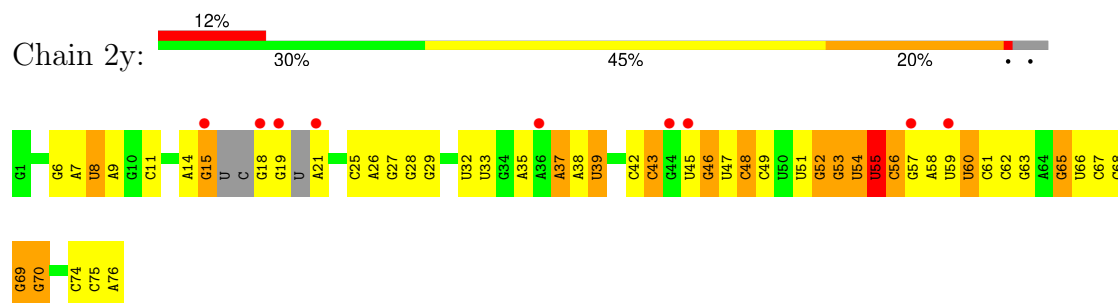
• Molecule 54: A- and E-site Deacylated tRNAphe



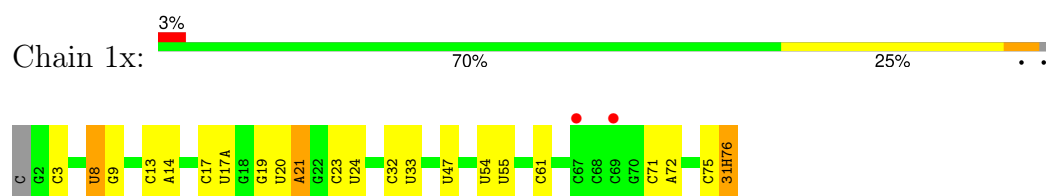
• Molecule 54: A- and E-site Deacylated tRNAphe



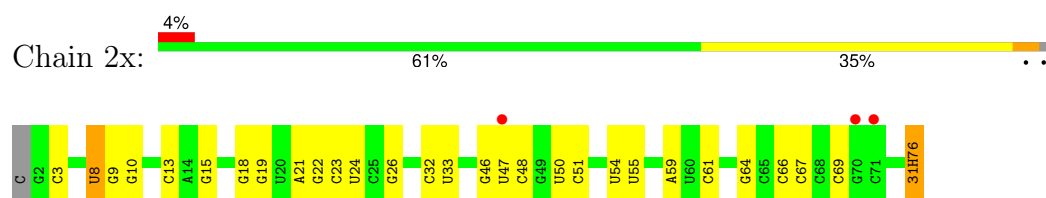
- Molecule 54: A- and E-site Deacylated tRNA^{phe}



- Molecule 55: P-site Aminoacyl-tRNA fMet-tRNA^{met}



- Molecule 55: P-site Aminoacyl-tRNA fMet-tRNA^{met}



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.01Å 449.04Å 621.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.89 – 2.60 121.89 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (121.89-2.60) 97.0 (121.89-2.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.216 , 0.261 0.218 , 0.262	Depositor DCC
R_{free} test set	86389 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	299649	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: OMU, K, MA6, ZN, G7M, 5MC, PSU, 5MU, MIA, M2G, 8AH, 0TD, UR3, 4SU, 4OC, SF4, 2MG, 31H, WC9, MG, OMG, OMC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.28	0/69011	0.45	1/107720 (0.0%)
1	2A	0.21	1/67295 (0.0%)	0.40	1/105042 (0.0%)
2	1B	0.22	0/2882	0.39	0/4494
2	2B	0.18	0/2879	0.36	0/4487
3	1D	0.26	0/2186	0.49	0/2944
3	2D	0.22	0/2186	0.43	0/2944
4	1E	0.27	0/1592	0.51	0/2149
4	2E	0.22	0/1592	0.47	0/2149
5	1F	0.25	0/1619	0.48	0/2193
5	2F	0.21	0/1615	0.47	2/2188 (0.1%)
6	1G	0.21	0/1448	0.43	0/1957
6	2G	0.22	0/1453	0.42	0/1963
7	1H	0.22	0/1356	0.43	0/1834
7	2H	0.19	0/1356	0.37	0/1834
8	1I	0.24	0/1112	0.42	0/1514
8	2I	0.20	0/1079	0.43	0/1475
9	1N	0.25	0/1144	0.47	0/1543
9	2N	0.18	0/1144	0.39	0/1543
10	1O	0.25	0/943	0.46	0/1269
10	2O	0.20	0/943	0.43	0/1269
11	1P	0.25	0/1152	0.52	0/1533
11	2P	0.21	0/1152	0.45	0/1533
12	1Q	0.28	0/1143	0.48	0/1527
12	2Q	0.19	0/1143	0.40	0/1527
13	1R	0.27	0/982	0.50	0/1312
13	2R	0.22	0/982	0.48	0/1312
14	1S	0.22	0/883	0.46	0/1176
14	2S	0.19	0/880	0.44	0/1172
15	1T	0.24	0/1105	0.46	0/1477
15	2T	0.20	0/1097	0.42	0/1468
16	1U	0.29	0/977	0.47	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.19	0/977	0.39	0/1301
17	1V	0.26	0/782	0.47	0/1049
17	2V	0.19	0/782	0.39	0/1049
18	1W	0.27	0/897	0.46	0/1205
18	2W	0.22	0/897	0.40	0/1205
19	1X	0.26	0/764	0.50	0/1025
19	2X	0.22	0/764	0.49	2/1025 (0.2%)
20	1Y	0.23	0/819	0.48	0/1095
20	2Y	0.20	0/819	0.49	0/1095
21	1Z	0.21	0/1267	0.47	0/1717
21	2Z	0.22	0/1299	0.45	0/1763
22	10	0.26	0/662	0.49	0/881
22	20	0.21	0/662	0.43	0/881
23	11	0.23	0/762	0.40	0/1014
23	21	0.22	0/762	0.42	0/1014
24	12	0.24	0/590	0.42	0/781
24	22	0.18	0/590	0.38	0/781
25	13	0.25	0/474	0.46	0/635
25	23	0.18	0/469	0.43	0/630
26	14	0.26	0/565	0.57	0/761
26	24	0.24	0/545	0.55	0/737
27	15	0.29	0/469	0.50	0/635
27	25	0.22	0/469	0.48	0/635
28	16	0.25	0/460	0.44	0/613
28	26	0.23	0/456	0.45	0/608
29	17	0.29	0/426	0.52	0/561
29	27	0.24	0/426	0.50	0/561
30	18	0.26	0/525	0.48	0/691
30	28	0.22	0/525	0.40	0/691
31	19	0.28	0/310	0.52	0/407
31	29	0.19	0/310	0.42	0/407
32	1a	0.20	0/35795	0.38	0/55864
32	2a	0.20	0/35886	0.38	4/56005 (0.0%)
33	1b	0.21	0/1881	0.52	0/2542
33	2b	0.22	0/1860	0.47	0/2518
34	1c	0.20	0/1572	0.45	0/2126
34	2c	0.25	0/1566	0.41	0/2119
35	1d	0.18	0/1685	0.42	0/2262
35	2d	0.20	0/1704	0.43	0/2284
36	1e	0.21	0/1145	0.46	0/1543
36	2e	0.27	0/1149	0.47	0/1548
37	1f	0.19	0/823	0.40	0/1115
37	2f	0.20	0/829	0.39	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1250	0.39	0/1679
38	2g	0.18	0/1254	0.40	0/1683
39	1h	0.19	0/1108	0.42	0/1494
39	2h	0.19	0/1108	0.41	0/1494
40	1i	0.20	0/1002	0.47	0/1346
40	2i	0.22	0/997	0.52	0/1343
41	1j	0.26	0/722	0.46	0/982
41	2j	0.23	0/727	0.51	0/988
42	1k	0.18	0/844	0.42	0/1145
42	2k	0.18	0/848	0.40	0/1149
43	1l	0.22	0/937	0.44	0/1260
43	2l	0.18	0/937	0.40	0/1260
44	1m	0.20	0/969	0.48	1/1302 (0.1%)
44	2m	0.20	0/961	0.45	0/1291
45	1n	0.20	0/501	0.44	0/664
45	2n	0.20	0/501	0.42	0/664
46	1o	0.20	0/739	0.38	0/985
46	2o	0.17	0/739	0.38	0/985
47	1p	0.19	0/697	0.44	0/939
47	2p	0.20	0/693	0.46	0/935
48	1q	0.19	0/836	0.39	0/1117
48	2q	0.18	0/836	0.38	0/1117
49	1r	0.20	0/560	0.40	0/746
49	2r	0.18	0/560	0.39	0/746
50	1s	0.19	0/667	0.49	0/900
50	2s	0.24	0/661	0.55	0/893
51	1t	0.20	0/730	0.51	0/965
51	2t	0.21	0/729	0.46	0/965
52	1u	0.20	0/203	0.46	0/266
52	2u	0.27	0/203	0.56	0/266
53	1v	0.21	0/310	0.33	0/480
53	2v	0.19	0/310	0.34	0/480
54	1w	0.28	1/1606 (0.1%)	0.40	0/2497
54	1y	0.28	2/1606 (0.1%)	0.38	0/2497
54	2w	0.31	2/1556 (0.1%)	0.41	0/2418
54	2y	0.28	2/1583 (0.1%)	0.40	0/2459
55	1x	0.27	0/1700	0.40	0/2650
55	2x	0.25	0/1700	0.39	0/2650
All	All	0.23	8/316640 (0.0%)	0.42	11/474051 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	2F	0	1
33	1b	0	2
38	2g	0	1
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	OMU	O3'-P	5.62	1.61	1.56
54	2w	46	G7M	O3'-P	5.57	1.61	1.56
54	1y	8	4SU	O3'-P	5.36	1.61	1.56
54	2w	8	4SU	O3'-P	5.30	1.61	1.56
54	2y	46	G7M	O3'-P	5.30	1.61	1.56
54	1y	46	G7M	O3'-P	5.18	1.61	1.56
54	1w	8	4SU	O3'-P	5.16	1.61	1.56
54	2y	8	4SU	O3'-P	5.01	1.61	1.56

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1992	G	C2'-C3'-O3'	6.70	119.54	109.50
32	2a	1272	G	N1-C2-N2	-5.92	98.45	116.20
32	2a	1263	C	N1-C2-O2	5.49	135.36	118.90
5	2F	21	ALA	CA-C-N	5.37	131.36	121.70
5	2F	21	ALA	C-N-CA	5.37	131.36	121.70
44	1m	106	ASN	CB-CA-C	-5.36	110.38	116.54
19	2X	94	GLY	CA-C-N	5.31	131.26	121.70
19	2X	94	GLY	C-N-CA	5.31	131.26	121.70
32	2a	1272	G	N3-C2-N2	5.16	135.38	119.90
32	2a	1065	U	P-O3'-C3'	5.10	127.84	120.20
1	2A	1992	G	C2'-C3'-O3'	5.08	117.12	109.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	122	PHE	Peptide
33	1b	124	SER	Peptide
5	2F	20	LEU	Peptide
38	2g	78	ARG	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	61853	0	31183	617	0
1	2A	60323	0	30413	682	0
2	1B	2577	0	1305	21	0
2	2B	2575	0	1303	33	0
3	1D	2136	0	2217	56	0
3	2D	2136	0	2218	33	0
4	1E	1559	0	1618	31	0
4	2E	1559	0	1618	34	0
5	1F	1584	0	1625	33	0
5	2F	1580	0	1619	38	0
6	1G	1423	0	1436	37	0
6	2G	1428	0	1438	57	0
7	1H	1330	0	1407	31	0
7	2H	1330	0	1407	26	0
8	1I	1097	0	1140	34	0
8	2I	1064	0	1082	27	0
9	1N	1117	0	1184	22	0
9	2N	1117	0	1184	16	0
10	1O	933	0	996	21	0
10	2O	933	0	996	35	0
11	1P	1135	0	1212	29	0
11	2P	1135	0	1212	32	0
12	1Q	1122	0	1179	16	0
12	2Q	1122	0	1179	25	0
13	1R	968	0	1033	17	0
13	2R	968	0	1033	23	0
14	1S	873	0	927	16	0
14	2S	870	0	923	30	0
15	1T	1091	0	1151	13	0
15	2T	1083	0	1136	28	0
16	1U	959	0	1019	13	0
16	2U	959	0	1019	17	0
17	1V	771	0	830	14	0
17	2V	771	0	830	16	0
18	1W	886	0	940	12	0
18	2W	886	0	940	19	0
19	1X	750	0	814	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2X	750	0	814	22	0
20	1Y	806	0	881	23	0
20	2Y	806	0	881	17	0
21	1Z	1240	0	1240	37	0
21	2Z	1271	0	1273	43	0
22	10	653	0	674	14	0
22	20	653	0	674	11	0
23	11	755	0	826	7	0
23	21	755	0	826	18	0
24	12	588	0	643	5	0
24	22	588	0	643	18	0
25	13	469	0	518	12	0
25	23	464	0	514	12	0
26	14	552	0	533	36	0
26	24	532	0	503	29	0
27	15	455	0	465	4	0
27	25	455	0	465	9	0
28	16	453	0	473	9	0
28	26	449	0	469	3	0
29	17	418	0	467	9	0
29	27	418	0	467	11	0
30	18	517	0	582	16	0
30	28	517	0	582	12	0
31	19	307	0	335	2	0
31	29	307	0	335	7	0
32	1a	32246	0	16295	374	0
32	2a	32327	0	16338	457	0
33	1b	1846	0	1867	72	0
33	2b	1825	0	1828	83	0
34	1c	1548	0	1535	42	0
34	2c	1542	0	1517	54	0
35	1d	1655	0	1672	57	0
35	2d	1674	0	1714	43	0
36	1e	1129	0	1185	38	0
36	2e	1133	0	1191	49	0
37	1f	810	0	804	24	0
37	2f	816	0	808	16	0
38	1g	1231	0	1238	20	0
38	2g	1235	0	1249	23	0
39	1h	1088	0	1126	32	0
39	2h	1088	0	1126	27	0
40	1i	983	0	986	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	2i	978	0	966	38	0
41	1j	709	0	650	24	0
41	2j	714	0	672	37	0
42	1k	829	0	825	15	0
42	2k	833	0	836	23	0
43	1l	932	0	981	12	0
43	2l	932	0	981	20	0
44	1m	958	0	1002	28	0
44	2m	950	0	988	43	0
45	1n	492	0	528	12	0
45	2n	492	0	529	14	0
46	1o	728	0	760	16	0
46	2o	728	0	760	20	0
47	1p	681	0	697	19	0
47	2p	677	0	686	22	0
48	1q	823	0	891	13	0
48	2q	823	0	891	14	0
49	1r	555	0	618	9	0
49	2r	555	0	618	11	0
50	1s	652	0	662	27	0
50	2s	646	0	644	34	0
51	1t	728	0	798	21	0
51	2t	727	0	796	20	0
52	1u	199	0	208	5	0
52	2u	199	0	208	6	0
53	1v	277	0	140	1	0
53	2v	277	0	140	2	0
54	1w	1592	0	818	31	0
54	1y	1585	0	803	25	0
54	2w	1544	0	787	20	0
54	2y	1565	0	794	37	0
55	1x	1635	0	839	7	0
55	2x	1635	0	839	12	0
56	10	8	0	0	0	0
56	11	6	0	0	0	0
56	12	2	0	0	0	0
56	13	3	0	0	0	0
56	14	1	0	0	0	0
56	15	10	0	0	0	0
56	16	1	0	0	0	0
56	17	6	0	0	0	0
56	18	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	19	1	0	0	0	0
56	1A	1096	0	0	0	0
56	1B	36	0	0	0	0
56	1D	14	0	0	0	0
56	1E	15	0	0	0	0
56	1F	15	0	0	0	0
56	1G	5	0	0	0	0
56	1H	1	0	0	0	0
56	1I	1	0	0	0	0
56	1N	6	0	0	0	0
56	1O	5	0	0	0	0
56	1P	5	0	0	0	0
56	1Q	6	0	0	0	0
56	1R	6	0	0	0	0
56	1S	3	0	0	0	0
56	1T	2	0	0	0	0
56	1U	9	0	0	0	0
56	1V	6	0	0	0	0
56	1W	7	0	0	0	0
56	1X	7	0	0	0	0
56	1Y	5	0	0	0	0
56	1Z	4	0	0	0	0
56	1a	210	0	0	0	0
56	1b	1	0	0	0	0
56	1d	1	0	0	0	0
56	1e	2	0	0	0	0
56	1f	2	0	0	0	0
56	1k	1	0	0	0	0
56	1l	2	0	0	0	0
56	1m	1	0	0	0	0
56	1n	2	0	0	0	0
56	1p	1	0	0	0	0
56	1t	1	0	0	0	0
56	1w	8	0	0	0	0
56	1x	15	0	0	0	0
56	1y	1	0	0	0	0
56	20	4	0	0	0	0
56	21	1	0	0	0	0
56	23	2	0	0	0	0
56	25	6	0	0	0	0
56	26	1	0	0	0	0
56	27	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	28	3	0	0	0	0
56	2A	844	0	0	0	0
56	2B	19	0	0	0	0
56	2D	8	0	0	0	0
56	2E	9	0	0	0	0
56	2F	8	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	1	0	0	0	0
56	2P	2	0	0	0	0
56	2Q	4	0	0	0	0
56	2R	4	0	0	0	0
56	2T	3	0	0	0	0
56	2U	2	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	2Z	1	0	0	0	0
56	2a	225	0	0	0	0
56	2d	2	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	1	0	0	0	0
56	2l	5	0	0	0	0
56	2m	1	0	0	0	0
56	2q	3	0	0	0	0
56	2t	1	0	0	0	0
56	2v	3	0	0	0	0
56	2w	6	0	0	0	0
56	2x	7	0	0	0	0
56	2y	7	0	0	0	0
57	1A	1	0	0	0	0
57	2A	1	0	0	0	0
58	1A	34	0	0	1	0
58	2A	34	0	0	1	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	2	0
60	2d	8	0	0	0	0
61	10	11	0	0	0	0
61	11	9	0	0	0	0
61	12	3	0	0	0	0
61	13	5	0	0	0	0
61	14	1	0	0	0	0
61	15	5	0	0	0	0
61	16	3	0	0	0	0
61	17	8	0	0	0	0
61	18	7	0	0	0	0
61	1A	1907	0	0	82	0
61	1B	59	0	0	3	0
61	1D	26	0	0	0	0
61	1E	28	0	0	2	0
61	1F	17	0	0	0	0
61	1G	2	0	0	0	0
61	1H	2	0	0	1	0
61	1N	4	0	0	0	0
61	1O	4	0	0	1	0
61	1P	23	0	0	1	0
61	1Q	5	0	0	0	0
61	1R	10	0	0	2	0
61	1S	3	0	0	1	0
61	1T	8	0	0	0	0
61	1U	14	0	0	0	0
61	1V	7	0	0	0	0
61	1W	7	0	0	2	0
61	1X	6	0	0	0	0
61	1Y	2	0	0	1	0
61	1Z	1	0	0	0	0
61	1a	267	0	0	18	0
61	1b	1	0	0	0	0
61	1e	1	0	0	0	0
61	1j	1	0	0	0	0
61	1l	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6l	1n	1	0	0	0	0
6l	1q	2	0	0	0	0
6l	1v	4	0	0	0	0
6l	1w	15	0	0	0	0
6l	1x	10	0	0	0	0
6l	1y	2	0	0	0	0
6l	20	3	0	0	0	0
6l	21	8	0	0	1	0
6l	23	1	0	0	0	0
6l	27	4	0	0	0	0
6l	28	3	0	0	0	0
6l	29	1	0	0	0	0
6l	2A	1000	0	0	74	0
6l	2B	18	0	0	0	0
6l	2D	17	0	0	0	0
6l	2E	10	0	0	0	0
6l	2F	12	0	0	0	0
6l	2O	2	0	0	0	0
6l	2P	8	0	0	0	0
6l	2Q	2	0	0	0	0
6l	2R	2	0	0	0	0
6l	2T	4	0	0	0	0
6l	2U	2	0	0	0	0
6l	2V	1	0	0	0	0
6l	2W	3	0	0	0	0
6l	2X	1	0	0	0	0
6l	2Y	2	0	0	0	0
6l	2a	172	0	0	13	0
6l	2d	2	0	0	0	0
6l	2e	1	0	0	0	0
6l	2i	1	0	0	0	0
6l	2j	2	0	0	0	0
6l	2l	4	0	0	1	0
6l	2p	1	0	0	0	0
6l	2q	1	0	0	0	0
6l	2r	1	0	0	0	0
6l	2t	2	0	0	1	0
6l	2v	3	0	0	0	0
6l	2w	3	0	0	0	0
6l	2x	4	0	0	1	0
6l	2y	4	0	0	0	0
All	All	299649	0	196683	4079	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 (4079) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.32	1.26
1:1A:1082:U:O4	1:1A:1086:A:N1	1.99	0.95
54:2y:55:PSU:HN1	54:2y:57:G:H5''	1.32	0.93
1:1A:1062:G:H1	1:1A:1077:A:H61	1.02	0.93
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.49	0.93
1:1A:2427:C:OP1	61:1A:4102:HOH:O	1.85	0.93
54:2y:18:G:N2	54:2y:55:PSU:HN3	1.69	0.91
54:2y:18:G:N2	54:2y:55:PSU:N3	2.17	0.90
1:1A:1082:U:N3	1:1A:1086:A:N6	2.01	0.90
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.04	0.90
29:17:24:THR:HG22	29:17:27:GLY:H	1.36	0.89
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.53	0.89
9:1N:123:TYR:HH	9:1N:130:HIS:HE2	1.13	0.88
54:2y:18:G:H22	54:2y:55:PSU:HN3	0.90	0.87
1:2A:2319:G:H22	14:2S:3:ARG:HH11	1.20	0.87
54:1w:26:A:H61	54:1w:44:G:H1	1.21	0.86
1:1A:1057:A:H61	1:1A:1081:U:H3	1.23	0.85
32:2a:953:G:H5'	32:2a:965:A:H61	1.42	0.85
32:1a:376:G:H5''	47:1p:5:ARG:HG2	1.58	0.84
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.10	0.84
32:1a:664:G:H22	32:1a:741:G:H1	1.26	0.84
1:2A:1689:A:H62	1:2A:1698:A:H2	1.22	0.83
32:1a:1314:C:OP2	50:1s:4:SER:OG	1.96	0.83
1:2A:1204:A:H2	1:2A:1241:A:H62	1.28	0.82
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.43	0.82
1:1A:1602:U:O4	61:1A:4103:HOH:O	1.98	0.82
32:1a:1125:U:H4'	41:1j:5:ARG:HH22	1.45	0.82
40:2i:28:VAL:HG12	40:2i:63:ILE:HB	1.62	0.81
22:10:10:THR:HG22	22:10:12:ASN:H	1.44	0.81
11:1P:126:VAL:HG12	11:1P:148:LEU:HD22	1.60	0.81
32:1a:1086:U:H3	32:1a:1099:G:H22	1.24	0.81
1:1A:826:U:OP1	61:1A:4102:HOH:O	1.99	0.81
1:1A:1669:A:OP2	61:1A:4104:HOH:O	1.98	0.81
32:1a:299:G:O6	61:1a:1901:HOH:O	1.99	0.81
32:2a:1278:U:H5'	32:2a:1279:A:H5'	1.60	0.80
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.62	0.80
32:2a:1272:G:N2	32:2a:1273:G:N7	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1651:G:OP1	13:2R:40:LYS:NZ	2.15	0.80
33:1b:33:TYR:HB2	33:1b:43:ASP:HB2	1.64	0.79
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.64	0.79
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.65	0.79
1:1A:2222:G:O6	61:1A:4107:HOH:O	2.01	0.79
32:2a:1099:G:OP2	33:2b:144:ARG:NH2	2.16	0.79
32:2a:1086:U:H3	32:2a:1099:G:H22	1.27	0.78
10:1O:48:PRO:HB3	32:1a:1422:G:H5''	1.63	0.78
32:2a:975:A:H4'	32:2a:976:G:H5''	1.65	0.78
54:1y:19:G:N2	54:1y:56:C:N3	2.31	0.78
23:21:32:LYS:O	61:21:201:HOH:O	2.02	0.78
1:2A:486:C:O2'	18:2W:60:ASN:ND2	2.16	0.78
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.66	0.78
1:1A:792:G:O6	61:1A:4105:HOH:O	2.00	0.77
26:14:56:VAL:HB	26:14:60:GLN:HG3	1.66	0.77
1:2A:948:G:OP1	61:2A:3903:HOH:O	2.01	0.77
32:1a:953:G:H5'	32:1a:965:A:H61	1.49	0.77
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.65	0.77
1:2A:570:G:O6	61:2A:3904:HOH:O	2.02	0.77
1:2A:1568:G:N7	61:2A:3942:HOH:O	2.18	0.77
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.18	0.77
1:1A:1332:G:OP1	61:1A:4106:HOH:O	2.01	0.77
5:2F:120:GLU:HG3	5:2F:122:LYS:HG2	1.67	0.76
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.18	0.76
44:2m:23:TYR:HB3	44:2m:67:GLU:HA	1.67	0.76
33:1b:118:LEU:HB3	33:1b:142:LEU:HD12	1.67	0.76
32:2a:1316:G:H22	32:2a:1319:A:H5''	1.51	0.76
1:1A:1057:A:N6	1:1A:1081:U:H3	1.83	0.76
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.17	0.76
16:1U:75:ASN:OD1	16:1U:78:THR:OG1	2.03	0.76
1:2A:248:G:OP1	61:2A:3905:HOH:O	2.04	0.76
1:1A:2051:A:OP2	61:1A:4109:HOH:O	2.04	0.75
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.66	0.75
32:2a:972:C:O2'	41:2j:55:LYS:O	2.05	0.75
1:2A:2448:A:OP1	61:2A:3904:HOH:O	2.03	0.75
1:2A:963:U:OP2	61:2A:3903:HOH:O	2.04	0.75
44:1m:3:ARG:HG2	44:1m:8:GLU:HA	1.68	0.75
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.68	0.75
1:2A:106:C:H1'	20:2Y:1:MET:HE2	1.68	0.75
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.68	0.75
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:544:G:OP1	35:2d:59:ARG:NH2	2.19	0.75
39:2h:10:LEU:HD23	39:2h:83:ILE:HG12	1.67	0.75
1:2A:981:A:OP1	61:2A:3908:HOH:O	2.05	0.74
21:2Z:31:ARG:HH11	21:2Z:94:GLU:HG2	1.52	0.74
1:1A:1014:U:OP2	61:1A:4108:HOH:O	2.04	0.74
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.20	0.74
33:2b:16:HIS:HB2	33:2b:204:ASN:HD22	1.50	0.74
48:2q:7:THR:HG22	48:2q:58:GLU:HG2	1.66	0.74
32:1a:975:A:H4'	32:1a:976:G:H5''	1.68	0.74
7:2H:86:GLU:OE1	7:2H:130:ARG:NH1	2.21	0.74
32:2a:1224:G:OP1	61:2a:1903:HOH:O	2.05	0.74
41:2j:6:ILE:HG12	41:2j:98:ILE:HG22	1.69	0.74
1:1A:1176:G:N2	1:1A:1178:C:OP2	2.16	0.74
1:1A:2499:C:OP1	61:1A:4111:HOH:O	2.05	0.74
1:2A:2100:G:H1	1:2A:2189:U:H3	1.35	0.74
32:2a:596:C:OP2	61:2a:1904:HOH:O	2.05	0.74
32:2a:278:G:OP2	48:2q:41:LYS:NZ	2.20	0.74
33:1b:195:ASP:O	39:1h:68:ARG:NH2	2.21	0.74
44:1m:80:ARG:NH1	50:1s:65:ASN:O	2.21	0.74
1:2A:792:G:O6	61:2A:3909:HOH:O	2.06	0.74
1:1A:530:G:N1	1:1A:2023:G:OP1	2.20	0.74
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.52	0.74
41:1j:8:LEU:HD22	41:1j:96:ILE:HG22	1.69	0.73
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.52	0.73
32:2a:664:G:H22	32:2a:741:G:H1	1.35	0.73
34:2c:58:GLU:HB3	41:2j:92:THR:HG21	1.70	0.73
44:2m:31:LYS:HA	44:2m:34:LEU:HD12	1.69	0.73
1:2A:1508:A:H4'	1:2A:1509(A):A:C5	2.24	0.73
32:2a:1271:G:N2	32:2a:1272:G:N7	2.35	0.73
32:1a:504:C:OP1	61:1a:1902:HOH:O	2.05	0.73
32:1a:1025:U:O2	32:1a:1036:G:O6	2.07	0.73
37:1f:100:ASN:HB2	49:1r:28:GLU:HA	1.69	0.73
1:2A:1271:G:OP2	61:2A:3907:HOH:O	2.05	0.73
1:2A:1973:G:OP1	61:2A:3910:HOH:O	2.06	0.73
32:2a:1151:A:HO2'	32:2a:1152:A:H8	1.34	0.73
1:1A:956:G:O6	61:1A:4112:HOH:O	2.06	0.73
1:2A:1812:A:OP2	61:2A:3906:HOH:O	2.05	0.73
35:2d:8:VAL:HG22	35:2d:21:LEU:HD13	1.71	0.73
1:1A:1607:C:O2	61:1A:4113:HOH:O	2.07	0.73
1:1A:2821:A:OP2	61:1R:301:HOH:O	2.06	0.73
1:2A:1024:G:OP2	61:2A:3911:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:25:40:LYS:NZ	27:25:44:THR:O	2.22	0.73
1:2A:883:G:N1	1:2A:894:C:O2	2.15	0.73
32:1a:558:G:OP1	61:1a:1901:HOH:O	2.06	0.73
11:2P:126:VAL:HG12	11:2P:148:LEU:HD22	1.70	0.73
44:2m:52:GLU:HG2	44:2m:55:ARG:HH21	1.54	0.73
1:1A:409:C:OP1	61:1A:4110:HOH:O	2.05	0.72
3:1D:2:ALA:N	3:1D:200:ASP:OD2	2.22	0.72
1:1A:2235:G:N7	61:1A:4158:HOH:O	2.22	0.72
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.69	0.72
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.36	0.72
1:2A:2125:G:N3	1:2A:2173:A:N6	2.38	0.72
32:2a:1312:G:H5'	50:2s:5:LEU:HD11	1.70	0.72
40:2i:128:ARG:NH2	55:2x:33:U:OP2	2.23	0.72
26:14:55:ARG:H	26:14:56:VAL:HA	1.55	0.72
32:1a:1027:C:C2	32:1a:1034:G:N2	2.57	0.72
14:2S:105:ALA:HB1	14:2S:110:LEU:HD23	1.71	0.72
1:2A:987:G:OP2	61:2A:3912:HOH:O	2.07	0.72
32:2a:1106:G:H5''	34:2c:172:ARG:HG2	1.70	0.72
32:1a:1036:G:H5''	32:1a:1037:C:C5	2.25	0.72
32:1a:1198:G:OP1	61:1a:1904:HOH:O	2.07	0.72
1:1A:2107:C:H42	1:1A:2182:G:H1	1.36	0.72
1:2A:1670:C:OP1	61:2A:3913:HOH:O	2.08	0.72
9:1N:91:LEU:HG	9:1N:98:VAL:HG21	1.71	0.72
32:2a:1239:A:H62	32:2a:1299:A:H62	1.38	0.72
1:2A:500:G:N1	1:2A:503:A:OP2	2.23	0.72
1:1A:2790:A:H5'	1:1A:2893:G:H21	1.54	0.71
32:2a:1191:A:H5''	34:2c:4:LYS:HE3	1.71	0.71
33:2b:8:LYS:HD2	33:2b:9:GLU:H	1.54	0.71
44:2m:34:LEU:HD13	44:2m:41:PRO:HB3	1.71	0.71
32:1a:1469:G:N7	61:1a:1916:HOH:O	2.23	0.71
32:2a:673:G:H2'	32:2a:674:G:C8	2.25	0.71
32:2a:1108:G:O6	61:2a:1906:HOH:O	2.07	0.71
33:1b:69:LEU:HB3	33:1b:162:ILE:HG22	1.73	0.71
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.24	0.71
33:1b:17:PHE:HB3	33:1b:44:LEU:HD11	1.72	0.71
18:2W:11:ARG:NH1	18:2W:99:ARG:O	2.22	0.71
14:1S:61:ASN:HB3	14:1S:64:GLU:HB2	1.72	0.71
32:1a:1224:G:OP1	61:1a:1906:HOH:O	2.08	0.71
32:2a:944:G:OP1	61:2a:1905:HOH:O	2.07	0.71
1:1A:1648:C:OP1	61:1A:4115:HOH:O	2.08	0.71
32:1a:812:C:O2	61:1a:1903:HOH:O	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1505:G:OP2	61:1a:1905:HOH:O	2.08	0.71
32:2a:598:U:O4	61:2a:1904:HOH:O	2.08	0.71
1:1A:1671:U:O4	61:1A:4104:HOH:O	2.09	0.71
9:1N:13:TRP:CE2	9:1N:133:GLN:HG2	2.25	0.71
26:14:55:ARG:N	26:14:56:VAL:HA	2.06	0.71
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.25	0.71
11:1P:35:HIS:O	61:1P:301:HOH:O	2.09	0.70
1:2A:888:C:OP1	44:2m:93:ARG:NH1	2.24	0.70
1:1A:370:G:OP2	61:1A:4114:HOH:O	2.08	0.70
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.72	0.70
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.71	0.70
1:1A:192:C:OP1	61:1A:4118:HOH:O	2.09	0.70
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	1.73	0.70
1:1A:1013:C:OP2	61:1A:4108:HOH:O	2.07	0.70
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	1.73	0.70
1:2A:1345:C:OP2	61:2A:3916:HOH:O	2.09	0.70
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.73	0.70
1:2A:2592:G:OP1	61:2A:3914:HOH:O	2.08	0.70
47:2p:18:ARG:HD3	47:2p:35:LYS:HD2	1.71	0.70
40:2i:88:TYR:HD2	40:2i:89:ASN:HB2	1.56	0.70
12:1Q:18:LYS:O	12:1Q:98:LYS:NZ	2.16	0.70
1:2A:975:C:OP1	61:2A:3919:HOH:O	2.10	0.70
1:2A:1971:A:OP1	61:2A:3917:HOH:O	2.09	0.70
5:2F:103:LYS:HA	5:2F:106:ARG:HG3	1.74	0.70
6:1G:72:ARG:HH12	6:1G:87:PRO:HG3	1.56	0.70
1:2A:323:G:HO2'	1:2A:1205:U:H3	1.36	0.70
32:2a:1189:C:OP1	41:2j:51:ARG:NH2	2.25	0.70
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.74	0.70
33:2b:204:ASN:HD21	33:2b:207:ALA:HB3	1.55	0.70
1:1A:2128:C:H42	1:1A:2160:G:H1	1.35	0.70
6:1G:18:GLU:HG3	6:1G:22:ARG:HD2	1.73	0.70
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.55	0.70
40:1i:23:ASN:OD1	40:1i:23:ASN:N	2.25	0.70
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.05	0.70
1:1A:1041:C:H42	1:1A:1114:G:H1	1.39	0.69
35:1d:7:PRO:HB2	35:1d:10:ARG:HD2	1.73	0.69
47:1p:15:PRO:HD2	47:1p:42:ARG:HD2	1.74	0.69
11:2P:29:LYS:HD2	11:2P:30:THR:HG23	1.74	0.69
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.74	0.69
1:1A:1622:G:OP2	61:1A:4117:HOH:O	2.09	0.69
1:1A:1647:G:OP1	61:1A:4115:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:99:G:OP2	61:1B:302:HOH:O	2.10	0.69
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.25	0.69
1:2A:1358:G:OP2	61:2A:3915:HOH:O	2.09	0.69
1:2A:1648:C:OP1	61:2A:3907:HOH:O	2.10	0.69
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.73	0.69
11:1P:39:LYS:HB2	11:1P:45:LEU:HD13	1.73	0.69
32:1a:812:C:N3	61:1a:1917:HOH:O	2.24	0.69
33:2b:178:ARG:HH22	39:2h:68:ARG:HH12	1.40	0.69
32:1a:1377:A:HO2'	38:1g:2:ALA:N	1.90	0.69
26:24:53:GLU:HG2	26:24:55:ARG:H	1.58	0.69
41:2j:89:ASP:N	41:2j:89:ASP:OD1	2.25	0.69
1:1A:2702:U:OP1	61:1A:4116:HOH:O	2.08	0.69
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	1.74	0.69
21:1Z:163:LEU:HD23	21:1Z:167:PRO:HG3	1.75	0.69
1:1A:2276:G:N7	61:1A:4165:HOH:O	2.24	0.69
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.24	0.69
47:2p:15:PRO:HD2	47:2p:42:ARG:HD3	1.74	0.69
33:1b:30:ARG:HH21	33:1b:194:PRO:HB2	1.57	0.69
54:1w:26:A:N6	54:1w:44:G:H1	1.89	0.69
54:1y:8:4SU:H4'	54:1y:48:C:H4'	1.75	0.69
13:2R:67:LEU:HD13	13:2R:76:VAL:HG21	1.74	0.69
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.25	0.69
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.40	0.69
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.25	0.69
1:2A:2592:G:OP2	61:2A:3918:HOH:O	2.10	0.69
2:2B:4:C:H42	2:2B:117:G:H1	1.41	0.69
32:2a:1002:G:C2	32:2a:1003:G:H1'	2.28	0.69
10:1O:110:GLY:HA2	10:1O:112:MET:HE2	1.74	0.69
1:1A:2090:G:O6	61:1A:4121:HOH:O	2.11	0.68
1:1A:2131:G:N2	1:1A:2158:A:N1	2.41	0.68
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.41	0.68
35:1d:53:ASP:N	35:1d:53:ASP:OD1	2.23	0.68
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.25	0.68
15:2T:109:GLU:HG2	15:2T:112:ARG:HH22	1.59	0.68
32:1a:1499:A:OP2	61:1a:1905:HOH:O	2.12	0.68
1:2A:602:G:O2'	1:2A:655:A:N6	2.27	0.68
1:2A:1024:G:HO2'	1:2A:1144:G:HO2'	1.39	0.68
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	1.75	0.68
1:1A:1937:A:H1'	1:1A:1939:5MU:H72	1.75	0.68
1:1A:2428:G:OP1	61:1A:4102:HOH:O	2.11	0.68
47:2p:58:TYR:O	47:2p:61:SER:OG	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1m:3:ARG:HD2	44:1m:9:ILE:HG12	1.76	0.68
1:2A:890:A:H2'	1:2A:892:G:H8	1.58	0.68
1:2A:2269:A:OP1	61:2A:3921:HOH:O	2.11	0.68
32:1a:266:G:H5''	32:1a:268:C:H41	1.59	0.68
32:1a:407:G:OP1	35:1d:115:ARG:NH2	2.27	0.68
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.74	0.68
6:1G:135:LEU:HD13	6:1G:140:ILE:HD11	1.76	0.68
26:14:13:ARG:HB3	26:14:30:GLU:HG2	1.76	0.68
1:2A:2394:C:N3	54:2y:76:A:O2'	2.25	0.68
44:1m:23:TYR:HB3	44:1m:67:GLU:HA	1.76	0.68
1:2A:2432:A:OP2	61:2A:3920:HOH:O	2.11	0.68
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.76	0.68
17:2V:55:ALA:HA	17:2V:101:GLY:HA2	1.76	0.68
34:2c:47:LEU:HB2	34:2c:52:LEU:HD22	1.75	0.68
1:1A:248:G:OP1	61:1A:4119:HOH:O	2.10	0.67
1:1A:881:G:N2	1:1A:897:C:O2	2.26	0.67
1:1A:1039:G:H1	1:1A:1116:C:H42	1.42	0.67
10:1O:35:VAL:HG21	10:1O:69:ILE:HD13	1.74	0.67
18:1W:92:ARG:NH1	61:1W:301:HOH:O	2.26	0.67
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.76	0.67
1:1A:1702:G:N7	61:1A:4178:HOH:O	2.26	0.67
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.75	0.67
32:1a:1303:C:OP1	61:1a:1908:HOH:O	2.12	0.67
32:2a:157:G:H1	32:2a:164:U:H3	1.41	0.67
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.76	0.67
32:2a:165:C:H2'	32:2a:166:G:H8	1.58	0.67
36:2e:20:GLN:OE1	36:2e:25:ARG:NH1	2.28	0.67
42:2k:48:ILE:O	42:2k:50:TYR:N	2.27	0.67
5:1F:24:LEU:HD23	5:1F:115:ALA:HA	1.76	0.67
32:1a:574:A:OP2	61:1a:1907:HOH:O	2.11	0.67
1:1A:422:A:OP2	61:1A:4114:HOH:O	2.12	0.67
1:1A:2759:G:N7	61:1A:4186:HOH:O	2.27	0.67
7:1H:56:SER:OG	7:1H:57:ASP:N	2.26	0.67
9:1N:123:TYR:OH	9:1N:130:HIS:NE2	2.17	0.67
1:2A:2079:U:OP1	23:21:21:ARG:NH2	2.24	0.67
32:2a:266:G:H5''	32:2a:268:C:H41	1.60	0.67
21:1Z:1:MET:HG3	21:1Z:56:VAL:H	1.60	0.67
1:2A:370:G:OP2	61:2A:3923:HOH:O	2.12	0.67
33:2b:98:LEU:HB2	33:2b:101:MET:HE3	1.76	0.67
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.26	0.67
1:2A:857:C:OP1	22:20:77:ARG:NH2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1778:U:OP1	61:1A:4122:HOH:O	2.12	0.67
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.30	0.67
2:1B:23:G:O6	61:1B:301:HOH:O	2.10	0.67
1:1A:842:G:N7	61:1A:4179:HOH:O	2.26	0.66
2:2B:87:G:N2	2:2B:90:A:OP2	2.24	0.66
14:2S:78:LEU:HD11	14:2S:109:GLY:HA3	1.77	0.66
1:1A:429:A:OP2	61:1A:4123:HOH:O	2.13	0.66
9:1N:46:VAL:HG23	9:1N:48:MET:HG2	1.76	0.66
25:13:55:ARG:HH22	25:13:57:GLU:HB2	1.60	0.66
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.29	0.66
14:2S:68:GLN:HA	14:2S:71:ARG:HD3	1.78	0.66
32:2a:677:U:H3	32:2a:713:G:H22	1.43	0.66
32:2a:1126:U:H3	41:2j:40:LEU:HD11	1.61	0.66
33:2b:71:VAL:HB	33:2b:164:VAL:HG12	1.75	0.66
46:2o:4:THR:N	46:2o:7:GLU:OE2	2.26	0.66
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.28	0.66
1:2A:1023:U:OP2	61:2A:3911:HOH:O	2.13	0.66
26:24:61:ARG:NH1	26:24:62:ARG:O	2.29	0.66
34:2c:162:GLN:NE2	53:2v:24:A:O2'	2.29	0.66
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.76	0.66
35:2d:20:TYR:HD1	35:2d:26:CYS:HB3	1.61	0.66
39:2h:86:ILE:HG21	39:2h:133:LEU:HD13	1.78	0.66
1:1A:615:G:OP1	5:1F:40:GLN:NE2	2.29	0.66
1:1A:2344:U:OP1	28:16:37:ARG:NH1	2.28	0.66
1:1A:2550:G:OP1	61:1A:4104:HOH:O	2.12	0.66
32:1a:437:U:H5''	35:1d:155:LEU:HD21	1.76	0.66
5:2F:12:LEU:HG	5:2F:124:LEU:HD11	1.78	0.66
32:2a:1255:G:N7	41:2j:43:ARG:NH2	2.42	0.66
32:2a:64:G:H4'	32:2a:65:U:H3'	1.76	0.66
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.75	0.66
41:2j:40:LEU:HB2	41:2j:69:ASN:HB3	1.76	0.66
1:1A:2585:U:OP1	61:1A:4127:HOH:O	2.14	0.66
18:1W:13:SER:HB3	18:1W:16:LYS:HD2	1.78	0.66
1:1A:1975:G:OP2	61:1A:4128:HOH:O	2.14	0.66
3:1D:183:ARG:HG3	3:1D:270:ILE:HD13	1.78	0.66
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.61	0.66
1:2A:832:G:H5'	11:2P:45:LEU:HD11	1.77	0.66
8:2I:40:THR:O	8:2I:44:LEU:HB2	1.96	0.66
36:2e:20:GLN:NE2	36:2e:21:ALA:O	2.28	0.66
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.77	0.66
54:1y:53:G:H3'	54:1y:54:5MU:H73	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.12	0.66
36:2e:100:VAL:O	36:2e:107:ARG:NH2	2.26	0.66
1:1A:1865:G:OP1	61:1A:4125:HOH:O	2.13	0.65
32:1a:159:G:N2	32:1a:162:A:OP2	2.30	0.65
32:1a:405:U:O4	35:1d:2:GLY:N	2.29	0.65
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.78	0.65
7:1H:101:ARG:HH22	7:1H:122:THR:HA	1.62	0.65
1:2A:2125:G:N1	1:2A:2172:U:OP1	2.22	0.65
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.28	0.65
1:2A:2524:G:N7	61:2A:3989:HOH:O	2.29	0.65
1:1A:882:G:H1	1:1A:894:C:H42	1.44	0.65
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.29	0.65
33:1b:22:LYS:HA	33:1b:40:HIS:HE1	1.61	0.65
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.79	0.65
16:2U:66:ASN:HD21	16:2U:70:ARG:HH21	1.43	0.65
40:2i:21:PRO:HA	40:2i:59:PHE:HA	1.78	0.65
32:2a:1010:G:H2'	32:2a:1011:G:H8	1.62	0.65
1:1A:1243:G:O3'	11:1P:7:ARG:NH2	2.29	0.65
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.79	0.65
32:2a:504:C:OP1	61:2a:1907:HOH:O	2.13	0.65
2:1B:66:A:H61	2:1B:109:C:H5'	1.62	0.65
3:1D:147:LEU:HD13	3:1D:155:LEU:HD21	1.78	0.65
41:1j:46:ARG:NH2	41:1j:64:GLU:OE1	2.30	0.65
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.15	0.65
43:2l:71:PRO:O	43:2l:102:ARG:NH1	2.26	0.65
1:1A:271(L):U:H4'	8:1I:50:ARG:HH22	1.59	0.65
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	1.78	0.65
32:2a:381:C:OP1	61:2a:1909:HOH:O	2.15	0.65
14:1S:14:VAL:O	14:1S:18:ILE:HG12	1.97	0.65
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.60	0.65
1:2A:2602:A:OP1	61:2A:3925:HOH:O	2.14	0.65
32:2a:56:U:H2'	32:2a:57:G:C8	2.32	0.65
1:1A:1023:U:OP2	61:1A:4124:HOH:O	2.13	0.65
1:2A:1830:C:OP2	61:2A:3927:HOH:O	2.14	0.65
21:2Z:55:HIS:HE1	21:2Z:135:GLU:HB2	1.61	0.65
42:2k:87:THR:O	42:2k:87:THR:OG1	2.12	0.65
1:2A:307:G:H21	1:2A:330:A:H62	1.45	0.65
1:1A:2573:C:OP1	61:1A:4129:HOH:O	2.15	0.64
26:14:16:CYS:SG	26:14:17:GLY:N	2.70	0.64
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.30	0.64
4:2E:119:ARG:HD2	4:2E:160:TYR:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2R:104:ARG:HG3	13:2R:111:LEU:HD21	1.77	0.64
54:2y:51:U:H3	54:2y:63:G:H1	1.44	0.64
1:1A:2243:U:OP1	61:1A:4118:HOH:O	2.15	0.64
5:1F:28:ILE:HG21	11:1P:1:MET:HE1	1.79	0.64
39:1h:86:ILE:HD12	39:1h:133:LEU:HD22	1.79	0.64
32:2a:1518:MA6:H93	32:2a:1519:MA6:H92	1.78	0.64
34:2c:47:LEU:HD12	34:2c:70:VAL:HG11	1.77	0.64
1:1A:1062:G:H1	1:1A:1077:A:N6	1.86	0.64
6:1G:126:ASP:HB2	6:1G:130:ASN:H	1.62	0.64
34:2c:179:ARG:NH1	34:2c:206:GLU:OE1	2.24	0.64
35:2d:175:SER:HB3	35:2d:186:LEU:HD11	1.79	0.64
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.33	0.64
37:1f:36:ARG:NH1	37:1f:66:GLU:OE2	2.29	0.64
35:2d:43:HIS:HB3	35:2d:46:LYS:HD2	1.79	0.64
1:1A:1054:A:H61	1:1A:1105:U:H3	1.45	0.64
35:1d:107:ARG:HH21	35:1d:194:LEU:HD21	1.62	0.64
41:1j:49:VAL:HG23	45:1n:41:ARG:HB2	1.80	0.64
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.15	0.64
3:1D:71:ASP:HB2	3:1D:103:ARG:HH12	1.61	0.64
32:1a:836:G:OP1	49:1r:61:LYS:NZ	2.27	0.64
1:2A:692:C:O2'	3:2D:38:LYS:NZ	2.30	0.64
32:2a:165:C:H2'	32:2a:166:G:C8	2.32	0.64
34:2c:182:ILE:HG22	34:2c:203:PHE:HA	1.79	0.64
36:2e:10:MET:HE2	36:2e:55:VAL:HG21	1.80	0.64
36:2e:57:LYS:HG2	36:2e:61:TYR:CE2	2.33	0.64
1:2A:10:G:H1'	1:2A:2801(A):A:H62	1.62	0.64
1:2A:2499:C:OP2	61:2A:3929:HOH:O	2.15	0.64
4:2E:7:VAL:HG23	4:2E:51:PHE:HE2	1.63	0.64
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.78	0.64
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.33	0.64
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.30	0.64
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.79	0.64
41:2j:44:VAL:HG13	41:2j:66:ARG:HB3	1.80	0.64
32:1a:573:A:OP2	61:1a:1907:HOH:O	2.15	0.64
37:1f:2:ARG:HD2	37:1f:69:GLU:HB3	1.80	0.64
40:1i:79:LEU:HG	40:1i:83:ARG:HD2	1.79	0.64
1:2A:2280:G:O6	61:2A:3924:HOH:O	2.14	0.64
32:2a:176:C:OP1	51:2t:29:LYS:NZ	2.31	0.64
38:2g:113:GLU:HG2	38:2g:119:ARG:HG2	1.79	0.64
1:2A:1349:A:OP1	61:2A:3928:HOH:O	2.15	0.64
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:20:LEU:HD23	5:2F:21:ALA:H	1.62	0.64
6:2G:48:GLU:O	6:2G:51:ARG:NH1	2.31	0.64
40:1i:51:ARG:HG3	40:1i:56:LEU:HD11	1.79	0.63
1:2A:892:G:H3'	1:2A:893:C:H4'	1.79	0.63
11:2P:91:PHE:O	11:2P:121:LYS:NZ	2.28	0.63
50:2s:77:THR:HG23	50:2s:78:ARG:HG3	1.79	0.63
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	1.79	0.63
32:2a:376:G:H5''	47:2p:5:ARG:HB2	1.80	0.63
33:2b:112:VAL:HG22	33:2b:149:LEU:HD13	1.80	0.63
25:13:26:LEU:O	25:13:35:ARG:NE	2.31	0.63
32:1a:504:C:OP1	61:1a:1909:HOH:O	2.15	0.63
46:1o:87:ILE:HG22	46:1o:88:ARG:H	1.63	0.63
1:2A:568:U:O4	61:2A:3922:HOH:O	2.12	0.63
1:2A:2114:A:H62	1:2A:2115:G:H21	1.46	0.63
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.79	0.63
41:2j:38:ILE:HD11	41:2j:71:LEU:HD23	1.80	0.63
31:19:17:ILE:HD13	31:19:26:ILE:HD13	1.81	0.63
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.33	0.63
8:1I:40:THR:O	8:1I:44:LEU:HB2	1.97	0.63
46:1o:16:ALA:HB1	46:1o:21:ASP:HB3	1.81	0.63
1:2A:2143:C:H42	1:2A:2148:G:H1	1.46	0.63
32:2a:563:A:O2'	61:2a:1908:HOH:O	2.15	0.63
37:2f:36:ARG:HH12	37:2f:38:GLU:HG3	1.62	0.63
1:1A:1269:A:N7	61:1A:4206:HOH:O	2.30	0.63
54:1y:13:C:H2'	54:1y:14:A:H5''	1.80	0.63
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.16	0.63
1:2A:2183:C:H2'	1:2A:2184:G:C8	2.33	0.63
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.31	0.63
44:1m:19:LEU:HD21	44:1m:56:LEU:HD21	1.81	0.63
1:2A:2431:U:OP2	61:2A:3920:HOH:O	2.15	0.63
1:2A:2801(A):A:O2'	1:2A:2895:U:H4'	1.99	0.63
19:2X:94:GLY:H	19:2X:95:LEU:HB2	1.62	0.63
32:2a:110:C:O2'	47:2p:25:ARG:O	2.17	0.63
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.34	0.63
54:1y:19:G:N1	54:1y:56:C:N4	2.45	0.63
1:2A:330:A:H2	1:2A:1210:A:HO2'	1.46	0.63
10:1O:97:ARG:NH1	32:1a:339:C:OP2	2.32	0.63
17:1V:43:GLU:OE1	17:1V:43:GLU:N	2.31	0.63
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.33	0.63
7:2H:8:PRO:HB3	7:2H:51:ARG:HG2	1.80	0.63
32:2a:1002:G:H1	32:2a:1038:C:H42	1.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1102:A:O3'	33:2b:96:ARG:NH2	2.31	0.63
32:2a:1263:C:N3	32:2a:1272:G:O6	2.32	0.63
1:1A:1009:A:OP2	9:1N:37:LYS:NZ	2.29	0.62
35:1d:65:ARG:HG3	35:1d:70:ILE:HG22	1.81	0.62
40:1i:16:ARG:HB2	40:1i:64:THR:HG22	1.81	0.62
32:2a:297:G:N2	32:2a:300:A:OP2	2.32	0.62
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.13	0.62
1:1A:2239:G:OP2	61:1A:4130:HOH:O	2.16	0.62
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.14	0.62
32:2a:1346:A:OP1	40:2i:120:ARG:NH1	2.32	0.62
1:1A:2361:A:OP2	30:18:26:LYS:NZ	2.30	0.62
32:1a:1414:U:H3	32:1a:1486:G:H1	1.46	0.62
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.64	0.62
32:2a:560:U:H5'	32:2a:566:G:N2	2.14	0.62
42:2k:43:SER:HB3	42:2k:68:ALA:HB2	1.80	0.62
50:2s:18:LYS:HB3	50:2s:31:ILE:HD13	1.80	0.62
1:2A:1754:C:OP1	15:2T:96:ARG:NH1	2.33	0.62
1:2A:1859:A:N6	1:2A:1883:G:O2'	2.33	0.62
32:2a:1228:C:OP1	44:2m:115:LYS:NZ	2.29	0.62
36:2e:33:VAL:HG13	36:2e:112:LEU:HD22	1.81	0.62
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.82	0.62
51:1t:10:LEU:HD12	51:1t:11:SER:H	1.64	0.62
1:2A:1021:A:H62	1:2A:1141:U:H3	1.47	0.62
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.31	0.62
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.33	0.62
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.79	0.62
46:2o:87:ILE:HG22	46:2o:88:ARG:H	1.64	0.62
1:1A:2099:U:H3	1:1A:2190:G:H1	1.48	0.62
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.82	0.62
32:1a:165:C:H2'	32:1a:166:G:H8	1.65	0.62
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.32	0.62
48:1q:53:LEU:HG	48:1q:82:MET:HE1	1.82	0.62
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.64	0.62
34:2c:44:GLU:HA	34:2c:52:LEU:HD23	1.80	0.62
1:1A:607:U:OP1	5:1F:102:PRO:HA	1.99	0.62
2:1B:76:G:N7	61:1B:304:HOH:O	2.31	0.62
7:1H:3:ARG:HG2	7:1H:6:ARG:HB2	1.80	0.62
20:2Y:77:PRO:HD3	20:2Y:106:LEU:HD23	1.81	0.62
32:2a:1251:A:H2'	32:2a:1252:A:C8	2.35	0.62
18:1W:4:LYS:HE3	18:1W:6:ILE:HD11	1.82	0.62
1:2A:100:G:O2'	24:22:7:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:23:40:THR:HG22	25:23:42:ALA:H	1.63	0.62
32:2a:974:A:OP2	45:2n:29:ARG:NH2	2.32	0.62
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.79	0.62
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.15	0.62
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.14	0.62
45:2n:23:ARG:NH1	45:2n:28:GLY:O	2.33	0.62
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.73	0.62
38:1g:151:TYR:HB3	38:1g:154:TYR:HD2	1.65	0.62
1:2A:1163:G:OP1	17:2V:24:LYS:NZ	2.31	0.61
30:28:28:GLY:O	30:28:36:LYS:NZ	2.33	0.61
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.64	0.61
39:2h:64:LYS:HG2	39:2h:79:VAL:HG21	1.81	0.61
10:2O:76:ALA:HB3	15:2T:75:ILE:HB	1.83	0.61
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.00	0.61
33:2b:19:HIS:HB2	33:2b:204:ASN:HB2	1.81	0.61
1:1A:1300:U:H4'	1:1A:1301:A:H5''	1.82	0.61
1:2A:2317:C:N4	1:2A:2318:G:O6	2.33	0.61
25:23:22:ALA:HB2	25:23:49:LYS:HD3	1.82	0.61
32:2a:1310:G:H5'	44:2m:77:ASN:HD21	1.65	0.61
8:1I:109:ILE:HG23	8:1I:130:TYR:CZ	2.36	0.61
40:2i:79:LEU:HG	40:2i:83:ARG:HD2	1.81	0.61
43:2l:56:ALA:HB2	43:2l:70:ILE:HD11	1.83	0.61
1:1A:2306:C:O2	61:1A:4120:HOH:O	2.11	0.61
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.82	0.61
1:2A:805:G:OP1	61:2A:3932:HOH:O	2.16	0.61
32:2a:179:A:H2'	32:2a:180:U:C6	2.35	0.61
41:2j:8:LEU:HB3	41:2j:96:ILE:HG23	1.82	0.61
7:1H:6:ARG:HH22	7:1H:54:ARG:HH22	1.46	0.61
1:2A:2316:C:O2'	6:2G:128:ARG:NH2	2.33	0.61
1:2A:2816:C:O3'	13:2R:99:LYS:NZ	2.34	0.61
32:2a:401:C:OP2	35:2d:73:ARG:NH2	2.24	0.61
32:2a:1271:G:C2	32:2a:1272:G:N7	2.69	0.61
1:2A:1379:A:H4'	1:2A:1380:G:OP2	1.99	0.61
6:2G:126:ASP:OD2	6:2G:130:ASN:ND2	2.23	0.61
34:2c:88:ARG:HA	34:2c:91:LEU:HD13	1.82	0.61
39:1h:34:GLU:OE1	39:1h:37:ARG:NH1	2.34	0.61
34:1c:57:ILE:HG12	34:1c:66:VAL:HG12	1.83	0.61
35:2d:173:TRP:CD2	35:2d:189:PRO:HB3	2.36	0.61
1:1A:2285:C:OP2	28:16:6:ARG:NH1	2.33	0.61
23:21:72:GLU:OE2	23:21:76:ARG:NH2	2.34	0.61
32:2a:620:C:C2	35:2d:135:LEU:HG	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.27	0.61
1:1A:859:G:O2'	1:1A:916:G:O6	2.17	0.60
7:1H:43:VAL:HG22	7:1H:52:VAL:HG22	1.83	0.60
41:1j:11:PHE:HE1	41:1j:67:THR:HG22	1.65	0.60
1:2A:370:G:N7	61:2A:3999:HOH:O	2.31	0.60
1:2A:492:A:H2'	1:2A:493:G:O4'	2.01	0.60
32:2a:45:U:H2'	32:2a:46:G:C8	2.36	0.60
6:1G:66:GLN:HG3	26:14:1:MET:HE1	1.82	0.60
32:1a:224:C:OP1	51:1t:74:LYS:NZ	2.32	0.60
32:1a:375:U:OP1	47:1p:69:THR:OG1	2.16	0.60
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.35	0.60
32:2a:957:U:O2'	32:2a:959:A:N7	2.29	0.60
32:2a:1010:G:C2	32:2a:1020:U:H1'	2.35	0.60
33:2b:63:MET:HG3	33:2b:225:ALA:HB1	1.83	0.60
4:1E:77:ILE:HD13	4:1E:195:LEU:HD13	1.83	0.60
32:1a:200:G:H1	32:1a:217:C:H42	1.48	0.60
34:1c:172:ARG:HG3	34:1c:174:PRO:HD3	1.83	0.60
24:22:16:LEU:O	24:22:67:LYS:NZ	2.34	0.60
32:2a:352:C:O2'	32:2a:354:G:OP1	2.18	0.60
54:2w:13:C:H4'	54:2w:14:A:OP1	2.01	0.60
32:1a:591:U:H2'	32:1a:592:G:H8	1.66	0.60
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.15	0.60
32:1a:1151:A:HO2'	32:1a:1152:A:H8	1.49	0.60
1:2A:397:G:N7	61:2A:3996:HOH:O	2.31	0.60
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.34	0.60
32:1a:742:G:OP2	46:1o:35:ARG:NH2	2.35	0.60
34:1c:6:HIS:CD2	34:1c:8:ILE:H	2.20	0.60
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.82	0.60
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.36	0.60
5:2F:33:LEU:HD22	5:2F:112:MET:HE3	1.84	0.60
6:2G:29:TRP:O	6:2G:33:ARG:NH1	2.34	0.60
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.83	0.60
1:1A:2250:G:OP1	12:1Q:85:LYS:NZ	2.31	0.60
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.34	0.60
54:1w:51:U:H2'	54:1w:52:G:C8	2.36	0.60
1:2A:500:G:H22	1:2A:503:A:H5'	1.65	0.60
21:2Z:45:ASP:OD1	21:2Z:49:ARG:NE	2.34	0.60
32:1a:700:G:N7	61:1a:1925:HOH:O	2.30	0.60
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.01	0.60
1:1A:247:G:H4'	1:1A:386:G:C5	2.37	0.60
1:1A:1176:G:H1'	1:1A:1177:A:H5''	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1315:C:OP2	61:1A:4106:HOH:O	2.16	0.60
9:1N:12:ARG:HH12	9:1N:138:LEU:HD11	1.67	0.60
13:1R:56:LYS:NZ	13:1R:87:TYR:O	2.27	0.60
1:1A:2206:G:H5''	1:1A:2207:G:C5	2.36	0.60
32:1a:542:G:H5'	35:1d:41:GLY:HA3	1.83	0.60
32:1a:969:A:OP1	41:1j:55:LYS:NZ	2.35	0.60
33:1b:47:THR:HA	33:1b:202:PRO:HG2	1.83	0.60
36:1e:81:GLU:HG2	36:1e:90:VAL:HG22	1.84	0.60
3:2D:71:ASP:HB2	3:2D:103:ARG:HH12	1.65	0.60
24:22:67:LYS:O	24:22:70:GLN:NE2	2.35	0.60
32:2a:692:U:O2'	32:2a:694:A:N7	2.25	0.60
46:2o:5:LYS:O	46:2o:9:GLN:HG2	2.02	0.60
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.02	0.60
1:1A:2431:U:OP1	61:1A:4131:HOH:O	2.16	0.60
1:1A:2636:U:OP1	4:1E:79:ARG:HD3	2.02	0.60
1:2A:1456:G:OP2	61:2A:3933:HOH:O	2.16	0.60
11:2P:89:ALA:HA	11:2P:121:LYS:HD3	1.84	0.60
32:2a:1055:A:N7	32:2a:1200:C:N4	2.50	0.60
1:1A:586:A:N1	1:1A:809:G:O2'	2.31	0.59
1:1A:1453:U:O2'	1:1A:1455:G:N7	2.35	0.59
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.84	0.59
20:1Y:17:SER:OG	20:1Y:71:LYS:NZ	2.29	0.59
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.84	0.59
49:1r:52:PRO:HB2	49:1r:54:ARG:HG2	1.83	0.59
1:2A:1607:C:N4	1:2A:1622:G:OP2	2.32	0.59
13:2R:104:ARG:HD2	13:2R:109:ALA:HB3	1.84	0.59
26:24:15:ILE:HG12	26:24:21:VAL:HG13	1.84	0.59
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.66	0.59
34:2c:20:SER:HB3	34:2c:22:TRP:HE1	1.65	0.59
32:1a:677:U:H3	32:1a:713:G:H22	1.49	0.59
33:1b:82:ARG:NH1	33:1b:86:GLU:OE2	2.35	0.59
21:2Z:154:ASP:N	21:2Z:154:ASP:OD1	2.35	0.59
1:2A:2138:C:H42	1:2A:2153:G:H1	1.50	0.59
15:2T:31:SER:OG	15:2T:85:LYS:NZ	2.34	0.59
33:2b:178:ARG:NH2	39:2h:74:PRO:HB3	2.17	0.59
35:2d:15:GLU:OE2	35:2d:66:ARG:NH1	2.35	0.59
36:2e:60:TYR:OH	36:2e:64:ARG:NH2	2.34	0.59
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.37	0.59
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.35	0.59
51:1t:26:ASN:OD1	51:1t:71:THR:OG1	2.15	0.59
1:2A:2504:U:OP2	61:2A:3930:HOH:O	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:16:CYS:HA	26:24:33:VAL:HG12	1.85	0.59
50:2s:53:ASN:OD1	50:2s:54:GLY:N	2.35	0.59
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.66	0.59
1:2A:1019:U:HO2'	1:2A:1021:A:H2	1.50	0.59
26:24:46:GLN:C	26:24:48:ARG:H	2.11	0.59
44:2m:16:ASP:OD1	44:2m:16:ASP:N	2.34	0.59
1:1A:2277:G:OP2	22:10:10:THR:HG21	2.02	0.59
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.84	0.59
50:1s:20:LEU:HD23	50:1s:23:ASN:HD22	1.67	0.59
1:2A:422:A:OP2	61:2A:3923:HOH:O	2.16	0.59
15:2T:30:VAL:HG22	15:2T:86:ILE:HG12	1.85	0.59
32:2a:1027:C:O2'	32:2a:1034:G:N2	2.35	0.59
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.38	0.59
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.38	0.59
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.02	0.59
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.37	0.59
40:1i:27:THR:HG23	40:1i:62:TYR:HA	1.84	0.59
43:1l:56:ALA:HB2	43:1l:70:ILE:HD11	1.85	0.59
10:2O:98:VAL:HG22	10:2O:118:ALA:HA	1.85	0.59
32:2a:976:G:H5'	32:2a:1358:U:O2'	2.03	0.59
33:2b:8:LYS:HA	33:2b:217:ARG:HD3	1.84	0.59
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.83	0.59
55:2x:76:31H:OP2	61:2x:201:HOH:O	2.16	0.59
50:1s:27:GLU:HB2	50:1s:28:LYS:HA	1.84	0.59
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.03	0.59
33:2b:195:ASP:O	39:2h:68:ARG:NH2	2.35	0.59
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.03	0.59
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.38	0.59
32:2a:1147:C:O2	40:2i:16:ARG:NH1	2.36	0.59
32:2a:1272:G:N2	32:2a:1273:G:C5	2.70	0.59
34:2c:22:TRP:CH2	34:2c:32:LEU:HB3	2.38	0.59
32:1a:73:G:H1	32:1a:96:U:H3	1.50	0.58
1:2A:97:C:OP1	24:22:2:LYS:NZ	2.36	0.58
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.33	0.58
33:2b:19:HIS:ND1	33:2b:206:ASP:OD2	2.36	0.58
32:1a:1348:U:H4'	40:1i:120:ARG:HD2	1.85	0.58
37:1f:11:ASN:HB3	37:1f:14:LEU:HG	1.85	0.58
54:1w:5:G:H2'	54:1w:6:G:C8	2.37	0.58
32:2a:1190:G:H5'	34:2c:176:HIS:CE1	2.37	0.58
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.39	0.58
54:2y:65:G:H2'	54:2y:66:U:C6	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:106:C:H1'	20:1Y:1:MET:HE2	1.85	0.58
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	1.86	0.58
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.85	0.58
1:2A:249:C:O2	30:28:12:LYS:NZ	2.31	0.58
1:2A:796:C:H2'	1:2A:797:C:C6	2.38	0.58
1:2A:1019:U:OP1	1:2A:1035:U:O2'	2.18	0.58
34:2c:152:ILE:HD11	34:2c:199:LYS:HZ2	1.67	0.58
3:1D:85:ASP:OD2	3:1D:88:ARG:NH1	2.36	0.58
32:1a:711:G:OP1	37:1f:54:LYS:NZ	2.35	0.58
8:2I:122:GLU:O	8:2I:126:TYR:OH	2.21	0.58
32:2a:1010:G:H2'	32:2a:1011:G:C8	2.39	0.58
50:1s:12:ASP:OD2	50:1s:35:SER:OG	2.20	0.58
32:2a:194:C:H2'	32:2a:195:A:H5''	1.85	0.58
44:2m:40:ASN:HD22	44:2m:43:THR:HG23	1.67	0.58
54:2y:8:4SU:H1'	54:2y:48:C:H1'	1.85	0.58
32:1a:1320:C:O2	50:1s:36:ARG:NH2	2.36	0.58
32:1a:1329:A:N7	52:1u:7:ARG:NH2	2.51	0.58
1:2A:987:G:O2'	1:2A:1000:A:N3	2.33	0.58
2:2B:2:C:H2'	2:2B:3:C:H6	1.67	0.58
10:2O:107:ARG:O	10:2O:112:MET:HE1	2.04	0.58
33:2b:130:ARG:O	33:2b:135:GLN:NE2	2.37	0.58
1:1A:484:C:H2'	1:1A:485:C:C6	2.39	0.58
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.84	0.58
35:1d:67:ILE:HD13	35:1d:196:LEU:HD22	1.84	0.58
37:1f:97:PHE:HD2	49:1r:31:LEU:HD11	1.69	0.58
51:1t:99:LEU:HA	51:1t:100:ILE:O	2.03	0.58
1:2A:1337:G:OP2	19:2X:73:ARG:NH2	2.36	0.58
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.29	0.58
14:1S:39:ILE:HB	14:1S:49:VAL:HG13	1.86	0.58
22:10:46:LYS:NZ	22:10:75:LEU:O	2.27	0.58
1:2A:851:U:H5'	25:23:49:LYS:HD2	1.86	0.58
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.68	0.58
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.86	0.58
32:2a:444:C:H2'	32:2a:445:G:C8	2.39	0.58
32:2a:779:C:H2'	32:2a:780:A:O4'	2.04	0.58
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.34	0.58
11:2P:138:LEU:HD23	11:2P:145:PRO:HB3	1.85	0.58
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.86	0.58
1:1A:1693:U:O2'	3:1D:14:ARG:NH2	2.36	0.58
1:1A:2108:C:H2'	1:1A:2109:U:C6	2.39	0.58
10:1O:63:VAL:HG12	10:1O:106:LEU:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:139:VAL:HG12	21:1Z:140:ASP:H	1.68	0.58
54:1w:23:A:H3'	54:1w:24:G:H8	1.69	0.58
1:2A:1783:A:OP2	61:2A:3937:HOH:O	2.17	0.58
32:2a:444:C:H2'	32:2a:445:G:H8	1.68	0.58
33:2b:20:GLU:HG3	33:2b:189:ASP:HB2	1.85	0.58
44:2m:122:LYS:HG3	44:2m:123:ALA:H	1.69	0.58
1:1A:1506:C:H2'	1:1A:1507:A:H8	1.68	0.57
1:1A:2849:U:OP2	15:1T:95:ARG:NH1	2.37	0.57
4:1E:31:CYS:HB3	4:1E:49:LEU:HG	1.85	0.57
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.12	0.57
32:1a:560:U:O2'	32:1a:561:U:OP2	2.15	0.57
34:1c:59:ARG:HG2	34:1c:64:VAL:HB	1.85	0.57
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.85	0.57
40:2i:85:LEU:HB3	40:2i:92:TYR:HD2	1.68	0.57
1:1A:1455:G:O2'	1:1A:2853:C:OP1	2.17	0.57
32:1a:757:U:H2'	32:1a:758:G:O4'	2.03	0.57
33:1b:55:PHE:HE1	33:1b:218:ALA:HA	1.69	0.57
37:1f:39:LYS:HB2	37:1f:64:GLN:HB3	1.86	0.57
6:2G:65:GLY:HA2	26:24:7:PRO:HG2	1.85	0.57
7:2H:45:VAL:HG13	7:2H:50:VAL:HG22	1.86	0.57
11:2P:94:GLU:OE2	11:2P:124:LYS:NZ	2.29	0.57
32:2a:1128:C:O2'	32:2a:1129:C:OP1	2.22	0.57
33:2b:155:LEU:HD21	33:2b:159:PRO:HD3	1.86	0.57
46:2o:7:GLU:OE1	46:2o:38:ARG:NH2	2.37	0.57
1:2A:668:G:H5'	1:2A:669:G:OP2	2.05	0.57
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.39	0.57
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.22	0.57
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.37	0.57
15:2T:41:ARG:NH2	32:2a:346:G:OP1	2.36	0.57
32:2a:1071:C:H2'	32:2a:1072:G:C8	2.38	0.57
1:1A:516:C:OP1	27:15:13:LYS:NZ	2.38	0.57
1:1A:1371:G:O6	61:1A:4126:HOH:O	2.14	0.57
1:1A:1721:G:H1'	1:1A:1741:A:H61	1.67	0.57
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.39	0.57
50:1s:22:LEU:HB3	50:1s:27:GLU:HB3	1.86	0.57
11:2P:19:VAL:HG12	11:2P:27:HIS:HB3	1.87	0.57
25:23:8:LEU:HG	25:23:31:LEU:HD23	1.86	0.57
32:2a:189(F):U:O2	48:2q:63:ARG:NH2	2.37	0.57
1:1A:2629:A:O2'	1:1A:2630:G:OP2	2.16	0.57
35:1d:18:LYS:NZ	35:1d:26:CYS:O	2.32	0.57
39:1h:83:ILE:HG13	39:1h:137:VAL:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:120:ALA:O	33:2b:125:PRO:HD2	2.04	0.57
38:2g:59:LEU:O	38:2g:63:LYS:HB2	2.05	0.57
40:2i:56:LEU:HD23	40:2i:56:LEU:H	1.69	0.57
54:2y:14:A:H61	54:2y:21:A:H2	1.52	0.57
1:1A:2575:C:OP2	61:1A:4129:HOH:O	2.16	0.57
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.68	0.57
32:1a:545:C:OP1	35:1d:61:LYS:NZ	2.33	0.57
32:1a:1060:C:H5''	41:1j:51:ARG:HG2	1.85	0.57
33:1b:12:GLU:HB2	33:1b:213:LEU:HD21	1.87	0.57
1:2A:568:U:O4	61:2A:3940:HOH:O	2.18	0.57
1:2A:918:A:N3	2:2B:80:U:O2'	2.34	0.57
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.38	0.57
32:2a:782:A:OP1	61:2a:1911:HOH:O	2.17	0.57
1:1A:668:G:H5'	1:1A:669:G:OP2	2.03	0.57
7:1H:3:ARG:HH11	7:1H:4:ILE:H	1.51	0.57
10:1O:73:ASP:HB2	15:1T:82:LEU:HD13	1.87	0.57
26:24:26:SER:OG	26:24:27:THR:N	2.35	0.57
39:2h:21:LYS:O	39:2h:65:TYR:OH	2.19	0.57
44:2m:80:ARG:NH2	50:2s:65:ASN:O	2.38	0.57
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.86	0.57
14:1S:59:LYS:O	61:1S:301:HOH:O	2.17	0.57
20:1Y:15:VAL:HG21	20:1Y:42:VAL:HG11	1.87	0.57
38:1g:106:GLN:O	38:1g:110:GLN:HG2	2.04	0.57
1:2A:1508:A:H4'	1:2A:1509(A):A:C6	2.40	0.57
1:2A:1693:U:O2'	3:2D:14:ARG:NH2	2.37	0.57
35:2d:99:SER:HB3	35:2d:139:ARG:HG3	1.85	0.57
41:2j:42:THR:HG22	41:2j:66:ARG:HB2	1.87	0.57
48:2q:40:LYS:HD3	48:2q:42:TYR:CZ	2.40	0.57
50:2s:49:ILE:HG22	50:2s:62:ILE:HD11	1.87	0.57
8:1I:5:LEU:H	8:1I:5:LEU:HD12	1.70	0.57
26:14:34:GLU:HG2	26:14:35:VAL:HG12	1.87	0.57
26:14:53:GLU:HG3	26:14:54:GLY:H	1.70	0.57
32:1a:1291:G:OP1	38:1g:41:ARG:NH1	2.38	0.57
33:1b:211:ILE:O	33:1b:215:LEU:HB2	2.05	0.57
2:2B:83:G:H5''	25:23:52:HIS:CD2	2.40	0.57
32:2a:407:G:H5''	35:2d:115:ARG:HB3	1.87	0.57
32:2a:628:G:H2'	32:2a:629:G:C8	2.40	0.57
32:2a:1524:C:OP1	42:2k:120:ARG:NH1	2.37	0.57
33:2b:8:LYS:HD2	33:2b:9:GLU:N	2.19	0.57
34:2c:6:HIS:HD2	34:2c:8:ILE:H	1.53	0.57
34:2c:69:HIS:HA	34:2c:104:GLN:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1079:C:H2'	1:1A:1080:C:O4'	2.05	0.57
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.03	0.57
34:1c:73:PRO:HB3	34:1c:103:VAL:HG11	1.86	0.57
42:1k:87:THR:O	42:1k:87:THR:OG1	2.21	0.57
1:2A:1356:G:OP2	61:2A:3939:HOH:O	2.18	0.57
16:2U:49:HIS:HA	16:2U:52:ARG:HB2	1.86	0.57
32:2a:1251:A:N1	32:2a:1354:C:O2'	2.37	0.57
32:2a:1310:G:H5'	44:2m:77:ASN:ND2	2.18	0.57
47:2p:1:MET:HE3	47:2p:3:LYS:HD3	1.85	0.57
1:1A:2128:C:H2'	1:1A:2129:C:O4'	2.04	0.56
13:1R:118:GLU:H	13:1R:118:GLU:CD	2.12	0.56
32:1a:438:G:H4'	35:1d:123:HIS:ND1	2.20	0.56
32:1a:1302:U:C6	44:1m:17:VAL:HG11	2.40	0.56
32:2a:1218:C:OP2	45:2n:9:LYS:NZ	2.38	0.56
54:2y:9:A:H4'	54:2y:46:G7M:H5'	1.87	0.56
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.40	0.56
21:1Z:52:SER:O	21:1Z:54:HIS:N	2.37	0.56
32:1a:640:A:O2'	39:1h:115:SER:O	2.23	0.56
1:2A:890:A:H2'	1:2A:892:G:C8	2.39	0.56
1:2A:1352:U:OP1	61:2A:3936:HOH:O	2.17	0.56
1:2A:2712(A):A:OP2	61:2A:3934:HOH:O	2.17	0.56
32:2a:826:C:O2	39:2h:15:ASN:ND2	2.38	0.56
54:2y:14:A:O2'	54:2y:15:G:OP1	2.23	0.56
1:1A:817:C:OP1	61:1A:4132:HOH:O	2.17	0.56
1:1A:2262:U:OP1	1:1A:2387:U:O2'	2.20	0.56
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.87	0.56
9:1N:62:VAL:HG22	9:1N:66:LYS:HD2	1.88	0.56
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.23	0.56
32:1a:1194:U:H4'	36:1e:22:GLY:HA2	1.87	0.56
32:1a:1353:G:OP1	52:1u:10:ARG:NH1	2.38	0.56
35:1d:173:TRP:CD2	35:1d:189:PRO:HG3	2.39	0.56
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.23	0.56
1:2A:1031:G:H5''	31:29:8:LYS:HE3	1.86	0.56
1:2A:1031:G:H21	31:29:36:GLN:HE22	1.53	0.56
1:2A:2108:C:H42	1:2A:2181:G:H1	1.51	0.56
1:2A:2133:G:O2'	1:2A:2157:G:N2	2.39	0.56
6:2G:173:LEU:HB3	6:2G:178:PHE:CD2	2.40	0.56
11:2P:39:LYS:HB2	11:2P:45:LEU:HD13	1.87	0.56
17:2V:4:ILE:HD12	17:2V:39:LEU:HB3	1.87	0.56
32:2a:1095:U:H5''	32:2a:1109:C:O2	2.04	0.56
32:2a:1292:U:H2'	32:2a:1293:G:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:7:THR:O	40:2i:83:ARG:NH1	2.30	0.56
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.38	0.56
10:1O:13:ASN:OD1	10:1O:97:ARG:N	2.38	0.56
1:2A:700:G:O2'	1:2A:1632:A:N3	2.30	0.56
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.86	0.56
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	1.87	0.56
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.41	0.56
9:2N:58:ASP:OD1	9:2N:58:ASP:N	2.33	0.56
32:2a:56:U:H2'	32:2a:57:G:H8	1.71	0.56
32:2a:1020:U:H2'	32:2a:1021:G:C8	2.40	0.56
33:2b:178:ARG:HH22	39:2h:68:ARG:NH1	2.04	0.56
34:2c:123:GLN:O	34:2c:128:PHE:HB2	2.06	0.56
1:1A:2218:U:O4'	23:11:52:ARG:NH2	2.38	0.56
1:1A:2582:G:OP1	61:1A:4133:HOH:O	2.18	0.56
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.38	0.56
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.69	0.56
35:1d:178:VAL:C	35:1d:180:GLY:H	2.13	0.56
4:2E:163:GLU:HG2	4:2E:164:ARG:N	2.19	0.56
6:2G:46:ALA:HA	6:2G:49:ASP:O	2.06	0.56
32:2a:224:C:H2'	32:2a:225:C:H6	1.71	0.56
32:2a:576:G:OP1	61:2a:1910:HOH:O	2.17	0.56
32:2a:745:C:OP1	32:2a:851:G:O2'	2.17	0.56
34:2c:142:MET:HA	34:2c:146:ALA:HB3	1.87	0.56
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.88	0.56
1:1A:271(I):G:H2'	1:1A:271(J):C:C2	2.40	0.56
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.41	0.56
47:1p:71:ARG:O	47:1p:75:ARG:N	2.38	0.56
1:2A:1316:U:H2'	1:2A:1317:A:H8	1.70	0.56
1:2A:1358:G:O2'	1:2A:1373:A:N6	2.35	0.56
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.70	0.56
32:2a:1292:U:H2'	32:2a:1293:G:H8	1.70	0.56
1:1A:731:C:OP2	61:1A:4134:HOH:O	2.18	0.56
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.88	0.56
42:1k:79:SER:HA	42:1k:104:GLN:HG2	1.88	0.56
32:2a:1060:C:C5	34:2c:2:GLY:HA3	2.40	0.56
42:2k:99:GLN:HG2	42:2k:105:VAL:HG21	1.87	0.56
1:1A:1430:C:H2'	1:1A:1431:U:C6	2.40	0.56
6:1G:137:GLU:HG2	6:1G:152:LEU:HD23	1.87	0.56
7:1H:7:LEU:HD12	7:1H:8:PRO:HD2	1.88	0.56
10:1O:68:GLU:HB3	10:1O:78:ARG:HB2	1.87	0.56
21:1Z:7:ALA:HB2	21:1Z:59:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1j:30:SER:HB3	41:1j:81:THR:HG23	1.86	0.56
41:1j:38:ILE:HD11	41:1j:71:LEU:HB3	1.87	0.56
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.40	0.56
23:21:50:ARG:HG2	23:21:59:THR:HG23	1.87	0.56
32:2a:377:G:OP1	47:2p:3:LYS:NZ	2.37	0.56
1:1A:1092:C:H2'	1:1A:1093:G:H5'	1.88	0.56
32:1a:112:G:OP2	47:1p:27:LYS:NZ	2.38	0.56
32:1a:946:A:H2'	32:1a:947:G:C8	2.41	0.56
34:1c:87:LEU:O	34:1c:91:LEU:N	2.35	0.56
51:1t:57:ARG:HH12	51:1t:100:ILE:HD12	1.71	0.56
1:2A:1647:G:OP1	61:2A:3907:HOH:O	2.18	0.56
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	1.88	0.56
32:2a:619:U:N3	35:2d:134:ASP:OD1	2.33	0.56
1:1A:987:G:O2'	1:1A:1000:A:N3	2.35	0.55
21:1Z:132:ASN:N	21:1Z:132:ASN:OD1	2.38	0.55
32:1a:1240:U:OP2	38:1g:116:ALA:N	2.39	0.55
6:2G:66:GLN:HE21	6:2G:92:VAL:HG22	1.71	0.55
36:2e:36:ASP:O	36:2e:38:GLN:N	2.37	0.55
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.41	0.55
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.07	0.55
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.88	0.55
32:1a:553:A:H5''	43:1l:24:VAL:HG21	1.87	0.55
36:1e:84:PHE:HB2	36:1e:134:ALA:HB2	1.89	0.55
38:1g:105:VAL:O	38:1g:109:ASN:ND2	2.36	0.55
1:2A:2557:G:H2'	1:2A:2558:C:C6	2.42	0.55
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.41	0.55
13:2R:20:LEU:HD11	13:2R:40:LYS:HD3	1.88	0.55
24:22:32:LEU:HD13	24:22:53:LEU:HB3	1.87	0.55
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.73	0.55
36:2e:20:GLN:HE21	36:2e:21:ALA:N	2.04	0.55
3:1D:137:PRO:O	3:1D:140:THR:OG1	2.24	0.55
32:1a:316:G:OP2	32:1a:351:G:O2'	2.24	0.55
32:1a:1239:A:H4'	32:1a:1240:U:H5''	1.89	0.55
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.06	0.55
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.05	0.55
1:2A:1218:C:OP2	16:2U:15:LYS:NZ	2.32	0.55
1:2A:1448:G:H2'	1:2A:1449:A:C8	2.42	0.55
32:2a:1069:C:O2'	32:2a:1192:C:H1'	2.07	0.55
32:2a:1244:C:H42	32:2a:1293:G:H1	1.53	0.55
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.42	0.55
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2f:91:VAL:HG11	49:2r:72:ARG:NH1	2.21	0.55
54:2y:18:G:N1	54:2y:55:PSU:C4	2.69	0.55
1:1A:881:G:H3'	1:1A:882:G:H8	1.72	0.55
33:1b:204:ASN:OD1	33:1b:205:ASP:N	2.39	0.55
41:1j:11:PHE:CE1	41:1j:67:THR:HG22	2.42	0.55
1:2A:1038:C:H42	1:2A:1117:G:H1	1.52	0.55
2:2B:3:C:H2'	2:2B:4:C:C6	2.42	0.55
6:2G:41:GLN:NE2	6:2G:153:ARG:HB3	2.21	0.55
6:2G:109:VAL:HG11	26:24:14:ILE:HG21	1.88	0.55
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.36	0.55
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.22	0.55
50:2s:61:TYR:CE2	50:2s:63:THR:HG22	2.41	0.55
1:1A:783:A:O2'	1:1A:785:G:OP1	2.22	0.55
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.89	0.55
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.04	0.55
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.41	0.55
26:24:50:VAL:HG11	44:2m:64:TRP:C	2.32	0.55
32:2a:17:U:H2'	32:2a:18:C:C6	2.41	0.55
32:2a:429:U:O3'	35:2d:22:LYS:NZ	2.34	0.55
1:1A:2629:A:H4'	1:1A:2629:A:OP1	2.07	0.55
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.88	0.55
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.07	0.55
32:1a:1028:C:H2'	32:1a:1029:C:O4'	2.06	0.55
1:2A:839:U:H2'	1:2A:840:C:C6	2.42	0.55
1:2A:1009:A:OP2	9:2N:37:LYS:NZ	2.31	0.55
1:2A:2807:G:H22	1:2A:2892:A:N6	2.05	0.55
2:2B:43:C:OP1	26:24:6:HIS:NE2	2.36	0.55
21:2Z:28:MET:HE1	21:2Z:61:LEU:HD21	1.87	0.55
32:2a:328:C:H4'	32:2a:329:A:H5'	1.89	0.55
32:2a:337:C:H2'	32:2a:338:A:C8	2.42	0.55
33:2b:102:LEU:HD13	33:2b:182:ILE:HD12	1.87	0.55
40:2i:9:ARG:H	40:2i:79:LEU:HD23	1.72	0.55
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.88	0.55
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	1.88	0.55
1:2A:2150:U:H2'	1:2A:2151:G:H8	1.72	0.55
1:2A:2892:A:H2'	1:2A:2893:G:H5'	1.89	0.55
29:27:8:ASN:HB3	29:27:11:LYS:HB3	1.89	0.55
32:2a:1367:C:H5''	40:2i:114:TYR:HB3	1.88	0.55
33:2b:54:THR:HG22	33:2b:199:TYR:HB3	1.88	0.55
54:2w:62:C:H2'	54:2w:63:G:C8	2.41	0.55
1:1A:536:A:H2'	1:1A:537:C:C6	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1434:A:H61	1:2A:1558:A:H62	1.55	0.55
20:2Y:38:ILE:HD11	20:2Y:66:PRO:HG3	1.89	0.55
32:2a:79:G:H1	32:2a:90:U:H3	1.55	0.55
32:2a:460:G:N2	32:2a:471:G:N7	2.55	0.55
32:2a:1190:G:H5'	34:2c:176:HIS:HE1	1.72	0.55
34:2c:8:ILE:HG12	34:2c:184:TYR:HB3	1.89	0.55
41:2j:16:LEU:HD13	41:2j:70:ARG:HG2	1.89	0.55
42:2k:73:MET:HA	42:2k:77:MET:H	1.70	0.55
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.07	0.55
1:1A:2336:A:H61	22:10:43:THR:CG2	2.20	0.55
32:1a:582:U:H2'	32:1a:583:A:H8	1.70	0.55
33:1b:204:ASN:OD1	33:1b:206:ASP:N	2.28	0.55
1:2A:332:A:O2'	1:2A:334:C:OP2	2.22	0.55
1:2A:2014:A:N1	61:2A:4008:HOH:O	2.33	0.55
1:2A:2895:U:H2'	1:2A:2896:C:O4'	2.07	0.55
1:1A:1456:G:OP2	61:1A:4135:HOH:O	2.18	0.54
1:1A:2492:U:H2'	1:1A:2493:U:H6	1.73	0.54
4:1E:29:GLY:HA3	61:1E:402:HOH:O	2.07	0.54
4:1E:122:PHE:O	61:1E:401:HOH:O	2.18	0.54
19:1X:32:PRO:HA	19:1X:77:LYS:HD3	1.89	0.54
40:1i:28:VAL:HG22	40:1i:63:ILE:HB	1.88	0.54
1:2A:1499:C:H2'	1:2A:1500:G:H8	1.73	0.54
1:2A:2576:G:OP1	61:2A:3941:HOH:O	2.18	0.54
6:2G:70:VAL:HA	6:2G:90:LEU:HD23	1.89	0.54
26:24:53:GLU:OE1	26:24:53:GLU:N	2.39	0.54
32:2a:148:G:H2'	32:2a:149:A:C8	2.41	0.54
32:2a:909:A:H2'	32:2a:910:C:O4'	2.07	0.54
39:2h:33:GLU:HG2	39:2h:48:TYR:CE1	2.42	0.54
17:1V:65:GLY:HA3	17:1V:91:TYR:CZ	2.41	0.54
32:1a:1429:C:H2'	32:1a:1430:C:C6	2.42	0.54
35:1d:119:GLN:HG2	35:1d:123:HIS:CD2	2.42	0.54
36:1e:105:VAL:HG21	36:1e:128:PRO:HB3	1.88	0.54
48:1q:6:LEU:HD13	48:1q:23:VAL:HG11	1.88	0.54
50:1s:80:TYR:CZ	50:1s:82:GLY:HA2	2.42	0.54
1:2A:570:G:H2'	1:2A:2030:A:C5	2.42	0.54
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.89	0.54
1:2A:1847:A:H3'	1:2A:1848:A:H5'	1.89	0.54
4:2E:54:GLN:HB3	4:2E:74:PRO:HB2	1.88	0.54
23:21:64:ALA:HA	23:21:67:ILE:HG13	1.89	0.54
33:2b:223:ILE:HA	33:2b:226:ARG:HD3	1.89	0.54
37:2f:61:LEU:HB3	37:2f:63:TYR:HE2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:13:A:N1	2:1B:69:G:O2'	2.34	0.54
37:1f:19:LEU:HD11	37:1f:59:TYR:CE1	2.42	0.54
2:2B:72:G:O2'	2:2B:105:A:N6	2.41	0.54
21:2Z:93:ASP:HB3	21:2Z:131:ARG:HH22	1.73	0.54
32:2a:539:A:OP2	43:2l:115:LYS:NZ	2.31	0.54
32:2a:862:C:H1'	32:2a:874:G:H5''	1.89	0.54
51:2t:9:ASN:OD1	51:2t:9:ASN:N	2.40	0.54
1:1A:218:A:C2	1:1A:235:U:H4'	2.43	0.54
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.41	0.54
1:1A:2888:C:H2'	1:1A:2889:C:H6	1.71	0.54
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.89	0.54
8:1I:93:THR:HG22	8:1I:119:PRO:HB3	1.89	0.54
11:1P:89:ALA:HA	11:1P:121:LYS:HD3	1.88	0.54
32:1a:867:G:O2'	32:1a:873:A:N1	2.37	0.54
34:1c:35:GLU:CD	34:1c:59:ARG:HH22	2.16	0.54
37:1f:21:LEU:O	37:1f:25:ILE:HG13	2.07	0.54
6:2G:5:VAL:HG13	6:2G:8:LYS:HE2	1.89	0.54
32:2a:141:A:H1'	32:2a:182:U:O2	2.07	0.54
32:2a:651:C:N4	32:2a:753:A:OP2	2.39	0.54
32:2a:1321:C:O2'	50:2s:77:THR:HG21	2.08	0.54
32:2a:1328:C:O2'	44:2m:29:ARG:NH2	2.40	0.54
1:1A:579:G:H2'	1:1A:580:C:C6	2.43	0.54
1:1A:882:G:H4'	54:1w:19:G:O6	2.07	0.54
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.39	0.54
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.88	0.54
13:1R:87:TYR:OH	13:1R:117:VAL:O	2.24	0.54
28:16:6:ARG:NE	28:16:24:GLU:OE2	2.36	0.54
32:1a:486:U:H2'	32:1a:487:A:C8	2.42	0.54
32:1a:922:G:H4'	36:1e:20:GLN:HA	1.88	0.54
1:2A:27:G:N2	1:2A:512:G:H1'	2.22	0.54
1:2A:203:C:OP2	61:2A:3938:HOH:O	2.17	0.54
1:2A:1268:A:OP1	61:2A:3945:HOH:O	2.19	0.54
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.43	0.54
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	1.89	0.54
10:2O:71:ARG:NE	10:2O:105:GLU:OE2	2.40	0.54
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.07	0.54
45:1n:21:TYR:HE1	45:1n:23:ARG:HE	1.53	0.54
48:1q:58:GLU:O	48:1q:74:LEU:N	2.36	0.54
1:2A:955:C:OP1	12:2Q:87:LYS:NZ	2.37	0.54
32:2a:1152:A:OP1	41:2j:70:ARG:NH2	2.35	0.54
58:1A:4098:WC9:CBE	54:1w:76:A:H5'	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:91:PHE:O	11:1P:121:LYS:NZ	2.31	0.54
25:13:23:LEU:HD13	25:13:50:VAL:HG11	1.89	0.54
32:1a:974:A:H8	32:1a:974:A:OP1	1.90	0.54
32:1a:1343:G:H1'	40:1i:121:ARG:NH1	2.23	0.54
35:1d:178:VAL:HG12	35:1d:179:GLU:H	1.73	0.54
1:2A:1843:C:H5'	3:2D:253:GLN:OE1	2.08	0.54
54:2y:18:G:O6	54:2y:56:C:N4	2.40	0.54
10:1O:36:GLY:O	61:1O:301:HOH:O	2.19	0.54
28:16:19:ARG:NH1	28:16:52:VAL:HG21	2.23	0.54
42:1k:48:ILE:O	42:1k:50:TYR:N	2.38	0.54
1:2A:392:C:H5''	1:2A:409:C:H5''	1.89	0.54
8:2I:75:LEU:HD13	8:2I:105:HIS:HD2	1.72	0.54
21:2Z:171:ILE:HD12	21:2Z:172:ALA:H	1.71	0.54
32:2a:7:G:H5'	32:2a:298:A:O4'	2.08	0.54
32:2a:662:G:H2'	32:2a:663:A:C8	2.42	0.54
1:1A:784:A:N6	3:1D:229:VAL:HG11	2.22	0.54
1:1A:1019:U:OP1	1:1A:1035:U:O2'	2.23	0.54
1:1A:1055:G:H1	1:1A:1104:C:H42	1.56	0.54
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.43	0.54
1:1A:1341:U:O2	19:1X:80:ILE:HD12	2.08	0.54
21:1Z:136:PHE:O	21:1Z:137:ILE:HG13	2.07	0.54
32:1a:524:G:H2'	32:1a:525:C:C6	2.42	0.54
55:1x:75:C:H2'	55:1x:76:31H:H1'	1.88	0.54
1:2A:276:A:H5''	1:2A:277:C:H5'	1.88	0.54
8:2I:62:LYS:HA	8:2I:133:HIS:HE1	1.72	0.54
21:2Z:124:ILE:HD11	21:2Z:165:VAL:HG21	1.89	0.54
25:23:6:VAL:HG22	25:23:56:VAL:HG12	1.89	0.54
32:2a:881:G:P	43:2l:12:ARG:HH22	2.31	0.54
32:2a:1458:G:OP1	51:2t:35:THR:OG1	2.21	0.54
34:2c:134:ILE:HG23	34:2c:151:VAL:HB	1.90	0.54
1:1A:242:G:C8	30:18:5:LYS:HG2	2.42	0.54
1:1A:1762:A:H2'	61:1A:5706:HOH:O	2.08	0.54
35:1d:154:ASN:HA	35:1d:159:ARG:HH21	1.73	0.54
1:2A:212:G:H2'	1:2A:213:A:O4'	2.08	0.54
1:2A:1336:A:H2'	1:2A:1337:G:H8	1.73	0.54
1:2A:1799:G:O2'	3:2D:181:GLU:OE2	2.22	0.54
1:2A:2378:A:O2'	14:2S:21:THR:HG21	2.08	0.54
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.08	0.54
3:2D:17:THR:HG1	3:2D:205:VAL:H	1.56	0.54
32:2a:1071:C:H2'	32:2a:1072:G:H8	1.73	0.54
37:2f:82:ARG:HB2	37:2f:85:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:13:LYS:HA	44:2m:44:ARG:HH11	1.71	0.54
1:1A:363(C):G:H2'	1:1A:363(D):G:C8	2.43	0.53
1:1A:1803:A:H4'	3:1D:259:THR:HG23	1.89	0.53
1:1A:2874:C:OP1	61:1A:4137:HOH:O	2.19	0.53
33:1b:163:PHE:HD1	33:1b:185:ILE:HG13	1.73	0.53
1:2A:271(M):G:H4'	1:2A:271(N):U:OP1	2.08	0.53
10:2O:87:ILE:HD12	10:2O:91:LEU:HA	1.90	0.53
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.41	0.53
1:1A:1139:G:OP2	9:1N:70:LYS:NZ	2.39	0.53
1:1A:2161:C:O2'	1:1A:2162:G:H5''	2.07	0.53
32:1a:1525:G:OP1	42:1k:120:ARG:NH2	2.42	0.53
1:2A:1603:A:OP1	61:2A:3946:HOH:O	2.19	0.53
1:2A:2166:G:H3'	1:2A:2167:U:H5''	1.90	0.53
6:2G:114:ILE:HB	6:2G:117:PHE:HD1	1.73	0.53
6:2G:124:SER:O	6:2G:124:SER:OG	2.22	0.53
32:2a:1194:U:H4'	36:2e:22:GLY:HA2	1.90	0.53
33:2b:118:LEU:HD21	33:2b:141:GLU:HB3	1.90	0.53
41:2j:32:ALA:HB1	41:2j:33:GLN:HA	1.88	0.53
1:1A:1075:C:H2'	1:1A:1076:C:H5'	1.89	0.53
1:1A:1673:U:OP1	61:1A:4136:HOH:O	2.19	0.53
32:1a:8:A:N6	35:1d:205:GLU:O	2.40	0.53
32:1a:452:A:H4'	47:1p:72:ARG:CZ	2.39	0.53
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.43	0.53
35:1d:15:GLU:OE2	35:1d:59:ARG:NH1	2.42	0.53
54:1y:42:C:H2'	54:1y:43:C:H6	1.71	0.53
1:2A:468:G:N7	29:27:39:ARG:NH2	2.52	0.53
1:2A:1359:A:H2	1:2A:1372:U:O4	1.92	0.53
8:2I:72:LEU:HA	8:2I:75:LEU:HD12	1.89	0.53
32:2a:532:A:N6	32:2a:1206:G:O2'	2.41	0.53
32:2a:1109:C:H2'	32:2a:1110:A:O4'	2.09	0.53
54:2w:18:G:O2'	54:2w:57:G:N2	2.32	0.53
1:1A:55:G:O2'	1:1A:127:A:N1	2.36	0.53
1:1A:588:U:H2'	1:1A:589:C:C6	2.44	0.53
1:1A:796:C:H2'	1:1A:797:C:C6	2.43	0.53
1:1A:1702:G:H2'	1:1A:1703:G:O4'	2.09	0.53
1:1A:1798:U:H5'	3:1D:259:THR:CG2	2.36	0.53
1:1A:2128:C:N4	1:1A:2160:G:H1	2.03	0.53
32:1a:582:U:H2'	32:1a:583:A:C8	2.44	0.53
40:1i:15:ALA:HA	40:1i:65:VAL:HG12	1.90	0.53
1:2A:600:G:O3'	5:2F:108:LYS:HE3	2.07	0.53
26:24:46:GLN:O	26:24:48:ARG:N	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1226:C:O2'	44:2m:111:LYS:NZ	2.41	0.53
1:1A:801:G:O6	5:1F:53:THR:OG1	2.24	0.53
1:1A:1062:G:N2	1:1A:1077:A:N1	2.48	0.53
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.44	0.53
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.43	0.53
13:1R:56:LYS:HE2	13:1R:94:TYR:OH	2.09	0.53
32:1a:652:U:O4	32:1a:752:G:O2'	2.26	0.53
1:2A:288:C:H2'	1:2A:289:A:H8	1.73	0.53
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.71	0.53
6:2G:114:ILE:HA	6:2G:140:ILE:HD11	1.90	0.53
18:2W:57:ASN:HA	18:2W:61:ASN:HD22	1.74	0.53
26:24:58:ARG:HH21	50:2s:69:HIS:CE1	2.27	0.53
32:2a:21:G:H2'	32:2a:22:G:C8	2.44	0.53
32:2a:737:A:H2'	32:2a:738:C:C6	2.42	0.53
32:2a:950:U:H2'	32:2a:951:G:C8	2.44	0.53
40:2i:43:ALA:HA	40:2i:74:ILE:HD13	1.90	0.53
1:1A:264:C:O2'	1:1A:265:A:H2'	2.08	0.53
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.44	0.53
32:1a:1005:A:OP2	32:1a:1006:C:N4	2.42	0.53
1:2A:2115:G:O2'	1:2A:2117:A:N7	2.38	0.53
1:2A:2123:G:H2'	1:2A:2124:G:C8	2.44	0.53
7:2H:149:ARG:HD2	7:2H:164:TYR:CE2	2.43	0.53
32:2a:407:G:OP1	35:2d:115:ARG:NH2	2.42	0.53
32:2a:509:A:N3	32:2a:543:C:O2'	2.36	0.53
1:1A:1783:A:H5'	1:1A:2608:G:H4'	1.90	0.53
32:1a:165:C:H2'	32:1a:166:G:C8	2.43	0.53
32:1a:436:C:H2'	32:1a:437:U:C6	2.43	0.53
32:1a:1149:C:H2'	32:1a:1150:U:C6	2.44	0.53
34:1c:131:ARG:NH1	34:1c:166:GLU:HG3	2.23	0.53
51:1t:33:ILE:O	51:1t:37:SER:OG	2.19	0.53
21:2Z:93:ASP:HA	21:2Z:131:ARG:HH12	1.74	0.53
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.24	0.53
32:2a:920:U:H2'	32:2a:921:U:C6	2.44	0.53
44:2m:91:ARG:NE	44:2m:97:PRO:O	2.40	0.53
51:2t:10:LEU:HG	51:2t:12:ALA:H	1.73	0.53
1:1A:1876:A:H2'	1:1A:1877:A:C8	2.43	0.53
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.43	0.53
32:1a:17:U:H2'	32:1a:18:C:C6	2.44	0.53
35:1d:117:ALA:O	35:1d:121:VAL:HG23	2.08	0.53
1:2A:652(A):A:H3'	1:2A:652(B):A:H5''	1.90	0.53
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2162:G:H5''	1:2A:2172:U:H2'	1.89	0.53
1:2A:2820:A:C5	13:2R:4:LEU:HD11	2.43	0.53
10:2O:35:VAL:HG13	10:2O:65:THR:HG23	1.91	0.53
15:2T:51:ARG:HG3	15:2T:98:LYS:HD2	1.90	0.53
18:2W:65:LEU:HD12	18:2W:68:ARG:HD2	1.89	0.53
33:2b:8:LYS:HA	33:2b:217:ARG:HH11	1.74	0.53
41:2j:8:LEU:HG	41:2j:70:ARG:HB2	1.89	0.53
54:2y:8:4SU:O4'	54:2y:48:C:O2'	2.21	0.53
1:1A:1312:U:OP2	19:1X:63:LYS:NZ	2.42	0.53
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.27	0.53
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.42	0.53
1:2A:309:G:N3	1:2A:329:G:O2'	2.40	0.53
1:2A:1784:A:O2'	61:2A:3944:HOH:O	2.18	0.53
14:2S:25:ARG:NH1	14:2S:42:ASP:OD2	2.42	0.53
20:2Y:16:ALA:HB2	20:2Y:73:ARG:HG3	1.91	0.53
32:2a:316:G:OP2	32:2a:351:G:O2'	2.24	0.53
1:1A:784:A:O4'	3:1D:227:ASN:ND2	2.41	0.53
1:1A:2359:C:H2'	1:1A:2360:A:O4'	2.08	0.53
5:1F:9:ILE:HD13	5:1F:22:ALA:HB3	1.91	0.53
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.09	0.53
19:1X:2:LYS:NZ	19:1X:38:GLU:OE2	2.39	0.53
32:1a:45:U:H2'	32:1a:46:G:C8	2.44	0.53
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.41	0.53
1:2A:1449:A:HO2'	1:2A:1529:G:H21	1.55	0.53
6:2G:18:GLU:OE2	6:2G:22:ARG:HD3	2.09	0.53
8:2I:82:ARG:NH2	8:2I:90:GLY:H	2.07	0.53
21:2Z:53:ILE:HG22	21:2Z:71:VAL:HG23	1.91	0.53
32:2a:405:U:O4	35:2d:2:GLY:N	2.42	0.53
32:2a:715:A:H2'	32:2a:716:A:C8	2.44	0.53
1:1A:674:G:O2'	5:1F:74:ARG:HD3	2.09	0.52
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.45	0.52
1:1A:1952:A:OP1	10:1O:44:LYS:NZ	2.29	0.52
6:1G:18:GLU:OE2	6:1G:22:ARG:NH1	2.30	0.52
6:1G:27:ASN:HB3	6:1G:30:GLU:HG3	1.91	0.52
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	1.91	0.52
32:1a:539:A:H2'	32:1a:540:G:C8	2.44	0.52
32:1a:1112:C:H1'	34:1c:179:ARG:HH11	1.74	0.52
33:1b:201:ILE:HG21	33:1b:214:ILE:HG21	1.91	0.52
40:1i:8:GLY:O	40:1i:15:ALA:N	2.40	0.52
46:1o:37:ASN:O	46:1o:41:GLU:HG2	2.09	0.52
55:1x:17:C:OP2	55:1x:17(A):U:O2'	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:625:G:O6	11:2P:107:LYS:NZ	2.32	0.52
1:2A:1325:G:OP1	1:2A:1647:G:O2'	2.21	0.52
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.24	0.52
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.09	0.52
32:2a:8:A:H5'	36:2e:101:ILE:HG22	1.91	0.52
33:2b:17:PHE:HB3	33:2b:44:LEU:HD11	1.89	0.52
1:1A:467:G:OP1	29:17:33:ARG:NH1	2.43	0.52
1:1A:1060:U:H3	1:1A:1088:A:H8	1.57	0.52
5:1F:107:LYS:HD2	5:1F:206:ILE:HA	1.91	0.52
29:17:46:VAL:HG22	29:17:48:LYS:HG3	1.90	0.52
32:1a:1352:C:H2'	32:1a:1353:G:C8	2.44	0.52
54:1y:23:A:H2'	54:1y:24:G:C8	2.44	0.52
1:2A:2103:C:H2'	1:2A:2104:G:C8	2.44	0.52
4:2E:111:ARG:HG2	4:2E:118:LYS:HD3	1.91	0.52
24:22:10:LEU:HD21	24:22:59:ARG:HG2	1.91	0.52
38:2g:54:THR:O	38:2g:56:GLN:N	2.39	0.52
1:1A:2161:C:HO2'	1:1A:2162:G:H5''	1.74	0.52
5:1F:31:HIS:NE2	5:1F:35:GLU:OE2	2.42	0.52
7:1H:6:ARG:HH22	7:1H:54:ARG:NH2	2.06	0.52
12:1Q:30:GLY:HA2	12:1Q:107:ALA:HB2	1.91	0.52
15:1T:65:LYS:HG2	15:1T:66:VAL:N	2.23	0.52
26:14:46:GLN:O	26:14:48:ARG:N	2.40	0.52
40:1i:9:ARG:HG2	40:1i:14:VAL:HG12	1.91	0.52
1:2A:892:G:H3'	1:2A:893:C:C5'	2.39	0.52
1:2A:1866:C:H2'	1:2A:1876:A:O4'	2.10	0.52
1:2A:2299:G:N1	1:2A:2318:G:N7	2.58	0.52
4:2E:59:VAL:HG22	4:2E:64:LYS:HG3	1.92	0.52
6:2G:113:ARG:HH11	26:24:33:VAL:HG23	1.75	0.52
14:2S:58:LEU:HD13	14:2S:65:VAL:HB	1.91	0.52
32:2a:289:G:OP2	61:2a:1912:HOH:O	2.19	0.52
39:2h:38:ILE:HD13	39:2h:41:ARG:HH21	1.74	0.52
54:2y:53:G:H3'	54:2y:54:5MU:H71	1.91	0.52
32:1a:266:G:H2'	32:1a:266:G:N3	2.24	0.52
32:1a:691:G:H2'	32:1a:692:U:C6	2.45	0.52
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.09	0.52
1:2A:2319:G:H22	14:2S:3:ARG:NH1	1.99	0.52
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.25	0.52
4:2E:1:MET:HE3	4:2E:199:ARG:HB3	1.91	0.52
10:2O:24:VAL:HG13	10:2O:33:ALA:HB2	1.91	0.52
33:2b:118:LEU:HD23	33:2b:142:LEU:HB2	1.90	0.52
37:2f:30:LEU:HD23	37:2f:75:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:299:A:OP2	61:1A:4138:HOH:O	2.19	0.52
1:1A:2572:A:C8	4:1E:144:ARG:HD3	2.44	0.52
26:14:54:GLY:N	26:14:55:ARG:HA	2.23	0.52
32:1a:56:U:H2'	32:1a:57:G:C8	2.45	0.52
33:1b:121:LEU:HD12	33:1b:126:GLU:HG3	1.92	0.52
36:1e:61:TYR:HA	36:1e:64:ARG:HD2	1.91	0.52
43:1l:60:LEU:HD11	43:1l:66:VAL:HG22	1.90	0.52
1:2A:1359:A:H2'	1:2A:1360:A:H5'	1.92	0.52
1:2A:2064:C:H2'	1:2A:2065:C:C6	2.44	0.52
1:2A:2105:C:H2'	1:2A:2106:G:H8	1.73	0.52
1:2A:2171:A:N3	1:2A:2172:U:N3	2.57	0.52
1:2A:2741:A:H2'	1:2A:2742:C:O4'	2.10	0.52
1:1A:271(L):U:H4'	8:1I:50:ARG:HH12	1.75	0.52
23:11:89:GLU:O	23:11:93:GLU:HG2	2.10	0.52
32:1a:688:G:H2'	32:1a:689:C:H6	1.75	0.52
34:1c:89:GLU:OE1	34:1c:90:GLU:N	2.42	0.52
36:1e:106:PRO:O	36:1e:110:LEU:HG	2.10	0.52
46:1o:82:ILE:O	46:1o:86:GLY:N	2.42	0.52
1:2A:744:G:OP1	4:2E:132:HIS:ND1	2.41	0.52
1:2A:893:C:H5'	1:2A:894:C:C5	2.45	0.52
10:2O:26:LYS:O	10:2O:30:ALA:HB2	2.09	0.52
32:2a:646:U:H2'	32:2a:647:C:C6	2.45	0.52
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.10	0.52
39:2h:39:LEU:HB3	39:2h:45:ILE:HD11	1.91	0.52
42:2k:81:ASP:OD1	42:2k:107:SER:OG	2.20	0.52
46:2o:26:GLU:HG3	46:2o:81:LEU:HD13	1.92	0.52
1:1A:1062:G:C4	1:1A:1088:A:H2'	2.44	0.52
1:1A:1283:G:N2	1:1A:1286:A:OP2	2.43	0.52
1:1A:2153:G:H2'	1:1A:2154:G:C8	2.45	0.52
8:1I:69:LYS:HA	8:1I:138:ILE:HD12	1.92	0.52
9:1N:96:GLU:H	9:1N:96:GLU:CD	2.17	0.52
21:1Z:44:PHE:CZ	21:1Z:86:VAL:HG11	2.45	0.52
32:1a:100:C:H2'	32:1a:101:A:C8	2.44	0.52
33:1b:207:ALA:HB3	33:1b:210:SER:HB2	1.90	0.52
40:1i:21:PRO:HA	40:1i:59:PHE:HA	1.90	0.52
1:2A:271(A):A:N1	1:2A:272(D):G:O2'	2.38	0.52
1:2A:1426:G:O2'	1:2A:1572:A:N6	2.41	0.52
1:2A:2340:G:H2'	1:2A:2341:G:H8	1.75	0.52
54:2w:68:C:H2'	54:2w:69:G:C8	2.45	0.52
1:1A:234:C:H2'	1:1A:235:U:H6	1.75	0.52
1:1A:2889:C:H2'	1:1A:2891:G:O4'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:3:ARG:NH1	7:1H:4:ILE:H	2.06	0.52
31:19:25:VAL:HB	31:19:34:GLN:HB2	1.90	0.52
32:1a:405:U:H5''	32:1a:495:A:H2	1.74	0.52
32:1a:591:U:H2'	32:1a:592:G:C8	2.45	0.52
47:1p:74:LEU:HD22	47:1p:79:VAL:HG21	1.92	0.52
1:2A:2849:U:O4	15:2T:23:ARG:NH2	2.42	0.52
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.09	0.52
32:2a:261:U:OP2	51:2t:79:ARG:NH2	2.43	0.52
32:2a:926:G:H3'	32:2a:1505:G:H21	1.75	0.52
32:2a:1060:C:H2'	32:2a:1061:G:H8	1.74	0.52
32:2a:1346:A:N1	32:2a:1374:A:H5''	2.25	0.52
40:2i:50:LEU:HA	40:2i:53:VAL:HG22	1.91	0.52
44:2m:13:LYS:NZ	44:2m:21:TYR:OH	2.43	0.52
54:2w:18:G:HO2'	54:2w:57:G:H22	1.53	0.52
1:1A:831:G:O2'	11:1P:38:GLN:OE1	2.25	0.52
33:1b:76:GLN:NE2	33:1b:206:ASP:OD1	2.43	0.52
47:1p:53:VAL:HB	47:1p:79:VAL:HG13	1.92	0.52
50:1s:63:THR:OG1	50:1s:65:ASN:OD1	2.27	0.52
1:2A:288:C:H2'	1:2A:289:A:C8	2.45	0.52
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.09	0.52
1:2A:1225:G:H4'	17:2V:84:LYS:HG2	1.91	0.52
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.21	0.52
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.45	0.52
4:2E:77:ILE:HD13	4:2E:195:LEU:HD22	1.92	0.52
32:2a:222:U:H2'	32:2a:223:U:C6	2.44	0.52
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.45	0.52
33:2b:88:ALA:HB1	33:2b:222:ILE:HD11	1.90	0.52
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.45	0.52
2:1B:8:U:O3'	14:1S:25:ARG:NH2	2.42	0.52
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.92	0.52
32:1a:501:C:H2'	32:1a:502:G:C8	2.45	0.52
2:2B:14:U:OP2	2:2B:70:C:O2'	2.22	0.52
5:2F:13:SER:OG	5:2F:16:GLY:O	2.24	0.52
6:2G:170:ARG:NH2	6:2G:182:LYS:O	2.43	0.52
9:2N:96:GLU:CD	9:2N:96:GLU:H	2.17	0.52
32:2a:736:C:H2'	32:2a:737:A:C8	2.45	0.52
36:2e:10:MET:HA	36:2e:32:VAL:HG22	1.92	0.52
54:2y:9:A:O2'	54:2y:11:C:N4	2.30	0.52
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.45	0.51
1:1A:2355:C:H1'	22:10:39:ARG:HH21	1.75	0.51
8:1I:77:LEU:O	8:1I:143:SER:N	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:96:U:H2'	32:1a:97:G:C8	2.45	0.51
32:1a:966:M2G:HM13	32:1a:967:5MC:H1'	1.91	0.51
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.93	0.51
46:1o:39:LEU:HD13	46:1o:56:LEU:HB2	1.91	0.51
1:2A:1141:U:OP2	9:2N:63:THR:OG1	2.20	0.51
5:2F:18:ARG:NH1	5:2F:127:GLU:OE2	2.43	0.51
32:2a:457:C:H2'	32:2a:458:C:H6	1.75	0.51
32:2a:973:G:H3'	32:2a:974:A:H5''	1.92	0.51
39:2h:49:GLU:HG2	39:2h:62:TYR:HE2	1.75	0.51
1:1A:444:C:H5''	61:1A:4745:HOH:O	2.09	0.51
1:1A:1069:A:H1'	1:1A:1096:A:H4'	1.92	0.51
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.25	0.51
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.25	0.51
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.45	0.51
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.92	0.51
32:1a:783:C:OP1	32:1a:1515:C:O2'	2.26	0.51
32:1a:828:A:H2'	32:1a:829:G:O4'	2.10	0.51
32:1a:966:M2G:O2'	40:1i:127:LYS:O	2.28	0.51
36:1e:85:GLY:C	36:1e:87:SER:H	2.18	0.51
50:1s:32:LYS:HA	50:1s:50:ALA:HB3	1.91	0.51
1:2A:483:A:O2'	20:2Y:49:VAL:O	2.24	0.51
7:2H:157:TYR:CE1	7:2H:172:LYS:HG3	2.45	0.51
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.92	0.51
21:2Z:75:ASN:HB2	21:2Z:85:HIS:HB3	1.92	0.51
42:2k:85:ARG:HD3	42:2k:113:PRO:HD3	1.93	0.51
44:2m:19:LEU:HB3	44:2m:25:ILE:HG21	1.93	0.51
50:2s:22:LEU:HD13	50:2s:31:ILE:HD11	1.93	0.51
1:1A:628:G:H2'	1:1A:629:G:C8	2.45	0.51
1:1A:2854:G:H2'	1:1A:2855:C:C6	2.45	0.51
8:1I:101:LEU:HD12	8:1I:107:VAL:HB	1.92	0.51
35:1d:187:ARG:NH1	35:1d:190:ASP:OD1	2.43	0.51
1:2A:639:U:H2'	1:2A:640:C:C6	2.46	0.51
1:2A:1537:G:H2'	1:2A:1538:G:H8	1.75	0.51
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.75	0.51
50:2s:51:VAL:O	50:2s:58:VAL:N	2.43	0.51
1:1A:1881:C:H2'	1:1A:1882:C:H6	1.76	0.51
1:1A:2837:G:H21	13:1R:45:ARG:HH12	1.58	0.51
32:1a:1202:G:O4'	45:1n:29:ARG:NH1	2.44	0.51
34:1c:22:TRP:CZ2	45:1n:54:PRO:HG2	2.45	0.51
36:1e:113:ALA:HB3	36:1e:115:VAL:HG23	1.92	0.51
10:2O:7:TYR:HE2	10:2O:20:MET:HE3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1002:G:N3	32:2a:1003:G:H1'	2.24	0.51
34:2c:148:GLY:HA3	34:2c:172:ARG:O	2.10	0.51
1:1A:271(O):C:H2'	1:1A:271(P):C:C6	2.46	0.51
1:1A:1041:C:N4	1:1A:1114:G:H1	2.06	0.51
1:1A:2107:C:N4	1:1A:2182:G:H1	2.05	0.51
3:1D:35:LYS:HE2	3:1D:64:ILE:HG12	1.92	0.51
18:1W:86:LEU:HD22	18:1W:96:ILE:HD11	1.92	0.51
26:14:53:GLU:HB2	26:14:55:ARG:C	2.35	0.51
36:1e:78:HIS:CD2	39:1h:104:ARG:HD2	2.46	0.51
1:2A:236:C:H2'	1:2A:237:C:C6	2.46	0.51
1:2A:646:A:H2'	1:2A:647:G:O4'	2.10	0.51
1:2A:2042:A:OP1	61:2A:3948:HOH:O	2.19	0.51
1:2A:2822:G:O2'	1:2A:2825:C:N4	2.43	0.51
2:2B:94:C:H2'	2:2B:95:C:C6	2.46	0.51
10:2O:63:VAL:HG23	10:2O:64:ARG:HG3	1.93	0.51
25:23:4:LEU:O	25:23:36:VAL:HA	2.11	0.51
32:2a:1051:C:H2'	32:2a:1052:U:C6	2.45	0.51
33:2b:27:LYS:HB2	33:2b:194:PRO:HD2	1.91	0.51
44:2m:50:GLU:HA	44:2m:53:VAL:HG22	1.91	0.51
1:1A:9:U:H3	1:1A:2629:A:H2	1.58	0.51
1:1A:880:G:H8	1:1A:880:G:OP2	1.94	0.51
8:1I:72:LEU:C	8:1I:74:ASN:H	2.18	0.51
32:1a:486:U:H2'	32:1a:487:A:H8	1.76	0.51
32:1a:642:A:N3	39:1h:113:SER:OG	2.41	0.51
48:1q:26:GLN:OE1	48:1q:37:LYS:NZ	2.43	0.51
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.10	0.51
1:2A:2206:G:H8	1:2A:2207:G:N7	2.09	0.51
3:2D:106:ILE:HD11	3:2D:144:ALA:HB2	1.91	0.51
4:2E:96:PHE:O	4:2E:175:VAL:HG21	2.10	0.51
19:2X:11:PRO:HB3	19:2X:92:LEU:HD11	1.92	0.51
40:2i:99:LEU:HB3	40:2i:101:PHE:CD2	2.45	0.51
1:1A:1670:C:OP2	61:1A:4104:HOH:O	2.19	0.51
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.09	0.51
26:14:18:CYS:SG	26:14:20:ASN:HB2	2.50	0.51
32:1a:975:A:H5'	32:1a:975:A:H8	1.76	0.51
34:1c:124:ILE:HG22	34:1c:130:VAL:HG22	1.91	0.51
36:1e:92:LYS:HB3	36:1e:119:LEU:HB2	1.93	0.51
36:1e:96:PRO:HA	36:1e:117:ASP:OD2	2.11	0.51
44:1m:40:ASN:O	44:1m:43:THR:OG1	2.28	0.51
10:2O:119:PRO:HB2	15:2T:68:TYR:CE2	2.46	0.51
12:2Q:11:LYS:NZ	12:2Q:88:GLY:O	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:73:GLN:O	21:2Z:87:ASP:N	2.42	0.51
32:2a:695:A:OP2	42:2k:53:SER:OG	2.29	0.51
32:2a:1228:C:H2'	32:2a:1229:A:H8	1.75	0.51
33:2b:125:PRO:O	33:2b:127:ILE:N	2.43	0.51
37:2f:6:VAL:HG22	37:2f:90:VAL:HG13	1.91	0.51
38:2g:80:VAL:HB	38:2g:85:TYR:HE2	1.75	0.51
55:2x:66:C:H2'	55:2x:67:C:O4'	2.11	0.51
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.92	0.51
12:1Q:138:ASP:N	12:1Q:138:ASP:OD1	2.42	0.51
32:1a:1152:A:OP1	41:1j:68:HIS:ND1	2.44	0.51
37:1f:35:ALA:HA	37:1f:67:MET:HB3	1.91	0.51
54:1w:4:C:H2'	54:1w:5:G:H8	1.76	0.51
6:2G:83:ARG:O	6:2G:85:GLY:N	2.44	0.51
23:21:76:ARG:NH1	23:21:97:LEU:O	2.44	0.51
32:2a:825:G:H2'	32:2a:826:C:C6	2.46	0.51
32:2a:921:U:O2	36:2e:19:MET:HB2	2.11	0.51
32:2a:1060:C:O2'	41:2j:56:HIS:ND1	2.43	0.51
32:2a:1129:C:H5'	40:2i:16:ARG:HH22	1.76	0.51
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.46	0.51
37:2f:50:TYR:CE2	49:2r:77:GLY:HA2	2.45	0.51
40:2i:50:LEU:HD13	40:2i:56:LEU:HA	1.92	0.51
7:1H:101:ARG:NH2	7:1H:122:THR:HA	2.25	0.51
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.10	0.51
32:1a:341:C:H2'	32:1a:342:C:C6	2.46	0.51
32:1a:431:A:H2'	32:1a:432:A:O4'	2.10	0.51
35:1d:65:ARG:NH1	35:1d:72:GLU:OE1	2.39	0.51
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.46	0.51
12:2Q:85:LYS:HD3	22:20:7:LEU:HD13	1.93	0.51
15:2T:55:ASN:HD22	15:2T:58:ASN:HB2	1.76	0.51
32:2a:1299:A:H2'	32:2a:1299:A:N3	2.26	0.51
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.25	0.51
33:2b:18:GLY:HA2	33:2b:42:ILE:HG13	1.93	0.51
35:2d:25:ARG:HA	35:2d:28:SER:HB3	1.92	0.51
39:2h:51:VAL:HG21	39:2h:60:ARG:NH1	2.26	0.51
46:2o:11:VAL:HG21	46:2o:34:LEU:HD22	1.93	0.51
55:2x:23:C:H2'	55:2x:24:U:C6	2.46	0.51
1:1A:754:C:H2'	1:1A:755:C:C6	2.46	0.51
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.28	0.51
32:1a:78:G:O6	32:1a:92:C:N4	2.43	0.51
52:1u:6:ARG:HG2	52:1u:15:ARG:HD2	1.93	0.51
1:2A:793:A:OP2	1:2A:2071:A:O2'	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.74	0.51
1:2A:2306:C:N4	6:2G:42:GLY:O	2.42	0.51
12:2Q:65:PHE:HB2	12:2Q:105:GLU:HB2	1.93	0.51
29:27:24:THR:HG22	29:27:26:GLY:H	1.75	0.51
32:2a:448:A:P	32:2a:485:G:H22	2.34	0.51
33:2b:8:LYS:O	33:2b:9:GLU:HB2	2.10	0.51
55:2x:15:G:H2'	55:2x:59:A:N1	2.26	0.51
1:1A:603:A:O4'	1:1A:655:A:N6	2.44	0.50
1:1A:630:G:OP1	30:18:47:LYS:NZ	2.37	0.50
1:1A:1173:G:OP2	1:1A:1173:G:H2'	2.10	0.50
6:1G:126:ASP:OD2	6:1G:130:ASN:ND2	2.36	0.50
6:1G:144:ILE:HA	6:1G:148:MET:HE1	1.92	0.50
21:1Z:28:MET:HE2	21:1Z:35:ARG:HB2	1.93	0.50
32:1a:7:G:H5'	32:1a:298:A:O4'	2.11	0.50
35:1d:134:ASP:OD1	35:1d:134:ASP:N	2.44	0.50
54:1y:4:C:H2'	54:1y:5:G:O4'	2.11	0.50
1:2A:637:A:OP1	11:2P:133:SER:OG	2.21	0.50
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.75	0.50
1:2A:2431:U:OP1	61:2A:3951:HOH:O	2.19	0.50
18:2W:19:LEU:HB3	27:25:25:LEU:HG	1.92	0.50
32:2a:707:C:OP1	42:2k:85:ARG:NH1	2.43	0.50
32:2a:1144:G:N2	32:2a:1146:A:H62	2.10	0.50
33:2b:114:ARG:HA	33:2b:117:GLU:HB2	1.93	0.50
39:2h:6:ILE:O	39:2h:10:LEU:HD12	2.11	0.50
45:2n:24:CYS:HB2	45:2n:40:CYS:HB3	1.93	0.50
50:2s:32:LYS:HA	50:2s:50:ALA:HB3	1.92	0.50
54:2w:21:A:O2'	54:2w:22:G:OP1	2.28	0.50
32:1a:453:A:C5	32:1a:454:C:C4	3.00	0.50
36:1e:100:VAL:HG13	36:1e:107:ARG:NH1	2.27	0.50
1:2A:247:G:H4'	1:2A:386:G:C5	2.45	0.50
1:2A:1171:G:H22	1:2A:1178:C:N4	2.09	0.50
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.46	0.50
32:2a:1427:U:H2'	32:2a:1428:A:C8	2.46	0.50
33:2b:185:ILE:HA	33:2b:199:TYR:HB2	1.93	0.50
50:2s:11:VAL:HG12	50:2s:13:ASP:H	1.76	0.50
54:2y:55:PSU:O2	54:2y:57:G:H3'	2.11	0.50
1:1A:732:C:OP1	61:1A:4141:HOH:O	2.20	0.50
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.11	0.50
10:1O:26:LYS:O	10:1O:30:ALA:HB2	2.10	0.50
32:1a:1323:G:H4'	32:1a:1363:C:N3	2.26	0.50
34:1c:79:ARG:O	34:1c:82:GLU:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:173:TRP:CE3	35:1d:174:LEU:HG	2.46	0.50
36:1e:7:GLU:OE2	36:1e:37:ARG:NH2	2.44	0.50
37:1f:86:ARG:O	37:1f:87:ARG:HG2	2.11	0.50
39:1h:35:ILE:HD11	39:1h:134:ILE:HG21	1.92	0.50
1:2A:1342:A:OP2	61:2A:3947:HOH:O	2.19	0.50
19:2X:1:MET:H3	24:22:29:LYS:HE3	1.77	0.50
20:2Y:39:VAL:HB	20:2Y:42:VAL:HB	1.92	0.50
32:2a:359:U:H2'	32:2a:360:A:C8	2.47	0.50
32:2a:859:A:H2'	32:2a:860:A:O4'	2.11	0.50
32:2a:1272:G:N2	32:2a:1273:G:C8	2.79	0.50
32:2a:1381:U:H1'	38:2g:79:ARG:HG2	1.92	0.50
54:2w:9:A:H8	54:2w:11:C:H41	1.58	0.50
1:1A:2067:G:N7	61:1A:4230:HOH:O	2.34	0.50
1:1A:2492:U:H2'	1:1A:2493:U:C6	2.46	0.50
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.46	0.50
1:1A:2722:G:OP2	61:1A:4140:HOH:O	2.20	0.50
33:1b:51:LEU:HD22	33:1b:55:PHE:HE2	1.76	0.50
1:2A:910:A:H2'	1:2A:911:A:C8	2.47	0.50
1:2A:981:A:N1	1:2A:2027:G:O2'	2.35	0.50
1:2A:1671:U:OP2	61:2A:3913:HOH:O	2.20	0.50
5:2F:32:LEU:HD22	5:2F:112:MET:HE2	1.92	0.50
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.47	0.50
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.11	0.50
32:2a:1226:C:H2'	44:2m:103:THR:HB	1.93	0.50
33:2b:17:PHE:HA	33:2b:44:LEU:HD21	1.93	0.50
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.91	0.50
50:2s:66:MET:HB2	50:2s:74:PHE:CZ	2.47	0.50
1:1A:2747:G:O6	1:1A:2755:C:H5''	2.11	0.50
5:1F:185:ASP:OD1	5:1F:188:ARG:NH1	2.36	0.50
32:1a:458:C:H2'	32:1a:460:G:O4'	2.12	0.50
38:1g:78:ARG:HG3	38:1g:79:ARG:H	1.76	0.50
1:2A:190:A:OP2	23:21:39:LYS:HE3	2.11	0.50
1:2A:709:U:H2'	1:2A:710:G:C8	2.47	0.50
1:2A:1183:G:H5''	25:23:30:ARG:NH2	2.27	0.50
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.92	0.50
1:2A:2130:U:H2'	1:2A:2131:G:H21	1.76	0.50
1:2A:2811:G:H22	1:2A:2891:G:H1'	1.76	0.50
2:2B:66:A:N6	2:2B:108:U:H3'	2.27	0.50
26:24:16:CYS:SG	26:24:17:GLY:N	2.84	0.50
26:24:45:GLY:C	26:24:47:GLN:H	2.19	0.50
32:2a:664:G:N2	32:2a:741:G:H1	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1320:C:N3	50:2s:36:ARG:NH2	2.55	0.50
33:2b:230:VAL:HG12	33:2b:232:PRO:HD2	1.94	0.50
1:1A:292:C:H2'	1:1A:293:U:C6	2.47	0.50
1:1A:628:G:H5''	30:18:18:ALA:HB2	1.92	0.50
1:1A:793:A:OP2	1:1A:2071:A:O2'	2.28	0.50
5:1F:14:PRO:HD2	5:1F:127:GLU:OE1	2.11	0.50
19:1X:92:LEU:O	19:1X:95:LEU:HB2	2.12	0.50
20:1Y:34:LYS:NZ	61:1Y:301:HOH:O	2.43	0.50
32:1a:1016:A:H2'	32:1a:1017:G:O4'	2.12	0.50
32:1a:1530:G:H2'	32:1a:1531:A:C8	2.46	0.50
34:1c:47:LEU:HD12	34:1c:68:VAL:HG11	1.94	0.50
35:1d:111:ALA:HB2	35:1d:120:LEU:HD12	1.93	0.50
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.94	0.50
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.47	0.50
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.29	0.50
3:2D:168:ARG:HG2	3:2D:173:VAL:HG12	1.93	0.50
4:2E:1:MET:HB3	4:2E:83:ASP:O	2.12	0.50
5:2F:158:THR:HB	5:2F:195:ASP:HB2	1.93	0.50
26:24:24:THR:OG1	26:24:25:TYR:N	2.44	0.50
32:2a:986:A:H2'	32:2a:987:G:O4'	2.12	0.50
33:2b:87:ARG:NH2	33:2b:220:ASP:OD2	2.37	0.50
35:2d:116:GLN:HE22	35:2d:161:ASN:HD21	1.60	0.50
35:2d:140:VAL:HG11	35:2d:146:ILE:HD11	1.93	0.50
40:2i:55:ALA:HA	40:2i:58:HIS:HD2	1.76	0.50
41:2j:35:SER:HB3	41:2j:73:ASP:HB2	1.92	0.50
1:1A:483:A:O2'	20:1Y:49:VAL:O	2.23	0.50
1:1A:534:U:H2'	1:1A:535:C:C6	2.47	0.50
1:1A:1187:G:H5''	17:1V:81:TYR:CE1	2.47	0.50
1:1A:2182:G:H2'	1:1A:2183:C:C6	2.46	0.50
1:1A:2853:C:H2'	1:1A:2854:G:C8	2.46	0.50
5:1F:165:ARG:HA	5:1F:168:ARG:HD2	1.93	0.50
32:1a:148:G:H2'	32:1a:149:A:H8	1.76	0.50
32:1a:250:A:H4'	32:1a:251:G:O5'	2.11	0.50
32:1a:1136:U:H5''	32:1a:1137:C:C5	2.47	0.50
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	1.92	0.50
1:2A:2135:A:C5	1:2A:2136:C:H5	2.30	0.50
1:2A:2141:G:H2'	1:2A:2142:C:O4'	2.12	0.50
1:2A:2547:U:O2	10:2O:23:ARG:NH2	2.45	0.50
15:2T:50:ILE:HD13	15:2T:64:ARG:HB2	1.93	0.50
16:2U:8:VAL:O	16:2U:12:ARG:HG3	2.11	0.50
18:2W:12:ILE:O	18:2W:101:SER:OG	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:29:10:ILE:HD12	31:29:32:HIS:HA	1.93	0.50
1:1A:191:A:H2'	1:1A:192:C:C6	2.46	0.50
1:1A:1048:A:N1	1:1A:1112:G:O2'	2.38	0.50
1:1A:2445:G:OP1	5:1F:74:ARG:NH2	2.43	0.50
26:14:16:CYS:HB2	26:14:36:CYS:HB3	1.93	0.50
32:1a:110:C:H2'	32:1a:111:G:O4'	2.12	0.50
32:1a:584:G:H2'	32:1a:585:G:C8	2.46	0.50
46:1o:3:ILE:HG21	46:1o:34:LEU:HD21	1.94	0.50
50:1s:31:ILE:O	50:1s:50:ALA:N	2.43	0.50
54:1y:42:C:H2'	54:1y:43:C:C6	2.47	0.50
1:2A:81:G:O2'	1:2A:295:G:O2'	2.30	0.50
1:2A:597:U:H2'	1:2A:598:G:C8	2.47	0.50
10:2O:112:MET:O	10:2O:116:SER:OG	2.30	0.50
10:2O:120:GLU:HB2	15:2T:68:TYR:HE2	1.76	0.50
15:2T:24:PRO:HA	15:2T:49:VAL:HG12	1.93	0.50
26:24:60:GLN:O	26:24:62:ARG:NH1	2.44	0.50
32:2a:718:G:O6	49:2r:74:ARG:NH1	2.45	0.50
32:2a:1263:C:H1'	32:2a:1273:G:N2	2.26	0.50
41:2j:9:ARG:O	41:2j:16:LEU:HD21	2.11	0.50
55:2x:50:U:H2'	55:2x:51:C:C6	2.47	0.50
1:1A:642:G:N2	1:1A:645:C:OP2	2.42	0.50
32:1a:92:C:H2'	32:1a:93:G:C8	2.47	0.50
1:2A:411:G:C5	11:2P:72:PRO:HB3	2.47	0.50
1:2A:2166:G:O6	1:2A:2171:A:N6	2.45	0.50
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.27	0.50
1:2A:2655:G:O2'	1:2A:2664:G:O6	2.28	0.50
1:2A:2711:A:OP2	61:2A:3934:HOH:O	2.19	0.50
3:2D:183:ARG:HG3	3:2D:270:ILE:HD13	1.93	0.50
6:2G:167:GLU:OE1	6:2G:167:GLU:N	2.43	0.50
12:2Q:18:LYS:O	12:2Q:98:LYS:NZ	2.29	0.50
23:21:3:LYS:HB2	23:21:61:ARG:HH22	1.77	0.50
32:2a:1103:C:P	33:2b:96:ARG:HH22	2.35	0.50
33:2b:47:THR:HG23	33:2b:202:PRO:HG2	1.94	0.50
33:2b:144:ARG:NH2	33:2b:148:TYR:OH	2.44	0.50
47:2p:26:ARG:HG3	47:2p:27:LYS:O	2.12	0.50
48:2q:15:MET:HB3	48:2q:18:THR:HB	1.94	0.50
1:1A:72:U:OP1	61:1A:4142:HOH:O	2.20	0.49
1:1A:1052:C:H2'	1:1A:1053:C:C6	2.47	0.49
1:1A:1054:A:N6	1:1A:1105:U:H3	2.08	0.49
1:1A:1744:C:H2'	1:1A:1745:C:C6	2.47	0.49
1:1A:2153:G:H2'	1:1A:2154:G:H8	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2377:A:O2'	14:1S:112:PHE:O	2.25	0.49
1:1A:2467:C:H4'	12:1Q:123:HIS:CD2	2.47	0.49
1:1A:2864:G:OP1	15:1T:119:LYS:HD2	2.11	0.49
32:1a:1187:G:H4'	40:1i:111:ARG:HH11	1.76	0.49
34:1c:13:GLY:HA3	45:1n:57:ARG:HH12	1.77	0.49
35:1d:200:GLU:O	35:1d:203:VAL:HG12	2.12	0.49
54:1y:58:A:H4'	54:1y:59:U:OP1	2.12	0.49
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.47	0.49
6:2G:41:GLN:O	6:2G:43:LEU:N	2.44	0.49
32:2a:130:A:H1'	32:2a:263:A:O2'	2.12	0.49
32:2a:1278:U:H5'	32:2a:1279:A:C5'	2.36	0.49
33:2b:33:TYR:HB3	33:2b:41:ILE:HD11	1.94	0.49
48:2q:45:HIS:CD2	48:2q:47:PRO:HG3	2.47	0.49
54:2w:27:G:H2'	54:2w:28:G:C8	2.47	0.49
1:1A:299:A:N1	1:1A:322:A:O2'	2.36	0.49
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.47	0.49
22:10:24:LYS:O	22:10:25:ARG:NH1	2.40	0.49
32:1a:880:C:OP1	43:1l:8:ASN:ND2	2.42	0.49
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.37	0.49
1:2A:27:G:O2'	1:2A:28:A:OP2	2.28	0.49
1:2A:479:A:N3	1:2A:481:G:H5''	2.27	0.49
1:2A:652(T):C:H2'	1:2A:652(U):G:C8	2.47	0.49
1:2A:877:U:O2'	1:2A:900:A:N6	2.45	0.49
1:2A:2782:G:OP2	61:2A:3953:HOH:O	2.20	0.49
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	1.94	0.49
32:2a:15:G:H21	36:2e:18:ARG:HA	1.77	0.49
32:2a:1388:C:H2'	32:2a:1389:C:C6	2.47	0.49
44:2m:16:ASP:HB3	44:2m:34:LEU:HD11	1.93	0.49
8:1I:93:THR:H	8:1I:96:ASP:HB2	1.77	0.49
9:1N:67:LEU:HB3	9:1N:88:GLU:HG3	1.94	0.49
20:1Y:47:LYS:HE2	20:1Y:48:ALA:O	2.12	0.49
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.47	0.49
32:1a:767:A:H2'	32:1a:768:A:O4'	2.12	0.49
33:1b:24:TRP:CZ3	33:1b:26:PRO:HA	2.47	0.49
51:1t:18:GLN:O	51:1t:22:ARG:HG3	2.12	0.49
1:2A:2650:U:H2'	1:2A:2651:C:C6	2.47	0.49
32:2a:1013:G:O2'	32:2a:1015:A:N7	2.41	0.49
32:2a:1359:C:H1'	32:2a:1362:C:H41	1.77	0.49
1:1A:396:G:H1'	23:11:42:GLN:HB3	1.94	0.49
8:1I:57:ARG:HG3	8:1I:61:ARG:HH21	1.76	0.49
26:14:63:TYR:N	26:14:63:TYR:CD1	2.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:1p:40:ASP:OD2	47:1p:44:THR:OG1	2.22	0.49
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.28	0.49
1:2A:2130:U:H2'	1:2A:2131:G:N2	2.27	0.49
1:2A:2238:G:H5''	61:2A:4035:HOH:O	2.11	0.49
3:2D:132:PRO:HD3	3:2D:190:TYR:CZ	2.46	0.49
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.26	0.49
7:2H:24:VAL:HG21	7:2H:72:ILE:HG12	1.95	0.49
10:2O:68:GLU:HB3	10:2O:78:ARG:HB2	1.94	0.49
12:2Q:35:VAL:HG22	12:2Q:102:VAL:HG22	1.93	0.49
22:20:23:VAL:HG22	22:20:38:VAL:HG22	1.94	0.49
32:2a:259:G:OP2	51:2t:83:ARG:NH1	2.46	0.49
36:2e:78:HIS:H	36:2e:78:HIS:CD2	2.31	0.49
38:2g:78:ARG:HE	38:2g:79:ARG:HE	1.60	0.49
1:1A:2791:C:H2'	1:1A:2792:G:H8	1.76	0.49
3:1D:61:LEU:O	3:1D:63:ARG:NH1	2.45	0.49
32:1a:200:G:H1	32:1a:217:C:N4	2.09	0.49
33:1b:22:LYS:HA	33:1b:40:HIS:CE1	2.43	0.49
35:1d:162:LEU:HD13	35:1d:181:MET:HG2	1.95	0.49
1:2A:568:U:H5'	1:2A:945:A:N1	2.27	0.49
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.47	0.49
1:2A:2722:G:H5'	13:2R:4:LEU:HD12	1.94	0.49
6:2G:41:GLN:HG3	6:2G:154:GLY:O	2.12	0.49
32:2a:310:G:OP2	47:2p:27:LYS:NZ	2.35	0.49
32:2a:390:C:H4'	47:2p:28:ARG:HH21	1.78	0.49
1:1A:271(L):U:H4'	8:1I:50:ARG:NH2	2.28	0.49
1:1A:483:A:H5''	20:1Y:50:ARG:HH11	1.76	0.49
1:1A:1264:G:OP1	27:15:19:ARG:NH2	2.27	0.49
6:1G:98:ARG:CZ	26:14:1:MET:HE3	2.42	0.49
32:1a:67:C:H4'	32:1a:172:A:O4'	2.12	0.49
35:1d:88:VAL:O	35:1d:92:VAL:HG23	2.12	0.49
46:1o:26:GLU:OE1	46:1o:77:ARG:NH2	2.39	0.49
1:2A:892:G:H3'	1:2A:893:C:C4'	2.41	0.49
1:2A:2096:U:H3	1:2A:2193:G:H1	1.60	0.49
12:2Q:43:THR:HG22	12:2Q:94:VAL:HG12	1.93	0.49
14:2S:11:LYS:HG3	14:2S:91:PRO:HB3	1.95	0.49
32:2a:689:C:H2'	32:2a:690:G:O4'	2.13	0.49
32:2a:1142:G:H2'	32:2a:1143:G:O4'	2.13	0.49
32:2a:1314:C:OP2	50:2s:4:SER:OG	2.09	0.49
32:2a:1478:C:H2'	32:2a:1479:C:H6	1.76	0.49
33:2b:186:ALA:HB3	33:2b:197:VAL:HG13	1.95	0.49
39:2h:12:ARG:HD2	39:2h:26:VAL:HG13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:42:GLU:HG3	39:2h:109:ILE:HD13	1.94	0.49
50:2s:28:LYS:HB3	50:2s:29:ARG:HA	1.95	0.49
1:1A:692:C:O2'	3:1D:38:LYS:NZ	2.43	0.49
1:1A:774:A:N3	1:1A:774:A:H2'	2.27	0.49
1:1A:897:C:H5'	54:1w:56:C:OP1	2.12	0.49
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.48	0.49
4:1E:52:LEU:O	4:1E:76:ARG:N	2.41	0.49
8:1I:107:VAL:HG12	8:1I:109:ILE:HG12	1.95	0.49
23:11:75:GLU:OE1	23:11:78:LYS:NZ	2.41	0.49
32:1a:171:A:H2'	32:1a:172:A:C8	2.48	0.49
33:1b:115:LEU:HD11	33:1b:146:GLN:HG3	1.93	0.49
34:1c:85:ARG:O	34:1c:89:GLU:HG3	2.13	0.49
35:1d:61:LYS:HD3	35:1d:206:PHE:CE2	2.48	0.49
36:1e:110:LEU:HD13	36:1e:118:ILE:HD13	1.95	0.49
45:1n:23:ARG:CZ	45:1n:30:ALA:HB2	2.43	0.49
1:2A:643:A:N1	1:2A:2369:A:O2'	2.45	0.49
1:2A:774:A:H2'	1:2A:774:A:N3	2.28	0.49
1:2A:1599:C:H5'	19:2X:35:THR:HG22	1.93	0.49
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.45	0.49
1:2A:2805:G:H2'	1:2A:2807:G:H8	1.76	0.49
12:2Q:32:TYR:OH	12:2Q:133:ARG:NH2	2.46	0.49
32:2a:1228:C:P	44:2m:108:ARG:HH22	2.35	0.49
33:2b:16:HIS:CB	33:2b:210:SER:HB2	2.40	0.49
49:2r:22:VAL:HB	49:2r:56:THR:HA	1.95	0.49
54:2y:55:PSU:N1	54:2y:57:G:H5''	2.15	0.49
1:1A:1044:G:H5'	1:1A:1045:A:OP2	2.13	0.49
1:1A:2497:A:H5''	61:1A:4276:HOH:O	2.12	0.49
7:1H:157:TYR:CE1	7:1H:172:LYS:HG3	2.47	0.49
28:16:12:GLU:OE1	28:16:19:ARG:NH1	2.45	0.49
32:1a:1086:U:H3	32:1a:1099:G:N2	2.02	0.49
33:1b:72:GLY:HA3	33:1b:81:VAL:HG11	1.93	0.49
38:1g:50:ILE:HG22	38:1g:58:PRO:HG3	1.95	0.49
44:1m:15:VAL:HG13	44:1m:43:THR:O	2.13	0.49
55:1x:8:4SU:O2	55:1x:21:A:H2	1.94	0.49
1:2A:531:C:OP1	1:2A:561:G:N1	2.39	0.49
1:2A:2125:G:H1'	1:2A:2173:A:N6	2.27	0.49
1:2A:2439:A:H5'	1:2A:2439:A:C8	2.47	0.49
32:2a:23:C:OP2	32:2a:561:U:N3	2.34	0.49
35:2d:4:TYR:OH	35:2d:7:PRO:O	2.28	0.49
46:2o:39:LEU:HD13	46:2o:56:LEU:HB2	1.94	0.49
54:2w:33:U:N3	54:2w:36:A:OP2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.11	0.49
1:1A:1087:G:H2'	1:1A:1089:G:C8	2.48	0.49
1:1A:1266:G:O2'	1:1A:2012:G:O6	2.28	0.49
1:1A:2090:G:N7	61:1A:4237:HOH:O	2.35	0.49
1:1A:2102:U:H3	1:1A:2187:G:H1	1.61	0.49
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.28	0.49
32:1a:1272:G:H2'	32:1a:1273:G:O4'	2.13	0.49
32:1a:1391:U:O2'	32:1a:1532:U:OP1	2.27	0.49
36:1e:98:THR:HG22	36:1e:99:GLY:H	1.78	0.49
1:2A:2483:C:N3	12:2Q:124:LYS:NZ	2.59	0.49
2:2B:9:G:H1	2:2B:112:U:H3	1.59	0.49
2:2B:106:G:H5'	21:2Z:31:ARG:HG2	1.95	0.49
18:2W:14:PRO:O	18:2W:18:ARG:HG3	2.13	0.49
38:2g:113:GLU:CG	38:2g:119:ARG:HG2	2.42	0.49
41:2j:85:LEU:HD12	41:2j:86:MET:N	2.28	0.49
48:2q:13:ASP:OD1	48:2q:13:ASP:N	2.44	0.49
1:1A:526:A:O2'	1:1A:2043:C:O2	2.30	0.49
1:1A:634:C:H2'	1:1A:635:C:C6	2.47	0.49
1:1A:880:G:H1	1:1A:898:C:N4	2.11	0.49
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.48	0.49
1:1A:2693:A:H2'	1:1A:2694:G:C8	2.46	0.49
15:1T:117:ASP:OD2	15:1T:120:ARG:NE	2.40	0.49
32:1a:446:G:H1	32:1a:488:C:H42	1.59	0.49
34:1c:61:ALA:C	34:1c:63:ASN:H	2.21	0.49
38:1g:28:ASN:HD21	38:1g:36:LYS:NZ	2.11	0.49
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.48	0.49
6:2G:5:VAL:HG22	6:2G:8:LYS:H	1.78	0.49
12:2Q:1:MET:N	12:2Q:1:MET:HE3	2.28	0.49
21:2Z:77:ASP:N	21:2Z:82:ARG:O	2.38	0.49
32:2a:553:A:H5''	43:2l:24:VAL:HG21	1.95	0.49
32:2a:1186:G:H4'	40:2i:110:GLU:OE2	2.13	0.49
39:2h:6:ILE:HD12	39:2h:35:ILE:HD12	1.95	0.49
54:2y:25:C:H2'	54:2y:26:A:C8	2.48	0.49
1:1A:981:A:N1	1:1A:2027:G:O2'	2.42	0.48
1:1A:992:C:OP1	17:1V:74:LYS:NZ	2.43	0.48
1:1A:2771:C:H2'	1:1A:2772:C:C6	2.48	0.48
4:1E:48:GLN:NE2	4:1E:78:LEU:HD13	2.28	0.48
24:12:2:LYS:O	24:12:6:VAL:HG23	2.13	0.48
32:1a:1025:U:C2	32:1a:1036:G:O6	2.66	0.48
37:1f:68:PRO:HG2	37:1f:71:ARG:HD2	1.94	0.48
43:1l:117:ARG:HB3	43:1l:122:THR:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:320:A:H4'	1:2A:322:A:N7	2.28	0.48
1:2A:572:A:OP2	17:2V:78:LYS:NZ	2.46	0.48
1:2A:662:G:H5''	11:2P:16:ARG:HG2	1.95	0.48
1:2A:855:G:O2'	22:20:27:GLU:OE2	2.23	0.48
1:2A:1311:G:H2'	29:27:47:ARG:HH22	1.78	0.48
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.47	0.48
1:2A:2561:A:H4'	10:2O:22:ILE:HD11	1.94	0.48
8:2I:82:ARG:HH21	8:2I:90:GLY:H	1.60	0.48
32:2a:339:C:H2'	32:2a:340:U:C6	2.47	0.48
32:2a:1256:A:OP1	34:2c:26:LYS:NZ	2.40	0.48
34:2c:121:ALA:O	34:2c:125:GLU:HG2	2.13	0.48
50:2s:44:MET:O	50:2s:47:HIS:HB2	2.13	0.48
1:1A:484:C:H2'	1:1A:485:C:H6	1.77	0.48
1:1A:1075:C:C2'	1:1A:1076:C:H5'	2.44	0.48
5:1F:24:LEU:HB3	5:1F:115:ALA:HB2	1.95	0.48
32:1a:109:A:H2'	32:1a:326:G:N2	2.28	0.48
32:1a:738:C:OP1	37:1f:4:TYR:OH	2.28	0.48
33:1b:134:GLU:O	33:1b:138:LEU:HG	2.13	0.48
1:2A:278:A:H61	1:2A:362:U:H3	1.61	0.48
1:2A:1257:C:H4'	5:2F:83:PHE:CD1	2.48	0.48
1:2A:2343:C:O2'	1:2A:2373:G:O2'	2.29	0.48
5:2F:108:LYS:O	5:2F:112:MET:HG3	2.13	0.48
21:2Z:55:HIS:CE1	21:2Z:135:GLU:HB2	2.46	0.48
32:2a:7:G:O2'	36:2e:120:THR:O	2.31	0.48
32:2a:983:A:N1	32:2a:1222:G:N2	2.60	0.48
32:2a:1002:G:H1	32:2a:1038:C:N4	2.11	0.48
32:2a:1273:G:H3'	32:2a:1274:G:H8	1.77	0.48
33:2b:53:ARG:HA	33:2b:56:ARG:HH11	1.78	0.48
33:2b:163:PHE:HA	33:2b:185:ILE:O	2.13	0.48
1:1A:41:C:H2'	1:1A:42:G:O4'	2.13	0.48
1:1A:185:U:H4'	1:1A:218:A:H4'	1.96	0.48
1:1A:2629:A:HO2'	1:1A:2630:G:P	2.35	0.48
5:1F:39:TRP:CZ2	5:1F:43:LYS:HE2	2.47	0.48
11:1P:59:LEU:HD11	30:18:10:ALA:HA	1.95	0.48
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.62	0.48
21:1Z:153:SER:HB3	21:1Z:167:PRO:HB3	1.95	0.48
32:1a:269:C:H2'	32:1a:270:A:C8	2.48	0.48
32:1a:1229:A:OP2	44:1m:114:ARG:HD3	2.13	0.48
34:1c:66:VAL:HG23	34:1c:101:LEU:HA	1.94	0.48
1:2A:652:C:C2'	1:2A:652(A):A:H5'	2.43	0.48
1:2A:1668:A:O2'	1:2A:1674:G:N7	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.48	0.48
21:2Z:45:ASP:CG	21:2Z:49:ARG:HE	2.20	0.48
32:2a:137:C:H2'	32:2a:138:G:H8	1.78	0.48
32:2a:458:C:H2'	32:2a:460:G:O4'	2.12	0.48
36:2e:7:GLU:CD	36:2e:37:ARG:HH21	2.20	0.48
41:2j:69:ASN:O	41:2j:70:ARG:NH1	2.40	0.48
50:2s:36:ARG:HD2	50:2s:52:TYR:O	2.13	0.48
1:1A:583:G:OP2	16:1U:10:ARG:HD2	2.14	0.48
1:1A:910:A:N1	1:1A:2277:G:H1'	2.29	0.48
26:14:26:SER:OG	26:14:27:THR:N	2.44	0.48
32:1a:300:A:H2'	32:1a:301:G:O4'	2.13	0.48
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.42	0.48
32:1a:1189:C:OP1	41:1j:51:ARG:NH2	2.37	0.48
1:2A:1187:G:O6	61:2A:3949:HOH:O	2.19	0.48
1:2A:2376:A:H2'	1:2A:2377:A:O4'	2.13	0.48
32:2a:625:G:H4'	47:2p:16:HIS:CD2	2.48	0.48
32:2a:1221:G:OP1	32:2a:1320:C:N4	2.44	0.48
35:2d:20:TYR:CD1	35:2d:26:CYS:HB3	2.44	0.48
36:2e:42:GLY:HA2	36:2e:65:ASN:O	2.13	0.48
40:2i:99:LEU:HB3	40:2i:101:PHE:CE2	2.48	0.48
43:2l:88:GLY:O	43:2l:99:HIS:HD2	1.96	0.48
54:2w:51:U:H2'	54:2w:52:G:C8	2.48	0.48
1:1A:1271:G:OP2	61:1A:4115:HOH:O	2.20	0.48
1:1A:1740:G:H2'	1:1A:1741:A:C8	2.48	0.48
1:1A:1916:A:OP2	61:1A:4146:HOH:O	2.20	0.48
1:1A:2316:C:O2'	6:1G:128:ARG:NH2	2.47	0.48
13:1R:9:LYS:O	13:1R:17:ARG:NH1	2.45	0.48
21:1Z:53:ILE:HG22	21:1Z:71:VAL:HG12	1.95	0.48
21:1Z:80:ARG:HD3	21:1Z:82:ARG:HH11	1.77	0.48
32:1a:108:G:P	32:1a:326:G:H22	2.36	0.48
33:1b:140:HIS:O	33:1b:144:ARG:HG3	2.12	0.48
37:1f:23:LYS:HA	37:1f:26:ILE:HD12	1.95	0.48
42:1k:33:THR:HA	42:1k:39:PRO:HA	1.95	0.48
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.14	0.48
1:2A:38:A:H2'	1:2A:39:C:C6	2.48	0.48
1:2A:645:C:H5''	1:2A:646:A:OP2	2.14	0.48
1:2A:829:A:N7	1:2A:2248:C:H5'	2.28	0.48
1:2A:1300:U:H4'	1:2A:1301:A:H5'	1.94	0.48
6:2G:63:ILE:HD11	6:2G:144:ILE:HD11	1.96	0.48
33:2b:121:LEU:HA	33:2b:125:PRO:HB2	1.95	0.48
35:2d:59:ARG:NH1	35:2d:59:ARG:HA	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2f:8:ILE:HD12	37:2f:26:ILE:HD13	1.95	0.48
44:2m:52:GLU:HG2	44:2m:55:ARG:NH2	2.25	0.48
49:2r:58:LEU:HB3	49:2r:62:GLU:HB2	1.95	0.48
54:2w:62:C:H2'	54:2w:63:G:H8	1.78	0.48
1:1A:2386:C:H2'	1:1A:2387:U:C6	2.49	0.48
32:1a:748:C:H4'	32:1a:749:C:O5'	2.13	0.48
54:1y:56:C:H2'	54:1y:57:G:O4'	2.13	0.48
1:2A:657:U:H2'	1:2A:658:C:C6	2.48	0.48
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.14	0.48
1:2A:1926:U:O2'	1:2A:1928:A:N7	2.37	0.48
1:2A:2334:G:H5'	14:2S:9:ARG:HG2	1.96	0.48
8:2I:75:LEU:HD13	8:2I:105:HIS:CD2	2.48	0.48
32:2a:157:G:H2'	32:2a:158:G:C8	2.49	0.48
32:2a:1427:U:H2'	32:2a:1428:A:H8	1.77	0.48
33:2b:165:VAL:HG23	33:2b:187:LEU:HD22	1.96	0.48
1:1A:548:A:H61	17:1V:18:LEU:HA	1.77	0.48
1:1A:1022:G:OP2	9:1N:65:LYS:NZ	2.45	0.48
1:1A:1971:A:C4	3:1D:241:PRO:HD3	2.49	0.48
1:1A:2155:G:H2'	1:1A:2155:G:N3	2.28	0.48
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.25	0.48
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.14	0.48
19:1X:44:GLU:HG3	19:1X:51:VAL:HG23	1.96	0.48
30:18:26:LYS:HD2	30:18:48:PHE:CD2	2.49	0.48
32:1a:667:G:H4'	46:1o:51:HIS:ND1	2.28	0.48
32:1a:1108:G:OP1	34:1c:175:LEU:HB2	2.14	0.48
34:1c:44:GLU:HA	34:1c:52:LEU:HD23	1.95	0.48
43:1l:40:VAL:HG11	43:1l:77:LEU:O	2.14	0.48
1:2A:900:A:HO2'	1:2A:901:A:P	2.35	0.48
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.12	0.48
8:2I:50:ARG:HA	8:2I:53:ALA:HB3	1.95	0.48
12:2Q:57:HIS:HD2	12:2Q:117:ALA:HB2	1.79	0.48
13:2R:1:MET:HB2	13:2R:1:MET:HE3	1.77	0.48
32:2a:266:G:H2'	32:2a:266:G:N3	2.27	0.48
34:2c:138:VAL:HG22	34:2c:151:VAL:HG23	1.96	0.48
42:2k:45:GLY:O	42:2k:50:TYR:HB2	2.14	0.48
43:2l:84:LEU:HB2	43:2l:105:TYR:CE2	2.49	0.48
46:2o:62:GLN:NE2	46:2o:65:ARG:HH21	2.11	0.48
54:2y:25:C:H2'	54:2y:26:A:H8	1.79	0.48
1:1A:847:U:OP2	61:1A:4144:HOH:O	2.20	0.48
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.49	0.48
1:1A:1942:5MC:OP2	1:1A:1943:U:O2'	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2031:A:C6	1:1A:2498:C:H1'	2.49	0.48
1:1A:2405:G:O2'	1:1A:2406:U:OP1	2.30	0.48
8:1I:38:LEU:HG	8:1I:40:THR:HG22	1.94	0.48
1:2A:271(K):U:H4'	1:2A:271(L):U:OP1	2.12	0.48
1:2A:1721:G:H8	1:2A:1741:A:H62	1.60	0.48
2:2B:13:A:N1	2:2B:69:G:O2'	2.45	0.48
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.49	0.48
32:2a:109:A:C6	32:2a:326:G:C6	3.02	0.48
32:2a:523:A:H61	43:2l:92:0TD:CG	2.26	0.48
32:2a:975:A:N1	41:2j:48:THR:HB	2.28	0.48
32:2a:1148:U:H2'	32:2a:1149:C:O4'	2.13	0.48
37:2f:97:PHE:HD2	49:2r:31:LEU:HD11	1.77	0.48
42:2k:73:MET:HG2	42:2k:103:LEU:HD21	1.94	0.48
1:1A:615:G:OP2	5:1F:43:LYS:NZ	2.42	0.48
32:1a:501:C:H2'	32:1a:502:G:H8	1.78	0.48
36:1e:18:ARG:HH11	36:1e:27:ARG:HH12	1.62	0.48
38:1g:64:GLN:HB3	38:1g:128:ALA:HB1	1.94	0.48
54:1w:71:G:H2'	54:1w:71:G:N3	2.29	0.48
1:2A:324:A:N6	1:2A:338:G:O2'	2.45	0.48
1:2A:438:G:H2'	1:2A:440:G:C8	2.49	0.48
1:2A:910:A:N1	1:2A:2277:G:H1'	2.28	0.48
1:2A:1019:U:O2'	1:2A:1021:A:H2	1.97	0.48
1:2A:2336:A:H61	22:20:43:THR:CG2	2.27	0.48
1:2A:2497:A:H5''	61:2A:4288:HOH:O	2.13	0.48
1:2A:2801(A):A:N3	1:2A:2895:U:O2'	2.44	0.48
6:2G:45:GLU:H	6:2G:45:GLU:HG2	1.32	0.48
21:2Z:36:LYS:HB2	21:2Z:36:LYS:HE3	1.73	0.48
32:2a:966:M2G:HM23	32:2a:967:5MC:H1'	1.96	0.48
32:2a:1010:G:N1	32:2a:1020:U:H1'	2.29	0.48
32:2a:1280:A:H5'	41:2j:40:LEU:HD22	1.95	0.48
32:2a:1307:U:H2'	32:2a:1308:U:C6	2.49	0.48
34:2c:152:ILE:HD11	34:2c:199:LYS:NZ	2.28	0.48
47:2p:28:ARG:HG2	47:2p:29:ASP:OD1	2.14	0.48
1:1A:286:C:H2'	1:1A:287:C:H6	1.79	0.48
1:1A:2712:U:OP1	1:1A:2714:G:H4'	2.13	0.48
1:1A:2790:A:H5''	1:1A:2791:C:H5'	1.95	0.48
5:1F:135:LYS:HB2	5:1F:138:GLU:HG3	1.95	0.48
7:1H:136:ILE:H	7:1H:136:ILE:HD13	1.79	0.48
32:1a:189(C):C:H2'	32:1a:189(D):C:O4'	2.13	0.48
32:1a:236:G:H5''	48:1q:42:TYR:OH	2.14	0.48
33:1b:78:GLN:O	33:1b:81:VAL:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:172:PRO:C	35:1d:174:LEU:H	2.22	0.48
37:1f:33:TYR:OH	37:1f:78:GLU:HG3	2.14	0.48
54:1w:23:A:H3'	54:1w:24:G:C8	2.49	0.48
54:1y:36:A:H2'	54:1y:37:MIA:O4'	2.14	0.48
1:2A:71:A:H4'	1:2A:72:U:H5''	1.96	0.48
1:2A:800:A:H8	1:2A:800:A:OP1	1.97	0.48
1:2A:1709:U:H2'	1:2A:1710:C:C6	2.49	0.48
1:2A:2584:U:O4	61:2A:3943:HOH:O	2.18	0.48
1:2A:2889:C:H2'	1:2A:2891:G:O4'	2.14	0.48
6:2G:170:ARG:NH1	6:2G:174:GLU:OE1	2.47	0.48
32:2a:109:A:H5'	32:2a:110:C:C5	2.48	0.48
1:1A:768:G:O2'	1:1A:1379:A:N1	2.39	0.47
3:1D:71:ASP:HB3	3:1D:103:ARG:HH22	1.79	0.47
26:14:61:ARG:NH1	50:1s:42:PRO:HD3	2.29	0.47
32:1a:519:C:OP2	43:1l:50:SER:OG	2.24	0.47
32:1a:598:U:H4'	39:1h:94:TYR:CD2	2.49	0.47
36:1e:152:ARG:HA	39:1h:64:LYS:NZ	2.29	0.47
42:1k:62:GLN:HB2	42:1k:93:GLN:HG3	1.96	0.47
1:2A:489:G:N7	18:2W:49:LYS:NZ	2.62	0.47
11:2P:59:LEU:HD11	30:28:10:ALA:HA	1.96	0.47
32:2a:618:C:O2	32:2a:622:A:N6	2.47	0.47
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.96	0.47
32:2a:974:A:P	45:2n:29:ARG:HH21	2.38	0.47
32:2a:1259:C:C4	32:2a:1260:C:H1'	2.49	0.47
38:2g:15:ASP:HB3	38:2g:24:THR:HG23	1.96	0.47
41:2j:81:THR:C	41:2j:83:GLU:N	2.72	0.47
1:1A:1419:A:O2'	1:1A:1421:G:N7	2.46	0.47
1:1A:1840:G:N7	61:1A:4233:HOH:O	2.35	0.47
1:1A:2693:A:H2'	1:1A:2694:G:H8	1.79	0.47
2:1B:105:A:P	21:1Z:72:ARG:HH12	2.37	0.47
5:1F:133:ASN:N	5:1F:138:GLU:OE1	2.42	0.47
32:1a:598:U:H2'	32:1a:599:C:C6	2.49	0.47
32:1a:1530:G:H4'	32:1a:1530:G:OP1	2.14	0.47
34:1c:190:ARG:HA	34:1c:195:VAL:HG23	1.95	0.47
39:1h:73:ASP:OD1	39:1h:75:ARG:NE	2.47	0.47
40:1i:48:GLU:HA	40:1i:51:ARG:HD3	1.96	0.47
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.49	0.47
8:2I:12:LEU:HD22	8:2I:19:VAL:HG21	1.96	0.47
10:2O:49:ARG:NH1	32:2a:1422:G:O3'	2.38	0.47
32:2a:160:A:H1'	32:2a:344:A:C5	2.48	0.47
32:2a:611:A:H2	32:2a:629:G:H22	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1129:C:H5''	32:2a:1130:A:OP1	2.14	0.47
34:2c:138:VAL:HG11	34:2c:169:ALA:HA	1.96	0.47
48:2q:53:LEU:HD12	48:2q:53:LEU:HA	1.77	0.47
55:2x:10:G:N2	55:2x:26:G:H1'	2.30	0.47
54:2y:61:C:H2'	54:2y:62:C:C6	2.48	0.47
1:1A:886:C:O2'	1:1A:890:A:N6	2.47	0.47
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.29	0.47
1:1A:2376:A:H2'	1:1A:2377:A:O4'	2.14	0.47
1:1A:2639:A:O3'	9:1N:97:ARG:NH2	2.44	0.47
15:1T:108:ARG:HA	15:1T:111:ARG:NH1	2.29	0.47
32:1a:396:G:O2'	32:1a:398:C:OP1	2.32	0.47
32:1a:736:C:H2'	32:1a:737:A:C8	2.49	0.47
32:1a:881:G:OP2	43:1l:12:ARG:NH2	2.46	0.47
32:1a:1027:C:C4	32:1a:1034:G:N1	2.82	0.47
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.49	0.47
43:1l:89:ARG:HH12	43:1l:91:LYS:HG2	1.79	0.47
44:1m:3:ARG:HG3	44:1m:4:ILE:H	1.79	0.47
1:2A:375:C:H2'	1:2A:376:C:C6	2.50	0.47
32:2a:142:G:H2'	32:2a:143:A:C8	2.50	0.47
32:2a:1330:U:H4'	44:2m:23:TYR:CE1	2.49	0.47
32:2a:1360:A:H2'	32:2a:1361:G:O4'	2.15	0.47
40:2i:47:LEU:HB3	40:2i:50:LEU:HD21	1.96	0.47
54:2y:6:G:H1	54:2y:67:C:H42	1.61	0.47
1:1A:816:C:H2'	1:1A:817:C:H6	1.80	0.47
1:1A:882:G:H4'	54:1w:19:G:C6	2.50	0.47
1:1A:1750:G:O2'	1:1A:2860:A:N1	2.36	0.47
19:1X:44:GLU:HG2	19:1X:49:VAL:O	2.13	0.47
24:12:41:ILE:HG13	24:12:43:GLN:HG3	1.95	0.47
26:14:49:PHE:HB3	26:14:50:VAL:H	1.55	0.47
32:1a:1148:U:O4'	40:1i:16:ARG:HD2	2.14	0.47
39:1h:35:ILE:HG12	39:1h:111:ILE:HG21	1.95	0.47
44:1m:3:ARG:HG3	44:1m:4:ILE:N	2.29	0.47
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.15	0.47
55:1x:23:C:H2'	55:1x:24:U:C6	2.50	0.47
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.50	0.47
1:2A:922:U:H2'	1:2A:923:C:C6	2.48	0.47
1:2A:1773:A:H5'	61:2A:4461:HOH:O	2.14	0.47
1:2A:2116:G:N1	1:2A:2162:G:OP1	2.47	0.47
1:2A:2774:C:H2'	1:2A:2775:A:O4'	2.15	0.47
3:2D:3:VAL:HG22	3:2D:17:THR:HB	1.96	0.47
13:2R:100:LEU:HD21	13:2R:113:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2T:99:LEU:O	15:2T:102:ILE:HG23	2.15	0.47
25:23:59:VAL:HG12	25:23:60:GLU:H	1.80	0.47
51:2t:72:LEU:HD23	51:2t:77:ALA:HB2	1.96	0.47
54:2y:14:A:N3	54:2y:14:A:H2'	2.28	0.47
1:1A:574:C:N3	4:1E:145:LYS:NZ	2.53	0.47
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.29	0.47
1:1A:2576:G:H1'	61:1A:4199:HOH:O	2.14	0.47
32:1a:1243:C:H2'	32:1a:1244:C:C6	2.48	0.47
54:1y:40:C:H2'	54:1y:41:C:C6	2.49	0.47
1:2A:200:U:O2	1:2A:386:G:N2	2.47	0.47
1:2A:1146:C:H2'	1:2A:1147:C:H6	1.79	0.47
1:2A:1227:G:OP1	16:2U:13:LYS:HE3	2.14	0.47
1:2A:1297:C:OP2	61:2A:3952:HOH:O	2.20	0.47
1:2A:2309:A:H2'	1:2A:2310:A:C8	2.49	0.47
1:2A:2689:U:P	1:2A:2719:G:H22	2.38	0.47
12:2Q:57:HIS:CE1	12:2Q:116:GLU:HG2	2.49	0.47
32:2a:137:C:H2'	32:2a:138:G:C8	2.50	0.47
32:2a:827:U:H5''	32:2a:828:A:OP2	2.14	0.47
32:2a:1014:A:C2	32:2a:1219:U:H1'	2.50	0.47
32:2a:1411:C:H2'	32:2a:1412:C:H6	1.79	0.47
34:2c:101:LEU:HD22	34:2c:102:ASN:H	1.80	0.47
50:2s:65:ASN:OD1	50:2s:65:ASN:N	2.45	0.47
51:2t:67:ALA:HA	51:2t:72:LEU:O	2.15	0.47
1:1A:1709:U:H2'	1:1A:1710:C:C6	2.49	0.47
1:1A:1851:U:H2'	1:1A:1852:C:O4'	2.14	0.47
2:1B:43:C:H5''	26:14:1:MET:HE2	1.97	0.47
2:1B:75:G:H22	21:1Z:73:GLN:NE2	2.11	0.47
3:1D:4:LYS:HE2	3:1D:6:PHE:CE1	2.49	0.47
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.96	0.47
21:1Z:8:TYR:HB2	21:1Z:38:TYR:CE2	2.50	0.47
21:1Z:65:GLN:HB3	21:1Z:67:LEU:HD21	1.97	0.47
21:1Z:91:LEU:HD22	21:1Z:130:PRO:HB3	1.96	0.47
32:1a:1278:U:H5''	32:1a:1279:A:O4'	2.15	0.47
32:1a:1333:A:H2'	32:1a:1334:G:O4'	2.15	0.47
36:1e:144:THR:O	36:1e:148:VAL:HG13	2.15	0.47
42:1k:34:ASP:HB2	42:1k:35:PRO:HD2	1.97	0.47
54:1w:19:G:H4'	54:1w:20:U:OP1	2.13	0.47
1:2A:848:G:H2'	1:2A:849:A:C8	2.49	0.47
1:2A:2156:G:H2'	1:2A:2157:G:C2	2.50	0.47
1:2A:2853:C:H2'	1:2A:2854:G:C8	2.50	0.47
4:2E:170:LEU:HB3	4:2E:184:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:102:PRO:HB2	5:2F:105:VAL:HG23	1.95	0.47
8:2I:45:LYS:O	8:2I:49:ALA:N	2.39	0.47
32:2a:881:G:OP2	43:2l:12:ARG:NH2	2.47	0.47
32:2a:1169:A:H2'	32:2a:1170:A:C8	2.50	0.47
1:1A:234:C:H2'	1:1A:235:U:C6	2.49	0.47
1:1A:388:G:O2'	1:1A:389:G:N7	2.45	0.47
1:1A:1062:G:H2'	1:1A:1063:G:C8	2.50	0.47
1:1A:1155:A:OP1	16:1U:55:ARG:HD2	2.14	0.47
1:1A:1430:C:H2'	1:1A:1431:U:H6	1.79	0.47
1:1A:2134:A:H2'	1:1A:2159:G:O2'	2.15	0.47
1:1A:2254:C:OP2	61:1A:4145:HOH:O	2.20	0.47
1:1A:2271:G:OP1	22:10:18:ALA:HB1	2.15	0.47
1:1A:2836:U:H2'	1:1A:2837:G:C8	2.50	0.47
3:1D:6:PHE:HE2	3:1D:18:VAL:HG13	1.79	0.47
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.49	0.47
9:1N:121:LYS:HD3	9:1N:130:HIS:CE1	2.49	0.47
10:1O:49:ARG:NH2	32:1a:1423:G:OP1	2.35	0.47
11:1P:88:LEU:HD22	11:1P:95:VAL:HG11	1.96	0.47
12:1Q:12:GLN:HG3	12:1Q:73:PRO:HD2	1.96	0.47
22:10:18:ALA:HB3	22:10:20:ARG:NH1	2.30	0.47
32:1a:436:C:H2'	32:1a:437:U:H6	1.79	0.47
32:1a:445:G:H2'	32:1a:446:G:O4'	2.13	0.47
32:1a:530:G:H1'	54:1w:35:A:O2'	2.15	0.47
32:1a:942:G:H21	40:1i:124:GLN:NE2	2.13	0.47
32:1a:1030(D):A:H2'	32:1a:1031:G:H4'	1.97	0.47
41:1j:50:ILE:HA	41:1j:60:ARG:HD3	1.95	0.47
43:1l:60:LEU:HD21	43:1l:85:ILE:HD13	1.96	0.47
1:2A:884:C:H3'	1:2A:885:C:C6	2.50	0.47
1:2A:2507:C:H5''	1:2A:2573:C:N4	2.29	0.47
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.49	0.47
1:2A:2557:G:H2'	1:2A:2558:C:H6	1.79	0.47
2:2B:75:G:H22	21:2Z:73:GLN:HE21	1.61	0.47
2:2B:94:C:H2'	2:2B:95:C:H6	1.79	0.47
3:2D:70:TRP:CE2	3:2D:150:LYS:HD3	2.50	0.47
5:2F:132:VAL:HA	5:2F:138:GLU:HB3	1.95	0.47
5:2F:143:ALA:HB1	5:2F:148:LEU:HB2	1.95	0.47
7:2H:113:VAL:HG11	7:2H:151:ILE:HG21	1.97	0.47
11:2P:1:MET:HE3	11:2P:1:MET:HB2	1.74	0.47
12:2Q:24:GLY:HA2	12:2Q:67:ARG:NH2	2.30	0.47
16:2U:69:CYS:HB3	16:2U:74:LEU:HD12	1.96	0.47
19:2X:30:VAL:HG21	19:2X:39:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:22:51:ARG:HE	24:22:51:ARG:HB2	1.60	0.47
32:2a:404:U:H2'	32:2a:405:U:C6	2.49	0.47
32:2a:953:G:N7	44:2m:104:ARG:NH2	2.63	0.47
32:2a:1130:A:H5''	40:2i:18:PHE:CE2	2.50	0.47
32:2a:1286:A:H2'	32:2a:1287:A:H4'	1.97	0.47
32:2a:1394:A:N1	32:2a:1500:A:O2'	2.46	0.47
34:2c:113:ALA:HB2	34:2c:202:ILE:HG13	1.96	0.47
34:2c:131:ARG:NH2	36:2e:50:GLU:HG3	2.29	0.47
36:2e:39:GLY:HA2	36:2e:69:VAL:HG13	1.96	0.47
44:2m:4:ILE:HD11	44:2m:22:ILE:HD11	1.97	0.47
44:2m:82:MET:O	44:2m:93:ARG:NH2	2.48	0.47
47:2p:23:ASP:OD1	47:2p:25:ARG:HG2	2.15	0.47
1:1A:1056:G:H5''	1:1A:1057:A:H4'	1.96	0.47
4:1E:5:LEU:HD21	4:1E:79:ARG:HB3	1.96	0.47
5:1F:126:VAL:HG21	5:1F:129:PHE:CZ	2.50	0.47
8:1I:43:ASN:HA	8:1I:46:ALA:HB3	1.96	0.47
19:1X:34:ALA:HA	19:1X:38:GLU:OE1	2.14	0.47
32:1a:920:U:H2'	32:1a:921:U:C6	2.49	0.47
32:1a:1101:A:H4'	32:1a:1102:A:O5'	2.14	0.47
36:1e:77:PRO:HD2	36:1e:142:LEU:HD22	1.97	0.47
1:2A:264:C:H4'	1:2A:428:A:C2	2.50	0.47
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.50	0.47
1:2A:2439:A:H5'	1:2A:2439:A:H8	1.80	0.47
2:2B:119:G:H5'	2:2B:120:A:OP2	2.15	0.47
4:2E:181:LEU:HD12	4:2E:181:LEU:HA	1.66	0.47
8:2I:83:ALA:HB3	8:2I:123:LEU:HD11	1.96	0.47
26:24:10:VAL:HG22	26:24:11:PRO:HD2	1.96	0.47
29:27:1:MET:HE3	29:27:3:ARG:NH2	2.30	0.47
32:2a:224:C:H2'	32:2a:225:C:C6	2.48	0.47
32:2a:1226:C:H4'	50:2s:80:TYR:CZ	2.49	0.47
32:2a:1228:C:OP1	44:2m:108:ARG:NH2	2.33	0.47
32:2a:1286:A:H2	52:2u:18:TYR:OH	1.98	0.47
54:2y:58:A:O2'	54:2y:60:U:OP2	2.25	0.47
1:1A:37:C:H2'	1:1A:38:A:C8	2.50	0.47
1:1A:249:C:O2	30:18:12:LYS:NZ	2.39	0.47
1:1A:2206:G:H3'	1:1A:2207:G:N7	2.30	0.47
12:1Q:60:ARG:HH21	54:1w:53:G:P	2.37	0.47
21:1Z:45:ASP:O	21:1Z:49:ARG:HB2	2.15	0.47
32:1a:116:A:H61	32:1a:313:A:H1'	1.80	0.47
32:1a:353:A:H5'	32:1a:353:A:H8	1.80	0.47
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1441:G:H5''	32:1a:1442:G:O5'	2.15	0.47
33:1b:51:LEU:HD21	33:1b:201:ILE:HG23	1.96	0.47
36:1e:74:GLY:HA3	36:1e:116:THR:HG22	1.97	0.47
36:1e:84:PHE:CE1	36:1e:133:TYR:HB3	2.50	0.47
49:1r:26:LEU:HD11	49:1r:42:ARG:HD3	1.95	0.47
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.32	0.47
1:2A:2811:G:N2	1:2A:2891:G:H1'	2.29	0.47
5:2F:95:ARG:NH1	5:2F:97:TYR:OH	2.48	0.47
16:2U:74:LEU:HD13	16:2U:79:PHE:HB2	1.96	0.47
32:2a:457:C:H2'	32:2a:458:C:C6	2.50	0.47
32:2a:742:G:OP2	46:2o:35:ARG:NH2	2.47	0.47
32:2a:839:U:H3'	32:2a:840:C:C6	2.50	0.47
32:2a:1005:A:H5''	32:2a:1006:C:C5	2.50	0.47
32:2a:1244:C:N4	32:2a:1293:G:H1	2.13	0.47
34:2c:7:PRO:O	34:2c:11:ARG:NH1	2.47	0.47
43:2l:7:ILE:O	43:2l:11:VAL:HG23	2.15	0.47
54:2y:18:G:N2	54:2y:58:A:C4	2.83	0.47
1:1A:1173:G:N2	1:1A:1177:A:OP2	2.47	0.47
1:1A:2788:C:P	4:1E:61:ARG:HH21	2.37	0.47
2:1B:66:A:N6	2:1B:109:C:H5'	2.30	0.47
12:1Q:125:LEU:HD12	12:1Q:129:THR:HG21	1.97	0.47
21:1Z:92:SER:OG	21:1Z:93:ASP:N	2.48	0.47
32:1a:993:G:H2'	32:1a:995:C:H41	1.80	0.47
34:1c:172:ARG:NH2	34:1c:206:GLU:OE2	2.47	0.47
44:1m:14:ARG:HG2	44:1m:44:ARG:HE	1.79	0.47
54:1y:63:G:H2'	54:1y:64:A:O4'	2.15	0.47
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.50	0.47
1:2A:2278:A:OP2	22:20:12:ASN:ND2	2.47	0.47
2:2B:115:G:O4'	14:2S:47:THR:HB	2.15	0.47
9:2N:85:ILE:HG21	9:2N:90:MET:HE2	1.96	0.47
14:2S:64:GLU:H	14:2S:64:GLU:HG3	1.35	0.47
32:2a:1183:A:O2'	32:2a:1184:G:OP1	2.31	0.47
32:2a:1241:G:H2'	32:2a:1242:C:C6	2.50	0.47
32:2a:1263:C:C4	32:2a:1272:G:O6	2.68	0.47
32:2a:1316:G:N2	32:2a:1319:A:H5''	2.25	0.47
33:2b:149:LEU:O	33:2b:153:ARG:HB3	2.15	0.47
41:2j:8:LEU:HA	41:2j:96:ILE:HA	1.96	0.47
44:2m:108:ARG:HD3	44:2m:108:ARG:HA	1.55	0.47
51:2t:9:ASN:O	51:2t:10:LEU:HB2	2.15	0.47
1:1A:956:G:H2'	1:1A:957:A:H2'	1.97	0.46
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:106:LEU:HD12	6:1G:110:ALA:HB3	1.97	0.46
8:1I:77:LEU:HG	8:1I:101:LEU:HD22	1.97	0.46
8:1I:109:ILE:HD12	8:1I:130:TYR:CE2	2.50	0.46
14:1S:5:THR:OG1	14:1S:8:GLU:HG3	2.14	0.46
22:10:10:THR:HG22	22:10:12:ASN:N	2.20	0.46
24:12:51:ARG:HD3	24:12:55:ARG:NH1	2.30	0.46
32:1a:308:C:H2'	32:1a:309:G:C8	2.50	0.46
32:1a:1326:C:H2'	32:1a:1327:C:C6	2.51	0.46
36:1e:82:VAL:HG21	36:1e:138:ALA:HA	1.98	0.46
41:1j:5:ARG:HH21	41:1j:73:ASP:CG	2.24	0.46
48:1q:45:HIS:NE2	48:1q:47:PRO:HG3	2.30	0.46
51:1t:36:LEU:HD13	51:1t:58:LYS:HG3	1.97	0.46
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.42	0.46
1:2A:1851:U:H2'	1:2A:1852:C:O4'	2.15	0.46
15:2T:6:LEU:HD23	15:2T:6:LEU:HA	1.78	0.46
20:2Y:8:LYS:HD3	20:2Y:97:ARG:NH1	2.29	0.46
21:2Z:53:ILE:HA	21:2Z:71:VAL:HG23	1.96	0.46
32:2a:580:U:H2'	32:2a:581:G:O4'	2.16	0.46
32:2a:1388:C:H2'	32:2a:1389:C:H6	1.80	0.46
33:2b:16:HIS:CE1	33:2b:203:GLY:HA2	2.50	0.46
35:2d:104:VAL:HG21	35:2d:140:VAL:HG21	1.96	0.46
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.49	0.46
1:1A:2106:G:H1	1:1A:2183:C:H42	1.62	0.46
1:1A:2804:C:H2'	1:1A:2805:G:H8	1.81	0.46
5:1F:172:TRP:CD1	5:1F:172:TRP:H	2.34	0.46
11:1P:97:PRO:HD3	11:1P:126:VAL:O	2.15	0.46
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.51	0.46
32:1a:189(D):C:H2'	32:1a:189(E):U:O4'	2.15	0.46
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.98	0.46
33:1b:36:ARG:C	33:1b:38:GLY:H	2.24	0.46
35:1d:8:VAL:O	35:1d:11:LEU:HB2	2.15	0.46
40:1i:96:LEU:HD22	40:1i:101:PHE:HD2	1.80	0.46
54:1w:51:U:H2'	54:1w:52:G:H8	1.80	0.46
1:2A:1503:U:H2'	1:2A:1504:C:C6	2.51	0.46
1:2A:1614:A:P	1:2A:1614:A:H8	2.38	0.46
1:2A:1957:C:H2'	1:2A:1958:C:C6	2.49	0.46
10:2O:98:VAL:HG13	10:2O:117:LEU:HB2	1.96	0.46
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.16	0.46
32:2a:562:C:H1'	43:2l:15:ARG:HB3	1.96	0.46
34:2c:101:LEU:HD22	34:2c:102:ASN:N	2.30	0.46
37:2f:100:ASN:HB2	49:2r:28:GLU:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:2q:45:HIS:HB3	48:2q:72:ARG:HG2	1.95	0.46
50:2s:72:GLY:HA2	50:2s:75:ALA:HB3	1.98	0.46
55:2x:50:U:H3	55:2x:64:G:H1	1.63	0.46
1:1A:503:A:H4'	1:1A:504:U:H5''	1.97	0.46
1:1A:922:U:H2'	1:1A:923:C:C6	2.50	0.46
1:1A:1359:A:H2'	1:1A:1360:A:H5'	1.97	0.46
1:1A:1448:G:H1'	1:1A:1528:A:N1	2.31	0.46
1:1A:1506:C:H2'	1:1A:1507:A:C8	2.48	0.46
3:1D:69:ARG:C	3:1D:71:ASP:H	2.22	0.46
6:1G:143:GLU:HG3	26:14:31:ILE:HD11	1.98	0.46
26:14:53:GLU:HB2	26:14:55:ARG:O	2.15	0.46
32:1a:408:A:H2'	32:1a:409:G:O4'	2.15	0.46
39:1h:95:VAL:HB	39:1h:99:GLU:HB2	1.96	0.46
50:1s:51:VAL:HG21	50:1s:71:LEU:HB3	1.96	0.46
1:2A:699:A:H2'	1:2A:700:G:O4'	2.16	0.46
1:2A:1364:G:N7	23:21:3:LYS:HD2	2.31	0.46
1:2A:1686:C:H2'	1:2A:1687:G:O4'	2.15	0.46
9:2N:15:LEU:HD12	9:2N:53:VAL:HB	1.98	0.46
32:2a:1347:G:H5''	40:2i:107:ARG:HB3	1.96	0.46
38:2g:78:ARG:HH21	38:2g:79:ARG:HE	1.64	0.46
38:2g:78:ARG:O	38:2g:84:ASN:HA	2.14	0.46
50:2s:49:ILE:H	50:2s:62:ILE:HD11	1.80	0.46
51:2t:25:ARG:HG2	51:2t:29:LYS:HE2	1.98	0.46
54:2w:51:U:H3	54:2w:63:G:H1	1.62	0.46
1:1A:747:U:O2	1:1A:2014:A:H1'	2.16	0.46
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.81	0.46
1:1A:2447:G:N2	1:1A:2450:A:OP2	2.47	0.46
9:1N:35:ARG:HD3	9:1N:37:LYS:HD2	1.97	0.46
18:1W:46:PHE:O	18:1W:50:VAL:HG23	2.15	0.46
25:13:7:LYS:HE3	25:13:32:GLN:NE2	2.31	0.46
32:1a:8:A:H5'	36:1e:101:ILE:HG22	1.97	0.46
32:1a:1529:G:H4'	32:1a:1530:G:OP2	2.15	0.46
39:1h:116:LYS:HD3	39:1h:127:LEU:HD13	1.97	0.46
54:1y:37:MIA:H2'	54:1y:38:A:C8	2.50	0.46
1:2A:479:A:H4'	1:2A:480:A:OP1	2.15	0.46
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.50	0.46
1:2A:1891:G:O6	61:2A:3950:HOH:O	2.19	0.46
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.16	0.46
6:2G:8:LYS:HD3	6:2G:100:TRP:CD1	2.50	0.46
6:2G:102:PHE:O	6:2G:106:LEU:N	2.49	0.46
11:2P:38:GLN:O	11:2P:40:SER:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2W:57:ASN:HA	18:2W:61:ASN:ND2	2.30	0.46
29:27:24:THR:HG22	29:27:26:GLY:N	2.31	0.46
32:2a:117:G:OP2	61:2a:1912:HOH:O	2.21	0.46
32:2a:406:G:O3'	35:2d:3:ARG:NH2	2.46	0.46
32:2a:520:A:N1	32:2a:536:C:H1'	2.30	0.46
33:2b:231:GLU:H	33:2b:232:PRO:CD	2.29	0.46
34:2c:164:ARG:NH1	34:2c:166:GLU:OE1	2.48	0.46
35:2d:64:LEU:HB2	35:2d:198:VAL:HG11	1.97	0.46
41:2j:6:ILE:HB	41:2j:72:VAL:HG13	1.98	0.46
1:1A:700:G:O2'	1:1A:1632:A:N3	2.42	0.46
1:1A:1268:A:C2	1:1A:2013:A:C4	3.04	0.46
1:1A:1846:G:H5''	1:1A:1847:A:OP2	2.16	0.46
1:1A:1965:C:OP1	1:1A:1966:A:O2'	2.31	0.46
13:1R:8:ARG:NH1	13:1R:43:GLU:OE2	2.44	0.46
18:1W:62:HIS:O	18:1W:64:MET:HG3	2.16	0.46
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.30	0.46
32:1a:670:G:H2'	32:1a:671:G:O4'	2.15	0.46
36:1e:12:LEU:HD21	36:1e:14:ARG:HD3	1.97	0.46
39:1h:121:ASP:O	39:1h:125:ARG:HG3	2.15	0.46
1:2A:1374:G:C6	1:2A:1375:C:C4	3.03	0.46
1:2A:2218:U:O2	23:21:52:ARG:NH1	2.48	0.46
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.50	0.46
1:2A:2772:C:H2'	1:2A:2773:C:C6	2.51	0.46
26:24:53:GLU:HG2	26:24:55:ARG:N	2.27	0.46
32:2a:160:A:H2'	32:2a:161:A:O4'	2.15	0.46
32:2a:435:C:H2'	32:2a:436:C:H6	1.80	0.46
32:2a:502:G:H2'	32:2a:503:C:O4'	2.16	0.46
32:2a:1011:G:H2'	32:2a:1012:U:O4'	2.16	0.46
32:2a:1060:C:H5''	41:2j:51:ARG:HB3	1.97	0.46
32:2a:1157:A:H5'	32:2a:1158:C:C6	2.50	0.46
40:2i:85:LEU:HB3	40:2i:92:TYR:CD2	2.49	0.46
48:2q:27:PHE:CE1	48:2q:36:ILE:HD11	2.50	0.46
1:1A:1092:C:C2'	1:1A:1093:G:H5'	2.44	0.46
1:1A:2390:U:P	30:18:35:GLN:HE22	2.39	0.46
1:1A:2789:C:O2	1:1A:2894:G:N1	2.42	0.46
32:1a:673:G:H2'	32:1a:674:G:C8	2.51	0.46
32:1a:1030:C:N4	32:1a:1030(A):G:N3	2.64	0.46
39:1h:38:ILE:HD11	39:1h:118:VAL:O	2.15	0.46
1:2A:813:U:H2'	1:2A:814:C:C6	2.51	0.46
1:2A:2051:A:H5'	1:2A:2578:G:O4'	2.15	0.46
1:2A:2539:C:H4'	31:29:3:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2804:C:H2'	1:2A:2805:G:C8	2.51	0.46
2:2B:42:C:O2	6:2G:93:THR:N	2.44	0.46
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.58	0.46
11:2P:135:LEU:HA	11:2P:135:LEU:HD23	1.77	0.46
18:2W:11:ARG:NH2	18:2W:98:LYS:HD3	2.30	0.46
26:24:40:HIS:O	26:24:44:THR:OG1	2.31	0.46
32:2a:1026:G:H5'	32:2a:1027:C:O5'	2.15	0.46
32:2a:1328:C:H2'	32:2a:1329:A:O4'	2.15	0.46
41:2j:23:ILE:HG13	41:2j:24:VAL:N	2.31	0.46
1:1A:27:G:N2	1:1A:512:G:H1'	2.31	0.46
1:1A:1056:G:H5''	1:1A:1057:A:C4'	2.45	0.46
3:1D:71:ASP:CB	3:1D:103:ARG:HH12	2.26	0.46
7:1H:153:LYS:O	61:1H:301:HOH:O	2.21	0.46
8:1I:12:LEU:HD23	8:1I:12:LEU:HA	1.76	0.46
17:1V:24:LYS:HE2	17:1V:24:LYS:HB3	1.78	0.46
32:1a:276:G:O3'	48:1q:68:ARG:NH1	2.48	0.46
32:1a:382:A:H2'	32:1a:383:A:C8	2.50	0.46
32:1a:974:A:P	45:1n:29:ARG:HH21	2.39	0.46
33:1b:118:LEU:HD23	33:1b:142:LEU:HB2	1.97	0.46
34:1c:89:GLU:HG3	34:1c:89:GLU:H	1.61	0.46
42:1k:51:LYS:HA	42:1k:51:LYS:HD2	1.44	0.46
1:2A:818:G:OP2	61:2A:3949:HOH:O	2.21	0.46
1:2A:1311:G:H2'	29:27:47:ARG:NH2	2.31	0.46
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.51	0.46
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.15	0.46
12:2Q:137:TYR:CE1	21:2Z:83:PRO:HG3	2.50	0.46
32:2a:1320:C:H42	50:2s:36:ARG:HE	1.63	0.46
44:2m:4:ILE:HG13	44:2m:5:ALA:H	1.80	0.46
1:1A:639:U:H2'	1:1A:640:C:C6	2.51	0.46
1:1A:876:C:H2'	1:1A:877:U:O4'	2.16	0.46
1:1A:1176:G:H21	1:1A:1178:C:P	2.32	0.46
2:1B:2:C:H2'	2:1B:3:C:C6	2.51	0.46
16:1U:85:LYS:HE3	16:1U:116:ALA:O	2.15	0.46
17:1V:1:MET:HE2	17:1V:43:GLU:H	1.81	0.46
26:14:44:THR:OG1	26:14:47:GLN:HB2	2.15	0.46
32:1a:262:A:C6	32:1a:263:A:C6	3.04	0.46
33:1b:19:HIS:NE2	33:1b:20:GLU:HG3	2.30	0.46
33:1b:70:PHE:CD2	33:1b:163:PHE:HB3	2.51	0.46
34:1c:159:GLY:HA2	34:1c:193:TYR:CD1	2.51	0.46
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.47	0.46
51:1t:13:LEU:HD12	51:1t:14:LYS:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:817:C:O2'	1:2A:839:U:H5''	2.15	0.46
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.51	0.46
19:2X:94:GLY:N	19:2X:95:LEU:HB2	2.30	0.46
32:2a:109:A:H5'	32:2a:110:C:H5	1.80	0.46
33:2b:15:VAL:HG12	33:2b:209:ARG:HB3	1.98	0.46
36:2e:8:GLU:HG2	36:2e:34:VAL:HG23	1.98	0.46
39:2h:85:ARG:NH1	39:2h:87:SER:O	2.48	0.46
44:2m:70:LEU:O	44:2m:74:VAL:HG23	2.16	0.46
1:1A:329:G:OP2	20:1Y:71:LYS:HD2	2.16	0.46
1:1A:684:G:OP1	29:17:16:HIS:ND1	2.45	0.46
1:1A:1025:G:O2'	61:1A:4124:HOH:O	2.17	0.46
1:1A:1047:G:H2'	1:1A:1110:G:N2	2.31	0.46
1:1A:1310:G:OP2	29:17:9:ARG:NE	2.47	0.46
5:1F:7:TYR:CD2	5:1F:24:LEU:HB2	2.51	0.46
24:12:3:LEU:HD23	24:12:3:LEU:HA	1.74	0.46
32:1a:222:U:H2'	32:1a:223:U:C6	2.51	0.46
32:1a:523:A:N1	43:1l:92:0TD:H6	2.31	0.46
32:1a:881:G:P	43:1l:12:ARG:HH22	2.38	0.46
32:1a:1057:G:H2'	32:1a:1058:G:O4'	2.16	0.46
34:1c:134:ILE:HD11	34:1c:153:VAL:HB	1.97	0.46
1:2A:882:G:H22	1:2A:894:C:H42	1.62	0.46
1:2A:952:G:OP1	12:2Q:16:ARG:NH2	2.48	0.46
1:2A:2235:G:H2'	1:2A:2236:C:C6	2.51	0.46
1:2A:2340:G:H2'	1:2A:2341:G:C8	2.51	0.46
1:2A:2577:A:OP1	61:2A:3955:HOH:O	2.21	0.46
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.32	0.46
25:23:6:VAL:HG12	25:23:28:LEU:HD11	1.98	0.46
32:2a:67:C:H2'	32:2a:68:G:C8	2.51	0.46
32:2a:642:A:N3	39:2h:113:SER:OG	2.41	0.46
32:2a:974:A:H8	32:2a:974:A:OP1	1.98	0.46
32:2a:978:A:O2'	32:2a:1322:C:N3	2.46	0.46
33:2b:187:LEU:HA	33:2b:201:ILE:HB	1.96	0.46
36:2e:76:ILE:O	36:2e:93:PRO:HB3	2.16	0.46
37:2f:7:ASN:HB2	37:2f:89:MET:HB3	1.97	0.46
50:2s:80:TYR:CZ	50:2s:82:GLY:HA2	2.51	0.46
1:1A:271(D):G:H2'	1:1A:271(E):U:O4'	2.16	0.46
1:1A:907:U:O2'	12:1Q:101:ARG:NH2	2.39	0.46
1:1A:2732:G:H3'	1:1A:2733:A:O4'	2.15	0.46
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.70	0.46
25:13:4:LEU:O	25:13:36:VAL:HA	2.16	0.46
26:14:16:CYS:HB3	26:14:20:ASN:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:166:LYS:NZ	35:1d:179:GLU:OE2	2.46	0.46
1:2A:721:C:H2'	1:2A:722:A:C8	2.50	0.46
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.23	0.46
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.30	0.46
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.50	0.46
6:2G:106:LEU:HG	6:2G:111:LEU:CD1	2.46	0.46
15:2T:127:ALA:C	15:2T:129:ARG:H	2.24	0.46
32:2a:157:G:H2'	32:2a:158:G:H8	1.82	0.46
32:2a:828:A:H2'	32:2a:829:G:O4'	2.16	0.46
32:2a:1005:A:H3'	32:2a:1006:C:C6	2.51	0.46
35:2d:193:ASP:OD1	35:2d:193:ASP:N	2.49	0.46
1:1A:375:C:H2'	1:1A:376:C:C6	2.51	0.45
1:1A:1420:U:O2'	1:1A:1421:G:OP1	2.29	0.45
1:1A:2144:U:H3	1:1A:2147:G:H22	1.63	0.45
1:1A:2203:U:H4'	3:1D:151:LYS:HG2	1.98	0.45
3:1D:206:LEU:HA	3:1D:211:ARG:NH1	2.31	0.45
4:1E:34:VAL:HB	4:1E:48:GLN:HG2	1.97	0.45
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.15	0.45
12:1Q:81:VAL:HB	22:10:7:LEU:HD21	1.98	0.45
21:1Z:138:GLU:H	21:1Z:156:LYS:HZ2	1.64	0.45
32:1a:332:G:OP2	51:1t:10:LEU:HD23	2.16	0.45
32:1a:584:G:H5'	48:1q:91:ARG:NH2	2.31	0.45
32:1a:1280:A:OP1	41:1j:7:LYS:NZ	2.40	0.45
32:1a:1292:U:H2'	32:1a:1293:G:H8	1.80	0.45
33:1b:132:LYS:HA	33:1b:135:GLN:HB3	1.98	0.45
34:1c:53:ALA:HB2	34:1c:115:LEU:HD23	1.98	0.45
37:1f:50:TYR:OH	37:1f:87:ARG:NH2	2.48	0.45
51:1t:48:LYS:HD3	51:1t:48:LYS:HA	1.70	0.45
1:2A:414:C:H2'	1:2A:415:A:C8	2.51	0.45
1:2A:1231:G:H2'	1:2A:1232:G:H8	1.81	0.45
1:2A:1359:A:C2	1:2A:1372:U:O4	2.69	0.45
1:2A:1713:U:H2'	1:2A:1714:G:H8	1.80	0.45
1:2A:2019:A:N7	27:25:9:LYS:HE2	2.30	0.45
1:2A:2626:C:H2'	1:2A:2627:G:O4'	2.15	0.45
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.44	0.45
8:2I:26:ALA:HA	8:2I:30:LEU:HB2	1.97	0.45
11:2P:97:PRO:O	11:2P:101:VAL:HG23	2.15	0.45
26:24:13:ARG:HH12	26:24:23:GLU:HG2	1.81	0.45
32:2a:411:A:H2'	32:2a:413:G:C8	2.51	0.45
32:2a:1016:A:H2'	32:2a:1017:G:O4'	2.15	0.45
32:2a:1089:G:H1	32:2a:1096:C:H42	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1239:A:H62	32:2a:1299:A:N6	2.10	0.45
32:2a:1264:C:C4	32:2a:1272:G:O6	2.69	0.45
34:2c:155:GLY:O	34:2c:157:ILE:N	2.49	0.45
36:2e:99:GLY:O	36:2e:117:ASP:HA	2.15	0.45
40:2i:23:ASN:ND2	40:2i:25:LYS:HE2	2.31	0.45
43:2l:43:VAL:HG12	43:2l:44:THR:H	1.80	0.45
51:2t:100:ILE:HG22	51:2t:101:GLY:H	1.82	0.45
1:1A:492:A:H2'	1:1A:493:G:O4'	2.17	0.45
1:1A:528:A:O2'	1:1A:529:A:H5'	2.17	0.45
1:1A:528:A:OP2	9:1N:114:ARG:NH1	2.49	0.45
1:1A:686:G:OP1	29:17:11:LYS:NZ	2.49	0.45
1:1A:1108:U:H2'	1:1A:1109:C:O4'	2.16	0.45
1:1A:2296:U:OP2	14:1S:9:ARG:NH2	2.44	0.45
1:1A:2341:G:H2'	1:1A:2342:C:C6	2.52	0.45
26:14:14:ILE:HB	26:14:22:ILE:HB	1.98	0.45
27:15:40:LYS:NZ	27:15:44:THR:O	2.39	0.45
32:1a:192:U:O3'	51:1t:57:ARG:HD2	2.16	0.45
32:1a:262:A:H2'	32:1a:263:A:C8	2.51	0.45
32:1a:580:U:H2'	32:1a:581:G:O4'	2.15	0.45
32:1a:1002:G:C5	32:1a:1003:G:H1'	2.52	0.45
33:1b:24:TRP:CD1	33:1b:24:TRP:H	2.35	0.45
48:1q:22:LEU:HD11	48:1q:39:SER:HB2	1.97	0.45
51:1t:72:LEU:HD21	51:1t:80:ARG:HD2	1.97	0.45
1:2A:1357:U:H2'	1:2A:1358:G:O4'	2.15	0.45
1:2A:2768:C:O2'	9:2N:89:LYS:NZ	2.46	0.45
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.50	0.45
21:2Z:121:HIS:N	21:2Z:171:ILE:O	2.50	0.45
32:2a:964:A:N3	32:2a:969:A:O2'	2.46	0.45
32:2a:1008:C:C2	32:2a:1022:G:C2	3.04	0.45
33:2b:91:PRO:HG3	33:2b:154:LEU:HB3	1.97	0.45
40:2i:18:PHE:O	40:2i:61:ALA:HA	2.17	0.45
41:2j:55:LYS:O	41:2j:57:LYS:N	2.48	0.45
46:2o:87:ILE:O	46:2o:88:ARG:HB2	2.16	0.45
47:2p:76:GLN:HE21	47:2p:76:GLN:HB2	1.54	0.45
1:1A:184:C:H2'	1:1A:185:U:C6	2.51	0.45
1:1A:1297:C:O2'	1:1A:1302:A:N1	2.39	0.45
1:1A:1936:A:OP1	1:1A:1937:A:H5'	2.16	0.45
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.14	0.45
12:1Q:17:LEU:HD23	12:1Q:17:LEU:HA	1.82	0.45
32:1a:905:U:O4	61:1a:1912:HOH:O	2.20	0.45
33:1b:90:MET:HE2	33:1b:90:MET:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1k:81:ASP:OD1	42:1k:107:SER:HB3	2.16	0.45
48:1q:43:LEU:HD12	48:1q:68:ARG:HB2	1.99	0.45
50:1s:11:VAL:HG12	50:1s:12:ASP:H	1.81	0.45
1:2A:656:G:H2'	1:2A:657:U:O4'	2.16	0.45
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.15	0.45
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.17	0.45
8:2I:79:ILE:HD11	8:2I:142:VAL:HG12	1.99	0.45
19:2X:1:MET:N	24:22:29:LYS:HE3	2.31	0.45
21:2Z:51:ALA:O	21:2Z:52:SER:HB3	2.17	0.45
21:2Z:121:HIS:N	21:2Z:172:ALA:HB2	2.30	0.45
24:22:46:GLN:O	24:22:49:LYS:HG3	2.16	0.45
30:28:33:ASN:HA	30:28:36:LYS:HD2	1.97	0.45
32:2a:35:G:H2'	32:2a:36:C:C6	2.51	0.45
32:2a:1076:C:OP1	33:2b:179:LYS:NZ	2.49	0.45
32:2a:1149:C:O2'	32:2a:1280:A:N1	2.48	0.45
34:2c:32:LEU:O	34:2c:36:ASP:HB2	2.17	0.45
38:2g:79:ARG:O	38:2g:80:VAL:C	2.59	0.45
45:2n:3:ARG:NH2	45:2n:3:ARG:HA	2.31	0.45
1:1A:207:A:H2'	1:1A:208:C:O4'	2.16	0.45
1:1A:272:G:N7	1:1A:421:U:H2'	2.30	0.45
1:1A:363(C):G:H2'	1:1A:363(D):G:H8	1.80	0.45
7:1H:40:GLU:OE2	7:1H:60:ARG:NH1	2.49	0.45
18:1W:64:MET:HE3	18:1W:109:GLU:HG3	1.97	0.45
26:14:13:ARG:HE	26:14:13:ARG:HB2	1.55	0.45
40:1i:20:ARG:O	40:1i:60:ASP:N	2.45	0.45
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.51	0.45
32:2a:373:A:O2'	32:2a:451:A:N7	2.49	0.45
32:2a:922:G:N3	32:2a:1398:A:H2	2.14	0.45
35:2d:53:ASP:O	35:2d:57:ARG:HG2	2.17	0.45
51:2t:60:GLU:HG3	51:2t:81:LYS:HD2	1.97	0.45
54:2y:74:C:H2'	54:2y:75:C:C6	2.52	0.45
1:1A:481:G:OP2	20:1Y:47:LYS:HE3	2.15	0.45
1:1A:636:G:N7	11:1P:113:LYS:NZ	2.63	0.45
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.51	0.45
1:1A:1426:G:O2'	1:1A:1572:A:N6	2.46	0.45
1:1A:2722:G:H2'	1:1A:2723:C:C6	2.51	0.45
3:1D:228:PRO:HD3	3:1D:235:GLY:CA	2.46	0.45
32:1a:434:U:H2'	32:1a:435:C:C6	2.52	0.45
32:1a:438:G:H4'	35:1d:123:HIS:CE1	2.51	0.45
32:1a:1318:A:H5''	50:1s:3:ARG:NH1	2.31	0.45
33:1b:63:MET:HE3	33:1b:63:MET:HB2	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:1q:15:MET:HB3	48:1q:18:THR:HB	1.98	0.45
49:1r:47:THR:O	49:1r:83:GLU:N	2.39	0.45
54:1w:43:C:H2'	54:1w:44:G:C8	2.51	0.45
1:2A:764:A:N1	1:2A:1789:A:O2'	2.42	0.45
1:2A:784:A:C8	1:2A:792:G:C5	3.05	0.45
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.16	0.45
1:2A:2121:G:H2'	1:2A:2122:U:O4'	2.16	0.45
1:2A:2134:A:H2'	1:2A:2134:A:N3	2.31	0.45
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.52	0.45
2:2B:105:A:H5'	2:2B:106:G:OP2	2.16	0.45
6:2G:129:GLY:O	6:2G:161:THR:HB	2.16	0.45
8:2I:127:VAL:HA	8:2I:140:LEU:O	2.16	0.45
17:2V:24:LYS:HE2	17:2V:24:LYS:HB3	1.80	0.45
32:2a:110:C:H2'	32:2a:111:G:O4'	2.17	0.45
32:2a:926:G:O2'	53:2v:13:A:H1'	2.17	0.45
40:2i:32:ASP:HB3	40:2i:35:GLU:HB2	1.98	0.45
43:2l:53:ARG:HD2	43:2l:93:LEU:HD11	1.99	0.45
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.16	0.45
1:1A:2233:U:H2'	1:1A:2234:G:C8	2.51	0.45
32:1a:376:G:O3'	47:1p:5:ARG:HD2	2.16	0.45
32:1a:838:G:H1	32:1a:848:C:H42	1.64	0.45
1:2A:64:A:O3'	19:2X:71:GLY:HA3	2.17	0.45
1:2A:247:G:OP2	1:2A:249:C:N4	2.44	0.45
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.33	0.45
1:2A:1038:C:N4	1:2A:1117:G:H1	2.14	0.45
17:2V:29:PRO:HA	17:2V:61:VAL:HG22	1.98	0.45
17:2V:58:VAL:HB	17:2V:98:GLU:HG3	1.99	0.45
18:2W:2:GLU:OE2	18:2W:72:LYS:NZ	2.33	0.45
19:2X:9:LEU:HB2	19:2X:29:TRP:O	2.17	0.45
32:2a:586:C:O3'	39:2h:89:PRO:HB3	2.17	0.45
32:2a:838:G:H1	32:2a:848:C:N4	2.15	0.45
36:2e:103:GLY:O	36:2e:106:PRO:HD2	2.16	0.45
48:2q:6:LEU:HB2	48:2q:59:ILE:HG12	1.98	0.45
1:1A:548:A:N1	17:1V:18:LEU:HD12	2.31	0.45
1:1A:593:G:H4'	30:18:4:MET:HE2	1.97	0.45
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.52	0.45
1:1A:1359:A:C2	1:1A:1372:U:O4	2.70	0.45
2:1B:88:C:H2'	2:1B:89:G:O4'	2.17	0.45
5:1F:152:GLU:OE1	5:1F:191:ARG:HD2	2.17	0.45
26:14:57:GLU:HA	26:14:58:ARG:HA	1.65	0.45
32:1a:866:C:C4	32:1a:867:G:H1'	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1198:G:H2'	32:1a:1199:U:C6	2.52	0.45
35:1d:60:GLU:HG3	35:1d:202:LEU:HD12	1.99	0.45
38:1g:27:ILE:HA	38:1g:30:ILE:HD12	1.99	0.45
54:1y:37:MIA:H2'	54:1y:38:A:H8	1.82	0.45
1:2A:81:G:N7	61:2A:4018:HOH:O	2.35	0.45
1:2A:748:G:C8	18:2W:89:ALA:HB1	2.51	0.45
1:2A:2538:C:H2'	1:2A:2539:C:H6	1.82	0.45
11:2P:94:GLU:HG3	11:2P:124:LYS:HD2	1.98	0.45
21:2Z:53:ILE:C	21:2Z:70:LEU:HD11	2.42	0.45
32:2a:163:C:H2'	32:2a:164:U:C6	2.52	0.45
32:2a:501:C:H2'	32:2a:502:G:C8	2.52	0.45
32:2a:693:G:H2'	32:2a:694:A:C8	2.51	0.45
32:2a:1348:U:H2'	32:2a:1349:A:H8	1.82	0.45
32:2a:1411:C:H2'	32:2a:1412:C:C6	2.51	0.45
34:2c:179:ARG:NH1	34:2c:206:GLU:HB2	2.31	0.45
1:1A:2171:A:O2'	1:1A:2172:U:H5''	2.17	0.45
8:1I:6:LEU:HG	8:1I:36:ALA:HA	1.98	0.45
15:1T:127:ALA:C	15:1T:129:ARG:H	2.24	0.45
30:18:26:LYS:HG2	30:18:46:ARG:O	2.16	0.45
32:1a:636:U:H2'	32:1a:637:G:H8	1.82	0.45
32:1a:1223:C:P	50:1s:78:ARG:HH21	2.40	0.45
40:1i:80:GLY:O	40:1i:84:ALA:N	2.44	0.45
41:1j:46:ARG:HB2	41:1j:46:ARG:HH11	1.82	0.45
1:2A:307:G:N1	1:2A:310:A:OP2	2.45	0.45
11:2P:71:VAL:HG12	11:2P:72:PRO:HA	1.99	0.45
14:2S:11:LYS:O	14:2S:15:ARG:HB2	2.17	0.45
21:2Z:92:SER:O	21:2Z:130:PRO:HG3	2.15	0.45
32:2a:23:C:H5	32:2a:561:U:O4	2.00	0.45
32:2a:953:G:H2'	32:2a:954:G:O4'	2.17	0.45
32:2a:996:A:H2'	32:2a:997:U:O4'	2.16	0.45
32:2a:1352:C:OP1	52:2u:3:LYS:NZ	2.46	0.45
34:2c:155:GLY:HA3	34:2c:196:LEU:HD22	1.99	0.45
54:2w:63:G:H2'	54:2w:64:A:O4'	2.17	0.45
1:1A:897:C:N3	1:1A:898:C:N4	2.65	0.45
3:1D:73:VAL:HG13	3:1D:120:GLY:HA3	1.99	0.45
4:1E:59:VAL:O	4:1E:64:LYS:HE3	2.17	0.45
6:1G:34:LEU:HD12	6:1G:100:TRP:CZ3	2.52	0.45
6:1G:47:LYS:HG3	6:1G:48:GLU:N	2.31	0.45
32:1a:600:C:H2'	32:1a:601:C:C6	2.52	0.45
32:1a:1040:U:H2'	32:1a:1041:A:C8	2.52	0.45
32:1a:1525:G:P	42:1k:120:ARG:HH22	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:111:ALA:HA	35:1d:116:GLN:HE21	1.82	0.45
51:1t:77:ALA:O	51:1t:81:LYS:HG3	2.17	0.45
1:2A:7:G:H2'	1:2A:8:A:C8	2.52	0.45
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.17	0.45
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.35	0.45
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.52	0.45
1:2A:2727:G:O3'	10:2O:70:LYS:NZ	2.47	0.45
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.32	0.45
7:2H:145:ALA:HA	7:2H:148:ILE:HD12	1.99	0.45
9:2N:29:LYS:HD2	9:2N:140:VAL:HB	1.98	0.45
32:2a:1151:A:O2'	32:2a:1152:A:H8	1.96	0.45
32:2a:1347:G:H22	32:2a:1373:G:H2'	1.82	0.45
33:2b:160:ASP:O	33:2b:183:PRO:HD2	2.17	0.45
1:1A:53:A:H2'	1:1A:54:G:O4'	2.16	0.45
1:1A:592:G:O6	61:1A:4143:HOH:O	2.20	0.45
1:1A:1973:G:OP1	61:1A:4151:HOH:O	2.21	0.45
1:1A:2118:U:OP1	1:1A:2148:G:O2'	2.27	0.45
1:1A:2336:A:H61	22:10:43:THR:HG22	1.80	0.45
1:1A:2774:C:H2'	1:1A:2775:A:O4'	2.16	0.45
6:1G:67:LYS:H	26:14:6:HIS:CE1	2.35	0.45
16:1U:97:ASP:OD1	16:1U:101:ARG:HD2	2.16	0.45
17:1V:72:VAL:HB	17:1V:85:LYS:HG2	1.98	0.45
32:1a:1338:G:C6	32:1a:1339:A:C6	3.05	0.45
34:1c:150:LYS:HG3	34:1c:169:ALA:HB2	1.99	0.45
41:1j:81:THR:HA	41:1j:84:GLN:HB3	1.99	0.45
55:1x:71:C:H2'	55:1x:72:A:O4'	2.16	0.45
1:2A:14:A:H5''	1:2A:15:G:OP2	2.17	0.45
1:2A:41:C:H2'	1:2A:42:G:H8	1.81	0.45
1:2A:2114:A:H2	1:2A:2171:A:H61	1.64	0.45
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	1.99	0.45
32:2a:1129:C:OP1	40:2i:66:ARG:NH1	2.48	0.45
35:2d:60:GLU:OE1	35:2d:199:ASN:N	2.48	0.45
35:2d:199:ASN:HB3	35:2d:202:LEU:HD12	1.99	0.45
36:2e:144:THR:O	36:2e:148:VAL:HG23	2.17	0.45
37:2f:2:ARG:NE	37:2f:69:GLU:HG2	2.30	0.45
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.52	0.44
1:1A:2406:U:H2'	1:1A:2406:U:OP2	2.17	0.44
1:1A:2853:C:H2'	1:1A:2854:G:H8	1.81	0.44
6:1G:126:ASP:HB2	6:1G:130:ASN:O	2.16	0.44
11:1P:2:LYS:HE2	11:1P:2:LYS:HB3	1.70	0.44
11:1P:135:LEU:HD23	11:1P:135:LEU:HA	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:13:7:LYS:NZ	25:13:32:GLN:O	2.50	0.44
29:17:12:ARG:NH2	29:17:44:PRO:HB3	2.32	0.44
32:1a:328:C:H4'	32:1a:329:A:H5'	1.99	0.44
33:1b:73:THR:OG1	33:1b:170:GLU:OE1	2.30	0.44
33:1b:93:VAL:HG11	33:1b:97:TRP:CD1	2.52	0.44
34:1c:148:GLY:HA3	34:1c:172:ARG:O	2.16	0.44
36:1e:93:PRO:HG2	39:1h:105:ARG:NE	2.32	0.44
38:1g:144:MET:HE2	38:1g:144:MET:HB3	1.67	0.44
42:1k:70:LYS:HB2	42:1k:70:LYS:HE3	1.76	0.44
44:1m:108:ARG:HD3	44:1m:108:ARG:HA	1.60	0.44
1:2A:729:G:C6	3:2D:208:LYS:HB2	2.52	0.44
1:2A:858:U:O2	1:2A:2268:A:H2'	2.17	0.44
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.17	0.44
4:2E:59:VAL:HG23	4:2E:63:LEU:HB2	1.99	0.44
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.52	0.44
8:2I:3:VAL:HG12	8:2I:38:LEU:HA	1.98	0.44
12:2Q:32:TYR:CE1	12:2Q:133:ARG:HB2	2.52	0.44
16:2U:113:ALA:O	16:2U:117:GLN:HG2	2.18	0.44
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	1.99	0.44
32:2a:841:U:C5	32:2a:848:C:H1'	2.52	0.44
32:2a:902:G:H2'	32:2a:903:G:H8	1.81	0.44
32:2a:1280:A:O2'	32:2a:1281:U:H5'	2.18	0.44
32:2a:1288:A:N1	32:2a:1371:G:H1'	2.32	0.44
32:2a:1502:A:H5'	32:2a:1504:G:N7	2.31	0.44
41:2j:16:LEU:HD23	41:2j:16:LEU:HA	1.69	0.44
1:1A:657:U:H2'	1:1A:658:C:C6	2.52	0.44
1:1A:858:U:O2	1:1A:2268:A:H2'	2.18	0.44
1:1A:1006:C:C2	1:1A:1138:G:N2	2.85	0.44
1:1A:2116:G:H2'	1:1A:2117:A:C5	2.52	0.44
1:1A:2378:A:H2'	14:1S:21:THR:HG21	1.99	0.44
1:1A:2685:G:H5'	10:1O:68:GLU:OE2	2.17	0.44
2:1B:2:C:H2'	2:1B:3:C:H6	1.81	0.44
4:1E:181:LEU:HD12	4:1E:181:LEU:HA	1.80	0.44
10:1O:86:ILE:HG22	10:1O:94:ARG:HD3	1.99	0.44
39:1h:39:LEU:HB3	39:1h:45:ILE:HD11	2.00	0.44
1:2A:1782:C:O2'	1:2A:2609:U:H5''	2.17	0.44
7:2H:27:LYS:HG3	7:2H:32:GLU:HB3	1.98	0.44
10:2O:85:VAL:HG11	10:2O:114:ILE:HG12	1.99	0.44
15:2T:28:VAL:HG13	15:2T:86:ILE:HG23	1.99	0.44
35:2d:187:ARG:NH1	35:2d:190:ASP:H	2.15	0.44
43:2l:86:ARG:NH1	61:2l:301:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:108:ARG:NH2	44:2m:114:ARG:HA	2.32	0.44
52:2u:12:LYS:HB3	52:2u:17:THR:O	2.18	0.44
54:2y:33:U:H2'	54:2y:35:A:OP2	2.17	0.44
1:1A:84:A:H5''	20:1Y:8:LYS:HE3	1.99	0.44
1:1A:555:U:O2'	1:1A:556:G:N7	2.47	0.44
1:1A:1779:U:OP2	61:1A:4150:HOH:O	2.21	0.44
1:1A:1818:U:O4	3:1D:154:LYS:HD2	2.17	0.44
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.53	0.44
1:1A:2820:A:O2'	1:1A:2821:A:OP1	2.32	0.44
6:1G:34:LEU:HD23	6:1G:161:THR:HG22	2.00	0.44
12:1Q:103:MET:HE1	12:1Q:125:LEU:HD13	1.98	0.44
32:1a:392:G:H2'	32:1a:393:A:H8	1.82	0.44
32:1a:1039:C:H2'	32:1a:1040:U:H6	1.83	0.44
32:1a:1531:A:H8	32:1a:1531:A:O5'	2.00	0.44
34:1c:63:ASN:HB2	34:1c:98:ASN:HB2	1.99	0.44
35:1d:76:ARG:NE	35:1d:80:GLU:OE2	2.38	0.44
35:1d:81:GLU:CD	35:1d:139:ARG:HH22	2.25	0.44
36:1e:33:VAL:HG13	36:1e:112:LEU:HD12	1.99	0.44
44:1m:16:ASP:OD1	44:1m:16:ASP:N	2.45	0.44
50:1s:27:GLU:CD	50:1s:27:GLU:H	2.25	0.44
54:1w:63:G:H2'	54:1w:64:A:O4'	2.17	0.44
1:2A:1204:A:H61	1:2A:1240:U:H2'	1.83	0.44
1:2A:1412:A:H2'	1:2A:1413:G:H8	1.82	0.44
4:2E:31:CYS:HB2	4:2E:91:VAL:HB	1.99	0.44
14:2S:84:GLN:H	14:2S:111:GLU:HB2	1.82	0.44
26:24:44:THR:HG22	26:24:45:GLY:H	1.82	0.44
32:2a:108:G:C6	51:2t:15:ARG:HG2	2.52	0.44
32:2a:1343:G:H2'	32:2a:1344:C:C6	2.53	0.44
42:2k:17:GLY:O	42:2k:80:VAL:HA	2.18	0.44
1:1A:1104:C:H2'	1:1A:1105:U:O4'	2.17	0.44
1:1A:1588:C:H2'	1:1A:1589:C:C6	2.53	0.44
1:1A:1923:U:H2'	1:1A:1924:C:C6	2.51	0.44
1:1A:2046:G:H5'	27:15:19:ARG:HG3	2.00	0.44
1:1A:2629:A:H62	1:1A:2801(A):A:H1'	1.81	0.44
1:1A:2854:G:H2'	1:1A:2855:C:H6	1.81	0.44
3:1D:39:LYS:NZ	3:1D:57:GLY:O	2.50	0.44
5:1F:33:LEU:HD12	5:1F:33:LEU:HA	1.88	0.44
32:1a:560:U:HO2'	32:1a:561:U:P	2.36	0.44
32:1a:1010:G:H2'	32:1a:1011:G:H8	1.82	0.44
32:1a:1070:U:H2'	32:1a:1071:C:C6	2.53	0.44
32:1a:1095:U:P	32:1a:1108:G:H1	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:34:LEU:O	34:1c:38:ARG:HB2	2.18	0.44
39:1h:121:ASP:HB2	39:1h:125:ARG:HH21	1.82	0.44
1:2A:1193:G:OP1	11:2P:14:LYS:NZ	2.27	0.44
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.17	0.44
1:2A:2138:C:N4	1:2A:2153:G:H1	2.13	0.44
6:2G:20:ILE:HA	6:2G:25:TYR:HD2	1.82	0.44
32:2a:10:A:OP2	36:2e:126:ARG:HD2	2.17	0.44
32:2a:153:C:H2'	32:2a:154:C:C6	2.53	0.44
32:2a:228:A:H2'	32:2a:229:U:O4'	2.17	0.44
32:2a:1348:U:H4'	40:2i:120:ARG:HD2	2.00	0.44
32:2a:1442:G:O2'	32:2a:1442(A):G:H5'	2.17	0.44
33:2b:69:LEU:HB3	33:2b:162:ILE:CG2	2.47	0.44
41:2j:33:GLN:HE21	41:2j:33:GLN:HB3	1.61	0.44
44:2m:57:ARG:C	44:2m:59:TYR:H	2.26	0.44
1:1A:34:C:H5''	1:1A:35:G:OP2	2.16	0.44
1:1A:127:A:H5''	1:1A:128:C:C6	2.52	0.44
1:1A:489:G:N7	18:1W:49:LYS:NZ	2.66	0.44
1:1A:686:G:H8	29:17:6:GLN:O	2.00	0.44
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.83	0.44
1:1A:1865:G:N2	1:1A:1877:A:OP2	2.45	0.44
1:1A:2223:G:OP1	3:1D:172:TYR:OH	2.31	0.44
19:1X:88:LYS:NZ	19:1X:90:GLU:OE1	2.32	0.44
21:1Z:93:ASP:HB2	21:1Z:131:ARG:HH12	1.83	0.44
32:1a:711:G:H2'	32:1a:712:A:C8	2.53	0.44
32:1a:1262:C:H2'	32:1a:1263:C:C6	2.52	0.44
32:1a:1401:G:C2	32:1a:1402:4OC:H1'	2.52	0.44
33:1b:156:LYS:HA	33:1b:156:LYS:HD2	1.67	0.44
36:1e:102:ALA:HB2	36:1e:120:THR:HG21	2.00	0.44
40:1i:46:ALA:HA	40:1i:78:LYS:HB2	1.99	0.44
44:1m:11:ARG:HA	44:1m:45:VAL:HB	1.99	0.44
44:1m:15:VAL:O	44:1m:19:LEU:HD22	2.18	0.44
46:1o:62:GLN:HA	46:1o:62:GLN:HE21	1.82	0.44
48:1q:24:GLU:HG2	48:1q:25:ARG:N	2.33	0.44
54:1w:9:A:O2'	54:1w:10:G:N7	2.50	0.44
54:1w:18:G:HO2'	54:1w:57:G:H22	1.61	0.44
1:2A:900:A:O2'	1:2A:901:A:OP1	2.24	0.44
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.18	0.44
1:2A:1882:C:H2'	1:2A:1883:G:O4'	2.18	0.44
1:2A:2698:U:H2'	1:2A:2699:C:C6	2.53	0.44
6:2G:67:LYS:H	26:24:6:HIS:CE1	2.35	0.44
14:2S:5:THR:OG1	14:2S:8:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:949:A:H1'	32:2a:1364:U:H3	1.82	0.44
32:2a:1013:G:H2'	32:2a:1015:A:OP2	2.18	0.44
32:2a:1023:G:H3'	32:2a:1024:G:H8	1.82	0.44
32:2a:1194:U:H4'	36:2e:22:GLY:CA	2.46	0.44
35:2d:148:VAL:HG11	35:2d:158:ILE:HG21	1.99	0.44
38:2g:65:ALA:HB1	38:2g:127:ALA:HB3	2.00	0.44
42:2k:19:ALA:HB3	42:2k:82:VAL:HG22	1.99	0.44
49:2r:26:LEU:HD11	49:2r:42:ARG:HD3	1.99	0.44
10:1O:1:MET:HE2	10:1O:1:MET:HB3	1.81	0.44
10:1O:122:LEU:HD13	15:1T:72:VAL:HG11	1.98	0.44
14:1S:11:LYS:HD3	14:1S:91:PRO:HD3	1.98	0.44
19:1X:43:VAL:HG21	19:1X:81:VAL:HG21	1.98	0.44
22:10:43:THR:OG1	22:10:46:LYS:HG2	2.18	0.44
32:1a:948:C:OP1	44:1m:109:THR:OG1	2.35	0.44
32:1a:1037:C:H2'	32:1a:1038:C:H6	1.82	0.44
32:1a:1429:C:H2'	32:1a:1430:C:H6	1.82	0.44
39:1h:40:ALA:HA	39:1h:45:ILE:HG13	1.99	0.44
51:1t:10:LEU:HD13	51:1t:10:LEU:HA	1.86	0.44
1:2A:93:G:H2'	1:2A:94:C:C6	2.52	0.44
1:2A:196:A:N3	1:2A:196:A:H2'	2.33	0.44
1:2A:320:A:H4'	1:2A:322:A:C8	2.52	0.44
1:2A:1204:A:N6	1:2A:1240:U:H2'	2.33	0.44
1:2A:1417:C:H2'	1:2A:1418:G:O4'	2.18	0.44
32:2a:1232:U:OP1	40:2i:124:GLN:HG2	2.18	0.44
33:2b:216:SER:C	33:2b:218:ALA:H	2.26	0.44
35:2d:119:GLN:HE21	35:2d:119:GLN:HB3	1.53	0.44
44:2m:15:VAL:HG21	44:2m:48:LEU:HD11	2.00	0.44
48:2q:40:LYS:HD3	48:2q:42:TYR:OH	2.18	0.44
50:2s:33:THR:HG21	50:2s:49:ILE:HD11	1.99	0.44
1:1A:851:U:O2'	25:13:42:ALA:O	2.33	0.44
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.18	0.44
1:1A:1790:C:H2'	1:1A:1791:A:C5	2.52	0.44
1:1A:2180:U:C4	1:1A:2181:G:N7	2.86	0.44
1:1A:2506:U:O2'	54:1w:76:A:O2'	2.30	0.44
1:1A:2698:U:H2'	1:1A:2699:C:C6	2.53	0.44
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.32	0.44
6:1G:15:VAL:HG13	6:1G:175:LEU:HB2	1.99	0.44
11:1P:121:LYS:O	11:1P:123:LEU:N	2.51	0.44
32:1a:1003:G:C4	32:1a:1004:A:H2	2.36	0.44
33:1b:37:ASN:C	33:1b:39:ILE:H	2.24	0.44
33:1b:77:ALA:HB2	33:1b:211:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:534:U:H5'	16:2U:42:ALA:HB1	2.00	0.44
1:2A:1820:U:C2	3:2D:202:LYS:HD2	2.53	0.44
1:2A:1837:C:OP1	32:2a:784:C:H4'	2.18	0.44
1:2A:2815:C:H2'	1:2A:2816:C:H6	1.83	0.44
4:2E:56:PRO:C	4:2E:58:ARG:H	2.26	0.44
5:2F:40:GLN:NE2	5:2F:182:ASN:HB2	2.32	0.44
5:2F:148:LEU:HD13	5:2F:154:VAL:HG21	1.99	0.44
20:2Y:6:HIS:H	20:2Y:6:HIS:CD2	2.35	0.44
23:21:7:ILE:HG23	23:21:98:LEU:HD11	2.00	0.44
32:2a:44:G:C2	32:2a:45:U:H1'	2.53	0.44
32:2a:573:A:N3	32:2a:883:C:O2'	2.46	0.44
34:2c:152:ILE:HG22	34:2c:167:TRP:HB2	2.00	0.44
35:2d:173:TRP:CD1	35:2d:174:LEU:HG	2.52	0.44
36:2e:100:VAL:HG13	36:2e:118:ILE:HG22	1.99	0.44
40:2i:37:PHE:HA	40:2i:40:LEU:HD22	1.99	0.44
42:2k:34:ASP:HB3	42:2k:40:ILE:HD11	1.99	0.44
47:2p:4:ILE:HG12	47:2p:21:VAL:HG12	2.00	0.44
54:2y:14:A:H3'	54:2y:15:G:C8	2.52	0.44
1:1A:1051:G:H2'	1:1A:1052:C:O4'	2.18	0.44
1:1A:1223:G:N2	1:1A:1226:A:OP2	2.40	0.44
17:1V:81:TYR:C	17:1V:82:ARG:HD2	2.42	0.44
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.54	0.44
32:1a:438:G:O2'	32:1a:494:U:O4	2.32	0.44
32:1a:1054:C:C5	54:1w:34:G:H1'	2.53	0.44
33:1b:155:LEU:HD11	33:1b:159:PRO:HG3	1.99	0.44
35:1d:98:GLU:OE1	35:1d:103:ASN:ND2	2.50	0.44
1:2A:455:C:N3	1:2A:472:A:H2'	2.33	0.44
1:2A:1204:A:H2	1:2A:1241:A:N6	2.07	0.44
1:2A:1231:G:H2'	1:2A:1232:G:C8	2.52	0.44
1:2A:1557:C:H5''	1:2A:1558:A:OP2	2.17	0.44
1:2A:1653:G:H3'	13:2R:2:ARG:HD3	1.99	0.44
1:2A:2186:G:H2'	1:2A:2187:G:C8	2.53	0.44
1:2A:2359:C:H2'	1:2A:2360:A:O4'	2.18	0.44
2:2B:2:C:H2'	2:2B:3:C:C6	2.50	0.44
21:2Z:145:GLU:N	21:2Z:148:ASP:HB2	2.32	0.44
29:27:20:ALA:HA	29:27:23:ARG:HH21	1.82	0.44
32:2a:328:C:H4'	32:2a:329:A:C5'	2.47	0.44
32:2a:524:G:H2'	32:2a:525:C:C6	2.53	0.44
32:2a:546:G:OP1	35:2d:73:ARG:HG2	2.18	0.44
32:2a:1081:G:OP1	36:2e:18:ARG:HG2	2.18	0.44
32:2a:1203:C:H2'	32:2a:1204:A:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1369:C:H2'	32:2a:1370:G:C8	2.51	0.44
35:2d:116:GLN:NE2	35:2d:161:ASN:HD21	2.16	0.44
36:2e:95:ALA:O	36:2e:97:GLY:N	2.51	0.44
42:2k:62:GLN:O	42:2k:66:LEU:HG	2.17	0.44
1:1A:94:C:H2'	1:1A:94(A):G:O4'	2.18	0.44
1:1A:1062:G:O5'	1:1A:1070:A:O2'	2.32	0.44
1:1A:1670:C:O2	4:1E:129:HIS:NE2	2.43	0.44
1:1A:1698:A:C8	1:1A:1700:A:O4'	2.70	0.44
4:1E:119:ARG:HD2	4:1E:160:TYR:HB2	2.00	0.44
21:1Z:52:SER:C	21:1Z:54:HIS:N	2.76	0.44
32:1a:258:G:H2'	32:1a:259:G:H8	1.83	0.44
32:1a:410:G:OP1	35:1d:30:LYS:NZ	2.32	0.44
32:1a:841:U:OP2	32:1a:841:U:H6	2.01	0.44
35:1d:60:GLU:OE1	35:1d:199:ASN:N	2.46	0.44
38:1g:77:SER:HA	38:1g:85:TYR:O	2.18	0.44
39:1h:111:ILE:HB	39:1h:135:CYS:SG	2.58	0.44
42:1k:45:GLY:O	42:1k:50:TYR:HB2	2.18	0.44
47:1p:39:TYR:HD1	47:1p:49:LEU:HD13	1.83	0.44
1:2A:297:C:OP1	20:2Y:87:LYS:NZ	2.48	0.44
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.32	0.44
1:2A:1547:C:H2'	1:2A:1548:C:C6	2.53	0.44
1:2A:2126:A:N3	1:2A:2127:G:H1'	2.33	0.44
8:2I:87:LYS:HE3	8:2I:87:LYS:HB2	1.88	0.44
12:2Q:81:VAL:HB	22:20:7:LEU:HD21	2.00	0.44
14:2S:10:ARG:NE	14:2S:91:PRO:O	2.34	0.44
17:2V:14:VAL:HA	17:2V:18:LEU:HD23	2.00	0.44
18:2W:11:ARG:HD2	18:2W:11:ARG:HA	1.76	0.44
32:2a:410:G:OP1	35:2d:30:LYS:NZ	2.43	0.44
32:2a:979:C:O2	45:2n:19:ARG:HG2	2.18	0.44
32:2a:1316:G:N2	32:2a:1318:A:H3'	2.33	0.44
35:2d:76:ARG:O	35:2d:80:GLU:HG2	2.17	0.44
1:1A:64:A:O3'	19:1X:71:GLY:HA3	2.18	0.43
1:1A:292:C:H2'	1:1A:293:U:H6	1.83	0.43
1:1A:1607:C:H4'	1:1A:1608:A:O5'	2.18	0.43
61:1A:4360:HOH:O	3:1D:14:ARG:HD2	2.18	0.43
4:1E:119:ARG:HG2	4:1E:120:TRP:NE1	2.32	0.43
9:1N:61:ARG:HD3	9:1N:61:ARG:HA	1.89	0.43
11:1P:35:HIS:O	11:1P:36:LYS:O	2.36	0.43
19:1X:40:LYS:HG3	19:1X:51:VAL:HB	2.00	0.43
30:18:4:MET:HE3	30:18:63:PRO:HG3	2.00	0.43
32:1a:1025:U:O2	32:1a:1036:G:C6	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1035:A:C4	32:1a:1036:G:N2	2.86	0.43
36:1e:72:GLN:O	36:1e:75:THR:HG22	2.18	0.43
39:1h:112:LEU:HA	39:1h:134:ILE:HG12	1.99	0.43
47:1p:72:ARG:HG2	47:1p:73:LEU:HD23	2.00	0.43
54:1w:28:G:H2'	54:1w:29:G:C8	2.53	0.43
54:1y:44:G:H8	54:1y:44:G:OP2	2.00	0.43
1:2A:740:U:H2'	1:2A:741:G:C8	2.53	0.43
1:2A:909:A:C6	1:2A:912:C:C2	3.06	0.43
1:2A:1466:G:O3'	1:2A:1546:C:O2'	2.36	0.43
1:2A:2542:A:H4'	1:2A:2543:G:C8	2.53	0.43
1:2A:2585:U:O4	54:2w:76:A:O2'	2.36	0.43
2:2B:56:G:H4'	2:2B:57:A:H8	1.82	0.43
4:2E:59:VAL:HG23	4:2E:63:LEU:CB	2.48	0.43
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.53	0.43
13:2R:103:ARG:HD3	13:2R:108:GLY:O	2.17	0.43
21:2Z:93:ASP:OD2	21:2Z:93:ASP:N	2.51	0.43
38:2g:6:ARG:H	38:2g:6:ARG:HG3	1.39	0.43
38:2g:111:ARG:HD2	38:2g:123:GLU:HB2	1.99	0.43
51:2t:16:HIS:O	51:2t:19:SER:OG	2.27	0.43
54:2w:50:U:H3	54:2w:64:A:H61	1.66	0.43
54:2y:14:A:H3'	54:2y:15:G:H8	1.83	0.43
1:1A:829:A:N7	1:1A:2248:C:H5'	2.33	0.43
1:1A:1356:G:OP2	61:1A:4152:HOH:O	2.21	0.43
1:1A:1495:A:H2'	1:1A:1496:A:C8	2.53	0.43
1:1A:2537:U:H2'	1:1A:2538:C:C6	2.53	0.43
1:1A:2846:G:H2'	1:1A:2847:U:O4'	2.18	0.43
5:1F:40:GLN:HA	5:1F:43:LYS:HE3	1.99	0.43
7:1H:24:VAL:HG11	7:1H:43:VAL:HG11	2.00	0.43
7:1H:98:LEU:HD23	7:1H:102:ALA:O	2.18	0.43
15:1T:20:PRO:HD2	15:1T:86:ILE:HB	1.99	0.43
25:13:8:LEU:HG	25:13:31:LEU:HD23	2.00	0.43
32:1a:749:C:H2'	32:1a:750:G:H8	1.83	0.43
33:1b:170:GLU:O	33:1b:174:VAL:HG23	2.18	0.43
36:1e:68:GLU:OE1	36:1e:70:PRO:HG3	2.18	0.43
54:1y:9:A:H4'	54:1y:46:G7M:OP2	2.18	0.43
1:2A:84:A:H5'	20:2Y:8:LYS:HG2	2.00	0.43
1:2A:910:A:N3	1:2A:2264:C:O2'	2.41	0.43
7:2H:80:SER:OG	7:2H:81:GLU:OE2	2.23	0.43
20:2Y:19:LYS:HE3	20:2Y:20:TYR:CE2	2.53	0.43
25:23:5:LYS:HE3	25:23:34:GLU:OE2	2.18	0.43
32:2a:20:U:H2'	32:2a:21:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:411:A:H2'	32:2a:413:G:H8	1.83	0.43
32:2a:653:A:C8	39:2h:56:LYS:HG2	2.52	0.43
32:2a:657:G:O2'	46:2o:28:GLN:HG2	2.18	0.43
32:2a:730:G:C5	32:2a:731:G:H1'	2.53	0.43
32:2a:1261:A:H5'	32:2a:1283:G:O3'	2.18	0.43
32:2a:1265:G:C4	32:2a:1271:G:N2	2.87	0.43
33:2b:134:GLU:O	33:2b:138:LEU:HG	2.17	0.43
36:2e:53:LEU:HD12	36:2e:53:LEU:H	1.82	0.43
1:1A:444:C:H4'	5:1F:49:ALA:HB2	1.99	0.43
1:1A:754:C:H2'	1:1A:755:C:H6	1.83	0.43
1:1A:1815:A:P	3:1D:54:ARG:HH22	2.41	0.43
1:1A:2106:G:H2'	1:1A:2107:C:C6	2.53	0.43
6:1G:41:GLN:HG2	6:1G:154:GLY:O	2.18	0.43
6:1G:99:MET:HE2	6:1G:99:MET:HB3	1.94	0.43
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.32	0.43
19:1X:25:LYS:HA	19:1X:81:VAL:O	2.18	0.43
32:1a:178:C:H2'	32:1a:179:A:C8	2.52	0.43
32:1a:300:A:O2'	32:1a:564:C:N3	2.47	0.43
32:1a:1004:A:H61	32:1a:1037:C:H42	1.65	0.43
32:1a:1036:G:H5''	32:1a:1037:C:H5	1.80	0.43
32:1a:1072:G:H2'	32:1a:1073:U:C6	2.52	0.43
33:1b:23:ARG:H	33:1b:23:ARG:HG2	1.65	0.43
47:1p:50:LYS:HA	47:1p:50:LYS:HD2	1.81	0.43
1:2A:459:U:H5''	29:27:40:TRP:CD2	2.53	0.43
1:2A:900:A:H2'	1:2A:901:A:H8	1.83	0.43
1:2A:1027:A:C2	1:2A:2488:A:H5'	2.53	0.43
1:2A:1027:A:C6	1:2A:1126:A:C4	3.07	0.43
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.52	0.43
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.52	0.43
1:2A:1607:C:H5''	1:2A:1608:A:H5'	2.00	0.43
1:2A:1703:G:H2'	1:2A:1704:G:C8	2.53	0.43
1:2A:1937:A:O2'	1:2A:1939:5MU:OP2	2.35	0.43
1:2A:2355:C:H1'	22:20:39:ARG:HH21	1.83	0.43
7:2H:170:ARG:O	7:2H:171:LEU:HD23	2.19	0.43
10:2O:76:ALA:O	15:2T:74:ARG:HG3	2.18	0.43
14:2S:30:ARG:HB2	14:2S:35:ILE:HD12	2.00	0.43
16:2U:108:GLU:O	16:2U:112:ARG:HG2	2.18	0.43
32:2a:109:A:H2'	32:2a:326:G:N2	2.33	0.43
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.33	0.43
32:2a:1423:G:H2'	32:2a:1424:C:C6	2.53	0.43
34:2c:32:LEU:HD12	34:2c:32:LEU:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:40:ARG:NH2	34:2c:57:ILE:HD13	2.33	0.43
36:2e:24:ARG:H	36:2e:24:ARG:HG2	1.57	0.43
1:1A:305:U:H2'	1:1A:306:U:C6	2.54	0.43
1:1A:570:G:H2'	1:1A:2030:A:N7	2.33	0.43
1:1A:2391:G:O6	1:1A:2425:A:H8	2.01	0.43
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.99	0.43
24:12:51:ARG:HE	24:12:51:ARG:HB2	1.55	0.43
26:14:50:VAL:HG21	44:1m:64:TRP:C	2.43	0.43
26:14:59:PHE:CE2	50:1s:64:GLU:HB3	2.54	0.43
32:1a:977:A:H1'	32:1a:982:U:O4	2.17	0.43
33:1b:13:ALA:C	33:1b:15:VAL:H	2.27	0.43
38:1g:78:ARG:O	38:1g:84:ASN:HA	2.17	0.43
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	1.98	0.43
54:1w:4:C:H2'	54:1w:5:G:C8	2.52	0.43
1:2A:184:C:H2'	1:2A:185:U:C6	2.54	0.43
1:2A:667:U:O2	30:28:2:PRO:HD2	2.18	0.43
1:2A:2514:U:H2'	1:2A:2515:C:C6	2.53	0.43
8:2I:63:ALA:HA	8:2I:66:GLU:HB3	2.00	0.43
11:2P:3:LEU:HD23	11:2P:6:LEU:HD12	2.00	0.43
32:2a:825:G:H2'	32:2a:826:C:H6	1.82	0.43
32:2a:1149:C:H2'	32:2a:1150:U:C6	2.53	0.43
33:2b:218:ALA:O	33:2b:222:ILE:HG23	2.18	0.43
34:2c:36:ASP:O	34:2c:39:ILE:HB	2.18	0.43
37:2f:69:GLU:CD	37:2f:69:GLU:H	2.26	0.43
38:2g:6:ARG:HB2	38:2g:6:ARG:HH11	1.83	0.43
38:2g:27:ILE:HA	38:2g:30:ILE:HD12	2.01	0.43
1:1A:32:C:O2'	1:1A:33:U:H5'	2.17	0.43
1:1A:800:A:H8	1:1A:800:A:OP1	2.01	0.43
1:1A:828:U:C5	1:1A:2247:A:H4'	2.54	0.43
1:1A:884:C:H42	1:1A:892:G:H1	1.65	0.43
1:1A:1062:G:P	1:1A:1070:A:H1'	2.59	0.43
1:1A:2098:U:H3	1:1A:2191:G:H1	1.67	0.43
1:1A:2100:G:H1	1:1A:2189:U:H3	1.67	0.43
1:1A:2203:U:O4'	3:1D:151:LYS:HE2	2.18	0.43
1:1A:2705:A:O2'	1:1A:2852:G:OP1	2.23	0.43
8:1I:47:LEU:O	8:1I:51:ILE:HG13	2.19	0.43
8:1I:78:THR:HA	8:1I:143:SER:O	2.18	0.43
32:1a:175:C:H2'	32:1a:176:C:C6	2.53	0.43
32:1a:193:C:H2'	32:1a:194:C:C6	2.53	0.43
32:1a:721:G:H4'	32:1a:722:A:O4'	2.19	0.43
39:1h:114:THR:C	39:1h:116:LYS:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:801:G:O6	5:2F:53:THR:OG1	2.37	0.43
1:2A:1272:A:H3'	1:2A:1273:U:H5''	1.99	0.43
1:2A:2134:A:H62	1:2A:2157:G:H4'	1.83	0.43
1:2A:2379:G:P	14:2S:23:ARG:HH21	2.41	0.43
2:2B:104:U:O2'	21:2Z:72:ARG:HG2	2.19	0.43
3:2D:29:PRO:HA	3:2D:83:GLU:OE1	2.19	0.43
4:2E:54:GLN:N	4:2E:74:PRO:O	2.48	0.43
4:2E:143:ASN:HD22	4:2E:147:PRO:HD3	1.84	0.43
7:2H:7:LEU:HD23	7:2H:69:ARG:NH2	2.32	0.43
14:2S:67:ARG:HG2	14:2S:71:ARG:HD2	2.00	0.43
32:2a:396:G:O2'	32:2a:398:C:OP1	2.18	0.43
32:2a:583:A:H2'	32:2a:584:G:O4'	2.18	0.43
32:2a:1027:C:HO2'	32:2a:1034:G:H22	1.66	0.43
32:2a:1318:A:O2'	50:2s:37:ARG:HB2	2.19	0.43
34:2c:153:VAL:O	34:2c:165:THR:HA	2.18	0.43
41:2j:81:THR:C	41:2j:83:GLU:H	2.27	0.43
1:1A:1170:G:H1	1:1A:1179:C:H42	1.67	0.43
1:1A:1508:A:H4'	1:1A:1509(A):A:C5	2.53	0.43
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	2.00	0.43
6:1G:34:LEU:HD23	6:1G:34:LEU:HA	1.84	0.43
32:1a:67:C:H2'	32:1a:68:G:C8	2.54	0.43
32:1a:1183:A:O2'	32:1a:1184:G:OP1	2.33	0.43
32:1a:1252:A:H2'	32:1a:1253:G:O4'	2.18	0.43
34:1c:65:ALA:O	34:1c:66:VAL:HG13	2.18	0.43
40:1i:5:TYR:OH	40:1i:16:ARG:HG2	2.19	0.43
50:1s:27:GLU:HB2	50:1s:28:LYS:CA	2.47	0.43
54:1y:7:A:O2'	54:1y:49:C:OP2	2.34	0.43
54:1y:61:C:H2'	54:1y:62:C:C6	2.53	0.43
1:2A:108:U:H2'	1:2A:109:G:C8	2.54	0.43
1:2A:383:U:H2'	1:2A:385:C:H5	1.83	0.43
1:2A:795:C:H2'	1:2A:796:C:C6	2.53	0.43
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.45	0.43
3:2D:2:ALA:N	3:2D:200:ASP:OD2	2.50	0.43
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	2.00	0.43
8:2I:62:LYS:HG3	8:2I:133:HIS:CE1	2.54	0.43
21:2Z:152:ALA:O	21:2Z:155:LEU:HD13	2.18	0.43
22:20:11:ARG:O	22:20:14:ARG:NH1	2.51	0.43
23:21:59:THR:O	23:21:91:LYS:NZ	2.52	0.43
24:22:25:VAL:HG13	24:22:57:ILE:HG23	2.00	0.43
26:24:41:PRO:HG3	26:24:49:PHE:CZ	2.54	0.43
32:2a:362:G:N1	32:2a:365:U:OP2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:486:U:H2'	32:2a:487:A:C8	2.53	0.43
32:2a:983:A:H3'	32:2a:983:A:N3	2.34	0.43
32:2a:1111:A:H2'	32:2a:1112:C:C6	2.54	0.43
32:2a:1326:C:H2'	32:2a:1327:C:C6	2.53	0.43
32:2a:1397:C:OP2	36:2e:24:ARG:NH2	2.52	0.43
40:2i:4:TYR:CE1	40:2i:88:TYR:HA	2.53	0.43
1:1A:625:G:O6	11:1P:107:LYS:NZ	2.47	0.43
1:1A:662:G:OP1	11:1P:16:ARG:NE	2.52	0.43
1:1A:674:G:H1'	5:1F:74:ARG:HD3	2.00	0.43
1:1A:1271:G:O3'	1:1A:1272:A:H4'	2.17	0.43
1:1A:2154:G:C2	1:1A:2155:G:H1'	2.54	0.43
1:1A:2353:G:H1'	22:10:34:GLY:HA3	2.00	0.43
1:1A:2808:U:H5''	1:1A:2891:G:O6	2.19	0.43
2:1B:75:G:H22	21:1Z:73:GLN:HE22	1.66	0.43
4:1E:72:VAL:HG12	4:1E:73:GLU:O	2.19	0.43
7:1H:24:VAL:HG22	7:1H:35:VAL:HB	2.01	0.43
21:1Z:158:PRO:O	21:1Z:161:VAL:HG22	2.19	0.43
32:1a:679:C:H2'	32:1a:680:C:H6	1.84	0.43
32:1a:950:U:H2'	32:1a:951:G:H8	1.84	0.43
32:1a:1030:C:H42	32:1a:1031:G:H1	1.65	0.43
33:1b:51:LEU:O	33:1b:55:PHE:HD2	2.02	0.43
33:1b:93:VAL:HG21	33:1b:97:TRP:CD1	2.54	0.43
33:1b:97:TRP:CZ2	33:1b:102:LEU:HD13	2.54	0.43
33:1b:119:GLU:OE2	33:1b:146:GLN:NE2	2.52	0.43
34:1c:180:ALA:HB1	34:1c:203:PHE:CE1	2.54	0.43
36:1e:33:VAL:HG11	36:1e:108:ALA:HB1	2.00	0.43
37:1f:6:VAL:HG22	37:1f:90:VAL:HG22	2.01	0.43
44:1m:34:LEU:HD13	44:1m:41:PRO:HA	1.99	0.43
50:1s:36:ARG:NH2	50:1s:72:GLY:O	2.51	0.43
1:2A:608:A:H2'	1:2A:609:A:C8	2.53	0.43
1:2A:996:A:H4'	16:2U:91:ASP:OD2	2.18	0.43
1:2A:1210:A:H5'	1:2A:1210:A:N3	2.34	0.43
1:2A:2745:C:O2'	7:2H:139:GLN:O	2.36	0.43
20:2Y:68:HIS:ND1	20:2Y:70:SER:HB3	2.34	0.43
32:2a:857:C:H2'	32:2a:858:G:O4'	2.19	0.43
32:2a:1239:A:N6	32:2a:1299:A:H62	2.10	0.43
1:1A:118:A:C8	1:1A:119:A:C8	3.06	0.43
1:1A:1756:G:H4'	1:1A:1758:G:O4'	2.19	0.43
1:1A:2512:C:H2'	1:1A:2513:G:O4'	2.19	0.43
3:1D:2:ALA:O	3:1D:20:ASP:HB3	2.18	0.43
32:1a:148:G:H2'	32:1a:149:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:679:C:H2'	32:1a:680:C:C6	2.54	0.43
32:1a:690:G:C6	32:1a:691:G:C6	3.07	0.43
32:1a:1223:C:OP2	50:1s:78:ARG:NH2	2.46	0.43
32:1a:1292:U:H2'	32:1a:1293:G:C8	2.52	0.43
33:1b:44:LEU:HA	33:1b:47:THR:HG23	2.00	0.43
34:1c:33:LEU:O	34:1c:37:GLN:HG2	2.19	0.43
34:1c:122:GLU:O	34:1c:126:ARG:HD2	2.18	0.43
40:1i:85:LEU:O	40:1i:88:TYR:HB3	2.18	0.43
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.37	0.43
44:1m:67:GLU:HB3	44:1m:68:GLY:H	1.68	0.43
51:1t:74:LYS:HB2	51:1t:74:LYS:HE3	1.91	0.43
54:1y:19:G:H1	54:1y:56:C:N4	2.15	0.43
1:2A:387:U:OP2	23:21:20:ARG:NH1	2.52	0.43
1:2A:824:A:H1'	1:2A:2358:G:N7	2.34	0.43
1:2A:2512:C:H2'	1:2A:2513:G:O4'	2.18	0.43
15:2T:90:GLN:OE1	15:2T:121:ILE:HD11	2.19	0.43
32:2a:192:U:O2'	51:2t:60:GLU:OE1	2.25	0.43
32:2a:1004:A:C6	32:2a:1037:C:H1'	2.53	0.43
32:2a:1073:U:H2'	32:2a:1074:G:C8	2.54	0.43
37:2f:79:LEU:HB2	37:2f:88:VAL:HG21	2.00	0.43
38:2g:101:LEU:O	38:2g:105:VAL:HG23	2.17	0.43
40:2i:3:GLN:HE21	40:2i:20:ARG:CZ	2.31	0.43
1:1A:720:C:H2'	1:1A:721:C:H6	1.83	0.43
1:1A:807:U:OP2	11:1P:41:ARG:NH2	2.52	0.43
1:1A:880:G:H2'	1:1A:881:G:H8	1.84	0.43
1:1A:1071:G:O2'	1:1A:1089:G:H2'	2.18	0.43
1:1A:2649:U:H2'	1:1A:2650:U:C6	2.53	0.43
2:1B:37:C:H2'	2:1B:38:C:O4'	2.19	0.43
5:1F:136:THR:HA	5:1F:166:ALA:O	2.19	0.43
6:1G:41:GLN:HB3	6:1G:43:LEU:HD22	2.00	0.43
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.61	0.43
8:1I:77:LEU:HD23	8:1I:77:LEU:HA	1.71	0.43
15:1T:16:ARG:HB3	15:1T:18:ASP:OD1	2.19	0.43
15:1T:41:ARG:NH2	15:1T:43:GLN:HE21	2.16	0.43
21:1Z:138:GLU:HB2	21:1Z:156:LYS:NZ	2.34	0.43
23:11:50:ARG:HG2	23:11:59:THR:HG23	2.00	0.43
32:1a:195:A:H1'	32:1a:222:U:O2'	2.19	0.43
32:1a:567:G:H2'	32:1a:568:G:O4'	2.18	0.43
32:1a:857:C:H2'	32:1a:858:G:O4'	2.18	0.43
32:1a:1047:G:H5''	45:1n:4:LYS:HD3	2.01	0.43
33:1b:109:SER:HA	33:1b:112:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1e:90:VAL:O	36:1e:120:THR:HA	2.19	0.43
1:2A:265:A:C8	1:2A:266:G:H1'	2.54	0.43
1:2A:287:C:H2'	1:2A:288:C:C6	2.54	0.43
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.33	0.43
1:2A:2558:C:H2'	1:2A:2559:C:O4'	2.19	0.43
4:2E:50:GLY:HA3	4:2E:75:VAL:HG21	2.01	0.43
5:2F:157:VAL:HB	5:2F:194:MET:HG2	2.00	0.43
6:2G:32:PRO:HB3	6:2G:163:ALA:HB2	2.00	0.43
6:2G:77:ILE:HG22	6:2G:80:PHE:H	1.83	0.43
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	2.00	0.43
7:2H:46:GLU:HB3	7:2H:47:GLU:H	1.59	0.43
15:2T:8:LYS:HD3	15:2T:8:LYS:HA	1.78	0.43
18:2W:71:VAL:HA	18:2W:107:LEU:HD23	2.01	0.43
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.51	0.43
32:2a:242:C:H2'	32:2a:243:A:H5'	2.00	0.43
32:2a:685:G:C2	32:2a:686:U:C4	3.07	0.43
32:2a:955:U:O2'	50:2s:83:HIS:HD2	2.01	0.43
32:2a:1530:G:H2'	32:2a:1531:A:O4'	2.19	0.43
35:2d:155:LEU:HD23	35:2d:156:GLU:H	1.84	0.43
36:2e:143:ARG:HE	39:2h:77:GLU:CD	2.26	0.43
51:2t:77:ALA:O	51:2t:81:LYS:HG3	2.19	0.43
1:1A:657:U:H2'	1:1A:658:C:H6	1.84	0.43
1:1A:769:G:H5'	1:1A:1379:A:N6	2.34	0.43
1:1A:816:C:H2'	1:1A:817:C:C6	2.53	0.43
1:1A:2141:G:C6	1:1A:2142:C:C2	3.07	0.43
1:1A:2160:G:C6	1:1A:2161:C:N4	2.87	0.43
6:1G:60:LEU:HB3	6:1G:68:PRO:HG3	2.01	0.43
32:1a:216:G:H2'	32:1a:217:C:C6	2.53	0.43
32:1a:447:G:H2'	32:1a:485:G:N2	2.34	0.43
32:1a:695:A:H2'	32:1a:696:A:C8	2.54	0.43
32:1a:950:U:H2'	32:1a:951:G:C8	2.54	0.43
32:1a:1504:G:OP1	32:1a:1507:A:H4'	2.19	0.43
1:2A:103:A:H5'	24:22:3:LEU:HD11	2.01	0.43
1:2A:530:G:C5	1:2A:2022:U:H5''	2.54	0.43
1:2A:557:U:H2'	1:2A:558:G:C8	2.54	0.43
1:2A:614(B):G:H2'	5:2F:44:ARG:HH11	1.84	0.43
1:2A:624:C:OP1	61:2A:3954:HOH:O	2.21	0.43
1:2A:637:A:H2'	11:2P:117:GLU:OE1	2.19	0.43
1:2A:1139:G:O3'	9:2N:24:GLY:HA3	2.17	0.43
1:2A:1339:G:H5''	19:2X:16:LYS:HD3	2.01	0.43
1:2A:1354:A:H2'	1:2A:1355:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2135:A:C4	1:2A:2136:C:H5	2.37	0.43
5:2F:116:ASP:OD1	5:2F:119:ARG:NH2	2.51	0.43
6:2G:163:ALA:HB1	6:2G:168:GLU:HB2	2.00	0.43
10:2O:19:ILE:HG22	10:2O:43:VAL:HA	2.01	0.43
10:2O:119:PRO:HB2	15:2T:68:TYR:CZ	2.54	0.43
32:2a:438:G:O2'	32:2a:494:U:O4	2.32	0.43
32:2a:688:G:O2'	32:2a:704:A:N1	2.40	0.43
32:2a:1095:U:P	32:2a:1108:G:H1	2.42	0.43
32:2a:1457:G:H5''	51:2t:35:THR:HG21	2.01	0.43
36:2e:81:GLU:HG2	36:2e:90:VAL:HG22	2.01	0.43
36:2e:82:VAL:HG21	36:2e:138:ALA:HA	2.01	0.43
45:2n:37:PHE:CZ	45:2n:56:VAL:HG21	2.54	0.43
47:2p:1:MET:HE2	47:2p:1:MET:H3	1.84	0.43
47:2p:41:PRO:O	47:2p:43:LYS:HE2	2.19	0.43
50:2s:19:VAL:O	50:2s:23:ASN:ND2	2.52	0.43
55:2x:8:4SU:O5'	55:2x:8:4SU:H6	2.18	0.43
54:2y:52:G:H5'	54:2y:53:G:OP2	2.18	0.43
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.34	0.42
1:1A:1257:C:H4'	5:1F:83:PHE:CD1	2.54	0.42
1:1A:2032:G:OP2	1:1A:2454:G:O2'	2.30	0.42
1:1A:2038:G:O6	61:1A:4149:HOH:O	2.20	0.42
1:1A:2315:G:H2'	1:1A:2316:C:C6	2.53	0.42
7:1H:149:ARG:HD2	7:1H:164:TYR:CE2	2.53	0.42
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.19	0.42
11:1P:52:GLU:OE2	11:1P:58:THR:OG1	2.25	0.42
32:1a:8:A:N7	35:1d:208:SER:OG	2.47	0.42
32:1a:219:C:H2'	32:1a:220:G:O4'	2.18	0.42
32:1a:750:G:O2'	46:1o:21:ASP:OD1	2.37	0.42
32:1a:1179:A:O3'	40:1i:103:THR:HG23	2.19	0.42
33:1b:84:GLU:OE1	33:1b:216:SER:HA	2.19	0.42
39:1h:98:LYS:HB2	39:1h:98:LYS:HE3	1.73	0.42
41:1j:54:PHE:CD2	41:1j:55:LYS:HG2	2.54	0.42
1:2A:484:C:H2'	1:2A:485:C:C6	2.54	0.42
1:2A:631:A:H2'	1:2A:632:A:O4'	2.18	0.42
1:2A:859:G:O2'	1:2A:916:G:O6	2.36	0.42
1:2A:1026:U:OP1	61:2A:3911:HOH:O	2.21	0.42
1:2A:1321:A:H2'	1:2A:1322:A:C8	2.54	0.42
1:2A:1354:A:H5''	3:2D:38:LYS:HD3	2.01	0.42
1:2A:1580:A:H8	1:2A:1580:A:OP2	2.02	0.42
1:2A:1810:A:H2'	1:2A:1811:G:O4'	2.19	0.42
1:2A:2162:G:H2'	1:2A:2163:C:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:17:C:H2'	2:2B:18:G:O4'	2.19	0.42
7:2H:33:LEU:HD21	7:2H:136:ILE:HB	2.00	0.42
10:2O:63:VAL:HG12	10:2O:106:LEU:HD11	2.00	0.42
10:2O:96:THR:O	10:2O:117:LEU:HD22	2.19	0.42
10:2O:103:ALA:HB1	10:2O:105:GLU:OE1	2.19	0.42
32:2a:501:C:H2'	32:2a:502:G:H8	1.84	0.42
32:2a:1342:C:H4'	40:2i:125:TYR:HB3	2.01	0.42
33:2b:149:LEU:HD22	33:2b:152:PHE:HD2	1.84	0.42
1:1A:1053:C:H42	1:1A:1106:G:H1	1.68	0.42
1:1A:1094:U:H1'	1:1A:1097:U:C4	2.54	0.42
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.54	0.42
1:1A:1972:A:H2'	1:1A:1973:G:H8	1.83	0.42
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.52	0.42
1:1A:2888:C:H2'	1:1A:2889:C:C6	2.53	0.42
5:1F:144:LYS:HE3	5:1F:144:LYS:HB3	1.64	0.42
6:1G:25:TYR:HB3	6:1G:30:GLU:HB2	2.00	0.42
21:1Z:125:LEU:HG	21:1Z:164:ALA:HB3	2.00	0.42
26:14:41:PRO:HG3	26:14:49:PHE:CE2	2.54	0.42
32:1a:186:C:H2'	32:1a:187:C:C6	2.54	0.42
33:1b:108:ILE:O	33:1b:111:ARG:HB2	2.19	0.42
34:1c:63:ASN:HB3	34:1c:98:ASN:HD22	1.84	0.42
35:1d:107:ARG:NH2	35:1d:194:LEU:HD11	2.34	0.42
49:1r:25:THR:O	49:1r:26:LEU:HD12	2.19	0.42
52:1u:3:LYS:HB3	52:1u:14:TRP:CG	2.54	0.42
54:1w:48:C:C2	54:1w:59:U:H1'	2.54	0.42
1:2A:284:U:H2'	1:2A:285:C:C6	2.54	0.42
1:2A:2143:C:N4	1:2A:2148:G:H1	2.12	0.42
26:24:57:GLU:CB	26:24:58:ARG:HA	2.49	0.42
32:2a:397:A:H3'	32:2a:397:A:N3	2.34	0.42
32:2a:454:C:H5''	32:2a:455:C:OP2	2.19	0.42
32:2a:1120:G:C6	32:2a:1121:U:C4	3.08	0.42
32:2a:1469:G:H2'	32:2a:1470:G:C8	2.54	0.42
33:2b:178:ARG:O	39:2h:72:PRO:HD3	2.19	0.42
45:2n:37:PHE:HZ	45:2n:56:VAL:HG21	1.84	0.42
51:2t:18:GLN:O	51:2t:22:ARG:HG3	2.19	0.42
1:1A:839:U:H2'	1:1A:840:C:C6	2.54	0.42
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.54	0.42
1:1A:1814:G:C4'	3:1D:51:VAL:HG21	2.48	0.42
1:1A:2074:U:H2'	1:1A:2075:U:C6	2.54	0.42
1:1A:2119:A:O2'	1:1A:2120:G:H5''	2.19	0.42
3:1D:69:ARG:C	3:1D:71:ASP:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:48:GLN:HE21	4:1E:78:LEU:HD22	1.85	0.42
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	2.01	0.42
32:1a:945:G:OP1	61:1a:1914:HOH:O	2.21	0.42
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.54	0.42
32:1a:1486:G:H2'	32:1a:1487:G:O4'	2.19	0.42
34:1c:71:ALA:HA	34:1c:106:VAL:HG21	2.01	0.42
38:1g:26:PHE:CE2	38:1g:30:ILE:HD11	2.54	0.42
1:2A:48:G:O2'	1:2A:118:A:N1	2.47	0.42
1:2A:127:A:H5''	1:2A:128:C:C6	2.54	0.42
1:2A:1630:G:H2'	1:2A:1631:C:C6	2.54	0.42
1:2A:2038:G:H2'	1:2A:2039:C:O4'	2.18	0.42
1:2A:2483:C:H2'	1:2A:2484:G:O4'	2.19	0.42
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.55	0.42
1:2A:2675:A:H5'	10:2O:29:ASN:O	2.19	0.42
1:2A:2886:G:H2'	1:2A:2887:U:H6	1.84	0.42
8:2I:82:ARG:CZ	8:2I:82:ARG:H	2.31	0.42
9:2N:99:LEU:O	9:2N:103:VAL:HG23	2.19	0.42
9:2N:123:TYR:CZ	9:2N:129:PRO:HD2	2.54	0.42
15:2T:26:ASP:OD1	15:2T:120:ARG:NH2	2.32	0.42
21:2Z:39:VAL:HG21	21:2Z:44:PHE:HB2	2.00	0.42
22:20:18:ALA:HB3	22:20:20:ARG:NH1	2.34	0.42
22:20:53:MET:HG3	22:20:59:LEU:HD23	2.00	0.42
32:2a:552:U:H4'	43:2l:86:ARG:HD2	2.01	0.42
32:2a:748:C:H4'	32:2a:749:C:O5'	2.19	0.42
33:2b:52:GLU:HG2	33:2b:56:ARG:HH12	1.84	0.42
35:2d:18:LYS:HD3	35:2d:20:TYR:OH	2.19	0.42
35:2d:180:GLY:HA3	35:2d:182:LYS:HE3	2.01	0.42
36:2e:105:VAL:HB	36:2e:106:PRO:HD3	2.01	0.42
36:2e:110:LEU:HD21	36:2e:139:LEU:HD21	2.00	0.42
41:2j:9:ARG:HB3	41:2j:10:GLY:H	1.66	0.42
41:2j:44:VAL:HG22	41:2j:66:ARG:HB3	2.01	0.42
44:2m:115:LYS:HE2	44:2m:115:LYS:HB2	1.85	0.42
51:2t:22:ARG:NH2	61:2t:301:HOH:O	2.53	0.42
1:1A:484:C:OP1	20:1Y:51:VAL:HG22	2.19	0.42
1:1A:1113:U:H2'	1:1A:1114:G:H8	1.84	0.42
1:1A:1138:G:H2'	1:1A:1139:G:O4'	2.20	0.42
1:1A:1827:C:O2'	1:1A:1970:A:N3	2.46	0.42
1:1A:2037:G:H2'	1:1A:2038:G:C8	2.55	0.42
8:1I:5:LEU:HD11	8:1I:19:VAL:HG13	2.01	0.42
32:1a:625:G:H2'	32:1a:626:U:C6	2.55	0.42
32:1a:738:C:H2'	32:1a:739:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1318:A:H1'	50:1s:37:ARG:NH1	2.34	0.42
35:1d:155:LEU:HD12	35:1d:155:LEU:HA	1.81	0.42
39:1h:87:SER:HA	39:1h:93:VAL:HG23	2.01	0.42
40:1i:70:LYS:O	40:1i:74:ILE:HG13	2.20	0.42
1:2A:1032:A:H2	1:2A:1122:G:H22	1.66	0.42
1:2A:1834:U:H4'	1:2A:1969:A:C6	2.54	0.42
1:2A:2136:C:O2'	1:2A:2137:C:H6	2.02	0.42
1:2A:2758:A:OP2	61:2A:3957:HOH:O	2.22	0.42
1:2A:2885:C:O2'	27:25:34:PRO:HG3	2.19	0.42
7:2H:3:ARG:HH22	7:2H:65:HIS:HB3	1.84	0.42
18:2W:17:VAL:HG11	18:2W:103:ILE:HD11	2.02	0.42
24:22:2:LYS:O	24:22:6:VAL:HG23	2.19	0.42
31:29:22:ARG:HD3	31:29:35:ARG:HD2	2.01	0.42
32:2a:517:G:N3	32:2a:531:U:H5'	2.35	0.42
32:2a:615:C:H2'	32:2a:616:G:O4'	2.19	0.42
32:2a:779:C:O2'	42:2k:120:ARG:HD3	2.19	0.42
32:2a:1189:C:OP1	34:2c:5:ILE:HD12	2.19	0.42
32:2a:1260:C:O5'	32:2a:1284:C:H4'	2.19	0.42
33:2b:215:LEU:HD23	33:2b:215:LEU:HA	1.78	0.42
46:2o:64:ARG:HH11	46:2o:68:ARG:HH21	1.66	0.42
47:2p:43:LYS:HG2	47:2p:48:TRP:CG	2.54	0.42
54:2y:51:U:H2'	54:2y:52:G:C8	2.55	0.42
1:1A:336:C:O2'	20:1Y:35:TYR:OH	2.31	0.42
1:1A:568:U:O5'	1:1A:945:A:N6	2.52	0.42
1:1A:1209:G:OP2	61:1A:4155:HOH:O	2.22	0.42
1:1A:1664:A:OP1	61:1A:4153:HOH:O	2.21	0.42
1:1A:1794:U:H2'	1:1A:1795:C:H6	1.83	0.42
1:1A:1881:C:H2'	1:1A:1882:C:C6	2.53	0.42
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.54	0.42
18:1W:14:PRO:HA	18:1W:17:VAL:HG23	2.01	0.42
25:13:3:ARG:HB2	25:13:59:VAL:HG23	2.01	0.42
32:1a:828:A:OP1	39:1h:21:LYS:NZ	2.41	0.42
32:1a:922:G:C6	32:1a:923:A:C6	3.08	0.42
32:1a:1083:U:OP1	61:1a:1913:HOH:O	2.21	0.42
35:1d:17:VAL:HG12	35:1d:19:LEU:HD13	2.01	0.42
1:2A:515:A:H1'	1:2A:581:C:H1'	2.01	0.42
1:2A:826:U:H5''	1:2A:2428:G:O3'	2.20	0.42
1:2A:947:G:H2'	1:2A:948:G:C8	2.54	0.42
1:2A:962:G:OP1	61:2A:3903:HOH:O	2.22	0.42
1:2A:1759:A:H1'	1:2A:2711:A:C2	2.55	0.42
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:69:ARG:NH1	3:2D:128:GLY:O	2.35	0.42
8:2I:62:LYS:HA	8:2I:133:HIS:CE1	2.53	0.42
11:2P:83:VAL:O	11:2P:115:LEU:N	2.40	0.42
12:2Q:138:ASP:OD2	21:2Z:81:ARG:NH1	2.52	0.42
15:2T:105:LEU:HB2	15:2T:110:ILE:HG13	2.02	0.42
32:2a:340:U:H2'	32:2a:341:C:C6	2.55	0.42
32:2a:403:C:H2'	32:2a:404:U:H6	1.84	0.42
32:2a:452:A:HO2'	32:2a:453:A:H8	1.66	0.42
32:2a:757:U:H2'	32:2a:758:G:O4'	2.19	0.42
32:2a:1095:U:H2'	32:2a:1096:C:C6	2.54	0.42
32:2a:1216:G:H5''	45:2n:5:ALA:HB2	2.00	0.42
34:2c:139:GLN:O	34:2c:143:GLU:HB2	2.20	0.42
44:2m:59:TYR:HD2	44:2m:60:VAL:HG23	1.83	0.42
44:2m:79:LYS:HB3	44:2m:79:LYS:HE3	1.94	0.42
1:1A:303:U:H2'	1:1A:304:G:H8	1.84	0.42
1:1A:303:U:H2'	1:1A:304:G:C8	2.54	0.42
1:1A:478:A:C6	1:1A:480:A:C6	3.07	0.42
1:1A:1027:A:C6	1:1A:1126:A:C4	3.07	0.42
1:1A:1999:C:H4'	1:1A:2723:C:O2	2.19	0.42
1:1A:2137:C:H2'	1:1A:2138:C:C6	2.54	0.42
4:1E:9:VAL:HG13	15:1T:3:ARG:HG2	2.02	0.42
4:1E:54:GLN:HG2	4:1E:59:VAL:HG12	2.02	0.42
8:1I:72:LEU:HD23	8:1I:72:LEU:HA	1.81	0.42
32:1a:271:C:H2'	32:1a:272:C:C6	2.54	0.42
32:1a:332:G:H2'	32:1a:333:G:H8	1.84	0.42
32:1a:456:C:H2'	32:1a:457:C:C6	2.55	0.42
32:1a:688:G:H2'	32:1a:689:C:C6	2.55	0.42
32:1a:1456:G:O3'	51:1t:39:LYS:NZ	2.52	0.42
33:1b:97:TRP:HZ3	33:1b:176:GLU:OE2	2.02	0.42
35:1d:173:TRP:CE2	35:1d:189:PRO:HG3	2.53	0.42
37:1f:42:GLU:OE2	37:1f:59:TYR:OH	2.24	0.42
38:1g:115:ARG:HG3	38:1g:118:VAL:CG2	2.49	0.42
54:1y:66:U:C4	54:1y:67:C:C4	3.08	0.42
1:2A:30:G:H2'	1:2A:31:C:C6	2.55	0.42
1:2A:271(O):C:H2'	1:2A:271(P):C:C6	2.53	0.42
1:2A:315:G:H2'	1:2A:316:C:C6	2.55	0.42
2:2B:78:A:C2	2:2B:100:A:C4	3.08	0.42
3:2D:24:ILE:HD11	3:2D:84:TYR:HB2	2.02	0.42
4:2E:36:ARG:NH2	4:2E:88:GLY:O	2.52	0.42
7:2H:26:VAL:O	7:2H:32:GLU:HA	2.19	0.42
21:2Z:59:LEU:HD11	21:2Z:88:PHE:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:26:35:GLU:HG2	28:26:50:ARG:HD3	2.01	0.42
32:2a:571:U:O4	32:2a:864:A:N6	2.52	0.42
32:2a:1073:U:H2'	32:2a:1074:G:H8	1.85	0.42
32:2a:1247:U:H1'	32:2a:1291:G:N2	2.34	0.42
32:2a:1326:C:H2'	32:2a:1327:C:H6	1.85	0.42
32:2a:1326:C:OP1	52:2u:17:THR:OG1	2.37	0.42
1:1A:443:A:H5''	1:1A:444:C:OP1	2.20	0.42
1:1A:749:C:H4'	1:1A:1271:G:N3	2.35	0.42
1:1A:818:G:H4'	1:1A:838:C:O3'	2.19	0.42
1:1A:2470:G:OP1	12:1Q:56:ARG:NH2	2.53	0.42
2:1B:90:A:C5	2:1B:91:C:H1'	2.55	0.42
3:1D:92:ILE:HD12	3:1D:104:TYR:CD1	2.54	0.42
18:1W:25:ARG:NH2	18:1W:74:ALA:O	2.44	0.42
20:1Y:5:MET:HE2	20:1Y:5:MET:HB2	1.90	0.42
20:1Y:13:VAL:HB	20:1Y:72:VAL:HG13	2.01	0.42
32:1a:6:G:H4'	32:1a:298:A:H4'	2.00	0.42
32:1a:892:A:H2'	32:1a:893:C:C6	2.54	0.42
32:1a:1239:A:C4	32:1a:1298:C:N4	2.88	0.42
33:1b:19:HIS:CG	33:1b:20:GLU:N	2.87	0.42
33:1b:21:ARG:HB3	33:1b:38:GLY:O	2.19	0.42
38:1g:91:VAL:HB	38:1g:96:GLN:HG2	2.02	0.42
42:1k:91:ARG:NH1	42:1k:110:ASP:OD1	2.52	0.42
47:1p:29:ASP:OD1	47:1p:29:ASP:N	2.52	0.42
54:1y:58:A:O2'	54:1y:60:U:OP2	2.35	0.42
1:2A:143(A):C:H4'	19:2X:38:GLU:OE2	2.19	0.42
1:2A:754:C:H2'	1:2A:755:C:C6	2.55	0.42
1:2A:880:G:C2	1:2A:881:G:C8	3.07	0.42
1:2A:1750:G:N3	1:2A:2860:A:H2	2.17	0.42
1:2A:2138:C:H2'	1:2A:2139:C:O4'	2.19	0.42
1:2A:2896:C:C2	1:2A:2897:U:H5	2.38	0.42
6:2G:101:ILE:HG22	6:2G:105:LYS:HE2	2.00	0.42
7:2H:71:LEU:HA	7:2H:71:LEU:HD23	1.73	0.42
14:2S:80:LEU:HD12	14:2S:80:LEU:HA	1.91	0.42
32:2a:1509:C:H2'	32:2a:1510:U:O4'	2.19	0.42
33:2b:212:GLN:CD	33:2b:235:SER:HG	2.21	0.42
47:2p:17:TYR:HE2	47:2p:41:PRO:HG3	1.84	0.42
1:1A:1054:A:C6	1:1A:1055:G:C6	3.07	0.42
1:1A:1084:A:H2'	1:1A:1085:A:O4'	2.19	0.42
1:1A:1424:G:H2'	1:1A:1425:G:O4'	2.20	0.42
61:1A:5878:HOH:O	13:1R:31:HIS:HD2	2.03	0.42
11:1P:38:GLN:O	11:1P:39:LYS:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:93:ASP:HB3	21:1Z:131:ARG:HH22	1.85	0.42
26:14:69:LYS:HD2	26:14:69:LYS:HA	1.63	0.42
32:1a:176:C:H2'	32:1a:177:C:C6	2.55	0.42
32:1a:1206:G:H2'	32:1a:1207:2MG:O4'	2.19	0.42
32:1a:1269:A:H2	32:1a:1312:G:N3	2.17	0.42
32:1a:1465:C:H2'	32:1a:1466:C:O4'	2.20	0.42
53:1v:16:A:H2'	53:1v:17:U:O4'	2.19	0.42
1:2A:121:G:H4'	1:2A:149:A:H5'	2.01	0.42
1:2A:263:C:H2'	1:2A:264:C:O4'	2.20	0.42
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.19	0.42
1:2A:536:A:H2'	1:2A:537:C:C6	2.55	0.42
1:2A:1721:G:H2'	1:2A:1740:G:O6	2.19	0.42
1:2A:2108:C:N4	1:2A:2181:G:H1	2.17	0.42
1:2A:2291:U:OP1	1:2A:2380:C:O2'	2.36	0.42
1:2A:2317:C:N3	1:2A:2318:G:N7	2.68	0.42
4:2E:111:ARG:HG3	13:2R:1:MET:SD	2.59	0.42
5:2F:148:LEU:HD11	5:2F:193:VAL:HG21	2.02	0.42
6:2G:16:ARG:NE	6:2G:31:VAL:HG11	2.35	0.42
6:2G:41:GLN:HE21	6:2G:153:ARG:HB3	1.84	0.42
7:2H:102:ALA:HB2	7:2H:116:GLU:OE1	2.20	0.42
10:2O:25:LEU:HD23	10:2O:25:LEU:HA	1.89	0.42
19:2X:5:TYR:CE2	24:22:30:ARG:HB2	2.55	0.42
32:2a:1265:G:C6	32:2a:1266:G:C5	3.08	0.42
38:2g:132:GLY:O	38:2g:136:LYS:HG2	2.20	0.42
47:2p:53:VAL:HG13	47:2p:79:VAL:HG22	2.02	0.42
1:1A:459:U:H5''	29:17:40:TRP:CD2	2.55	0.42
1:1A:643:A:N1	1:1A:2369:A:O2'	2.51	0.42
1:1A:910:A:N3	1:1A:2264:C:O2'	2.47	0.42
1:1A:1540:U:H2'	1:1A:1541:G:O4'	2.19	0.42
1:1A:2615:U:H2'	1:1A:2616:C:H6	1.85	0.42
10:1O:49:ARG:HH12	32:1a:1423:G:P	2.43	0.42
25:13:8:LEU:HA	25:13:54:VAL:HG23	2.02	0.42
32:1a:308:C:H2'	32:1a:309:G:H8	1.85	0.42
32:1a:551:U:H2'	32:1a:552:U:C6	2.55	0.42
32:1a:1513:A:H2'	32:1a:1514:C:C6	2.55	0.42
33:1b:121:LEU:HD23	33:1b:138:LEU:HD13	2.02	0.42
36:1e:15:ARG:HD2	36:1e:26:PHE:CD1	2.55	0.42
39:1h:9:MET:HG3	39:1h:26:VAL:HG21	2.01	0.42
47:1p:57:ARG:O	47:1p:61:SER:HB3	2.18	0.42
1:2A:197:A:N6	1:2A:2430:A:H2'	2.34	0.42
1:2A:271(K):U:O2	8:2I:50:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:358:U:H2'	1:2A:359:A:C8	2.54	0.42
1:2A:783:A:OP2	61:2A:3956:HOH:O	2.22	0.42
1:2A:885:C:H2'	1:2A:886:C:O4'	2.19	0.42
1:2A:1031:G:N2	31:29:36:GLN:HE22	2.16	0.42
5:2F:126:VAL:HG21	5:2F:129:PHE:CZ	2.54	0.42
6:2G:15:VAL:HG13	6:2G:175:LEU:HB2	2.01	0.42
7:2H:46:GLU:N	7:2H:49:VAL:O	2.51	0.42
21:2Z:159:PRO:HA	21:2Z:161:VAL:HG12	2.02	0.42
25:23:2:PRO:HB2	25:23:3:ARG:H	1.62	0.42
32:2a:429:U:H1'	32:2a:430:A:H5''	2.02	0.42
32:2a:529:G:O6	43:2l:49:ASN:HA	2.20	0.42
32:2a:737:A:H2'	32:2a:738:C:H6	1.83	0.42
32:2a:1004:A:C8	32:2a:1025:U:O4	2.73	0.42
34:2c:119:ARG:HE	34:2c:140:ARG:NH2	2.18	0.42
36:2e:83:GLU:HA	36:2e:88:LYS:HA	2.02	0.42
42:2k:54:ARG:NH1	54:2y:39:PSU:O2'	2.53	0.42
50:2s:80:TYR:O	50:2s:81:ARG:HG2	2.19	0.42
1:1A:783:A:N3	1:1A:783:A:H2'	2.35	0.42
1:1A:1058:G:N2	1:1A:1080:C:N3	2.67	0.42
1:1A:1614:A:P	1:1A:1614:A:H8	2.43	0.42
1:1A:2144:U:H3'	1:1A:2146:C:N4	2.35	0.42
1:1A:2579:C:O5'	1:1A:2579:C:H6	2.03	0.42
2:1B:96:U:H2'	2:1B:97:G:C8	2.55	0.42
11:1P:38:GLN:HG2	11:1P:45:LEU:H	1.84	0.42
18:1W:92:ARG:NH2	61:1W:303:HOH:O	2.53	0.42
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	2.02	0.42
32:1a:369:C:OP2	32:1a:388:G:N1	2.47	0.42
32:1a:448:A:C4	32:1a:487:A:C2	3.07	0.42
32:1a:1367:C:H5'	41:1j:60:ARG:NH1	2.34	0.42
32:1a:1464:G:H2'	32:1a:1465:C:C6	2.54	0.42
33:1b:13:ALA:HB2	33:1b:44:LEU:HD13	2.01	0.42
33:1b:37:ASN:C	33:1b:39:ILE:N	2.78	0.42
33:1b:122:PHE:HZ	33:1b:135:GLN:HG3	1.84	0.42
35:1d:26:CYS:CB	60:1d:302:SF4:S1	3.08	0.42
35:1d:65:ARG:NH1	35:1d:72:GLU:HB2	2.35	0.42
35:1d:158:ILE:H	35:1d:158:ILE:HG13	1.46	0.42
39:1h:21:LYS:O	39:1h:65:TYR:OH	2.34	0.42
50:1s:32:LYS:HB3	50:1s:32:LYS:HE2	1.73	0.42
1:2A:306:U:H2'	1:2A:307:G:O4'	2.20	0.42
1:2A:870:A:P	12:2Q:6:ARG:HH21	2.42	0.42
1:2A:884:C:H3'	1:2A:885:C:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1790:C:O2'	3:2D:209:ALA:HB2	2.20	0.42
1:2A:2161:C:H2'	1:2A:2162:G:O4'	2.20	0.42
3:2D:58:HIS:HD1	3:2D:59:LYS:N	2.18	0.42
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	2.01	0.42
6:2G:44:GLY:HA2	6:2G:88:ILE:HG22	2.01	0.42
7:2H:3:ARG:HH21	7:2H:54:ARG:NH1	2.18	0.42
32:2a:1305:G:H5'	52:2u:4:GLY:HA3	2.01	0.42
36:2e:31:LEU:HD11	36:2e:43:LEU:HD11	2.02	0.42
38:2g:69:VAL:HG11	38:2g:134:ALA:HB1	2.02	0.42
39:2h:41:ARG:NH2	39:2h:123:GLU:OE2	2.53	0.42
41:2j:42:THR:HG23	41:2j:68:HIS:HA	2.02	0.42
42:2k:92:GLU:HA	42:2k:95:ILE:HD12	2.01	0.42
43:2l:37:CYS:SG	43:2l:81:SER:HB2	2.60	0.42
43:2l:56:ALA:O	43:2l:68:ALA:N	2.40	0.42
47:2p:9:PHE:N	47:2p:16:HIS:O	2.46	0.42
47:2p:43:LYS:HG2	47:2p:48:TRP:CD1	2.55	0.42
1:1A:458:G:O2'	1:1A:469:G:O6	2.36	0.41
1:1A:893:C:H2'	1:1A:894:C:C6	2.55	0.41
1:1A:975(A):G:O2'	1:1A:1156:A:N1	2.49	0.41
1:1A:1712:C:H2'	1:1A:1713:U:O4'	2.20	0.41
1:1A:1796:U:H2'	1:1A:1797:C:H6	1.85	0.41
1:1A:2833:G:H8	1:1A:2833:G:OP1	2.03	0.41
2:1B:73:A:N1	21:1Z:34:ASN:ND2	2.67	0.41
3:1D:35:LYS:HB2	3:1D:36:PRO:HD2	2.02	0.41
11:1P:90:ARG:NH1	11:1P:105:LEU:HD11	2.34	0.41
25:13:18:ASP:OD1	25:13:18:ASP:N	2.53	0.41
32:1a:741:G:H2'	32:1a:742:G:O4'	2.20	0.41
32:1a:947:G:H4'	44:1m:109:THR:HG23	2.01	0.41
40:1i:51:ARG:CG	40:1i:56:LEU:HD11	2.46	0.41
44:1m:79:LYS:HA	44:1m:82:MET:HE3	2.02	0.41
45:1n:3:ARG:HH21	45:1n:3:ARG:HA	1.84	0.41
54:1w:18:G:H4'	54:1w:60:U:C5	2.54	0.41
1:2A:478:A:N1	1:2A:500:G:H4'	2.34	0.41
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.54	0.41
1:2A:1265:A:C8	1:2A:1267:U:C2	3.08	0.41
1:2A:1924:C:H4'	55:2x:13:C:O2'	2.20	0.41
1:2A:2365:G:O6	30:28:39:LYS:HE3	2.19	0.41
1:2A:2516:G:H1	1:2A:2568:C:H42	1.68	0.41
1:2A:2649:U:H2'	1:2A:2650:U:C6	2.55	0.41
21:2Z:73:GLN:H	21:2Z:87:ASP:HB2	1.85	0.41
32:2a:359:U:H2'	32:2a:360:A:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:841:U:H6	32:2a:841:U:P	2.43	0.41
36:2e:7:GLU:OE2	36:2e:37:ARG:NH2	2.42	0.41
38:2g:125:MET:O	38:2g:129:GLU:HG2	2.19	0.41
1:1A:1368:G:C2	1:1A:1369:G:C8	3.08	0.41
1:1A:1570:A:H2'	1:1A:1571:A:C8	2.55	0.41
1:1A:1810:A:H2'	1:1A:1811:G:O4'	2.20	0.41
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	2.02	0.41
1:1A:2619:C:O2'	1:1A:2620:C:H5'	2.21	0.41
2:1B:31:C:H4'	6:1G:29:TRP:CH2	2.55	0.41
7:1H:121:ILE:HG12	7:1H:140:LYS:HD3	2.02	0.41
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.56	0.41
10:1O:2:ILE:HB	10:1O:33:ALA:HB3	2.01	0.41
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.55	0.41
17:1V:55:ALA:HA	17:1V:101:GLY:CA	2.43	0.41
25:13:39:ASP:OD1	25:13:44:ARG:HD2	2.19	0.41
32:1a:21:G:H2'	32:1a:22:G:C8	2.55	0.41
32:1a:36:C:H2'	32:1a:37:U:O4'	2.20	0.41
32:1a:1142:G:H2'	32:1a:1143:G:O4'	2.20	0.41
34:1c:24:ALA:HB2	34:1c:32:LEU:HD22	2.01	0.41
36:1e:95:ALA:HB1	36:1e:96:PRO:HD2	2.01	0.41
38:1g:103:TRP:HZ3	38:1g:138:LYS:HA	1.85	0.41
1:2A:1270:C:H5''	1:2A:1271:G:O5'	2.20	0.41
1:2A:1561:G:H2'	1:2A:1562:A:C8	2.54	0.41
1:2A:1919:A:O3'	32:2a:1517:G:H1'	2.20	0.41
1:2A:2135:A:C8	1:2A:2136:C:H5	2.38	0.41
1:2A:2740:A:C6	1:2A:2741:A:C6	3.08	0.41
1:2A:2887:U:H2'	1:2A:2888:C:H6	1.85	0.41
2:2B:43:C:H5''	26:24:1:MET:HG2	2.02	0.41
3:2D:154:LYS:HB2	3:2D:155:LEU:HD22	2.02	0.41
8:2I:58:LEU:O	8:2I:62:LYS:N	2.51	0.41
12:2Q:1:MET:HB3	12:2Q:44:ALA:HB1	2.01	0.41
15:2T:82:LEU:H	15:2T:82:LEU:HD12	1.84	0.41
27:25:20:ARG:HG2	27:25:23:HIS:ND1	2.35	0.41
32:2a:397:A:H5'	32:2a:398:C:OP1	2.20	0.41
32:2a:434:U:H2'	32:2a:435:C:C6	2.56	0.41
32:2a:827:U:C2	32:2a:874:G:N2	2.88	0.41
32:2a:853:G:H2'	32:2a:854:G:H8	1.86	0.41
32:2a:883:C:C2'	32:2a:884:U:H5'	2.50	0.41
32:2a:985:C:H2'	32:2a:986:A:C8	2.56	0.41
32:2a:1105:A:H2'	32:2a:1106:G:H8	1.85	0.41
33:2b:147:LYS:HG2	33:2b:148:TYR:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:110:ALA:HB3	39:2h:121:ASP:HB3	2.01	0.41
1:1A:601:C:O2'	1:1A:605:C:H5''	2.21	0.41
1:1A:857:C:N4	1:1A:858:U:O4	2.53	0.41
1:1A:1045:A:OP1	1:1A:1045:A:H4'	2.19	0.41
1:1A:1557:C:H5''	1:1A:1558:A:OP2	2.21	0.41
1:1A:2104:G:H2'	1:1A:2105:C:C6	2.55	0.41
1:1A:2181:G:HO2'	1:1A:2182:G:P	2.43	0.41
1:1A:2723:C:OP1	13:1R:3:HIS:ND1	2.53	0.41
8:1I:77:LEU:HD12	8:1I:97:ILE:HG23	2.01	0.41
19:1X:2:LYS:HD2	19:1X:2:LYS:HA	1.84	0.41
32:1a:748:C:O5'	32:1a:748:C:H6	2.03	0.41
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.56	0.41
35:1d:190:ASP:OD1	35:1d:190:ASP:N	2.52	0.41
46:1o:10:LYS:HB2	46:1o:10:LYS:HE3	1.68	0.41
1:2A:271(A):A:H8	1:2A:271(B):C:C6	2.38	0.41
1:2A:1857:G:C6	1:2A:1858:G:C6	3.08	0.41
1:2A:2347:C:H2'	1:2A:2348:U:C6	2.54	0.41
1:2A:2652:C:H2'	1:2A:2653:U:O4'	2.20	0.41
7:2H:3:ARG:HE	7:2H:54:ARG:HH12	1.69	0.41
9:2N:35:ARG:O	9:2N:42:TRP:NE1	2.52	0.41
17:2V:16:PRO:HG3	17:2V:99:ILE:HG13	2.02	0.41
20:2Y:20:TYR:CE2	20:2Y:43:ASN:HA	2.55	0.41
32:2a:114:U:O2'	32:2a:115:G:H5'	2.20	0.41
32:2a:391:G:C6	32:2a:392:G:C5	3.08	0.41
32:2a:945:G:C2	32:2a:946:A:C8	3.08	0.41
32:2a:1256:A:N1	32:2a:1278:U:H1'	2.35	0.41
33:2b:67:THR:HA	33:2b:90:MET:HE1	2.00	0.41
33:2b:230:VAL:HG12	33:2b:231:GLU:H	1.85	0.41
46:2o:64:ARG:HH11	46:2o:68:ARG:NH2	2.18	0.41
50:2s:50:ALA:HA	50:2s:59:PRO:HA	2.02	0.41
54:2w:74:C:C4	54:2w:75:C:C2	3.09	0.41
1:1A:576:U:H2'	1:1A:577:G:C8	2.56	0.41
1:1A:1152:C:H4'	16:1U:77:SER:HA	2.03	0.41
1:1A:2499:C:N3	61:1A:4257:HOH:O	2.37	0.41
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.56	0.41
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.19	0.41
3:1D:72:LYS:HB3	3:1D:75:ILE:HD12	2.02	0.41
3:1D:141:VAL:HG13	3:1D:162:SER:HB2	2.02	0.41
8:1I:33:ARG:C	8:1I:35:LEU:H	2.29	0.41
8:1I:77:LEU:HD13	8:1I:79:ILE:HD11	2.02	0.41
13:1R:65:LEU:HD23	13:1R:65:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1070:U:H2'	32:1a:1071:C:H6	1.85	0.41
32:1a:1346:A:OP1	40:1i:120:ARG:NH1	2.28	0.41
35:1d:107:ARG:HA	35:1d:107:ARG:HD2	1.88	0.41
35:1d:107:ARG:HH22	35:1d:194:LEU:HD11	1.85	0.41
45:1n:27:CYS:SG	45:1n:29:ARG:HB2	2.60	0.41
54:1w:5:G:H2'	54:1w:6:G:H8	1.82	0.41
1:2A:84:A:N1	1:2A:98:G:O2'	2.41	0.41
1:2A:652(B):A:N6	1:2A:655:A:O2'	2.50	0.41
1:2A:817:C:H2'	1:2A:818:G:O4'	2.20	0.41
1:2A:839:U:H2'	1:2A:840:C:H6	1.84	0.41
1:2A:1539:G:H2'	1:2A:1540:U:O4'	2.20	0.41
1:2A:1812:A:H5''	61:2A:3906:HOH:O	2.21	0.41
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.55	0.41
1:2A:2807:G:C2	1:2A:2893:G:O6	2.73	0.41
5:2F:11:VAL:HA	5:2F:125:LEU:O	2.21	0.41
6:2G:11:TYR:HB2	6:2G:176:LEU:HD21	2.00	0.41
11:2P:81:GLN:NE2	11:2P:105:LEU:O	2.49	0.41
12:2Q:78:PRO:HG2	12:2Q:81:VAL:HG11	2.03	0.41
19:2X:59:VAL:N	19:2X:76:ARG:O	2.46	0.41
30:28:62:LEU:HB3	30:28:65:GLU:HG2	2.02	0.41
32:2a:255:G:H4'	48:2q:17:LYS:HE3	2.03	0.41
32:2a:446:G:O6	61:2a:1914:HOH:O	2.21	0.41
32:2a:755:G:OP2	46:2o:65:ARG:HD2	2.20	0.41
32:2a:989:C:H42	32:2a:1216:G:H1	1.67	0.41
32:2a:1074:G:H1	32:2a:1083:U:H3	1.67	0.41
32:2a:1327:C:OP2	52:2u:12:LYS:NZ	2.46	0.41
32:2a:1478:C:H2'	32:2a:1479:C:C6	2.53	0.41
34:2c:6:HIS:HB3	45:2n:49:HIS:CD2	2.55	0.41
44:2m:122:LYS:HD2	44:2m:122:LYS:HA	1.94	0.41
54:2y:8:4SU:H2'	54:2y:46:G7M:N2	2.35	0.41
54:2y:28:G:H2'	54:2y:29:G:H8	1.85	0.41
1:1A:78:A:H2'	1:1A:79:G:C8	2.55	0.41
1:1A:139(A):G:O2'	1:1A:140:G:H5'	2.21	0.41
1:1A:479:A:N3	1:1A:481:G:H5''	2.35	0.41
2:1B:78:A:C2	2:1B:100:A:C4	3.07	0.41
3:1D:118:VAL:HG22	3:1D:119:ALA:H	1.85	0.41
7:1H:149:ARG:HH12	7:1H:167:GLU:CD	2.28	0.41
21:1Z:103:ARG:O	21:1Z:138:GLU:HA	2.21	0.41
32:1a:167:G:H2'	32:1a:168:G:C8	2.55	0.41
32:1a:625:G:H4'	47:1p:16:HIS:CD2	2.55	0.41
32:1a:791:G:N2	32:1a:1497:G:O3'	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:814:A:H2'	32:1a:816:A:H5''	2.03	0.41
32:1a:957:U:O2'	32:1a:959:A:N7	2.46	0.41
32:1a:973:G:H3'	32:1a:974:A:H5''	2.03	0.41
32:1a:1006:C:N3	32:1a:1023:G:N2	2.66	0.41
32:1a:1251:A:H2'	32:1a:1252:A:C8	2.54	0.41
32:1a:1264:C:H2'	32:1a:1265:G:C8	2.55	0.41
38:1g:15:ASP:O	38:1g:19:GLY:HA2	2.20	0.41
1:2A:16:G:H2'	1:2A:17:G:H8	1.86	0.41
1:2A:422:A:H2'	1:2A:423:A:C8	2.56	0.41
1:2A:2376:A:N3	14:2S:106:ARG:NH2	2.68	0.41
1:2A:2533:A:OP1	1:2A:2665:A:O2'	2.29	0.41
1:2A:2577:A:OP2	27:25:3:LYS:NZ	2.52	0.41
1:2A:2749:A:H3'	1:2A:2750:A:H2'	2.01	0.41
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.85	0.41
12:2Q:1:MET:HE3	12:2Q:1:MET:H3	1.86	0.41
20:2Y:43:ASN:CG	20:2Y:65:ALA:HB3	2.46	0.41
26:24:40:HIS:HB3	26:24:43:TYR:HB2	2.01	0.41
32:2a:309:G:H1'	32:2a:608:A:C2	2.56	0.41
32:2a:435:C:H2'	32:2a:436:C:C6	2.56	0.41
54:2w:18:G:H4'	54:2w:60:U:C5	2.55	0.41
55:2x:8:4SU:O2	55:2x:21:A:H2	2.02	0.41
54:2y:37:MIA:H2'	54:2y:38:A:O4'	2.21	0.41
1:1A:324:A:H2'	1:1A:325:G:O4'	2.20	0.41
1:1A:668:G:OP2	61:1A:4154:HOH:O	2.22	0.41
1:1A:1048:A:OP2	1:1A:1109:C:N4	2.51	0.41
1:1A:1082:U:C4	1:1A:1086:A:N1	2.84	0.41
1:1A:1316:U:H2'	1:1A:1317:A:C8	2.55	0.41
1:1A:1930:G:O2'	1:1A:1968:G:O6	2.29	0.41
3:1D:4:LYS:HG2	3:1D:18:VAL:HG22	2.03	0.41
3:1D:72:LYS:HB3	3:1D:72:LYS:HE3	1.88	0.41
7:1H:83:TYR:CE2	7:1H:138:LYS:HB2	2.56	0.41
12:1Q:10:ARG:HH11	12:1Q:11:LYS:HE3	1.85	0.41
13:1R:10:LEU:HD13	13:1R:40:LYS:HG2	2.01	0.41
20:1Y:21:LYS:HE2	20:1Y:21:LYS:HB3	1.87	0.41
28:16:8:LYS:HB2	28:16:54:ILE:HD13	2.03	0.41
32:1a:1004:A:N6	32:1a:1036:G:N2	2.69	0.41
32:1a:1071:C:H2'	32:1a:1072:G:H8	1.85	0.41
32:1a:1084:G:C5	32:1a:1085:U:C4	3.09	0.41
33:1b:121:LEU:HA	33:1b:126:GLU:HG3	2.02	0.41
36:1e:102:ALA:HB1	36:1e:106:PRO:HB2	2.03	0.41
38:1g:45:ASP:O	38:1g:49:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1m:65:LYS:O	44:1m:70:LEU:HG	2.21	0.41
1:2A:6:A:N3	9:2N:133:GLN:NE2	2.66	0.41
1:2A:956:G:N2	1:2A:959:A:H3'	2.35	0.41
1:2A:1991:U:H2'	1:2A:1992:G:H5''	2.01	0.41
1:2A:2563:U:N3	1:2A:2566:A:OP2	2.46	0.41
3:2D:206:LEU:HD22	3:2D:211:ARG:HG2	2.03	0.41
4:2E:111:ARG:HA	13:2R:1:MET:SD	2.60	0.41
6:2G:16:ARG:HD2	6:2G:16:ARG:HA	1.87	0.41
11:2P:63:PRO:HG2	30:28:25:MET:HB2	2.02	0.41
21:2Z:77:ASP:OD1	21:2Z:80:ARG:NH1	2.53	0.41
32:2a:189(C):C:H2'	32:2a:189(D):C:O4'	2.21	0.41
32:2a:772:U:H2'	32:2a:773:G:O4'	2.21	0.41
32:2a:1015:A:H2'	32:2a:1016:A:C8	2.56	0.41
38:2g:108:ALA:HA	38:2g:111:ARG:HD2	2.02	0.41
54:2w:23:A:H2'	54:2w:24:G:C8	2.55	0.41
1:1A:213:A:H2'	1:1A:214:G:O4'	2.21	0.41
1:1A:748:G:OP1	1:1A:2612:C:N4	2.53	0.41
1:1A:1055:G:H2'	1:1A:1056:G:O4'	2.20	0.41
1:1A:2108:C:H2'	1:1A:2109:U:H6	1.85	0.41
1:1A:2156:G:OP2	1:1A:2156:G:H8	2.04	0.41
1:1A:2164:C:H2'	1:1A:2165:G:H5'	2.03	0.41
1:1A:2751:G:H4'	7:1H:4:ILE:HD11	2.02	0.41
3:1D:6:PHE:CE2	3:1D:18:VAL:HG13	2.55	0.41
8:1I:77:LEU:HB2	8:1I:142:VAL:HG12	2.01	0.41
10:1O:68:GLU:CB	10:1O:78:ARG:HB2	2.51	0.41
26:14:58:ARG:HD2	44:1m:80:ARG:NH1	2.36	0.41
26:14:61:ARG:O	26:14:62:ARG:C	2.63	0.41
32:1a:1218:C:OP2	45:1n:9:LYS:NZ	2.34	0.41
33:1b:70:PHE:HD2	33:1b:163:PHE:HB3	1.85	0.41
37:1f:61:LEU:HB3	37:1f:63:TYR:HE2	1.85	0.41
37:1f:82:ARG:HB2	37:1f:85:VAL:HG23	2.03	0.41
54:1w:28:G:H2'	54:1w:29:G:H8	1.86	0.41
1:2A:579:G:H2'	1:2A:580:C:C6	2.56	0.41
1:2A:631:A:N3	1:2A:2415:G:O2'	2.48	0.41
1:2A:647:G:O5'	1:2A:647:G:H8	2.04	0.41
1:2A:686:G:N2	1:2A:788:A:H61	2.18	0.41
1:2A:752:A:H3'	29:27:1:MET:HE1	2.03	0.41
1:2A:839:U:H1'	1:2A:1191:G:H1'	2.01	0.41
1:2A:942:G:O2'	1:2A:1189:A:N3	2.53	0.41
1:2A:1130:U:O2	4:2E:149:ARG:NH2	2.53	0.41
1:2A:1264:G:H2'	1:2A:2014:A:N6	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2888:C:H2'	1:2A:2889:C:C6	2.56	0.41
2:2B:80:U:H2'	2:2B:81:G:C8	2.55	0.41
11:2P:38:GLN:C	11:2P:40:SER:H	2.28	0.41
13:2R:87:TYR:OH	13:2R:116:LEU:HB3	2.20	0.41
14:2S:84:GLN:HA	14:2S:111:GLU:HB2	2.03	0.41
15:2T:65:LYS:HG2	15:2T:66:VAL:N	2.34	0.41
21:2Z:40:ASP:OD2	21:2Z:43:GLU:N	2.36	0.41
24:22:49:LYS:HB3	24:22:49:LYS:HE2	1.86	0.41
32:2a:107:G:H2'	32:2a:108:G:O4'	2.21	0.41
32:2a:636:U:H2'	32:2a:637:G:C8	2.56	0.41
32:2a:1221:G:O3'	50:2s:77:THR:OG1	2.37	0.41
33:2b:216:SER:C	33:2b:218:ALA:N	2.79	0.41
34:2c:131:ARG:HH21	36:2e:50:GLU:HG3	1.86	0.41
36:2e:131:ILE:HD13	36:2e:131:ILE:HA	1.89	0.41
1:1A:251:A:C5	1:1A:252:G:H1'	2.55	0.41
1:1A:613:G:N2	1:1A:614(C):A:O2'	2.54	0.41
1:1A:1274:A:N3	1:1A:1297:C:H1'	2.35	0.41
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.29	0.41
1:1A:2121:G:H2'	1:1A:2122:U:C6	2.55	0.41
1:1A:2291:U:OP1	1:1A:2380:C:O2'	2.34	0.41
1:1A:2871:C:H5''	1:1A:2872:G:OP1	2.20	0.41
7:1H:126:PRO:HD2	7:1H:130:ARG:O	2.21	0.41
9:1N:59:LYS:O	9:1N:61:ARG:NH2	2.53	0.41
16:1U:19:LYS:O	16:1U:22:LYS:HG3	2.21	0.41
32:1a:113:G:H2'	32:1a:114:U:C6	2.56	0.41
32:1a:299:G:H2'	32:1a:300:A:C8	2.55	0.41
32:1a:814:A:N7	32:1a:816:A:C4	2.89	0.41
32:1a:901:A:C5	32:1a:902:G:H1'	2.56	0.41
32:1a:1004:A:H61	32:1a:1036:G:N2	2.19	0.41
32:1a:1032:G:H2'	32:1a:1033:G:O4'	2.21	0.41
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.56	0.41
33:1b:24:TRP:H	33:1b:24:TRP:HD1	1.68	0.41
33:1b:163:PHE:HA	33:1b:185:ILE:O	2.19	0.41
44:1m:50:GLU:HA	44:1m:53:VAL:HG22	2.02	0.41
1:2A:723:G:H2'	1:2A:724:U:O4'	2.21	0.41
1:2A:1337:G:H2'	1:2A:1338:G:H8	1.86	0.41
1:2A:1472:A:H61	1:2A:1519:G:H1'	1.86	0.41
1:2A:1913:A:H4'	1:2A:1914:C:O5'	2.20	0.41
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.20	0.41
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.55	0.41
1:2A:2116:G:H2'	1:2A:2117:A:C2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:8:U:H3	2:2B:113:G:H1	1.69	0.41
13:2R:95:THR:HG22	13:2R:116:LEU:HD23	2.02	0.41
19:2X:9:LEU:HA	24:22:36:ARG:HH21	1.86	0.41
19:2X:26:TYR:O	19:2X:81:VAL:HG23	2.21	0.41
21:2Z:31:ARG:HD3	21:2Z:94:GLU:OE2	2.21	0.41
23:21:80:LEU:HD12	23:21:80:LEU:HA	1.89	0.41
32:2a:1291:G:C6	32:2a:1292:U:C4	3.09	0.41
34:2c:56:ASP:C	34:2c:57:ILE:HD12	2.46	0.41
43:2l:10:LEU:O	43:2l:14:GLY:N	2.53	0.41
1:1A:22:C:H2'	1:1A:23:G:O4'	2.21	0.41
1:1A:26:G:H1'	1:1A:515:A:H61	1.86	0.41
1:1A:27:G:C2	1:1A:512:G:N3	2.89	0.41
1:1A:84:A:H5'	20:1Y:8:LYS:HB3	2.03	0.41
1:1A:284:U:H2'	1:1A:285:C:C6	2.55	0.41
1:1A:667:U:O2	30:18:2:PRO:HD2	2.21	0.41
1:1A:930:U:H4'	1:1A:931:G:O5'	2.21	0.41
1:1A:1427:A:H4'	1:1A:1428:C:O4'	2.21	0.41
1:1A:1580:A:H5'	1:1A:1581:G:OP2	2.21	0.41
1:1A:1799:G:O2'	3:1D:181:GLU:OE2	2.39	0.41
1:1A:1866:C:H2'	1:1A:1876:A:O4'	2.21	0.41
1:1A:1903:G:OP1	3:1D:241:PRO:HB2	2.21	0.41
1:1A:2097:C:H2'	1:1A:2098:U:H6	1.86	0.41
1:1A:2466:C:C2	1:1A:2485:G:C2	3.08	0.41
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.56	0.41
1:1A:2756:U:H1'	1:1A:2757:A:H5''	2.03	0.41
1:1A:2790:A:H3'	1:1A:2790:A:N3	2.36	0.41
2:1B:11:C:OP2	22:10:72:ARG:NH2	2.42	0.41
3:1D:26:LYS:HD3	3:1D:83:GLU:OE2	2.21	0.41
4:1E:49:LEU:HD12	4:1E:49:LEU:HA	1.82	0.41
6:1G:39:ILE:HB	6:1G:92:VAL:HG12	2.01	0.41
7:1H:11:VAL:HA	7:1H:12:PRO:HD3	1.94	0.41
13:1R:38:VAL:HG12	13:1R:42:LYS:HE3	2.02	0.41
21:1Z:1:MET:HG3	21:1Z:55:HIS:HB3	2.02	0.41
21:1Z:36:LYS:HB2	21:1Z:36:LYS:HE3	1.89	0.41
32:1a:399:G:H2'	32:1a:400:C:C6	2.56	0.41
32:1a:955:U:O2'	50:1s:83:HIS:HD2	2.03	0.41
32:1a:1006:C:H42	32:1a:1023:G:H1	1.64	0.41
32:1a:1053:G:N7	32:1a:1200:C:H5''	2.36	0.41
32:1a:1121:U:H2'	32:1a:1122:U:C6	2.56	0.41
32:1a:1170:A:H2'	32:1a:1171:G:O4'	2.20	0.41
32:1a:1361:G:H2'	32:1a:1362:C:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1379:G:N2	32:1a:1381:U:O4	2.50	0.41
33:1b:30:ARG:NH2	33:1b:194:PRO:HB2	2.31	0.41
33:1b:127:ILE:HG13	33:1b:130:ARG:CZ	2.51	0.41
33:1b:230:VAL:HG22	33:1b:232:PRO:HD2	2.03	0.41
34:1c:16:ARG:HE	34:1c:16:ARG:HB3	1.72	0.41
37:1f:39:LYS:HE3	37:1f:39:LYS:HB3	1.71	0.41
37:1f:67:MET:HE3	37:1f:72:VAL:HG22	2.03	0.41
37:1f:91:VAL:HG11	49:1r:72:ARG:NH1	2.36	0.41
41:1j:38:ILE:HD11	41:1j:71:LEU:HD23	2.02	0.41
54:1w:56:C:H2'	54:1w:57:G:O4'	2.21	0.41
54:1w:66:U:H2'	54:1w:67:C:C6	2.56	0.41
1:2A:207:A:H2'	1:2A:208:C:O4'	2.21	0.41
1:2A:322:A:C5	1:2A:340:A:C2	3.09	0.41
1:2A:348:G:H2'	1:2A:349:G:C8	2.56	0.41
1:2A:403:U:H4'	1:2A:404:C:H5'	2.03	0.41
1:2A:659:C:H2'	1:2A:660:G:H8	1.85	0.41
1:2A:742:G:H2'	1:2A:743:G:H8	1.86	0.41
1:2A:1181:C:H2'	1:2A:1182:A:H8	1.85	0.41
1:2A:1341:U:O2	19:2X:80:ILE:HD12	2.20	0.41
1:2A:1541:G:H3'	1:2A:1542:A:H2'	2.02	0.41
1:2A:1721:G:H3'	1:2A:1722:A:H2'	2.03	0.41
1:2A:2110:G:OP1	1:2A:2118:U:N3	2.54	0.41
1:2A:2224:G:H4'	1:2A:2226:C:C2	2.56	0.41
1:2A:2619:C:OP1	4:2E:152:LYS:NZ	2.32	0.41
1:2A:2815:C:H2'	1:2A:2816:C:C6	2.56	0.41
1:2A:2820:A:C6	13:2R:4:LEU:HD11	2.56	0.41
2:2B:42:C:O2'	6:2G:66:GLN:HG2	2.21	0.41
4:2E:112:GLY:O	4:2E:159:HIS:HA	2.21	0.41
6:2G:131:TYR:O	6:2G:159:VAL:HG23	2.21	0.41
10:2O:36:GLY:HA2	10:2O:106:LEU:HD23	2.03	0.41
12:2Q:39:PRO:HD3	12:2Q:99:PRO:HG3	2.03	0.41
14:2S:15:ARG:O	14:2S:19:LYS:HG2	2.21	0.41
32:2a:227:G:H2'	32:2a:228:A:C8	2.56	0.41
32:2a:257:G:H2'	32:2a:258:G:O4'	2.21	0.41
32:2a:604:G:H2'	32:2a:605:U:O4'	2.21	0.41
33:2b:36:ARG:O	33:2b:39:ILE:HG13	2.21	0.41
33:2b:51:LEU:HD23	33:2b:51:LEU:HA	1.90	0.41
33:2b:211:ILE:O	33:2b:215:LEU:HB2	2.21	0.41
34:2c:20:SER:HB3	34:2c:22:TRP:NE1	2.32	0.41
34:2c:53:ALA:HB2	34:2c:115:LEU:HD21	2.03	0.41
35:2d:67:ILE:HD13	35:2d:196:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2g:80:VAL:HB	38:2g:85:TYR:CE2	2.53	0.41
40:2i:16:ARG:HB2	40:2i:64:THR:HG23	2.03	0.41
42:2k:27:ASN:OD1	42:2k:28:THR:N	2.48	0.41
43:2l:84:LEU:HB2	43:2l:105:TYR:HE2	1.85	0.41
46:2o:35:ARG:O	46:2o:39:LEU:HB2	2.21	0.41
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.45	0.41
54:2w:12:U:H2'	54:2w:13:C:H5''	2.02	0.41
54:2w:27:G:H2'	54:2w:28:G:H8	1.86	0.41
54:2y:42:C:H2'	54:2y:43:C:H6	1.85	0.41
1:1A:1090:U:O2	1:1A:1102:C:H1'	2.20	0.41
1:1A:1695:G:H1'	3:1D:8:PRO:O	2.21	0.41
1:1A:1920:OMC:HM22	1:1A:1921:G:O4'	2.20	0.41
1:1A:2056:G:C2	1:1A:2057:A:C8	3.09	0.41
1:1A:2206:G:OP1	3:1D:68:LYS:NZ	2.53	0.41
1:1A:2298:A:H2'	1:1A:2299:G:O4'	2.21	0.41
11:1P:100:LEU:HD22	11:1P:105:LEU:HD12	2.03	0.41
14:1S:34:HIS:O	14:1S:97:ARG:NH2	2.54	0.41
21:1Z:1:MET:CG	21:1Z:56:VAL:H	2.31	0.41
30:18:52:LYS:N	30:18:53:PRO:HD2	2.36	0.41
32:1a:354:G:N2	32:1a:388:G:O2'	2.30	0.41
32:1a:1010:G:H2'	32:1a:1011:G:C8	2.56	0.41
35:1d:181:MET:HE3	35:1d:181:MET:HB2	1.98	0.41
36:1e:43:LEU:HD12	36:1e:43:LEU:HA	1.93	0.41
39:1h:28:ALA:HA	39:1h:59:LEU:HG	2.02	0.41
40:1i:43:ALA:HA	40:1i:74:ILE:HD13	2.03	0.41
42:1k:51:LYS:HE3	42:1k:55:LYS:NZ	2.35	0.41
54:1w:18:G:H4'	54:1w:60:U:C6	2.56	0.41
1:2A:125:G:O2'	29:27:48:LYS:NZ	2.54	0.41
1:2A:172:C:H2'	1:2A:173:G:H8	1.85	0.41
1:2A:310:A:H1'	1:2A:311:A:H2'	2.03	0.41
1:2A:614:U:H2'	1:2A:614(A):U:O4'	2.21	0.41
1:2A:1665:A:H2'	1:2A:1666:G:O4'	2.20	0.41
1:2A:1777:U:O2'	1:2A:1778:U:H5'	2.20	0.41
1:2A:2155:G:N7	1:2A:2156:G:C4	2.89	0.41
1:2A:2505:G:OP1	58:2A:3846:WC9:OAI	2.38	0.41
1:2A:2639:A:O3'	9:2N:97:ARG:NH2	2.54	0.41
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.21	0.41
1:2A:2859:G:H2'	1:2A:2860:A:C8	2.56	0.41
6:2G:41:GLN:O	6:2G:43:LEU:HD22	2.21	0.41
7:2H:3:ARG:HD2	7:2H:3:ARG:HA	1.73	0.41
9:2N:1:MET:HE1	16:2U:94:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2U:105:VAL:HG22	17:2V:45:THR:HB	2.03	0.41
21:2Z:92:SER:C	21:2Z:130:PRO:HG3	2.45	0.41
32:2a:736:C:H2'	32:2a:737:A:H8	1.85	0.41
32:2a:833:U:H2'	32:2a:834:C:C6	2.55	0.41
33:2b:55:PHE:HD1	33:2b:55:PHE:HA	1.79	0.41
34:2c:119:ARG:HH21	34:2c:140:ARG:NH1	2.19	0.41
37:2f:22:GLU:OE2	37:2f:84:ASN:ND2	2.40	0.41
50:2s:28:LYS:CB	50:2s:29:ARG:HA	2.51	0.41
1:1A:11:G:H2'	1:1A:12:U:H5'	2.03	0.40
1:1A:958:U:H5'	12:1Q:14:ARG:HD3	2.03	0.40
1:1A:1220:A:OP2	16:1U:19:LYS:NZ	2.44	0.40
1:1A:1341:U:C2	19:1X:80:ILE:HD12	2.56	0.40
1:1A:2164:C:C3'	1:1A:2165:G:H5'	2.51	0.40
9:1N:58:ASP:OD1	9:1N:58:ASP:N	2.46	0.40
21:1Z:103:ARG:O	21:1Z:139:VAL:HG23	2.22	0.40
32:1a:256:U:H2'	32:1a:257:G:O4'	2.21	0.40
32:1a:838:G:H1	32:1a:848:C:N4	2.19	0.40
32:1a:1006:C:N4	32:1a:1023:G:H1	2.19	0.40
34:1c:18:TRP:O	34:1c:54:ARG:NH2	2.51	0.40
35:1d:18:LYS:HG2	60:1d:302:SF4:S1	2.61	0.40
37:1f:12:PRO:HG3	37:1f:57:GLN:O	2.20	0.40
42:1k:32:ILE:HG13	42:1k:72:ALA:HB2	2.01	0.40
1:2A:1479:G:H5'	1:2A:1558:A:C2	2.56	0.40
1:2A:1857:G:C6	1:2A:1858:G:N1	2.89	0.40
1:2A:2390:U:P	30:28:35:GLN:HE22	2.44	0.40
1:2A:2838:G:C2	1:2A:2881:C:C2	3.09	0.40
9:2N:91:LEU:HG	9:2N:98:VAL:HG21	2.03	0.40
17:2V:24:LYS:HA	17:2V:92:THR:OG1	2.21	0.40
23:21:65:SER:OG	23:21:66:HIS:ND1	2.47	0.40
26:24:46:GLN:C	26:24:48:ARG:N	2.79	0.40
32:2a:241:C:H42	32:2a:285:G:H1	1.68	0.40
32:2a:499:A:H4'	32:2a:500:G:OP1	2.20	0.40
33:2b:58:ILE:H	33:2b:58:ILE:HG13	1.68	0.40
34:2c:188:LEU:HD12	34:2c:188:LEU:HA	1.90	0.40
36:2e:92:LYS:HB3	36:2e:119:LEU:HB2	2.02	0.40
48:2q:81:ARG:NH2	48:2q:84:LEU:HD21	2.36	0.40
1:1A:1173:G:N1	1:1A:1176:G:OP2	2.42	0.40
1:1A:2735:G:H2'	1:1A:2736:G:H8	1.86	0.40
3:1D:145:VAL:HG11	3:1D:175:LEU:HD11	2.02	0.40
4:1E:101:ARG:HA	4:1E:170:LEU:O	2.21	0.40
4:1E:111:ARG:HG2	4:1E:118:LYS:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:25:TYR:CZ	6:1G:32:PRO:HD3	2.56	0.40
6:1G:36:LYS:HD3	6:1G:95:ARG:HH12	1.87	0.40
9:1N:12:ARG:NH1	9:1N:138:LEU:HD11	2.34	0.40
13:1R:86:ARG:NH2	61:1R:302:HOH:O	2.25	0.40
14:1S:78:LEU:HD21	14:1S:109:GLY:O	2.21	0.40
32:1a:974:A:OP2	45:1n:29:ARG:NH2	2.53	0.40
32:1a:1137:C:H5'	32:1a:1138:G:C5	2.56	0.40
32:1a:1226:C:H4'	50:1s:80:TYR:OH	2.22	0.40
33:1b:102:LEU:HD23	33:1b:182:ILE:HD12	2.03	0.40
50:1s:40:ILE:HG21	50:1s:62:ILE:HG21	2.03	0.40
51:1t:100:ILE:H	51:1t:100:ILE:HG12	1.47	0.40
1:2A:208:C:H2'	1:2A:209:C:C6	2.57	0.40
1:2A:484:C:H2'	1:2A:485:C:H6	1.87	0.40
1:2A:2128:C:H6	1:2A:2128:C:O5'	2.03	0.40
1:2A:2319:G:N2	14:2S:3:ARG:HH11	2.02	0.40
4:2E:143:ASN:HB2	4:2E:147:PRO:HD2	2.04	0.40
10:2O:61:VAL:HG11	10:2O:114:ILE:HD13	2.03	0.40
11:2P:50:ARG:O	11:2P:52:GLU:HG3	2.21	0.40
13:2R:57:ARG:HH22	13:2R:61:HIS:HD2	1.70	0.40
32:2a:158:G:H2'	32:2a:159:G:H8	1.85	0.40
32:2a:341:C:H2'	32:2a:342:C:C6	2.56	0.40
32:2a:438:G:H4'	35:2d:123:HIS:HD1	1.87	0.40
32:2a:1055:A:C6	32:2a:1206:G:C5	3.10	0.40
32:2a:1181:G:O2'	32:2a:1182:G:N7	2.50	0.40
32:2a:1298:C:H2'	38:2g:114:ARG:NH2	2.35	0.40
33:2b:167:PRO:HD3	33:2b:187:LEU:O	2.21	0.40
35:2d:76:ARG:NE	35:2d:80:GLU:OE2	2.54	0.40
36:2e:109:ILE:O	36:2e:113:ALA:HB2	2.21	0.40
36:2e:115:VAL:HG21	36:2e:118:ILE:HD12	2.02	0.40
40:2i:5:TYR:OH	40:2i:16:ARG:HD2	2.21	0.40
42:2k:48:ILE:N	42:2k:48:ILE:HD12	2.36	0.40
45:2n:4:LYS:HE2	45:2n:4:LYS:HB3	1.95	0.40
54:2y:69:G:H5'	54:2y:70:G:OP2	2.21	0.40
1:1A:336:C:HO2'	20:1Y:35:TYR:HH	1.65	0.40
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.22	0.40
1:1A:2001:A:H2'	1:1A:2002:G:C8	2.56	0.40
1:1A:2002:G:OP2	13:1R:9:LYS:NZ	2.53	0.40
1:1A:2040:C:H2'	1:1A:2041:U:O4'	2.21	0.40
1:1A:2111:C:N4	1:1A:2144:U:O2'	2.54	0.40
19:1X:66:LEU:HD12	19:1X:66:LEU:HA	1.83	0.40
23:11:40:ARG:HE	23:11:40:ARG:HB2	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:40:HIS:HB3	26:14:43:TYR:HD2	1.86	0.40
32:1a:49:U:C2	32:1a:361:G:N2	2.90	0.40
32:1a:1151:A:O2'	32:1a:1152:A:H8	2.04	0.40
33:1b:16:HIS:HB2	33:1b:204:ASN:HB2	2.03	0.40
33:1b:47:THR:O	33:1b:51:LEU:HG	2.20	0.40
33:1b:60:ASP:O	33:1b:64:ARG:HG2	2.22	0.40
40:1i:49:PRO:HD3	40:1i:78:LYS:HG3	2.04	0.40
1:2A:116:C:H2'	1:2A:117:G:O4'	2.21	0.40
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.57	0.40
1:2A:348:G:H2'	1:2A:349:G:H8	1.85	0.40
1:2A:1499:C:H2'	1:2A:1500:G:C8	2.52	0.40
1:2A:2286:A:H4'	1:2A:2287:A:O4'	2.21	0.40
1:2A:2409:G:H2'	1:2A:2410:G:O4'	2.21	0.40
1:2A:2505:G:H2'	1:2A:2576:G:O6	2.21	0.40
1:2A:2543:G:H5'	1:2A:2767:C:OP1	2.22	0.40
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.57	0.40
1:2A:2781:A:H5''	1:2A:2782:G:H5'	2.03	0.40
6:2G:106:LEU:O	6:2G:110:ALA:HB3	2.21	0.40
6:2G:116:ASP:OD2	44:2m:68:GLY:HA3	2.20	0.40
10:2O:15:GLY:O	10:2O:47:ILE:HG12	2.21	0.40
10:2O:69:ILE:HD11	10:2O:105:GLU:OE2	2.21	0.40
15:2T:28:VAL:O	15:2T:46:GLU:HA	2.21	0.40
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.21	0.40
19:2X:24:GLY:O	19:2X:83:VAL:HG22	2.21	0.40
23:21:8:SER:HB3	23:21:66:HIS:CD2	2.56	0.40
32:2a:1207:2MG:C6	32:2a:1208:C:C4	3.09	0.40
33:2b:55:PHE:CE1	33:2b:218:ALA:HA	2.56	0.40
41:2j:8:LEU:HD11	41:2j:20:ALA:HB2	2.04	0.40
44:2m:24:GLY:HA3	44:2m:66:LEU:HD23	2.03	0.40
46:2o:16:ALA:HB1	46:2o:21:ASP:HB3	2.03	0.40
55:2x:15:G:N2	55:2x:21:A:N3	2.69	0.40
1:1A:143:G:H2'	1:1A:143(A):C:C6	2.57	0.40
1:1A:1005:C:H5''	61:1A:4217:HOH:O	2.21	0.40
1:1A:1323:U:H2'	1:1A:1324:G:H5'	2.04	0.40
1:1A:1478:G:O2'	1:1A:1558:A:N7	2.53	0.40
1:1A:1705:G:C6	1:1A:1706:U:C4	3.10	0.40
1:1A:2100:G:H2'	1:1A:2101:G:C8	2.56	0.40
1:1A:2235:G:H2'	1:1A:2236:C:C6	2.56	0.40
6:1G:56:ALA:HA	6:1G:59:GLU:HG2	2.04	0.40
21:1Z:48:PHE:HA	21:1Z:51:ALA:HB3	2.04	0.40
28:16:12:GLU:OE1	28:16:52:VAL:HG11	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:257:G:C6	32:1a:258:G:C5	3.09	0.40
32:1a:452:A:H4'	47:1p:72:ARG:NH1	2.36	0.40
32:1a:487:A:H2'	32:1a:488:C:O4'	2.22	0.40
32:1a:1039:C:H2'	32:1a:1040:U:C6	2.56	0.40
32:1a:1317:C:H2'	32:1a:1318:A:O4'	2.21	0.40
35:1d:178:VAL:C	35:1d:180:GLY:N	2.79	0.40
39:1h:87:SER:HB2	39:1h:93:VAL:HB	2.04	0.40
44:1m:44:ARG:HD3	44:1m:44:ARG:HA	1.86	0.40
51:1t:56:MET:HE3	51:1t:85:MET:HG2	2.01	0.40
54:1y:9:A:O3'	54:1y:45:U:O2'	2.38	0.40
54:1y:55:PSU:N3	54:1y:57:G:H5'	2.37	0.40
1:2A:358:U:H2'	1:2A:359:A:H8	1.86	0.40
1:2A:849:A:N6	1:2A:928:G:O2'	2.51	0.40
1:2A:1023:U:H4'	1:2A:1123:C:OP1	2.22	0.40
1:2A:2021:C:OP1	27:25:12:SER:OG	2.32	0.40
1:2A:2319:G:N2	14:2S:3:ARG:HD2	2.36	0.40
1:2A:2438:U:O2'	1:2A:2440:C:OP1	2.25	0.40
1:2A:2625:G:H2'	1:2A:2626:C:O4'	2.21	0.40
1:2A:2669:G:H2'	1:2A:2670:A:H8	1.86	0.40
2:2B:31:C:H4'	6:2G:29:TRP:CZ2	2.57	0.40
2:2B:34:U:OP1	6:2G:2:PRO:HG3	2.22	0.40
8:2I:51:ILE:HD12	8:2I:51:ILE:HA	1.86	0.40
10:2O:86:ILE:H	10:2O:86:ILE:HG12	1.75	0.40
18:2W:10:VAL:HG12	18:2W:12:ILE:HG22	2.03	0.40
21:2Z:54:HIS:ND1	21:2Z:101:PRO:HG3	2.36	0.40
32:2a:861:G:HO2'	32:2a:874:G:HO2'	1.67	0.40
32:2a:1391:U:H2'	32:2a:1392:G:C8	2.56	0.40
33:2b:219:VAL:O	33:2b:223:ILE:HG12	2.22	0.40
40:2i:26:VAL:HG22	40:2i:61:ALA:HB3	2.04	0.40
44:2m:65:LYS:HG2	44:2m:69:GLU:HB3	2.03	0.40
49:2r:58:LEU:HD12	49:2r:63:GLN:NE2	2.37	0.40
50:2s:20:LEU:HA	50:2s:23:ASN:HD22	1.87	0.40
1:1A:392:C:OP1	61:1A:4110:HOH:O	2.22	0.40
1:1A:495:G:C6	1:1A:496:G:C5	3.10	0.40
1:1A:1003:G:O2'	1:1A:1010:A:N1	2.49	0.40
1:1A:1471:A:H2'	1:1A:1472:A:C8	2.56	0.40
8:1I:134:PRO:C	8:1I:136:VAL:H	2.30	0.40
32:1a:119:A:H4'	32:1a:120:A:C8	2.57	0.40
32:1a:313:A:H2'	32:1a:314:C:C6	2.57	0.40
32:1a:392:G:H2'	32:1a:393:A:C8	2.55	0.40
32:1a:409:G:OP2	35:1d:22:LYS:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1057:G:C6	32:1a:1058:G:C4	3.10	0.40
32:1a:1134:G:H2'	32:1a:1134:G:N3	2.37	0.40
41:1j:34:VAL:HA	41:1j:73:ASP:O	2.21	0.40
46:1o:84:LYS:O	46:1o:84:LYS:HD3	2.21	0.40
47:1p:56:ALA:O	47:1p:60:LEU:HB2	2.22	0.40
1:2A:275:G:H2'	1:2A:276:A:C8	2.56	0.40
1:2A:844:C:C5	1:2A:845:G:C6	3.09	0.40
1:2A:996:A:O3'	16:2U:91:ASP:HB2	2.22	0.40
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.57	0.40
1:2A:1515:G:H2'	1:2A:1516:C:C6	2.56	0.40
1:2A:1713:U:H2'	1:2A:1714:G:C8	2.57	0.40
1:2A:2097:C:H2'	1:2A:2098:U:O4'	2.22	0.40
1:2A:2396:G:OP1	23:21:25:LYS:NZ	2.42	0.40
1:2A:2516:G:C6	1:2A:2517:C:N4	2.90	0.40
1:2A:2759:G:OP2	61:2A:3957:HOH:O	2.22	0.40
6:2G:127:GLY:HA2	6:2G:166:ASP:OD1	2.21	0.40
21:2Z:151:HIS:HB3	21:2Z:152:ALA:H	1.70	0.40
32:2a:614:A:H2'	32:2a:615:C:C6	2.57	0.40
32:2a:967:5MC:H2'	32:2a:968:A:N7	2.36	0.40
34:2c:18:TRP:HB2	34:2c:21:ARG:HG2	2.02	0.40
37:2f:4:TYR:CE1	37:2f:92:LYS:HG2	2.56	0.40
42:2k:110:ASP:HB3	49:2r:85:LEU:HB3	2.04	0.40
44:2m:73:GLU:O	44:2m:77:ASN:HB2	2.22	0.40
45:2n:32:SER:O	45:2n:40:CYS:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	1D	273/276 (99%)	255 (93%)	18 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2D	273/276 (99%)	257 (94%)	16 (6%)	0	100	100
4	1E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	24	46
4	2E	202/206 (98%)	187 (93%)	14 (7%)	1 (0%)	24	46
5	1F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	24	46
5	2F	201/210 (96%)	196 (98%)	1 (0%)	4 (2%)	6	12
6	1G	179/182 (98%)	167 (93%)	12 (7%)	0	100	100
6	2G	179/182 (98%)	153 (86%)	23 (13%)	3 (2%)	7	15
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	21	42
7	2H	172/180 (96%)	152 (88%)	20 (12%)	0	100	100
8	1I	144/148 (97%)	124 (86%)	20 (14%)	0	100	100
8	2I	144/148 (97%)	126 (88%)	17 (12%)	1 (1%)	18	38
9	1N	138/140 (99%)	134 (97%)	3 (2%)	1 (1%)	18	38
9	2N	138/140 (99%)	125 (91%)	11 (8%)	2 (1%)	9	19
10	1O	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
11	1P	147/150 (98%)	128 (87%)	15 (10%)	4 (3%)	4	7
11	2P	147/150 (98%)	132 (90%)	11 (8%)	4 (3%)	4	7
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
12	2Q	139/141 (99%)	126 (91%)	13 (9%)	0	100	100
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
14	2S	108/112 (96%)	99 (92%)	7 (6%)	2 (2%)	6	13
15	1T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	16	34
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	3 (3%)	2 (2%)	6	12
17	2V	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	6	12
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11	25
19	2X	93/96 (97%)	86 (92%)	7 (8%)	0	100	100
20	1Y	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
21	1Z	148/206 (72%)	130 (88%)	16 (11%)	2 (1%)	9	19
21	2Z	156/206 (76%)	128 (82%)	23 (15%)	5 (3%)	3	5
22	10	81/85 (95%)	81 (100%)	0	0	100	100
22	20	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
23	11	95/98 (97%)	89 (94%)	5 (5%)	1 (1%)	11	25
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	51 (90%)	6 (10%)	0	100	100
26	14	67/71 (94%)	52 (78%)	10 (15%)	5 (8%)	1	1
26	24	67/71 (94%)	53 (79%)	11 (16%)	3 (4%)	2	2
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	51 (100%)	0	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	200 (87%)	22 (10%)	7 (3%)	3	5
33	2b	229/256 (90%)	182 (80%)	39 (17%)	8 (4%)	3	4
34	1c	204/239 (85%)	182 (89%)	22 (11%)	0	100	100
34	2c	204/239 (85%)	170 (83%)	30 (15%)	4 (2%)	6	12
35	1d	206/209 (99%)	191 (93%)	13 (6%)	2 (1%)	12	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/209 (99%)	195 (95%)	9 (4%)	2 (1%)	12	28
36	1e	146/162 (90%)	129 (88%)	14 (10%)	3 (2%)	5	11
36	2e	146/162 (90%)	131 (90%)	12 (8%)	3 (2%)	5	11
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	146 (95%)	6 (4%)	1 (1%)	18	38
38	2g	153/156 (98%)	139 (91%)	12 (8%)	2 (1%)	9	21
39	1h	135/138 (98%)	126 (93%)	8 (6%)	1 (1%)	18	38
39	2h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
40	1i	125/128 (98%)	110 (88%)	14 (11%)	1 (1%)	16	34
40	2i	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
41	1j	95/105 (90%)	83 (87%)	9 (10%)	3 (3%)	3	5
41	2j	94/105 (90%)	79 (84%)	11 (12%)	4 (4%)	2	2
42	1k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	6	14
42	2k	112/129 (87%)	99 (88%)	11 (10%)	2 (2%)	6	14
43	1l	119/132 (90%)	107 (90%)	12 (10%)	0	100	100
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100	100
44	1m	121/126 (96%)	109 (90%)	11 (9%)	1 (1%)	16	34
44	2m	120/126 (95%)	104 (87%)	15 (12%)	1 (1%)	16	34
45	1n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
45	2n	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	15
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
46	2o	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
47	1p	80/88 (91%)	69 (86%)	11 (14%)	0	100	100
47	2p	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
48	1q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
48	2q	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
49	1r	66/88 (75%)	58 (88%)	8 (12%)	0	100	100
49	2r	66/88 (75%)	59 (89%)	7 (11%)	0	100	100
50	1s	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	4	8
50	2s	81/93 (87%)	68 (84%)	13 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1t	94/106 (89%)	84 (89%)	6 (6%)	4 (4%)	2	2
51	2t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	5	11
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11370/12128 (94%)	10431 (92%)	836 (7%)	103 (1%)	14	30

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	1P	36	LYS
21	1Z	53	ILE
26	14	62	ARG
33	1b	17	PHE
33	1b	125	PRO
42	1k	105	VAL
44	1m	67	GLU
51	1t	100	ILE
6	2G	84	LYS
11	2P	29	LYS
21	2Z	52	SER
33	2b	9	GLU
33	2b	17	PHE
33	2b	21	ARG
33	2b	126	GLU
33	2b	231	GLU
34	2c	91	LEU
38	2g	80	VAL
5	1F	130	ALA
7	1H	159	GLU
17	1V	43	GLU
17	1V	79	VAL
23	11	3	LYS
33	1b	126	GLU
35	1d	173	TRP
38	1g	52	GLU
40	1i	54	ASP
50	1s	81	ARG
5	2F	130	ALA
6	2G	42	GLY
17	2V	79	VAL
21	2Z	144	LEU

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Mol	Chain	Res	Type
26	24	48	ARG
38	2g	55	GLY
42	2k	49	GLY
51	2t	47	GLY
4	1E	52	LEU
11	1P	38	GLN
15	1T	37	GLY
26	14	49	PHE
41	1j	79	ARG
4	2E	52	LEU
6	2G	43	LEU
11	2P	36	LYS
14	2S	109	GLY
26	24	47	GLN
26	24	49	PHE
33	2b	20	GLU
33	2b	74	LYS
34	2c	92	ALA
34	2c	181	ASN
35	2d	18	LYS
41	2j	78	ASN
51	2t	95	ALA
11	1P	45	LEU
21	1Z	163	LEU
33	1b	155	LEU
35	1d	88	VAL
36	1e	85	GLY
39	1h	133	LEU
41	1j	78	ASN
5	2F	21	ALA
5	2F	168	ARG
8	2I	117	GLU
17	2V	53	GLU
21	2Z	93	ASP
33	2b	226	ARG
34	2c	156	ARG
41	2j	9	ARG
41	2j	77	PRO
41	2j	79	ARG
44	2m	67	GLU
9	1N	2	LYS
26	14	47	GLN

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Mol	Chain	Res	Type
26	14	59	PHE
33	1b	124	SER
41	1j	77	PRO
42	1k	49	GLY
51	1t	96	GLY
51	1t	102	GLY
5	2F	18	ARG
9	2N	2	LYS
11	2P	38	GLN
11	2P	45	LEU
36	2e	69	VAL
33	1b	37	ASN
33	1b	231	GLU
36	1e	69	VAL
36	1e	77	PRO
50	1s	27	GLU
9	2N	23	LEU
14	2S	84	GLN
35	2d	5	ILE
36	2e	96	PRO
42	2k	117	ASN
26	14	45	GLY
51	1t	47	GLY
21	2Z	146	ILE
21	2Z	171	ILE
45	2n	14	PRO
19	1X	94	GLY
36	2e	77	PRO
11	1P	122	PRO

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%)	207 (96%)	8 (4%)	30	57
3	2D	215/218 (99%)	207 (96%)	8 (4%)	30	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	1E	164/166 (99%)	157 (96%)	7 (4%)	26	51
4	2E	164/166 (99%)	154 (94%)	10 (6%)	17	37
5	1F	160/166 (96%)	142 (89%)	18 (11%)	5	12
5	2F	159/166 (96%)	141 (89%)	18 (11%)	5	12
6	1G	143/156 (92%)	133 (93%)	10 (7%)	14	31
6	2G	143/156 (92%)	128 (90%)	15 (10%)	6	14
7	1H	144/148 (97%)	133 (92%)	11 (8%)	12	27
7	2H	144/148 (97%)	134 (93%)	10 (7%)	14	32
8	1I	113/124 (91%)	96 (85%)	17 (15%)	3	5
8	2I	105/124 (85%)	88 (84%)	17 (16%)	2	4
9	1N	118/119 (99%)	113 (96%)	5 (4%)	26	52
9	2N	118/119 (99%)	111 (94%)	7 (6%)	18	38
10	1O	100/100 (100%)	97 (97%)	3 (3%)	36	64
10	2O	100/100 (100%)	90 (90%)	10 (10%)	7	16
11	1P	115/116 (99%)	104 (90%)	11 (10%)	8	17
11	2P	115/116 (99%)	110 (96%)	5 (4%)	26	51
12	1Q	111/111 (100%)	102 (92%)	9 (8%)	11	24
12	2Q	111/111 (100%)	108 (97%)	3 (3%)	39	67
13	1R	101/101 (100%)	96 (95%)	5 (5%)	22	46
13	2R	101/101 (100%)	95 (94%)	6 (6%)	18	38
14	1S	86/88 (98%)	78 (91%)	8 (9%)	8	18
14	2S	85/88 (97%)	76 (89%)	9 (11%)	6	14
15	1T	115/127 (91%)	110 (96%)	5 (4%)	26	51
15	2T	113/127 (89%)	107 (95%)	6 (5%)	20	43
16	1U	93/94 (99%)	87 (94%)	6 (6%)	15	35
16	2U	93/94 (99%)	89 (96%)	4 (4%)	26	51
17	1V	80/82 (98%)	76 (95%)	4 (5%)	22	46
17	2V	80/82 (98%)	76 (95%)	4 (5%)	22	46
18	1W	90/92 (98%)	87 (97%)	3 (3%)	33	61
18	2W	90/92 (98%)	88 (98%)	2 (2%)	45	72
19	1X	77/78 (99%)	76 (99%)	1 (1%)	61	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28	55
20	1Y	85/91 (93%)	75 (88%)	10 (12%)	5	10
20	2Y	85/91 (93%)	76 (89%)	9 (11%)	6	14
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11	24
21	2Z	137/179 (76%)	117 (85%)	20 (15%)	3	6
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	61 (94%)	4 (6%)	16	36
23	11	80/83 (96%)	74 (92%)	6 (8%)	12	28
23	21	80/83 (96%)	74 (92%)	6 (8%)	12	28
24	12	65/67 (97%)	61 (94%)	4 (6%)	16	36
24	22	65/67 (97%)	59 (91%)	6 (9%)	8	19
25	13	51/52 (98%)	44 (86%)	7 (14%)	3	7
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	25
26	14	59/63 (94%)	48 (81%)	11 (19%)	1	3
26	24	53/63 (84%)	41 (77%)	12 (23%)	1	1
27	15	50/52 (96%)	49 (98%)	1 (2%)	48	74
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	25
28	16	51/52 (98%)	47 (92%)	4 (8%)	11	26
28	26	50/52 (96%)	47 (94%)	3 (6%)	17	37
29	17	41/42 (98%)	39 (95%)	2 (5%)	22	47
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	17
30	18	54/55 (98%)	52 (96%)	2 (4%)	30	57
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	57
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	65
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	38
33	1b	192/220 (87%)	162 (84%)	30 (16%)	2	4
33	2b	187/220 (85%)	161 (86%)	26 (14%)	3	7
34	1c	142/188 (76%)	127 (89%)	15 (11%)	6	14
34	2c	140/188 (74%)	117 (84%)	23 (16%)	2	4
35	1d	169/181 (93%)	149 (88%)	20 (12%)	5	10
35	2d	173/181 (96%)	157 (91%)	16 (9%)	8	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	1e	113/123 (92%)	102 (90%)	11 (10%)	8	17
36	2e	114/123 (93%)	98 (86%)	16 (14%)	3	6
37	1f	84/90 (93%)	81 (96%)	3 (4%)	31	58
37	2f	85/90 (94%)	76 (89%)	9 (11%)	6	14
38	1g	119/127 (94%)	108 (91%)	11 (9%)	8	19
38	2g	120/127 (94%)	108 (90%)	12 (10%)	7	16
39	1h	114/119 (96%)	104 (91%)	10 (9%)	9	21
39	2h	114/119 (96%)	105 (92%)	9 (8%)	11	26
40	1i	90/99 (91%)	80 (89%)	10 (11%)	6	12
40	2i	89/99 (90%)	75 (84%)	14 (16%)	2	4
41	1j	66/92 (72%)	56 (85%)	10 (15%)	3	5
41	2j	69/92 (75%)	63 (91%)	6 (9%)	9	21
42	1k	82/99 (83%)	71 (87%)	11 (13%)	4	7
42	2k	83/99 (84%)	74 (89%)	9 (11%)	6	13
43	1l	96/108 (89%)	88 (92%)	8 (8%)	10	23
43	2l	96/108 (89%)	89 (93%)	7 (7%)	13	29
44	1m	93/101 (92%)	83 (89%)	10 (11%)	6	13
44	2m	92/101 (91%)	80 (87%)	12 (13%)	4	8
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	10
45	2n	49/50 (98%)	48 (98%)	1 (2%)	48	74
46	1o	78/80 (98%)	75 (96%)	3 (4%)	29	56
46	2o	78/80 (98%)	74 (95%)	4 (5%)	21	45
47	1p	69/74 (93%)	60 (87%)	9 (13%)	4	8
47	2p	68/74 (92%)	59 (87%)	9 (13%)	4	8
48	1q	94/97 (97%)	87 (93%)	7 (7%)	13	29
48	2q	94/97 (97%)	90 (96%)	4 (4%)	26	51
49	1r	59/77 (77%)	57 (97%)	2 (3%)	32	60
49	2r	59/77 (77%)	52 (88%)	7 (12%)	5	10
50	1s	69/80 (86%)	65 (94%)	4 (6%)	18	39
50	2s	67/80 (84%)	63 (94%)	4 (6%)	17	37
51	1t	70/82 (85%)	62 (89%)	8 (11%)	5	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	2t	70/82 (85%)	64 (91%)	6 (9%)	10	22
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	40
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	40
All	All	9303/10064 (92%)	8516 (92%)	787 (8%)	10	22

All (787) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	4	LYS
3	1D	140	THR
3	1D	141	VAL
3	1D	155	LEU
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	260	ARG
4	1E	47	VAL
4	1E	49	LEU
4	1E	59	VAL
4	1E	116	VAL
4	1E	154	LYS
4	1E	181	LEU
4	1E	195	LEU
5	1F	19	GLU
5	1F	24	LEU
5	1F	27	GLU
5	1F	28	ILE
5	1F	33	LEU
5	1F	57	VAL
5	1F	60	SER
5	1F	70	THR
5	1F	74	ARG
5	1F	106	ARG
5	1F	140	LEU
5	1F	144	LYS
5	1F	162	LEU
5	1F	168	ARG
5	1F	176	LEU
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL

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Mol	Chain	Res	Type
6	1G	3	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	31	VAL
6	1G	43	LEU
6	1G	133	LEU
6	1G	139	LEU
6	1G	148	MET
6	1G	159	VAL
6	1G	174	GLU
7	1H	2	SER
7	1H	23	ARG
7	1H	45	VAL
7	1H	56	SER
7	1H	57	ASP
7	1H	88	LEU
7	1H	90	LYS
7	1H	92	ILE
7	1H	95	ARG
7	1H	124	GLU
7	1H	136	ILE
8	1I	1	MET
8	1I	7	GLU
8	1I	10	GLU
8	1I	12	LEU
8	1I	20	ASP
8	1I	38	LEU
8	1I	40	THR
8	1I	47	LEU
8	1I	77	LEU
8	1I	85	GLU
8	1I	87	LYS
8	1I	92	VAL
8	1I	101	LEU
8	1I	108	THR
8	1I	129	THR
8	1I	133	HIS
8	1I	140	LEU
9	1N	1	MET
9	1N	38	HIS
9	1N	48	MET
9	1N	83	LYS

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Mol	Chain	Res	Type
9	1N	138	LEU
10	1O	28	SER
10	1O	98	VAL
10	1O	113	LYS
11	1P	15	ARG
11	1P	36	LYS
11	1P	45	LEU
11	1P	75	ILE
11	1P	77	ARG
11	1P	95	VAL
11	1P	98	GLU
11	1P	101	VAL
11	1P	126	VAL
11	1P	133	SER
11	1P	147	LEU
12	1Q	1	MET
12	1Q	7	MET
12	1Q	8	LYS
12	1Q	75	THR
12	1Q	89	ASN
12	1Q	109	VAL
12	1Q	110	THR
12	1Q	133	ARG
12	1Q	138	ASP
13	1R	15	SER
13	1R	36	THR
13	1R	67	LEU
13	1R	99	LYS
13	1R	114	VAL
14	1S	14	VAL
14	1S	38	GLN
14	1S	46	VAL
14	1S	49	VAL
14	1S	58	LEU
14	1S	68	GLN
14	1S	73	LEU
14	1S	110	LEU
15	1T	21	GLU
15	1T	28	VAL
15	1T	85	LYS
15	1T	96	ARG
15	1T	128	GLU

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Mol	Chain	Res	Type
16	1U	9	VAL
16	1U	31	SER
16	1U	74	LEU
16	1U	78	THR
16	1U	100	VAL
16	1U	110	VAL
17	1V	61	VAL
17	1V	73	SER
17	1V	79	VAL
17	1V	100	ARG
18	1W	11	ARG
18	1W	17	VAL
18	1W	50	VAL
19	1X	88	LYS
20	1Y	1	MET
20	1Y	7	VAL
20	1Y	8	LYS
20	1Y	21	LYS
20	1Y	31	LEU
20	1Y	43	ASN
20	1Y	47	LYS
20	1Y	72	VAL
20	1Y	86	ARG
20	1Y	99	CYS
21	1Z	1	MET
21	1Z	53	ILE
21	1Z	72	ARG
21	1Z	84	GLU
21	1Z	124	ILE
21	1Z	132	ASN
21	1Z	136	PHE
21	1Z	139	VAL
21	1Z	140	ASP
21	1Z	154	ASP
21	1Z	170	THR
23	11	21	ARG
23	11	40	ARG
23	11	46	LEU
23	11	59	THR
23	11	78	LYS
23	11	89	GLU
24	12	38	GLN

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Mol	Chain	Res	Type
24	12	40	SER
24	12	53	LEU
24	12	65	ASN
25	13	10	LYS
25	13	20	LYS
25	13	23	LEU
25	13	34	GLU
25	13	37	LEU
25	13	54	VAL
25	13	60	GLU
26	14	1	MET
26	14	10	VAL
26	14	33	VAL
26	14	49	PHE
26	14	50	VAL
26	14	52	THR
26	14	56	VAL
26	14	63	TYR
26	14	66	SER
26	14	67	TYR
26	14	69	LYS
27	15	6	VAL
28	16	5	VAL
28	16	6	ARG
28	16	19	ARG
28	16	44	ARG
29	17	24	THR
29	17	46	VAL
30	18	14	VAL
30	18	23	VAL
31	19	4	ARG
33	1b	7	VAL
33	1b	11	LEU
33	1b	12	GLU
33	1b	21	ARG
33	1b	23	ARG
33	1b	35	GLU
33	1b	39	ILE
33	1b	54	THR
33	1b	67	THR
33	1b	74	LYS
33	1b	93	VAL

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Mol	Chain	Res	Type
33	1b	101	MET
33	1b	112	VAL
33	1b	127	ILE
33	1b	156	LYS
33	1b	160	ASP
33	1b	172	ILE
33	1b	178	ARG
33	1b	185	ILE
33	1b	196	LEU
33	1b	200	ILE
33	1b	208	ILE
33	1b	210	SER
33	1b	212	GLN
33	1b	215	LEU
33	1b	221	LEU
33	1b	222	ILE
33	1b	223	ILE
33	1b	233	SER
33	1b	236	TYR
34	1c	3	ASN
34	1c	8	ILE
34	1c	15	THR
34	1c	38	ARG
34	1c	49	SER
34	1c	64	VAL
34	1c	66	VAL
34	1c	89	GLU
34	1c	101	LEU
34	1c	112	SER
34	1c	115	LEU
34	1c	182	ILE
34	1c	190	ARG
34	1c	195	VAL
34	1c	196	LEU
35	1d	17	VAL
35	1d	19	LEU
35	1d	31	CYS
35	1d	53	ASP
35	1d	59	ARG
35	1d	76	ARG
35	1d	104	VAL
35	1d	107	ARG

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Mol	Chain	Res	Type
35	1d	112	VAL
35	1d	119	GLN
35	1d	134	ASP
35	1d	135	LEU
35	1d	140	VAL
35	1d	157	LEU
35	1d	158	ILE
35	1d	160	GLN
35	1d	175	SER
35	1d	184	LYS
35	1d	190	ASP
35	1d	194	LEU
36	1e	10	MET
36	1e	31	LEU
36	1e	41	VAL
36	1e	51	VAL
36	1e	56	GLN
36	1e	64	ARG
36	1e	78	HIS
36	1e	79	GLU
36	1e	91	LEU
36	1e	98	THR
36	1e	100	VAL
37	1f	37	VAL
37	1f	45	LEU
37	1f	92	LYS
38	1g	12	LEU
38	1g	13	GLN
38	1g	32	ARG
38	1g	50	ILE
38	1g	53	LYS
38	1g	59	LEU
38	1g	61	VAL
38	1g	94	ARG
38	1g	104	LEU
38	1g	113	GLU
38	1g	115	ARG
39	1h	13	ILE
39	1h	18	ARG
39	1h	35	ILE
39	1h	45	ILE
39	1h	51	VAL

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Mol	Chain	Res	Type
39	1h	52	ASP
39	1h	60	ARG
39	1h	112	LEU
39	1h	121	ASP
39	1h	133	LEU
40	1i	23	ASN
40	1i	27	THR
40	1i	41	VAL
40	1i	53	VAL
40	1i	56	LEU
40	1i	64	THR
40	1i	86	VAL
40	1i	87	GLN
40	1i	92	TYR
40	1i	113	LYS
41	1j	5	ARG
41	1j	17	ASP
41	1j	21	GLN
41	1j	34	VAL
41	1j	44	VAL
41	1j	46	ARG
41	1j	49	VAL
41	1j	72	VAL
41	1j	81	THR
41	1j	84	GLN
42	1k	14	VAL
42	1k	18	ARG
42	1k	31	THR
42	1k	40	ILE
42	1k	48	ILE
42	1k	84	VAL
42	1k	87	THR
42	1k	91	ARG
42	1k	104	GLN
42	1k	109	VAL
42	1k	114	VAL
43	1l	18	VAL
43	1l	22	SER
43	1l	33	ARG
43	1l	42	THR
43	1l	62	SER
43	1l	78	GLN

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Mol	Chain	Res	Type
43	1l	83	VAL
43	1l	124	LYS
44	1m	4	ILE
44	1m	12	ASN
44	1m	17	VAL
44	1m	19	LEU
44	1m	43	THR
44	1m	47	ASP
44	1m	53	VAL
44	1m	109	THR
44	1m	117	VAL
44	1m	122	LYS
45	1n	13	THR
45	1n	15	LYS
45	1n	18	VAL
45	1n	25	VAL
45	1n	33	VAL
45	1n	35	ARG
46	1o	39	LEU
46	1o	62	GLN
46	1o	87	ILE
47	1p	11	SER
47	1p	20	VAL
47	1p	27	LYS
47	1p	29	ASP
47	1p	61	SER
47	1p	62	VAL
47	1p	67	THR
47	1p	75	ARG
47	1p	79	VAL
48	1q	7	THR
48	1q	15	MET
48	1q	60	ILE
48	1q	63	ARG
48	1q	73	VAL
48	1q	78	GLU
48	1q	85	VAL
49	1r	31	LEU
49	1r	46	GLU
50	1s	4	SER
50	1s	12	ASP
50	1s	28	LYS

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Mol	Chain	Res	Type
50	1s	41	VAL
51	1t	10	LEU
51	1t	24	LEU
51	1t	62	LEU
51	1t	71	THR
51	1t	72	LEU
51	1t	84	LEU
51	1t	90	GLN
51	1t	100	ILE
52	1u	20	LYS
3	2D	14	ARG
3	2D	24	ILE
3	2D	34	VAL
3	2D	64	ILE
3	2D	122	ASP
3	2D	242	ARG
3	2D	275	LYS
3	2D	276	LYS
4	2E	21	VAL
4	2E	38	THR
4	2E	59	VAL
4	2E	73	GLU
4	2E	90	THR
4	2E	94	GLU
4	2E	116	VAL
4	2E	134	ILE
4	2E	163	GLU
4	2E	181	LEU
5	2F	20	LEU
5	2F	23	ASP
5	2F	28	ILE
5	2F	33	LEU
5	2F	57	VAL
5	2F	70	THR
5	2F	107	LYS
5	2F	126	VAL
5	2F	132	VAL
5	2F	145	GLU
5	2F	154	VAL
5	2F	157	VAL
5	2F	161	GLU
5	2F	165	ARG

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Mol	Chain	Res	Type
5	2F	176	LEU
5	2F	183	VAL
5	2F	192	LEU
5	2F	197	ASP
6	2G	5	VAL
6	2G	20	ILE
6	2G	28	VAL
6	2G	43	LEU
6	2G	45	GLU
6	2G	51	ARG
6	2G	53	LEU
6	2G	70	VAL
6	2G	124	SER
6	2G	126	ASP
6	2G	139	LEU
6	2G	140	ILE
6	2G	149	VAL
6	2G	159	VAL
6	2G	165	THR
7	2H	16	SER
7	2H	23	ARG
7	2H	45	VAL
7	2H	57	ASP
7	2H	60	ARG
7	2H	65	HIS
7	2H	92	ILE
7	2H	104	GLU
7	2H	119	GLU
7	2H	136	ILE
8	2I	19	VAL
8	2I	20	ASP
8	2I	31	LEU
8	2I	38	LEU
8	2I	40	THR
8	2I	44	LEU
8	2I	77	LEU
8	2I	82	ARG
8	2I	92	VAL
8	2I	108	THR
8	2I	117	GLU
8	2I	125	GLU
8	2I	127	VAL

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Mol	Chain	Res	Type
8	2I	129	THR
8	2I	133	HIS
8	2I	142	VAL
8	2I	144	VAL
9	2N	10	GLU
9	2N	22	THR
9	2N	38	HIS
9	2N	58	ASP
9	2N	62	VAL
9	2N	83	LYS
9	2N	138	LEU
10	2O	21	CYS
10	2O	29	ASN
10	2O	69	ILE
10	2O	82	ASN
10	2O	85	VAL
10	2O	86	ILE
10	2O	91	LEU
10	2O	98	VAL
10	2O	102	VAL
10	2O	116	SER
11	2P	15	ARG
11	2P	45	LEU
11	2P	71	VAL
11	2P	98	GLU
11	2P	135	LEU
12	2Q	1	MET
12	2Q	75	THR
12	2Q	110	THR
13	2R	1	MET
13	2R	36	THR
13	2R	40	LYS
13	2R	67	LEU
13	2R	73	VAL
13	2R	111	LEU
14	2S	15	ARG
14	2S	17	ARG
14	2S	28	VAL
14	2S	36	TYR
14	2S	38	GLN
14	2S	58	LEU
14	2S	64	GLU

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Mol	Chain	Res	Type
14	2S	80	LEU
14	2S	110	LEU
15	2T	23	ARG
15	2T	40	THR
15	2T	66	VAL
15	2T	96	ARG
15	2T	102	ILE
15	2T	121	ILE
16	2U	5	LYS
16	2U	8	VAL
16	2U	55	ARG
16	2U	59	ARG
17	2V	7	THR
17	2V	28	GLU
17	2V	61	VAL
17	2V	79	VAL
18	2W	11	ARG
18	2W	17	VAL
19	2X	35	THR
19	2X	81	VAL
19	2X	95	LEU
20	2Y	1	MET
20	2Y	7	VAL
20	2Y	14	LEU
20	2Y	40	GLU
20	2Y	50	ARG
20	2Y	51	VAL
20	2Y	72	VAL
20	2Y	99	CYS
20	2Y	107	ASP
21	2Z	24	LEU
21	2Z	32	HIS
21	2Z	33	LEU
21	2Z	36	LYS
21	2Z	40	ASP
21	2Z	58	VAL
21	2Z	74	VAL
21	2Z	91	LEU
21	2Z	100	VAL
21	2Z	121	HIS
21	2Z	126	VAL
21	2Z	128	VAL

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Mol	Chain	Res	Type
21	2Z	129	SER
21	2Z	136	PHE
21	2Z	137	ILE
21	2Z	144	LEU
21	2Z	154	ASP
21	2Z	157	LEU
21	2Z	171	ILE
21	2Z	174	VAL
22	20	7	LEU
22	20	9	SER
22	20	10	THR
22	20	11	ARG
23	21	35	THR
23	21	40	ARG
23	21	46	LEU
23	21	53	VAL
23	21	59	THR
23	21	80	LEU
24	22	4	SER
24	22	19	VAL
24	22	34	GLU
24	22	53	LEU
24	22	59	ARG
24	22	70	GLN
25	23	37	LEU
25	23	54	VAL
25	23	56	VAL
25	23	59	VAL
26	24	10	VAL
26	24	26	SER
26	24	33	VAL
26	24	34	GLU
26	24	37	SER
26	24	44	THR
26	24	50	VAL
26	24	56	VAL
26	24	59	PHE
26	24	62	ARG
26	24	63	TYR
26	24	68	ARG
27	25	6	VAL
27	25	40	LYS

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Mol	Chain	Res	Type
27	25	58	LEU
27	25	59	GLU
28	26	5	VAL
28	26	9	LEU
28	26	19	ARG
29	27	1	MET
29	27	4	THR
29	27	46	VAL
29	27	48	LYS
30	28	14	VAL
30	28	23	VAL
31	29	7	VAL
31	29	18	ARG
33	2b	7	VAL
33	2b	8	LYS
33	2b	9	GLU
33	2b	16	HIS
33	2b	23	ARG
33	2b	37	ASN
33	2b	41	ILE
33	2b	58	ILE
33	2b	76	GLN
33	2b	90	MET
33	2b	94	ASN
33	2b	107	THR
33	2b	111	ARG
33	2b	115	LEU
33	2b	130	ARG
33	2b	136	VAL
33	2b	142	LEU
33	2b	158	LEU
33	2b	162	ILE
33	2b	164	VAL
33	2b	185	ILE
33	2b	189	ASP
33	2b	204	ASN
33	2b	222	ILE
33	2b	223	ILE
33	2b	230	VAL
34	2c	5	ILE
34	2c	14	ILE
34	2c	15	THR

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Mol	Chain	Res	Type
34	2c	16	ARG
34	2c	30	ARG
34	2c	32	LEU
34	2c	34	LEU
34	2c	43	LEU
34	2c	55	VAL
34	2c	58	GLU
34	2c	68	VAL
34	2c	70	VAL
34	2c	89	GLU
34	2c	103	VAL
34	2c	132	ARG
34	2c	142	MET
34	2c	152	ILE
34	2c	161	GLU
34	2c	182	ILE
34	2c	190	ARG
34	2c	191	THR
34	2c	198	VAL
34	2c	202	ILE
35	2d	5	ILE
35	2d	8	VAL
35	2d	34	GLU
35	2d	43	HIS
35	2d	49	ARG
35	2d	59	ARG
35	2d	78	LEU
35	2d	85	LYS
35	2d	107	ARG
35	2d	119	GLN
35	2d	127	THR
35	2d	150	GLU
35	2d	155	LEU
35	2d	162	LEU
35	2d	165	MET
35	2d	178	VAL
36	2e	6	PHE
36	2e	13	ILE
36	2e	18	ARG
36	2e	20	GLN
36	2e	24	ARG
36	2e	25	ARG

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Mol	Chain	Res	Type
36	2e	41	VAL
36	2e	51	VAL
36	2e	55	VAL
36	2e	64	ARG
36	2e	68	GLU
36	2e	73	ASN
36	2e	80	ILE
36	2e	83	GLU
36	2e	115	VAL
36	2e	149	GLU
37	2f	8	ILE
37	2f	17	SER
37	2f	37	VAL
37	2f	40	VAL
37	2f	63	TYR
37	2f	69	GLU
37	2f	70	ASP
37	2f	90	VAL
37	2f	94	GLN
38	2g	4	ARG
38	2g	6	ARG
38	2g	24	THR
38	2g	36	LYS
38	2g	78	ARG
38	2g	79	ARG
38	2g	85	TYR
38	2g	90	GLU
38	2g	91	VAL
38	2g	98	SER
38	2g	113	GLU
38	2g	139	GLU
39	2h	10	LEU
39	2h	22	GLU
39	2h	29	SER
39	2h	45	ILE
39	2h	51	VAL
39	2h	109	ILE
39	2h	112	LEU
39	2h	120	THR
39	2h	133	LEU
40	2i	50	LEU
40	2i	54	ASP

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Mol	Chain	Res	Type
40	2i	64	THR
40	2i	65	VAL
40	2i	75	ASP
40	2i	86	VAL
40	2i	89	ASN
40	2i	96	LEU
40	2i	99	LEU
40	2i	102	LEU
40	2i	108	VAL
40	2i	113	LYS
40	2i	114	TYR
40	2i	128	ARG
41	2j	8	LEU
41	2j	33	GLN
41	2j	38	ILE
41	2j	67	THR
41	2j	89	ASP
41	2j	96	ILE
42	2k	14	VAL
42	2k	30	VAL
42	2k	51	LYS
42	2k	53	SER
42	2k	81	ASP
42	2k	84	VAL
42	2k	87	THR
42	2k	101	SER
42	2k	117	ASN
43	2l	18	VAL
43	2l	36	VAL
43	2l	42	THR
43	2l	43	VAL
43	2l	66	VAL
43	2l	83	VAL
43	2l	117	ARG
44	2m	3	ARG
44	2m	16	ASP
44	2m	17	VAL
44	2m	19	LEU
44	2m	27	LYS
44	2m	32	GLU
44	2m	48	LEU
44	2m	60	VAL

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Mol	Chain	Res	Type
44	2m	62	ASN
44	2m	69	GLU
44	2m	90	LEU
44	2m	102	ARG
45	2n	33	VAL
46	2o	3	ILE
46	2o	7	GLU
46	2o	39	LEU
46	2o	87	ILE
47	2p	1	MET
47	2p	2	VAL
47	2p	4	ILE
47	2p	8	ARG
47	2p	20	VAL
47	2p	57	ARG
47	2p	60	LEU
47	2p	73	LEU
47	2p	74	LEU
48	2q	52	LYS
48	2q	60	ILE
48	2q	77	VAL
48	2q	78	GLU
49	2r	25	THR
49	2r	30	ASP
49	2r	31	LEU
49	2r	37	VAL
49	2r	46	GLU
49	2r	68	LYS
49	2r	86	VAL
50	2s	22	LEU
50	2s	31	ILE
50	2s	32	LYS
50	2s	47	HIS
51	2t	9	ASN
51	2t	24	LEU
51	2t	33	ILE
51	2t	46	GLU
51	2t	93	GLU
51	2t	100	ILE
52	2u	6	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (144) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	48	GLN
4	1E	121	ASN
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
8	1I	105	HIS
8	1I	139	GLN
11	1P	70	GLN
11	1P	81	GLN
12	1Q	12	GLN
12	1Q	57	HIS
12	1Q	123	HIS
13	1R	61	HIS
13	1R	71	GLN
14	1S	68	GLN
15	1T	43	GLN
15	1T	58	ASN
16	1U	94	ASN
19	1X	31	HIS
20	1Y	6	HIS
20	1Y	43	ASN
21	1Z	32	HIS
21	1Z	34	ASN
21	1Z	73	GLN
24	12	9	GLN
25	13	32	GLN
27	15	23	HIS
30	18	35	GLN
31	19	34	GLN
33	1b	40	HIS
33	1b	78	GLN
33	1b	94	ASN
34	1c	98	ASN
34	1c	123	GLN
34	1c	136	GLN
34	1c	162	GLN
35	1d	116	GLN
35	1d	123	HIS
35	1d	161	ASN
35	1d	201	GLN
36	1e	141	GLN
37	1f	64	GLN

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Mol	Chain	Res	Type
37	1f	73	ASN
38	1g	28	ASN
38	1g	86	GLN
40	1i	31	GLN
40	1i	124	GLN
41	1j	56	HIS
44	1m	77	ASN
44	1m	92	HIS
46	1o	9	GLN
46	1o	62	GLN
47	1p	14	ASN
49	1r	63	GLN
50	1s	23	ASN
50	1s	83	HIS
51	1t	9	ASN
51	1t	42	GLN
3	2D	87	ASN
3	2D	116	GLN
4	2E	48	GLN
4	2E	121	ASN
5	2F	75	HIS
6	2G	26	GLN
6	2G	27	ASN
6	2G	132	ASN
8	2I	54	GLN
8	2I	133	HIS
9	2N	69	GLN
10	2O	82	ASN
12	2Q	12	GLN
12	2Q	57	HIS
12	2Q	123	HIS
13	2R	13	HIS
13	2R	50	HIS
13	2R	71	GLN
14	2S	68	GLN
14	2S	95	HIS
15	2T	55	ASN
15	2T	58	ASN
15	2T	79	HIS
16	2U	66	ASN
16	2U	81	HIS
16	2U	94	ASN

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Mol	Chain	Res	Type
18	2W	62	HIS
19	2X	31	HIS
19	2X	82	GLN
20	2Y	6	HIS
20	2Y	43	ASN
21	2Z	55	HIS
21	2Z	65	GLN
22	20	35	ASN
24	22	46	GLN
25	23	32	GLN
26	24	20	ASN
30	28	35	GLN
31	29	36	GLN
33	2b	40	HIS
33	2b	95	GLN
33	2b	135	GLN
33	2b	204	ASN
34	2c	6	HIS
34	2c	123	GLN
34	2c	162	GLN
34	2c	170	GLN
34	2c	181	ASN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	201	GLN
36	2e	20	GLN
36	2e	141	GLN
37	2f	18	GLN
37	2f	100	ASN
38	2g	13	GLN
38	2g	28	ASN
38	2g	64	GLN
38	2g	86	GLN
38	2g	109	ASN
40	2i	3	GLN
40	2i	38	GLN
40	2i	58	HIS
40	2i	117	HIS
41	2j	21	GLN
41	2j	33	GLN
41	2j	84	GLN

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Mol	Chain	Res	Type
42	2k	38	ASN
42	2k	62	GLN
43	2l	49	ASN
43	2l	80	HIS
43	2l	99	HIS
46	2o	62	GLN
47	2p	76	GLN
48	2q	26	GLN
48	2q	45	HIS
49	2r	63	GLN
50	2s	23	ASN
50	2s	47	HIS
50	2s	69	HIS
50	2s	83	HIS
51	2t	42	GLN
51	2t	45	GLN
51	2t	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	436 (15%)	24 (0%)
1	2A	2791/2915 (95%)	476 (17%)	25 (0%)
2	1B	119/121 (98%)	7 (5%)	0
2	2B	118/121 (97%)	27 (22%)	0
32	1a	1497/1521 (98%)	241 (16%)	0
32	2a	1501/1521 (98%)	273 (18%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	1 (8%)	0
54	1w	72/76 (94%)	26 (36%)	0
54	1y	72/76 (94%)	29 (40%)	0
54	2w	69/76 (90%)	18 (26%)	0
54	2y	70/76 (92%)	19 (27%)	0
55	1x	74/77 (96%)	9 (12%)	0
55	2x	74/77 (96%)	10 (13%)	0
All	All	9345/9620 (97%)	1574 (16%)	49 (0%)

All (1574) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G

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Mol	Chain	Res	Type
1	1A	11	G
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	51	G
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	102	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	139	G
1	1A	173	G
1	1A	181	A
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	261	G
1	1A	269	U
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	271(P)	C
1	1A	271(S)	G
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(G)	C
1	1A	275	G
1	1A	279	C

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Mol	Chain	Res	Type
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	357	A
1	1A	363	G
1	1A	363(B)	G
1	1A	380	U
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	428	A
1	1A	443	A
1	1A	444	C
1	1A	448	U
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	551	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	586	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A

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Mol	Chain	Res	Type
1	1A	651	G
1	1A	652(A)	A
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	740	U
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	827	U
1	1A	828	U
1	1A	855	G
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	880	G
1	1A	882	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	889	C
1	1A	890	A
1	1A	896	A
1	1A	897	C
1	1A	899	A
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G

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Mol	Chain	Res	Type
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1038	C
1	1A	1041	C
1	1A	1044	G
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1057	A
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G
1	1A	1068	G
1	1A	1069	A
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1080	C
1	1A	1081	U
1	1A	1083	U
1	1A	1085	A
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G

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Mol	Chain	Res	Type
1	1A	1093	G
1	1A	1094	U
1	1A	1096	A
1	1A	1098	A
1	1A	1099	G
1	1A	1101	U
1	1A	1102	C
1	1A	1107	G
1	1A	1111	A
1	1A	1112	G
1	1A	1115	G
1	1A	1116	C
1	1A	1135	C
1	1A	1136	G
1	1A	1141	U
1	1A	1169	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1218	C
1	1A	1247	A
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1286	A
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1320	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1384	A
1	1A	1385	G
1	1A	1416	G
1	1A	1417	C

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Mol	Chain	Res	Type
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1542	A
1	1A	1543	C
1	1A	1558	A
1	1A	1559	G
1	1A	1569	A
1	1A	1578	U
1	1A	1581	G
1	1A	1584	C
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1634	A
1	1A	1648	C
1	1A	1658	C
1	1A	1664	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1746	G
1	1A	1756	G
1	1A	1763	G
1	1A	1764	G
1	1A	1769	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C

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Mol	Chain	Res	Type
1	1A	1786	A
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1817	G
1	1A	1829	A
1	1A	1847	A
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1919	A
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2110	G
1	1A	2113	U

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Mol	Chain	Res	Type
1	1A	2116	G
1	1A	2119	A
1	1A	2121	G
1	1A	2127	G
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2140	C
1	1A	2141	G
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2145	C
1	1A	2146	C
1	1A	2148	G
1	1A	2150	U
1	1A	2151	G
1	1A	2154	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2163	C
1	1A	2165	G
1	1A	2166	G
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2190	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G

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Mol	Chain	Res	Type
1	1A	2208	A
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2280	G
1	1A	2283	C
1	1A	2286	A
1	1A	2287	A
1	1A	2305	A
1	1A	2307	G
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2354	G
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
1	1A	2400	G
1	1A	2406	U
1	1A	2407	G
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2469	A
1	1A	2470	G
1	1A	2474	C
1	1A	2476	A
1	1A	2478	A

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Mol	Chain	Res	Type
1	1A	2490	G
1	1A	2498	C
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2549	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2574	G
1	1A	2585	U
1	1A	2601	C
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2657	A
1	1A	2689	U
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2744	G
1	1A	2757	A
1	1A	2758	A
1	1A	2764	A
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2790	A
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2804	C
1	1A	2805	G

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Mol	Chain	Res	Type
1	1A	2812	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2836	U
1	1A	2839	G
1	1A	2872	G
1	1A	2873	A
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
1	1A	2897	U
2	1B	2	C
2	1B	45	A
2	1B	56	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	50	A
32	1a	51	A
32	1a	52	G
32	1a	61	G
32	1a	65	U
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	115	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	163	C
32	1a	174	C
32	1a	182	U

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Mol	Chain	Res	Type
32	1a	189	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	203	U
32	1a	204	U
32	1a	222	U
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	306	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	347	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	405	U
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	441	A
32	1a	442	C
32	1a	452	A
32	1a	457	C
32	1a	458	C
32	1a	461	A
32	1a	470	C

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Mol	Chain	Res	Type
32	1a	471	G
32	1a	482	A
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	524	G
32	1a	527	G7M
32	1a	531	U
32	1a	532	A
32	1a	536	C
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	576	G
32	1a	577	G
32	1a	630	G
32	1a	631	G
32	1a	653	A
32	1a	657	G
32	1a	665	A
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	695	A
32	1a	702	A
32	1a	703	G
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	753	A
32	1a	755	G

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Mol	Chain	Res	Type
32	1a	766	A
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	857	C
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	960	U
32	1a	961	U
32	1a	966	M2G
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	996	A
32	1a	997	U
32	1a	999	C
32	1a	1000	U
32	1a	1001	A
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1010	G

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Mol	Chain	Res	Type
32	1a	1013	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1034	G
32	1a	1037	C
32	1a	1039	C
32	1a	1044	A
32	1a	1063	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1127	G
32	1a	1132	C
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1157	A
32	1a	1159	U
32	1a	1174	G
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G

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Mol	Chain	Res	Type
32	1a	1201	A
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1222	G
32	1a	1227	A
32	1a	1233	G
32	1a	1236	A
32	1a	1238	A
32	1a	1240	U
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1273	G
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1312	G
32	1a	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1370	G
32	1a	1394	A
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A

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Mol	Chain	Res	Type
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	24	A
54	1w	2	C
54	1w	3	C
54	1w	6	G
54	1w	7	A
54	1w	8	4SU
54	1w	9	A
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	25	C
54	1w	34	G
54	1w	46	G7M
54	1w	47	U
54	1w	48	C
54	1w	62	C
54	1w	63	G
54	1w	64	A
54	1w	68	C
54	1w	69	G
54	1w	71	G
54	1w	73	A
54	1w	74	C
54	1w	76	A
55	1x	3	C
55	1x	9	G
55	1x	13	C

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Mol	Chain	Res	Type
55	1x	14	A
55	1x	19	G
55	1x	20	U
55	1x	21	A
55	1x	47	U
55	1x	61	C
54	1y	6	G
54	1y	8	4SU
54	1y	13	C
54	1y	14	A
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	22	G
54	1y	23	A
54	1y	28	G
54	1y	34	G
54	1y	35	A
54	1y	44	G
54	1y	45	U
54	1y	46	G7M
54	1y	47	U
54	1y	48	C
54	1y	49	C
54	1y	50	U
54	1y	52	G
54	1y	53	G
54	1y	54	5MU
54	1y	56	C
54	1y	58	A
54	1y	64	A
54	1y	65	G
54	1y	66	U
54	1y	70	G
54	1y	73	A
1	2A	8	A
1	2A	11	G
1	2A	12	U
1	2A	14	A
1	2A	15	G
1	2A	34	C
1	2A	35	G

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Mol	Chain	Res	Type
1	2A	45	C
1	2A	51	G
1	2A	71	A
1	2A	72	U
1	2A	74	A
1	2A	75	G
1	2A	83	G
1	2A	84	A
1	2A	92	A
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	140	G
1	2A	141	A
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
1	2A	248	G
1	2A	250	G
1	2A	266	G
1	2A	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(P)	C
1	2A	272	G
1	2A	272(B)	G
1	2A	277	C

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Mol	Chain	Res	Type
1	2A	278	A
1	2A	283	A
1	2A	302	C
1	2A	311	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	354	G
1	2A	363(B)	G
1	2A	363(E)	U
1	2A	363(F)	A
1	2A	386	G
1	2A	396	G
1	2A	405	U
1	2A	406	G
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	501	A
1	2A	503	A
1	2A	505	A
1	2A	507	A
1	2A	508	G
1	2A	509	C
1	2A	521	G
1	2A	528	A
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	563	G
1	2A	568	U
1	2A	573	G

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Mol	Chain	Res	Type
1	2A	575	A
1	2A	588	U
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	651	G
1	2A	652	C
1	2A	652(A)	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(D)	C
1	2A	653	A
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	771	G
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	828	U
1	2A	832	G
1	2A	859	G

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Mol	Chain	Res	Type
1	2A	874	G
1	2A	875	G
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	882	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	903	C
1	2A	910	A
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	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	999	U
1	2A	1012	U
1	2A	1013	C
1	2A	1021	A
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U

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Mol	Chain	Res	Type
1	2A	1038	C
1	2A	1039	G
1	2A	1043	C
1	2A	1116	C
1	2A	1128	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1170	G
1	2A	1171	G
1	2A	1195	G
1	2A	1205	U
1	2A	1206	G
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1236	G
1	2A	1244	G
1	2A	1252	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1287	A
1	2A	1288	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
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	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1416	G
1	2A	1417	C

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Mol	Chain	Res	Type
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1495	A
1	2A	1496	A
1	2A	1497	U
1	2A	1505	C
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1547	C
1	2A	1554	A
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1608	A
1	2A	1610	A
1	2A	1616	A
1	2A	1648	C
1	2A	1650	G
1	2A	1654	A
1	2A	1664	A
1	2A	1667	G
1	2A	1674	G

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Mol	Chain	Res	Type
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1741	A
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1774	C
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1819	A
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	1896	G
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G

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Mol	Chain	Res	Type
1	2A	1992	G
1	2A	1993	U
1	2A	1996	C
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2070	G
1	2A	2096	U
1	2A	2099	U
1	2A	2104	G
1	2A	2111	C
1	2A	2113	U
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	2130	U
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C
1	2A	2140	C
1	2A	2141	G

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Mol	Chain	Res	Type
1	2A	2142	C
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G
1	2A	2150	U
1	2A	2151	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2162	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2171	A
1	2A	2172	U
1	2A	2174	C
1	2A	2176	A
1	2A	2178	C
1	2A	2180	U
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2268	A
1	2A	2275	C
1	2A	2278	A
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A

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Mol	Chain	Res	Type
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2383	G
1	2A	2385	C
1	2A	2396	G
1	2A	2406	U
1	2A	2414	G
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2434	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2469	A
1	2A	2476	A
1	2A	2478	A
1	2A	2484	G
1	2A	2491	U
1	2A	2492	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2554	U
1	2A	2555	U
1	2A	2562	U
1	2A	2564	A
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2602	A
1	2A	2609	U

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Mol	Chain	Res	Type
1	2A	2610	C
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2646	C
1	2A	2654	A
1	2A	2663	G
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2739	U
1	2A	2751	G
1	2A	2758	A
1	2A	2760	C
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2769	C
1	2A	2778	A
1	2A	2783	G
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	2803	C
1	2A	2810	A
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2839	G

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Mol	Chain	Res	Type
1	2A	2872	G
1	2A	2876	G
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2896	C
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	9	G
2	2B	12	C
2	2B	13	A
2	2B	17	C
2	2B	19	G
2	2B	20	C
2	2B	29	A
2	2B	34	U
2	2B	41	U
2	2B	42	C
2	2B	44	G
2	2B	53	A
2	2B	62	C
2	2B	63	G
2	2B	67	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	88	C
2	2B	91	C
2	2B	95	C
2	2B	108	U
2	2B	110	G
2	2B	120	A
32	2a	9	G
32	2a	15	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A

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Mol	Chain	Res	Type
32	2a	51	A
32	2a	52	G
32	2a	66	G
32	2a	73	G
32	2a	78	G
32	2a	80	G
32	2a	89	C
32	2a	101	A
32	2a	115	G
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	156	G
32	2a	163	C
32	2a	182	U
32	2a	188	C
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	231	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	345	C
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	355	C
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G

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Mol	Chain	Res	Type
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	454	C
32	2a	457	C
32	2a	461	A
32	2a	470	C
32	2a	484	G
32	2a	485	G
32	2a	495	A
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	527	G7M
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	536	C
32	2a	545	C
32	2a	547	A
32	2a	559	A
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C

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Mol	Chain	Res	Type
32	2a	607	A
32	2a	630	G
32	2a	631	G
32	2a	653	A
32	2a	657	G
32	2a	661	G
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	721	G
32	2a	723	U
32	2a	731	G
32	2a	733	A
32	2a	749	C
32	2a	755	G
32	2a	774	G
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	799	G
32	2a	816	A
32	2a	817	C
32	2a	819	A
32	2a	821	G
32	2a	827	U
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	859	A
32	2a	873	A
32	2a	874	G
32	2a	884	U
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	936	C

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Mol	Chain	Res	Type
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	966	M2G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	992	U
32	2a	993	G
32	2a	996	A
32	2a	997	U
32	2a	999	C
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	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(D)	A
32	2a	1032	G
32	2a	1033	G
32	2a	1035	A
32	2a	1036	G
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1041	A
32	2a	1044	A
32	2a	1045	C

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Mol	Chain	Res	Type
32	2a	1046	A
32	2a	1050	G
32	2a	1053	G
32	2a	1064	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1085	U
32	2a	1086	U
32	2a	1091	U
32	2a	1092	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1108	G
32	2a	1113	C
32	2a	1117	G
32	2a	1121	U
32	2a	1125	U
32	2a	1126	U
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1141	C
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1155	G
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1160	G
32	2a	1172	C
32	2a	1181	G
32	2a	1182	G

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Mol	Chain	Res	Type
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1201	A
32	2a	1202	G
32	2a	1211	U
32	2a	1213	A
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1270	C
32	2a	1273	G
32	2a	1276	G
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	1311	G
32	2a	1319	A
32	2a	1320	C
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1358	U
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1368	G
32	2a	1394	A
32	2a	1397	C
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	1492	A
32	2a	1497	G
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1519	MA6
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	24	A
54	2w	4	C
54	2w	6	G
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	31	A
54	2w	45	U
54	2w	46	G7M
54	2w	48	C
54	2w	58	A
54	2w	61	C
54	2w	64	A
54	2w	66	U
54	2w	68	C
54	2w	69	G
54	2w	71	G
54	2w	73	A
54	2w	74	C
55	2x	3	C
55	2x	9	G
55	2x	18	G
55	2x	19	G
55	2x	22	G
55	2x	46	G
55	2x	47	U
55	2x	48	C
55	2x	61	C
55	2x	69	C

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Mol	Chain	Res	Type
54	2y	7	A
54	2y	15	G
54	2y	19	G
54	2y	27	G
54	2y	43	C
54	2y	45	U
54	2y	47	U
54	2y	48	C
54	2y	49	C
54	2y	52	G
54	2y	53	G
54	2y	55	PSU
54	2y	56	C
54	2y	59	U
54	2y	60	U
54	2y	65	G
54	2y	68	C
54	2y	69	G
54	2y	70	G

All (49) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	746	A
1	1A	764	A
1	1A	974	G
1	1A	1067	A
1	1A	1174	A
1	1A	1176	G
1	1A	1420	U
1	1A	1508	A
1	1A	1608	A
1	1A	1663	C
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C

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Mol	Chain	Res	Type
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2629	A
1	1A	2756	U
1	2A	196	A
1	2A	228	A
1	2A	229	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	827	U
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1379	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	2116	G
1	2A	2126	A
1	2A	2406	U
1	2A	2439	A
1	2A	2689	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	8AH	2A	2503	56,1	22,26,27	1.68	5 (22%)	29,39,42	2.19	5 (17%)
54	4SU	1y	8	54	18,21,22	1.84	5 (27%)	25,30,33	1.88	4 (16%)
55	4SU	2x	8	55	18,21,22	2.02	5 (27%)	25,30,33	1.29	4 (16%)
1	5MU	2A	1939	56,1	19,22,23	1.45	6 (31%)	27,32,35	2.20	6 (22%)
54	PSU	2y	32	54	18,21,22	1.33	2 (11%)	21,30,33	1.95	3 (14%)
55	31H	1x	76	55,56	31,34,35	1.21	3 (9%)	35,47,50	2.37	11 (31%)
54	PSU	1y	55	54	18,21,22	1.36	2 (11%)	21,30,33	2.03	5 (23%)
55	PSU	2x	55	55	18,21,22	1.34	2 (11%)	21,30,33	1.97	4 (19%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	1.98	4 (19%)
1	OMC	2A	1920	1	19,22,23	0.80	0	25,31,34	0.91	1 (4%)
32	PSU	1a	516	32,56	18,21,22	1.42	2 (11%)	21,30,33	2.06	5 (23%)
1	PSU	2A	2605	1	18,21,22	1.34	3 (16%)	21,30,33	2.12	5 (23%)
32	5MC	1a	967	32	19,22,23	1.75	3 (15%)	26,32,35	1.15	2 (7%)
32	4OC	2a	1402	32	20,23,24	0.76	0	25,32,35	0.88	1 (4%)
1	5MC	2A	1962	56,1	19,22,23	1.67	3 (15%)	26,32,35	1.18	2 (7%)
55	5MC	2x	32	55	19,22,23	1.59	3 (15%)	26,32,35	1.31	4 (15%)
54	MIA	2y	37	54	21,24,32	1.59	3 (14%)	30,35,47	2.00	7 (23%)
32	UR3	2a	1498	32	19,22,23	1.04	1 (5%)	26,32,35	1.82	3 (11%)
43	0TD	2l	92	43	8,9,10	4.62	1 (12%)	6,11,13	2.31	3 (50%)
54	G7M	1y	46	54	23,26,27	1.58	3 (13%)	34,39,42	1.70	4 (11%)
1	PSU	2A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	2.01	3 (14%)
32	2MG	1a	1207	32,56	23,26,27	1.24	2 (8%)	33,38,41	2.25	8 (24%)
55	PSU	1x	55	55,56	18,21,22	1.35	2 (11%)	21,30,33	2.05	4 (19%)
54	PSU	1y	39	54	18,21,22	1.39	2 (11%)	21,30,33	1.84	3 (14%)
32	MA6	2a	1518	32	23,26,27	0.42	0	33,38,41	2.03	9 (27%)
32	M2G	1a	966	32	24,27,28	1.32	4 (16%)	33,40,43	1.84	6 (18%)
54	PSU	1y	32	54	18,21,22	1.35	2 (11%)	21,30,33	1.90	3 (14%)
1	5MC	1A	1962	56,1	19,22,23	1.81	3 (15%)	26,32,35	1.13	4 (15%)
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.16	9 (27%)
54	5MU	2w	54	54	19,22,23	1.39	5 (26%)	27,32,35	1.72	6 (22%)
32	5MC	2a	1404	32	19,22,23	1.73	3 (15%)	26,32,35	1.11	2 (7%)
54	G7M	2y	46	54	23,26,27	1.60	3 (13%)	34,39,42	1.89	5 (14%)
32	5MC	1a	1404	32	19,22,23	1.78	3 (15%)	26,32,35	1.27	3 (11%)
54	5MU	1w	54	54	19,22,23	1.40	5 (26%)	27,32,35	1.86	6 (22%)
55	4SU	1x	8	55	18,21,22	2.43	5 (27%)	25,30,33	1.83	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	5MU	2x	54	55	19,22,23	1.44	5 (26%)	27,32,35	1.94	6 (22%)
32	5MC	2a	967	32	19,22,23	1.68	3 (15%)	26,32,35	1.06	2 (7%)
54	PSU	1w	55	54	18,21,22	1.39	2 (11%)	21,30,33	2.03	4 (19%)
32	M2G	2a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.87	6 (18%)
32	UR3	1a	1498	32	19,22,23	1.01	2 (10%)	26,32,35	1.79	4 (15%)
55	5MC	1x	32	55	19,22,23	1.69	3 (15%)	26,32,35	1.20	3 (11%)
1	5MC	1A	1942	56,1	19,22,23	1.60	3 (15%)	26,32,35	1.26	2 (7%)
1	PSU	1A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	1.99	3 (14%)
54	MIA	1y	37	54	21,24,32	1.65	4 (19%)	30,35,47	2.01	7 (23%)
54	4SU	1w	8	54	18,21,22	1.85	5 (27%)	25,30,33	1.97	4 (16%)
54	PSU	1w	32	54,56	18,21,22	1.33	2 (11%)	21,30,33	1.90	3 (14%)
54	4SU	2y	8	54	18,21,22	1.69	4 (22%)	25,30,33	2.26	5 (20%)
54	PSU	2y	39	54	18,21,22	1.41	2 (11%)	21,30,33	1.69	3 (14%)
54	5MU	1y	54	54	19,22,23	1.48	5 (26%)	27,32,35	1.77	5 (18%)
1	OMU	1A	2552	56,1	19,22,23	1.29	4 (21%)	25,31,34	1.82	5 (20%)
32	MA6	2a	1519	32	23,26,27	0.44	0	33,38,41	2.06	9 (27%)
54	4SU	2w	8	54	18,21,22	1.73	5 (27%)	25,30,33	2.11	5 (20%)
32	G7M	1a	527	32,56	23,26,27	1.52	4 (17%)	34,39,42	1.62	5 (14%)
32	5MC	2a	1400	32	19,22,23	1.61	3 (15%)	26,32,35	1.22	3 (11%)
54	PSU	2w	55	54	18,21,22	1.42	2 (11%)	21,30,33	1.97	3 (14%)
54	5MU	2y	54	54	19,22,23	1.46	5 (26%)	27,32,35	1.90	6 (22%)
54	G7M	1w	46	54	23,26,27	1.59	3 (13%)	34,39,42	1.74	4 (11%)
32	MA6	1a	1518	32	23,26,27	0.41	0	33,38,41	2.03	9 (27%)
54	PSU	1w	39	54	18,21,22	1.39	2 (11%)	21,30,33	1.97	4 (19%)
1	8AH	1A	2503	56,1	22,26,27	1.61	5 (22%)	29,39,42	2.14	5 (17%)
1	5MU	2A	1915	56,1	19,22,23	1.46	5 (26%)	27,32,35	2.09	6 (22%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	0.97	1 (4%)
1	OMG	1A	2251	55,56,1	23,26,27	1.24	3 (13%)	32,38,41	1.89	5 (15%)
54	PSU	2w	39	54	18,21,22	1.36	2 (11%)	21,30,33	2.07	3 (14%)
32	2MG	2a	1207	32	23,26,27	1.24	3 (13%)	33,38,41	2.25	8 (24%)
1	5MU	1A	1915	1	19,22,23	1.41	5 (26%)	27,32,35	2.18	7 (25%)
54	MIA	1w	37	54	28,31,32	2.33	6 (21%)	38,44,47	2.78	12 (31%)
54	PSU	2w	32	54	18,21,22	1.37	2 (11%)	21,30,33	1.93	4 (19%)
55	5MU	1x	54	55,56	19,22,23	1.48	6 (31%)	27,32,35	1.87	8 (29%)
54	MIA	2w	37	54	24,27,32	2.00	6 (25%)	32,39,47	2.62	10 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	2A	2552	56,1	19,22,23	1.20	3 (15%)	25,31,34	1.76	5 (20%)
1	PSU	2A	1917	56,1	18,21,22	1.32	2 (11%)	21,30,33	1.95	4 (19%)
32	5MC	2a	1407	32,56	19,22,23	1.54	3 (15%)	26,32,35	1.16	3 (11%)
55	31H	2x	76	55,56,57,1	31,34,35	1.21	3 (9%)	35,47,50	1.95	9 (25%)
32	5MC	1a	1407	32	19,22,23	1.65	3 (15%)	26,32,35	1.15	2 (7%)
32	5MC	1a	1400	32	19,22,23	1.53	3 (15%)	26,32,35	1.10	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.77	0	25,32,35	0.95	1 (4%)
32	G7M	2a	527	32,56	23,26,27	1.52	4 (17%)	34,39,42	1.70	5 (14%)
1	PSU	1A	2605	56,1	18,21,22	1.40	3 (16%)	21,30,33	2.09	4 (19%)
54	PSU	2y	55	54	18,21,22	1.44	3 (16%)	21,30,33	1.95	5 (23%)
1	PSU	1A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	1.98	4 (19%)
54	G7M	2w	46	54	23,26,27	1.53	4 (17%)	34,39,42	1.59	4 (11%)
1	5MC	2A	1942	1	19,22,23	1.59	3 (15%)	26,32,35	1.12	2 (7%)
43	0TD	1l	92	43	8,9,10	4.53	1 (12%)	6,11,13	1.79	2 (33%)
1	OMG	2A	2251	55,56,1	23,26,27	1.22	3 (13%)	32,38,41	2.05	7 (21%)
1	5MU	1A	1939	56,1	19,22,23	1.43	6 (31%)	27,32,35	2.20	6 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	8AH	2A	2503	56,1	-	0/7/25/26	0/3/3/3
54	4SU	1y	8	54	-	3/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	56,1	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
55	31H	1x	76	55,56	-	5/22/40/41	0/3/3/3
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	0/9/29/30	0/2/2/2
1	5MC	2A	1962	56,1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	0/7/25/34	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	3/7/12/14	-
54	G7M	1y	46	54	-	1/7/25/26	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32,56	-	2/9/27/28	0/3/3/3
55	PSU	1x	55	55,56	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	56,1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
54	G7M	2y	46	54	-	2/7/25/26	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	56,1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	1/7/25/34	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54,56	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	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	-	2/7/25/26	0/2/2/2
1	OMU	1A	2552	56,1	-	0/9/27/28	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,56	-	3/7/25/26	0/3/3/3
32	5MC	2a	1400	32	-	1/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	8AH	1A	2503	56,1	-	1/7/25/26	0/3/3/3
1	5MU	2A	1915	56,1	-	1/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	OMG	1A	2251	55,56,1	-	0/9/27/28	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/15/33/34	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55,56	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/11/29/34	0/3/3/3
1	OMU	2A	2552	56,1	-	0/9/27/28	0/2/2/2
1	PSU	2A	1917	56,1	-	1/7/25/26	0/2/2/2
32	5MC	2a	1407	32,56	-	0/7/25/26	0/2/2/2
55	31H	2x	76	55,56,57,1	-	6/22/40/41	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	1/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
32	G7M	2a	527	32,56	-	3/7/25/26	0/3/3/3
1	PSU	1A	2605	56,1	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	3/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
1	OMG	2A	2251	55,56,1	-	0/9/27/28	0/3/3/3
1	5MU	1A	1939	56,1	-	0/7/25/26	0/2/2/2

All (258) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.64	1.69	1.82
43	1l	92	0TD	CB-SB	-12.37	1.69	1.82
54	1w	37	MIA	C2-S10	-7.07	1.69	1.75
1	1A	1962	5MC	C5-C4	6.82	1.49	1.44
54	1w	37	MIA	C13-C14	6.78	1.52	1.32
32	1a	967	5MC	C5-C4	6.55	1.49	1.44
32	1a	1404	5MC	C5-C4	6.38	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1404	5MC	C5-C4	6.35	1.48	1.44
55	1x	8	4SU	C4-N3	-6.33	1.31	1.37
32	2a	967	5MC	C5-C4	6.13	1.48	1.44
32	1a	1407	5MC	C5-C4	6.09	1.48	1.44
1	2A	1962	5MC	C5-C4	6.06	1.48	1.44
55	1x	32	5MC	C5-C4	5.97	1.48	1.44
54	2w	37	MIA	C2-S10	-5.88	1.70	1.75
32	2a	1400	5MC	C5-C4	5.77	1.48	1.44
1	2A	1942	5MC	C5-C4	5.65	1.48	1.44
1	1A	1942	5MC	C5-C4	5.64	1.48	1.44
55	2x	32	5MC	C5-C4	5.59	1.48	1.44
32	2a	1407	5MC	C5-C4	5.49	1.48	1.44
32	1a	1400	5MC	C5-C4	5.29	1.48	1.44
54	1y	37	MIA	C5-C4	5.29	1.48	1.39
54	2y	37	MIA	C5-C4	5.09	1.48	1.39
54	2w	37	MIA	C5-C4	5.04	1.48	1.39
54	1w	46	G7M	C5-N7	-4.90	1.33	1.39
54	2y	46	G7M	C5-N7	-4.87	1.33	1.39
54	1w	8	4SU	C4-S4	-4.85	1.60	1.68
32	1a	527	G7M	C5-N7	-4.85	1.33	1.39
55	1x	8	4SU	C4-S4	-4.80	1.60	1.68
54	1w	37	MIA	C5-C4	4.78	1.47	1.39
54	1y	46	G7M	C5-N7	-4.72	1.33	1.39
54	1y	8	4SU	C4-S4	-4.70	1.60	1.68
32	2a	527	G7M	C5-N7	-4.65	1.33	1.39
54	2y	8	4SU	C4-S4	-4.61	1.60	1.68
55	2x	8	4SU	C4-N3	-4.56	1.32	1.37
54	2w	8	4SU	C4-S4	-4.55	1.60	1.68
54	2w	46	G7M	C5-N7	-4.54	1.33	1.39
1	2A	2503	8AH	C5-C4	4.53	1.47	1.39
55	2x	8	4SU	C4-S4	-4.35	1.61	1.68
55	1x	8	4SU	C2-N3	-4.33	1.30	1.38
1	1A	2503	8AH	C5-C4	4.27	1.46	1.39
54	2w	55	PSU	C6-C5	4.18	1.39	1.35
55	1x	76	31H	C5-N7	-4.10	1.31	1.39
54	1w	55	PSU	C6-C5	4.04	1.39	1.35
55	2x	76	31H	C5-N7	-4.03	1.31	1.39
54	1y	39	PSU	C6-C5	3.88	1.39	1.35
54	1y	8	4SU	C4-N3	-3.80	1.33	1.37
54	1y	32	PSU	C6-C5	3.76	1.39	1.35
54	1y	55	PSU	C6-C5	3.74	1.39	1.35
54	2w	32	PSU	C6-C5	3.73	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	516	PSU	C6-C5	3.70	1.39	1.35
32	2a	516	PSU	C6-C5	3.69	1.39	1.35
55	2x	55	PSU	C6-C5	3.69	1.39	1.35
54	2w	39	PSU	C6-C5	3.67	1.39	1.35
54	2y	39	PSU	C6-C5	3.60	1.39	1.35
54	1w	32	PSU	C6-C5	3.59	1.39	1.35
1	1A	1917	PSU	C6-C5	3.58	1.39	1.35
54	2y	32	PSU	C6-C5	3.56	1.39	1.35
54	2y	46	G7M	C5-C4	3.56	1.47	1.38
54	1y	46	G7M	C5-C4	3.54	1.47	1.38
1	1A	1911	PSU	C6-C5	3.52	1.39	1.35
54	1w	8	4SU	C4-N3	-3.49	1.34	1.37
1	2A	1917	PSU	C6-C5	3.46	1.39	1.35
55	1x	55	PSU	C6-C5	3.40	1.39	1.35
1	2A	1911	PSU	C6-C5	3.38	1.39	1.35
1	1A	2605	PSU	C6-C5	3.36	1.39	1.35
1	2A	2605	PSU	C6-C5	3.35	1.39	1.35
55	2x	8	4SU	C2-N3	-3.35	1.32	1.38
54	1w	46	G7M	C5-C4	3.34	1.46	1.38
54	2w	46	G7M	C5-C4	3.34	1.46	1.38
1	2A	2503	8AH	C4-N9	-3.33	1.33	1.38
54	1w	39	PSU	C6-C5	3.30	1.38	1.35
54	2y	55	PSU	C6-C5	3.30	1.38	1.35
1	2A	2503	8AH	C8-N7	3.25	1.36	1.31
55	1x	8	4SU	C5-C4	-3.22	1.38	1.42
32	1a	527	G7M	C5-C4	3.19	1.46	1.38
32	2a	527	G7M	C5-C4	3.19	1.46	1.38
1	1A	2503	8AH	C4-N9	-3.16	1.34	1.38
1	2A	1915	5MU	C6-C5	3.14	1.39	1.34
1	1A	2251	OMG	C5-C4	3.14	1.47	1.38
55	2x	8	4SU	C5-C4	-3.11	1.38	1.42
54	2w	8	4SU	C4-N3	-3.11	1.34	1.37
32	2a	1207	2MG	C5-C4	3.11	1.47	1.38
32	1a	1207	2MG	C5-C4	3.10	1.47	1.38
55	1x	32	5MC	C6-C5	3.09	1.39	1.34
1	2A	2251	OMG	C5-C4	3.07	1.47	1.38
32	1a	966	M2G	C5-C4	3.07	1.47	1.38
32	2a	1404	5MC	C6-C5	3.06	1.39	1.34
32	2a	966	M2G	C5-C4	3.05	1.47	1.38
55	2x	76	31H	C5-C4	-3.04	1.33	1.39
54	2w	37	MIA	C5-C6	3.04	1.49	1.41
54	1y	54	5MU	C6-C5	2.98	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2503	8AH	C5-N7	-2.97	1.34	1.39
55	2x	54	5MU	C6-C5	2.96	1.39	1.34
55	1x	76	31H	C5-C6	-2.96	1.32	1.41
1	1A	1962	5MC	C6-C5	2.96	1.39	1.34
1	1A	2503	8AH	C8-N7	2.95	1.35	1.31
32	1a	966	M2G	C2-N2	2.92	1.40	1.35
1	1A	2503	8AH	C5-N7	-2.92	1.34	1.39
1	2A	1939	5MU	C4-N3	-2.90	1.33	1.38
54	2y	54	5MU	C6-C5	2.90	1.39	1.34
1	2A	2251	OMG	C6-N1	-2.90	1.33	1.38
32	1a	1404	5MC	C6-C5	2.89	1.39	1.34
1	2A	1942	5MC	C6-C5	2.89	1.39	1.34
54	2y	37	MIA	C5-C6	2.88	1.49	1.41
54	2y	55	PSU	C4-N3	-2.87	1.33	1.38
1	1A	1939	5MU	C6-C5	2.87	1.39	1.34
54	1y	37	MIA	C5-C6	2.87	1.49	1.41
32	1a	1400	5MC	C6-C5	2.86	1.39	1.34
54	2y	39	PSU	C4-N3	-2.84	1.33	1.38
55	1x	54	5MU	C4-C5	2.83	1.49	1.44
32	2a	966	M2G	C2-N2	2.83	1.40	1.35
1	1A	2251	OMG	C6-N1	-2.82	1.33	1.38
54	1w	54	5MU	C4-N3	-2.82	1.33	1.38
55	1x	54	5MU	C6-C5	2.81	1.39	1.34
55	1x	54	5MU	C4-N3	-2.80	1.33	1.38
1	2A	1939	5MU	C6-C5	2.79	1.39	1.34
32	1a	967	5MC	C6-C5	2.78	1.39	1.34
32	1a	1407	5MC	C6-C5	2.77	1.39	1.34
1	1A	1915	5MU	C6-C5	2.76	1.39	1.34
1	1A	1942	5MC	C6-C5	2.75	1.39	1.34
1	1A	1939	5MU	C4-N3	-2.74	1.33	1.38
54	2y	54	5MU	C2-N1	2.74	1.42	1.38
54	1w	39	PSU	C4-N3	-2.74	1.33	1.38
54	1w	54	5MU	C6-C5	2.74	1.39	1.34
54	1y	54	5MU	C4-N3	-2.72	1.33	1.38
1	1A	1915	5MU	C2-N1	2.71	1.42	1.38
54	1w	37	MIA	C5-C6	2.70	1.48	1.41
1	1A	2552	OMU	C4-N3	-2.69	1.34	1.38
32	2a	1407	5MC	C6-C5	2.68	1.39	1.34
54	1y	54	5MU	C2-N1	2.68	1.42	1.38
32	2a	1400	5MC	C6-C5	2.67	1.39	1.34
1	1A	1911	PSU	C4-N3	-2.66	1.33	1.38
1	2A	1915	5MU	C4-N3	-2.66	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	32	5MC	C6-C5	2.65	1.38	1.34
55	2x	54	5MU	C4-N3	-2.64	1.33	1.38
55	2x	54	5MU	C4-C5	2.63	1.49	1.44
32	2a	967	5MC	C6-C5	2.63	1.38	1.34
1	1A	1915	5MU	C4-C5	2.63	1.49	1.44
54	2y	8	4SU	C4-N3	-2.63	1.34	1.37
55	2x	76	31H	C5-C6	-2.62	1.33	1.41
54	2w	54	5MU	C4-N3	-2.62	1.33	1.38
54	2y	54	5MU	C4-N3	-2.61	1.34	1.38
1	2A	2552	OMU	C4-N3	-2.60	1.34	1.38
32	1a	516	PSU	C4-N3	-2.59	1.34	1.38
1	1A	2251	OMG	C5-N7	-2.59	1.33	1.39
1	1A	2605	PSU	C4-N3	-2.58	1.34	1.38
1	2A	1911	PSU	C4-N3	-2.58	1.34	1.38
54	1y	55	PSU	C4-N3	-2.58	1.34	1.38
1	2A	2605	PSU	C4-N3	-2.56	1.34	1.38
54	1y	39	PSU	C4-N3	-2.55	1.34	1.38
54	1w	8	4SU	C5-C4	-2.55	1.39	1.42
55	1x	55	PSU	C4-N3	-2.54	1.34	1.38
55	2x	55	PSU	C4-N3	-2.54	1.34	1.38
32	1a	966	M2G	C6-N1	-2.53	1.34	1.38
1	2A	1962	5MC	C6-C5	2.52	1.38	1.34
54	2w	54	5MU	C6-C5	2.52	1.38	1.34
1	2A	1915	5MU	C2-N1	2.51	1.42	1.38
54	2y	46	G7M	C6-N1	-2.51	1.34	1.38
32	2a	1498	UR3	C2-N1	2.49	1.42	1.38
55	1x	8	4SU	O2-C2	2.49	1.27	1.23
54	1w	46	G7M	C6-N1	-2.47	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.46	1.34	1.38
54	1w	55	PSU	C4-N3	-2.45	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.45	1.33	1.38
1	2A	1915	5MU	C4-C5	2.45	1.48	1.44
54	1w	32	PSU	C4-N3	-2.43	1.34	1.38
54	2w	32	PSU	C4-N3	-2.43	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.42	1.34	1.38
54	1w	37	MIA	C5-N7	-2.42	1.34	1.39
32	1a	527	G7M	C6-N1	-2.41	1.34	1.38
32	2a	527	G7M	C6-N1	-2.41	1.34	1.38
54	1w	8	4SU	C2-N1	2.40	1.42	1.38
54	2y	32	PSU	C4-N3	-2.38	1.34	1.38
54	2w	55	PSU	C4-N3	-2.38	1.34	1.38
55	2x	32	5MC	C6-N1	-2.37	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2552	OMU	C2-N3	-2.37	1.33	1.38
32	1a	1404	5MC	C6-N1	-2.37	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.37	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.37	1.34	1.38
54	2y	37	MIA	C8-N7	2.37	1.36	1.31
1	1A	1917	PSU	C4-N3	-2.37	1.34	1.38
32	2a	966	M2G	C6-N1	-2.35	1.34	1.38
54	2w	37	MIA	C5-N7	-2.35	1.34	1.39
54	2w	54	5MU	C4-C5	2.35	1.48	1.44
54	2y	8	4SU	C2-N1	2.35	1.42	1.38
54	1w	37	MIA	C8-N7	2.34	1.36	1.31
54	1y	8	4SU	C2-N3	-2.33	1.33	1.38
1	2A	1939	5MU	C6-N1	-2.31	1.34	1.38
54	1y	8	4SU	C5-C4	-2.31	1.39	1.42
54	2y	55	PSU	C2-N3	-2.31	1.33	1.37
54	1y	32	PSU	C4-N3	-2.31	1.34	1.38
54	2y	8	4SU	C5-C4	-2.31	1.39	1.42
1	1A	1939	5MU	C6-N1	-2.31	1.34	1.38
1	1A	1915	5MU	C4-N3	-2.31	1.34	1.38
54	1y	54	5MU	C4-C5	2.30	1.48	1.44
1	1A	1939	5MU	C4-C5	2.30	1.48	1.44
54	2w	39	PSU	C4-N3	-2.29	1.34	1.38
1	2A	1939	5MU	C4-C5	2.29	1.48	1.44
55	1x	76	31H	C5-C4	-2.29	1.35	1.39
54	1y	46	G7M	C6-N1	-2.29	1.34	1.38
54	1y	37	MIA	C8-N7	2.29	1.36	1.31
54	2w	8	4SU	C2-N1	2.29	1.42	1.38
1	1A	2552	OMU	C5-C4	-2.28	1.38	1.43
32	2a	967	5MC	C6-N1	-2.28	1.34	1.38
1	2A	2503	8AH	C5-C6	2.28	1.47	1.41
1	2A	2552	OMU	C2-N3	-2.27	1.34	1.38
32	2a	516	PSU	C4-N3	-2.27	1.34	1.38
54	1w	8	4SU	C2-N3	-2.27	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.26	1.34	1.38
54	2w	37	MIA	C2-N3	2.26	1.37	1.34
54	2w	8	4SU	C5-C4	-2.25	1.39	1.42
1	2A	1942	5MC	C6-N1	-2.25	1.34	1.38
54	2y	54	5MU	C2-N3	-2.24	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.23	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.22	1.34	1.38
54	1w	54	5MU	C4-C5	2.22	1.48	1.44
55	1x	32	5MC	C6-N1	-2.21	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2605	PSU	C2-N3	-2.21	1.33	1.37
54	2w	37	MIA	C8-N7	2.21	1.35	1.31
54	1y	37	MIA	C5-N7	-2.20	1.35	1.39
54	1y	54	5MU	C2-N3	-2.19	1.34	1.38
32	1a	1498	UR3	C2-N1	2.19	1.41	1.38
1	2A	2251	OMG	C5-N7	-2.19	1.34	1.39
1	1A	1962	5MC	C6-N1	-2.18	1.34	1.38
54	1w	54	5MU	C2-N3	-2.17	1.34	1.38
54	2w	54	5MU	C2-N1	2.17	1.41	1.38
55	2x	54	5MU	C2-N3	-2.15	1.34	1.38
1	2A	1939	5MU	C2-N1	2.15	1.41	1.38
32	1a	1400	5MC	C6-N1	-2.14	1.34	1.38
54	2w	54	5MU	C2-N3	-2.13	1.34	1.38
54	2y	54	5MU	C4-C5	2.13	1.48	1.44
1	1A	2503	8AH	C5-C6	2.13	1.46	1.41
55	1x	54	5MU	C2-N3	-2.13	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.12	1.34	1.38
55	2x	54	5MU	C2-N1	2.12	1.41	1.38
55	1x	54	5MU	C6-N1	-2.12	1.34	1.38
55	1x	54	5MU	C2-N1	2.12	1.41	1.38
54	1w	54	5MU	C2-N1	2.11	1.41	1.38
32	1a	967	5MC	C6-N1	-2.11	1.34	1.38
32	1a	966	M2G	C5-N7	-2.11	1.34	1.39
1	1A	2605	PSU	C2-N1	-2.10	1.33	1.36
54	2w	46	G7M	C6-N1	-2.10	1.34	1.38
1	1A	1939	5MU	C2-N1	2.08	1.41	1.38
1	1A	2552	OMU	C2-N1	2.08	1.41	1.38
32	2a	1404	5MC	C6-N1	-2.07	1.34	1.38
32	2a	1207	2MG	C5-N7	-2.07	1.34	1.39
32	1a	527	G7M	C4-N9	-2.07	1.32	1.38
54	2w	8	4SU	C2-N3	-2.06	1.34	1.38
54	1y	8	4SU	C6-C5	2.06	1.39	1.35
32	1a	1498	UR3	C6-C5	2.06	1.39	1.35
32	2a	527	G7M	C5-C6	2.05	1.48	1.43
1	2A	1915	5MU	C6-N1	-2.04	1.34	1.38
54	2w	46	G7M	C4-N9	-2.03	1.32	1.38
32	2a	966	M2G	C4-N9	-2.02	1.32	1.38
1	1A	1915	5MU	C6-N1	-2.02	1.34	1.38
1	2A	2552	OMU	C5-C4	-2.02	1.39	1.43
32	1a	1407	5MC	C6-N1	-2.01	1.34	1.38
55	2x	8	4SU	C6-C5	2.01	1.39	1.35

All (404) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	37	MIA	C12-C13-C14	-9.44	110.07	127.01
54	2w	37	MIA	C5-C4-N3	-9.22	117.47	127.18
1	2A	2503	8AH	C5-C4-N3	-8.19	118.56	127.18
54	1w	37	MIA	C5-C4-N3	-7.94	118.81	127.18
1	1A	2503	8AH	C5-C4-N3	-7.67	119.10	127.18
32	2a	1207	2MG	C2-N3-C4	7.28	121.11	112.00
54	2w	37	MIA	N3-C4-N9	7.27	136.22	126.99
32	1a	1207	2MG	C2-N3-C4	7.20	121.00	112.00
32	2a	1498	UR3	C4-N3-C2	-7.14	118.83	124.58
32	1a	1498	UR3	C4-N3-C2	-7.03	118.92	124.58
54	2y	8	4SU	C4-N3-C2	-6.73	120.87	127.31
1	2A	2605	PSU	N1-C2-N3	6.52	122.05	115.17
1	2A	2251	OMG	C5-C4-N3	-6.50	118.05	128.39
55	1x	55	PSU	N1-C2-N3	6.40	121.92	115.17
54	2w	8	4SU	C4-N3-C2	-6.39	121.19	127.31
54	1y	55	PSU	N1-C2-N3	6.36	121.88	115.17
55	1x	76	31H	O4'-C1'-N9	6.35	120.28	108.09
32	1a	516	PSU	N1-C2-N3	6.33	121.84	115.17
54	2y	46	G7M	N9-C4-N3	6.32	138.58	125.95
54	2w	39	PSU	N1-C2-N3	6.27	121.78	115.17
1	2A	1911	PSU	N1-C2-N3	6.24	121.75	115.17
54	1w	39	PSU	N1-C2-N3	6.22	121.72	115.17
54	1w	55	PSU	N1-C2-N3	6.18	121.69	115.17
54	1w	37	MIA	N3-C4-N9	6.18	134.83	126.99
32	2a	1207	2MG	C5-C4-N3	-6.10	118.68	128.39
54	2w	55	PSU	N1-C2-N3	6.10	121.60	115.17
32	2a	516	PSU	N1-C2-N3	6.08	121.58	115.17
1	1A	2605	PSU	N1-C2-N3	6.01	121.51	115.17
1	1A	2251	OMG	C5-C4-N3	-6.01	118.82	128.39
1	1A	1911	PSU	N1-C2-N3	6.01	121.50	115.17
54	2y	32	PSU	N1-C2-N3	5.99	121.48	115.17
54	1y	37	MIA	C5-C4-N3	-5.97	118.49	126.72
32	2a	966	M2G	C5-C4-N3	-5.97	118.89	128.39
54	2y	55	PSU	N1-C2-N3	5.94	121.43	115.17
32	1a	966	M2G	C5-C4-N3	-5.90	119.00	128.39
55	2x	55	PSU	N1-C2-N3	5.89	121.39	115.17
54	2y	46	G7M	C5-C4-N3	-5.89	117.01	128.15
54	2w	32	PSU	N1-C2-N3	5.89	121.38	115.17
32	1a	1207	2MG	C5-C4-N3	-5.88	119.03	128.39
54	1w	32	PSU	N1-C2-N3	5.83	121.32	115.17
1	1A	1917	PSU	N1-C2-N3	5.83	121.32	115.17
54	1w	46	G7M	N9-C4-N3	5.81	137.56	125.95
1	2A	1917	PSU	N1-C2-N3	5.81	121.29	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	37	MIA	C5-C4-N3	-5.80	118.73	126.72
54	1y	39	PSU	N1-C2-N3	5.74	121.23	115.17
54	1y	32	PSU	N1-C2-N3	5.73	121.21	115.17
54	1w	8	4SU	C5-C4-N3	5.67	120.02	114.75
55	1x	76	31H	N1-C2-N3	-5.64	120.05	128.58
54	1y	46	G7M	N9-C4-N3	5.60	137.14	125.95
55	2x	76	31H	N1-C2-N3	-5.57	120.15	128.58
54	1w	8	4SU	C4-N3-C2	-5.53	122.02	127.31
1	2A	1939	5MU	C4-N3-C2	-5.49	120.15	127.34
54	2y	8	4SU	C5-C4-N3	5.47	119.84	114.75
54	1y	8	4SU	C4-N3-C2	-5.45	122.09	127.31
1	1A	1939	5MU	C4-N3-C2	-5.44	120.20	127.34
32	2a	527	G7M	N9-C4-N3	5.42	136.79	125.95
32	2a	527	G7M	C5-C4-N3	-5.38	117.99	128.15
54	2w	8	4SU	C5-C4-N3	5.38	119.75	114.75
54	2y	39	PSU	N1-C2-N3	5.34	120.80	115.17
1	2A	1939	5MU	N3-C2-N1	5.32	121.81	114.89
54	1y	46	G7M	C5-C4-N3	-5.30	118.14	128.15
55	1x	76	31H	C5-C4-N3	-5.28	119.44	126.72
1	1A	1915	5MU	C4-N3-C2	-5.27	120.44	127.34
1	2A	1915	5MU	N3-C2-N1	5.10	121.53	114.89
1	2A	1915	5MU	C4-N3-C2	-5.06	120.71	127.34
1	2A	2251	OMG	C2-N3-C4	5.05	121.01	112.30
1	1A	1939	5MU	N3-C2-N1	5.03	121.43	114.89
54	1y	8	4SU	C5-C4-N3	5.02	119.42	114.75
1	2A	2251	OMG	N9-C4-N3	5.01	135.97	125.95
32	1a	1519	MA6	N1-C2-N3	-4.97	121.05	128.58
54	2w	46	G7M	N9-C4-N3	4.97	135.89	125.95
32	2a	1518	MA6	N1-C2-N3	-4.97	121.06	128.58
54	1w	46	G7M	C5-C4-N3	-4.95	118.79	128.15
32	1a	527	G7M	N9-C4-N3	4.95	135.85	125.95
54	1y	37	MIA	N3-C4-N9	4.94	135.57	127.17
1	1A	1915	5MU	N3-C2-N1	4.92	121.30	114.89
54	2y	46	G7M	C2-N3-C4	4.90	120.74	112.30
32	1a	527	G7M	C5-C4-N3	-4.89	118.92	128.15
1	1A	2251	OMG	C2-N3-C4	4.87	120.69	112.30
1	1A	1915	5MU	C5-C4-N3	4.84	119.53	115.32
32	2a	1519	MA6	N1-C2-N3	-4.84	121.26	128.58
32	1a	1518	MA6	N1-C2-N3	-4.82	121.29	128.58
1	2A	1939	5MU	C5-C4-N3	4.79	119.49	115.32
55	2x	76	31H	C5-C4-N3	-4.78	120.14	126.72
1	1A	1939	5MU	C5-C4-N3	4.78	119.47	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2552	OMU	C4-N3-C2	-4.77	120.69	126.61
54	2y	37	MIA	N3-C4-N9	4.76	135.26	127.17
32	2a	527	G7M	C2-N3-C4	4.74	120.47	112.30
32	2a	1519	MA6	C5-C4-N3	-4.69	120.25	126.72
1	2A	2552	OMU	C4-N3-C2	-4.68	120.80	126.61
54	2w	46	G7M	C5-C4-N3	-4.67	119.32	128.15
55	1x	54	5MU	N3-C2-N1	4.64	120.93	114.89
1	2A	2605	PSU	C4-N3-C2	-4.63	119.99	126.37
55	2x	54	5MU	N3-C2-N1	4.63	120.92	114.89
54	1y	46	G7M	C2-N3-C4	4.62	120.26	112.30
55	2x	54	5MU	C4-N3-C2	-4.60	121.31	127.34
32	1a	966	M2G	N9-C4-N3	4.56	135.07	125.95
1	2A	1915	5MU	C5-C4-N3	4.55	119.28	115.32
54	1w	54	5MU	N3-C2-N1	4.52	120.78	114.89
32	2a	966	M2G	C2-N3-C4	4.52	120.87	112.51
32	2a	1518	MA6	C5-C4-N3	-4.51	120.51	126.72
1	1A	1939	5MU	C5-C6-N1	-4.43	118.50	123.31
54	1w	54	5MU	C4-N3-C2	-4.42	121.55	127.34
32	2a	966	M2G	N9-C4-N3	4.41	134.77	125.95
1	1A	2503	8AH	N6-C6-N1	4.39	122.95	117.03
1	1A	2605	PSU	C4-N3-C2	-4.36	120.36	126.37
54	2w	46	G7M	C2-N3-C4	4.34	119.78	112.30
32	1a	1519	MA6	C5-C4-N3	-4.34	120.75	126.72
1	2A	2552	OMU	N3-C2-N1	4.33	120.53	114.89
54	2y	54	5MU	N3-C2-N1	4.32	120.52	114.89
54	1w	46	G7M	C2-N3-C4	4.32	119.73	112.30
55	2x	55	PSU	C4-N3-C2	-4.31	120.43	126.37
32	1a	527	G7M	C2-N3-C4	4.30	119.71	112.30
54	2y	8	4SU	N3-C2-N1	4.28	120.47	114.89
32	1a	966	M2G	C2-N3-C4	4.28	120.43	112.51
55	1x	54	5MU	C4-N3-C2	-4.28	121.73	127.34
1	1A	2552	OMU	N3-C2-N1	4.26	120.43	114.89
54	2w	39	PSU	C4-N3-C2	-4.25	120.52	126.37
32	1a	1519	MA6	C4-C5-N7	-4.25	105.72	110.58
54	1y	54	5MU	N3-C2-N1	4.24	120.42	114.89
54	2y	54	5MU	C4-N3-C2	-4.24	121.78	127.34
32	1a	1519	MA6	C5-N7-C8	4.23	110.10	103.45
1	1A	2251	OMG	N9-C4-N3	4.23	134.41	125.95
54	1y	55	PSU	C4-N3-C2	-4.20	120.59	126.37
55	1x	8	4SU	C6-C5-C4	-4.19	116.32	119.95
32	1a	516	PSU	C4-N3-C2	-4.19	120.60	126.37
1	1A	1939	5MU	O4-C4-C5	-4.17	120.14	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	8	4SU	S4-C4-N3	-4.16	115.86	120.20
55	1x	55	PSU	C4-N3-C2	-4.16	120.65	126.37
55	2x	54	5MU	C5-C4-N3	4.13	118.91	115.32
54	1w	37	MIA	C15-C14-C13	-4.11	110.33	122.66
1	1A	1911	PSU	C4-N3-C2	-4.11	120.71	126.37
54	2y	54	5MU	O4-C4-C5	-4.10	120.22	124.92
32	2a	516	PSU	C4-N3-C2	-4.10	120.73	126.37
1	1A	1915	5MU	O4-C4-C5	-4.09	120.23	124.92
55	1x	8	4SU	O2-C2-N1	4.09	128.12	122.80
32	1a	1519	MA6	C2-N1-C6	4.09	121.82	111.83
1	2A	1917	PSU	C4-N3-C2	-4.08	120.75	126.37
54	1w	54	5MU	C5-C4-N3	4.07	118.86	115.32
1	2A	2503	8AH	C4-C5-N7	-4.07	106.75	110.91
32	1a	1518	MA6	C2-N1-C6	4.07	121.77	111.83
32	2a	1518	MA6	C2-N1-C6	4.06	121.75	111.83
54	2y	54	5MU	C5-C4-N3	4.06	118.85	115.32
32	2a	1207	2MG	N9-C4-N3	4.05	134.06	125.95
54	2w	39	PSU	O2-C2-N1	-4.04	118.62	122.79
54	1w	55	PSU	C4-N3-C2	-4.04	120.80	126.37
1	1A	2605	PSU	O2-C2-N1	-4.03	118.63	122.79
1	1A	1917	PSU	C4-N3-C2	-4.02	120.83	126.37
1	2A	1911	PSU	O2-C2-N1	-4.02	118.64	122.79
32	1a	1207	2MG	C6-C5-N7	4.01	137.59	130.29
1	2A	1939	5MU	C5-C6-N1	-4.01	118.96	123.31
32	1a	1518	MA6	C5-C4-N3	-4.00	121.21	126.72
1	2A	1915	5MU	O4-C4-C5	-3.98	120.36	124.92
54	2w	8	4SU	N3-C2-N1	3.98	120.07	114.89
54	2y	55	PSU	C4-N3-C2	-3.98	120.89	126.37
54	2y	8	4SU	C5-C4-S4	-3.97	119.77	124.31
32	2a	1519	MA6	C2-N1-C6	3.96	121.51	111.83
1	2A	2503	8AH	C6-C5-N7	3.96	135.65	131.72
54	1w	32	PSU	C4-N3-C2	-3.96	120.92	126.37
1	2A	1911	PSU	C4-N3-C2	-3.92	120.97	126.37
54	1y	54	5MU	C4-N3-C2	-3.89	122.24	127.34
32	1a	1518	MA6	C5-N7-C8	3.89	109.56	103.45
54	2w	54	5MU	C5-C4-N3	3.88	118.70	115.32
54	2y	32	PSU	C4-N3-C2	-3.88	121.03	126.37
54	2w	32	PSU	C4-N3-C2	-3.87	121.04	126.37
1	2A	1939	5MU	O4-C4-C5	-3.84	120.53	124.92
54	1w	37	MIA	C16-C14-C13	-3.83	111.18	122.66
54	1y	8	4SU	N3-C2-N1	3.80	119.84	114.89
54	2w	37	MIA	C12-N6-C6	-3.80	119.33	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-3.80	95.54	102.36
1	2A	2552	OMU	C5-C4-N3	3.79	120.11	114.80
32	2a	1519	MA6	C5-N7-C8	3.78	109.39	103.45
1	1A	1917	PSU	O2-C2-N1	-3.77	118.91	122.79
32	2a	1519	MA6	C4-C5-N7	-3.76	106.28	110.58
55	1x	76	31H	N9-C8-N7	-3.76	108.60	113.94
32	1a	1518	MA6	N9-C8-N7	-3.75	108.61	113.94
54	2w	54	5MU	C4-N3-C2	-3.73	122.45	127.34
32	1a	1207	2MG	N9-C4-N3	3.73	133.41	125.95
54	1w	39	PSU	C4-N3-C2	-3.72	121.25	126.37
54	1y	37	MIA	C2-N3-C4	3.71	120.89	111.83
54	2w	54	5MU	N3-C2-N1	3.70	119.71	114.89
32	1a	1519	MA6	N9-C8-N7	-3.70	108.69	113.94
32	1a	967	5MC	C5-C6-N1	-3.70	119.30	123.31
54	2w	55	PSU	O2-C2-N1	-3.69	118.99	122.79
32	2a	1518	MA6	C5-N7-C8	3.68	109.23	103.45
54	1y	54	5MU	C5-C4-N3	3.67	118.51	115.32
32	2a	1518	MA6	C4-C5-N7	-3.66	106.39	110.58
32	2a	1404	5MC	C5-C6-N1	-3.66	119.34	123.31
55	2x	54	5MU	C5-C6-N1	-3.65	119.35	123.31
1	1A	2552	OMU	C5-C4-N3	3.64	119.91	114.80
54	1y	32	PSU	C4-N3-C2	-3.63	121.37	126.37
54	2y	37	MIA	C2-N3-C4	3.62	120.67	111.83
55	1x	76	31H	C5-N7-C8	3.62	109.13	103.45
32	2a	1207	2MG	C6-C5-N7	3.61	136.86	130.29
55	1x	54	5MU	C5-C4-N3	3.60	118.46	115.32
55	2x	32	5MC	C5-C6-N1	-3.60	119.40	123.31
32	1a	1407	5MC	C5-C6-N1	-3.59	119.41	123.31
32	2a	1400	5MC	C5-C6-N1	-3.59	119.42	123.31
1	1A	2503	8AH	C6-C5-N7	3.58	135.27	131.72
54	1y	54	5MU	O4-C4-C5	-3.58	120.83	124.92
54	2w	55	PSU	C4-N3-C2	-3.57	121.45	126.37
54	1y	32	PSU	O2-C2-N1	-3.57	119.10	122.79
54	1y	39	PSU	C4-N3-C2	-3.57	121.46	126.37
54	2w	37	MIA	C2-N3-C4	3.56	121.62	112.29
55	1x	55	PSU	O2-C2-N1	-3.55	119.13	122.79
1	2A	1917	PSU	O2-C2-N1	-3.53	119.14	122.79
55	1x	76	31H	C2-N3-C4	3.52	120.44	111.83
54	2y	32	PSU	O2-C2-N1	-3.52	119.16	122.79
1	2A	1962	5MC	C5-C6-N1	-3.52	119.50	123.31
54	2w	37	MIA	C4-C5-N7	-3.51	106.57	110.58
54	1w	54	5MU	O4-C4-C5	-3.51	120.90	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1498	UR3	C5-C4-N3	3.51	119.66	115.04
32	2a	1519	MA6	C2-N3-C4	3.50	120.37	111.83
54	1y	37	MIA	N3-C2-N1	-3.48	123.31	128.58
54	1w	37	MIA	C4-C5-N7	-3.48	106.60	110.58
32	1a	1518	MA6	C4-C5-N7	-3.48	106.61	110.58
32	1a	1404	5MC	C5-C6-N1	-3.48	119.54	123.31
32	2a	1518	MA6	C2-N3-C4	3.47	120.31	111.83
55	2x	76	31H	N9-C8-N7	-3.47	109.01	113.94
1	2A	1942	5MC	C5-C6-N1	-3.46	119.55	123.31
54	1w	39	PSU	O2-C2-N1	-3.45	119.23	122.79
54	1w	55	PSU	O2-C2-N1	-3.45	119.23	122.79
1	1A	2503	8AH	C4-C5-N7	-3.45	107.39	110.91
32	1a	516	PSU	O2-C2-N1	-3.44	119.25	122.79
55	1x	32	5MC	C5-C6-N1	-3.42	119.60	123.31
1	2A	2503	8AH	N6-C6-N1	3.40	121.61	117.03
32	1a	1519	MA6	C2-N3-C4	3.40	120.12	111.83
55	1x	8	4SU	C5-C4-N3	3.38	117.90	114.75
55	2x	54	5MU	O4-C4-C5	-3.37	121.06	124.92
32	1a	1404	5MC	C5-C4-N3	-3.35	118.32	121.75
54	1w	54	5MU	C5-C6-N1	-3.35	119.67	123.31
54	2y	37	MIA	N3-C2-N1	-3.35	123.52	128.58
1	2A	1915	5MU	C5-C6-N1	-3.32	119.71	123.31
54	2w	54	5MU	O4-C4-C5	-3.32	121.12	124.92
54	2y	37	MIA	C4-C5-N7	-3.31	106.80	110.58
54	1w	37	MIA	C6-C5-N7	3.30	136.03	132.43
54	2w	8	4SU	C5-C4-S4	-3.30	120.54	124.31
32	2a	966	M2G	C6-C5-N7	3.30	136.29	130.29
54	1w	8	4SU	N3-C2-N1	3.28	119.17	114.89
54	2y	54	5MU	C5-C6-N1	-3.28	119.75	123.31
1	1A	1942	5MC	C5-C6-N1	-3.27	119.76	123.31
1	1A	1942	5MC	C5-C4-N3	-3.26	118.41	121.75
32	2a	1519	MA6	N9-C8-N7	-3.26	109.31	113.94
55	2x	76	31H	C5-N7-C8	3.25	108.55	103.45
54	1w	37	MIA	C2-N3-C4	3.24	120.78	112.29
43	2l	92	0TD	OD2-CG-CB	3.24	120.16	113.15
1	1A	1911	PSU	O2-C2-N1	-3.23	119.45	122.79
32	1a	1518	MA6	C2-N3-C4	3.23	119.72	111.83
32	1a	1207	2MG	C4-C5-N7	-3.23	105.55	110.67
55	1x	54	5MU	C5-C6-N1	-3.22	119.82	123.31
55	2x	76	31H	C2-N3-C4	3.20	119.66	111.83
1	1A	2251	OMG	C6-C5-N7	3.20	136.11	130.29
32	2a	516	PSU	O2-C2-N1	-3.19	119.50	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1518	MA6	N9-C8-N7	-3.16	109.45	113.94
55	1x	32	5MC	C5-C4-N3	-3.16	118.51	121.75
54	1w	8	4SU	C5-C4-S4	-3.16	120.70	124.31
55	1x	76	31H	C4'-O4'-C1'	-3.12	102.58	109.47
1	1A	2552	OMU	O4-C4-C5	-3.12	119.78	125.16
32	2a	967	5MC	C5-C6-N1	-3.10	119.95	123.31
55	2x	76	31H	C4'-O4'-C1'	-3.08	102.66	109.47
54	1y	37	MIA	C4-C5-N7	-3.07	107.07	110.58
54	1y	54	5MU	C5-C6-N1	-3.06	119.99	123.31
1	1A	1915	5MU	C5-C6-N1	-3.04	120.01	123.31
32	1a	1400	5MC	C5-C4-N3	-3.02	118.66	121.75
54	2y	39	PSU	C4-N3-C2	-3.01	122.22	126.37
1	1A	1962	5MC	C5-C6-N1	-3.01	120.05	123.31
32	1a	966	M2G	C6-C5-N7	3.01	135.76	130.29
1	2A	2251	OMG	C6-C5-N7	3.00	135.75	130.29
54	1y	55	PSU	O2-C2-N1	-2.99	119.70	122.79
32	1a	1207	2MG	N1-C2-N2	2.99	119.61	116.56
54	2w	32	PSU	O2-C2-N1	-2.98	119.72	122.79
55	2x	8	4SU	C5-C4-N3	2.96	117.50	114.75
32	2a	1207	2MG	C4-C5-N7	-2.94	106.01	110.67
1	1A	2503	8AH	C2-N1-C6	2.93	122.60	118.10
32	1a	1400	5MC	C5-C6-N1	-2.93	120.13	123.31
32	2a	1407	5MC	C5-C4-N3	-2.92	118.76	121.75
54	1w	32	PSU	O2-C2-N1	-2.91	119.78	122.79
32	2a	1519	MA6	N3-C4-N9	2.89	132.09	127.17
55	2x	32	5MC	C5-C4-N3	-2.89	118.79	121.75
32	1a	1498	UR3	C5-C4-N3	2.89	118.84	115.04
55	2x	76	31H	C5-C4-N9	2.87	108.94	105.81
55	1x	76	31H	C4-C5-N7	-2.87	107.30	110.58
43	1l	92	0TD	OD2-CG-CB	2.87	119.34	113.15
32	2a	1207	2MG	N1-C2-N2	2.85	119.47	116.56
32	2a	1407	5MC	C5-C6-N1	-2.84	120.22	123.31
1	2A	1942	5MC	C5-C4-N3	-2.83	118.85	121.75
1	2A	2503	8AH	C2-N1-C6	2.80	122.41	118.10
54	1y	39	PSU	O2-C2-N1	-2.80	119.90	122.79
55	1x	76	31H	N3-C4-N9	2.79	131.92	127.17
1	1A	1962	5MC	C5-C4-N3	-2.77	118.92	121.75
32	1a	1518	MA6	N3-C4-N9	2.75	131.84	127.17
32	2a	1404	5MC	C5-C4-N3	-2.74	118.94	121.75
32	2a	1518	MA6	N3-C4-N9	2.74	131.83	127.17
55	1x	54	5MU	C5M-C5-C4	2.73	121.70	118.78
54	2w	54	5MU	C5-C6-N1	-2.72	120.36	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1962	5MC	C5-C4-N3	-2.69	119.00	121.75
55	2x	8	4SU	C1'-N1-C2	2.69	122.42	117.59
1	2A	2552	OMU	O4-C4-C5	-2.68	120.54	125.16
1	1A	1915	5MU	C5M-C5-C4	2.67	121.64	118.78
55	2x	8	4SU	C6-C5-C4	-2.65	117.66	119.95
54	2w	54	5MU	C5M-C5-C4	2.64	121.60	118.78
54	2y	37	MIA	C4-N9-C8	2.64	108.50	105.74
1	2A	2605	PSU	O2-C2-N1	-2.63	120.07	122.79
32	2a	966	M2G	C4-C5-N7	-2.63	106.50	110.67
1	1A	1939	5MU	O2-C2-N1	-2.63	119.38	122.80
32	2a	1519	MA6	C4-C5-C6	2.61	118.61	115.91
1	1A	2251	OMG	C4-C5-N7	-2.60	106.54	110.67
32	1a	1498	UR3	C6-N1-C2	-2.59	119.68	121.80
55	1x	54	5MU	O4-C4-C5	-2.59	121.95	124.92
55	1x	76	31H	C5-C4-N9	2.57	108.61	105.81
54	1w	46	G7M	O6-C6-C5	-2.56	122.29	128.01
54	2w	37	MIA	C5-N7-C8	2.55	107.46	103.45
54	1w	37	MIA	C5-N7-C8	2.54	107.45	103.45
32	1a	1402	4OC	C6-C5-C4	2.53	120.05	117.00
32	1a	967	5MC	C5-C4-N3	-2.53	119.17	121.75
54	1w	37	MIA	C4-N9-C8	2.50	108.37	105.74
54	2w	37	MIA	C6-C5-N7	2.50	135.16	132.43
55	1x	54	5MU	O2-C2-N1	-2.50	119.54	122.80
32	1a	1407	5MC	C5-C4-N3	-2.49	119.20	121.75
32	2a	1400	5MC	O2-C2-N3	-2.48	118.42	122.33
54	2y	37	MIA	C5-N7-C8	2.48	107.35	103.45
32	2a	1518	MA6	C4-C5-C6	2.47	118.46	115.91
54	1w	37	MIA	C2-N1-C6	2.46	122.21	117.54
1	2A	1939	5MU	O2-C2-N1	-2.45	119.60	122.80
55	2x	32	5MC	O2-C2-N3	-2.45	118.47	122.33
32	1a	1207	2MG	N2-C2-N3	-2.45	117.39	120.51
32	1a	1519	MA6	N3-C4-N9	2.45	131.33	127.17
55	2x	55	PSU	O2-C2-N1	-2.44	120.27	122.79
32	2a	967	5MC	C5-C4-N3	-2.42	119.27	121.75
32	1a	1518	MA6	C4-N9-C8	2.42	108.28	105.74
32	2a	1407	5MC	O2-C2-N3	-2.42	118.52	122.33
54	2y	55	PSU	C6-C5-C4	-2.41	116.55	118.17
32	1a	527	G7M	O6-C6-C5	-2.38	122.69	128.01
32	1a	1498	UR3	C3U-N3-C4	2.38	121.17	117.87
43	2l	92	0TD	OD1-CG-CB	-2.38	117.47	122.44
32	2a	1207	2MG	N2-C2-N3	-2.37	117.49	120.51
55	2x	76	31H	C4-C5-N7	-2.37	107.87	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1400	5MC	C5-C4-N3	-2.37	119.33	121.75
55	2x	8	4SU	O2-C2-N1	2.36	125.87	122.80
32	1a	966	M2G	C4-C5-N7	-2.36	106.93	110.67
54	2w	46	G7M	O6-C6-C5	-2.35	122.75	128.01
32	1a	966	M2G	O6-C6-C5	-2.34	120.36	126.53
32	1a	1519	MA6	C4-C5-C6	2.33	118.32	115.91
32	1a	1404	5MC	O2-C2-N3	-2.33	118.66	122.33
55	1x	76	31H	C3'-N3'-C	-2.33	119.66	123.20
55	2x	54	5MU	O2-C2-N1	-2.33	119.77	122.80
1	2A	2605	PSU	C5-C6-N1	-2.31	118.93	122.14
54	2y	46	G7M	O6-C6-C5	-2.29	122.89	128.01
55	1x	8	4SU	O2-C2-N3	-2.28	117.27	121.49
1	2A	1915	5MU	O2-C2-N1	-2.28	119.82	122.80
1	1A	1920	OMC	O2-C2-N3	-2.28	118.73	122.33
1	2A	2251	OMG	C4-C5-N7	-2.28	107.05	110.67
54	2y	8	4SU	O2-C2-N1	-2.28	119.83	122.80
55	1x	32	5MC	O2-C2-N3	-2.27	118.75	122.33
55	2x	55	PSU	C5-C6-N1	-2.27	118.99	122.14
54	2y	55	PSU	O2-C2-N1	-2.26	120.45	122.79
32	1a	516	PSU	O4'-C1'-C2'	2.26	108.28	105.15
54	2y	39	PSU	O2-C2-N1	-2.26	120.46	122.79
1	2A	2251	OMG	O6-C6-C5	-2.26	120.57	126.53
54	1y	46	G7M	O6-C6-C5	-2.25	122.98	128.01
54	1y	37	MIA	C5-N7-C8	2.25	106.99	103.45
54	1y	55	PSU	C5-C6-N1	-2.25	119.02	122.14
1	2A	2605	PSU	O2-C2-N3	-2.24	117.88	121.86
54	1w	37	MIA	N3-C2-N1	-2.24	122.92	127.00
54	2w	37	MIA	N3-C2-N1	-2.24	122.92	127.00
54	2w	37	MIA	C2-N1-C6	2.23	121.77	117.54
1	1A	1962	5MC	O2-C2-N3	-2.22	118.83	122.33
55	2x	76	31H	N3-C4-N9	2.20	130.92	127.17
54	1w	39	PSU	C5-C6-N1	-2.20	119.09	122.14
55	1x	55	PSU	C5-C6-N1	-2.19	119.09	122.14
54	1w	54	5MU	O2-C2-N1	-2.19	119.95	122.80
54	1y	37	MIA	C4-N9-C8	2.18	108.03	105.74
1	2A	2251	OMG	C5-C6-N1	2.18	118.79	113.25
55	1x	54	5MU	C5M-C5-C6	-2.17	119.91	122.85
1	1A	2605	PSU	C5-C6-N1	-2.17	119.13	122.14
32	2a	527	G7M	C5-C6-N1	2.15	116.29	111.84
1	2A	2552	OMU	O2-C2-N1	-2.15	120.00	122.80
1	1A	1915	5MU	O2-C2-N1	-2.15	120.00	122.80
54	2w	32	PSU	C6-C5-C4	-2.14	116.73	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	G7M	O6-C6-C5	-2.14	123.23	128.01
1	1A	1962	5MC	CM5-C5-C6	-2.14	119.96	122.85
32	2a	1402	4OC	C6-C5-C4	2.14	119.58	117.00
32	2a	1498	UR3	C1'-N1-C2	2.13	120.53	117.04
1	1A	2552	OMU	C1'-N1-C2	2.13	121.41	117.59
55	2x	32	5MC	C1'-N1-C6	-2.12	117.66	121.15
54	1y	55	PSU	O4'-C1'-C2'	2.11	108.07	105.15
54	2y	55	PSU	O2-C2-N3	-2.11	118.12	121.86
1	2A	1917	PSU	C5-C6-N1	-2.10	119.22	122.14
1	1A	1911	PSU	C5-C6-N1	-2.09	119.24	122.14
32	2a	966	M2G	O6-C6-C5	-2.08	121.04	126.53
32	2a	516	PSU	O4'-C1'-C2'	2.07	108.02	105.15
32	1a	1207	2MG	C8-N7-C5	2.06	107.94	104.26
43	1l	92	0TD	OD1-CG-CB	-2.06	118.13	122.44
55	1x	8	4SU	C4-N3-C2	2.06	129.29	127.31
1	2A	1920	OMC	O2-C2-N3	-2.05	119.10	122.33
54	2w	37	MIA	C1'-N9-C8	-2.04	122.57	127.09
54	2w	8	4SU	C1'-N1-C2	2.04	121.25	117.59
32	1a	516	PSU	C5-C6-N1	-2.03	119.33	122.14
54	2y	54	5MU	C1'-N1-C2	2.02	121.22	117.59
54	2y	46	G7M	C5-C6-N1	2.01	115.99	111.84
32	1a	527	G7M	C5-C6-N1	2.01	115.99	111.84
54	1y	8	4SU	C5-C4-S4	-2.00	122.02	124.31
54	1w	55	PSU	C5-C6-N1	-2.00	119.36	122.14
32	2a	1207	2MG	C2-N1-C6	-2.00	122.13	124.55

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	C12-C13-C14-C16
55	1x	76	31H	CB-CA-N-CN
54	1y	8	4SU	O4'-C4'-C5'-O5'
54	1y	46	G7M	C4'-C5'-O5'-P
32	2a	1519	MA6	O4'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
54	2y	55	PSU	C2'-C1'-C5-C6
55	1x	76	31H	C3'-C4'-C5'-O5'
55	2x	76	31H	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
54	2y	55	PSU	C3'-C4'-C5'-O5'
54	2y	55	PSU	O4'-C4'-C5'-O5'
55	1x	76	31H	O4'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
54	1y	54	5MU	O4'-C4'-C5'-O5'
55	2x	76	31H	O4'-C4'-C5'-O5'
55	1x	76	31H	CB-CG-SD-CE
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
55	2x	76	31H	C4'-C5'-O5'-P
32	2a	527	G7M	O4'-C4'-C5'-O5'
54	1w	46	G7M	C4'-C5'-O5'-P
55	1x	76	31H	C4'-C5'-O5'-P
32	1a	1519	MA6	C3'-C4'-C5'-O5'
55	2x	76	31H	N-CA-CB-CG
55	2x	76	31H	C-CA-CB-CG
54	2y	46	G7M	O4'-C1'-N9-C4
54	1y	37	MIA	C3'-C4'-C5'-O5'
55	2x	76	31H	CB-CG-SD-CE
54	2w	46	G7M	C4'-C5'-O5'-P
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
1	2A	1915	5MU	O4'-C4'-C5'-O5'
1	2A	1917	PSU	O4'-C4'-C5'-O5'
43	1l	92	0TD	SB-CB-CG-OD1
43	2l	92	0TD	SB-CB-CG-OD1
54	1y	54	5MU	C3'-C4'-C5'-O5'
32	2a	527	G7M	C4'-C5'-O5'-P
32	1a	527	G7M	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C4'-C5'-O5'
54	2y	46	G7M	O4'-C1'-N9-C8
43	1l	92	0TD	CA-CB-SB-CSB
43	2l	92	0TD	CA-CB-SB-CSB
32	1a	527	G7M	O4'-C4'-C5'-O5'
54	1y	8	4SU	C4'-C5'-O5'-P
32	1a	1519	MA6	C4'-C5'-O5'-P
1	1A	2503	8AH	C4'-C5'-O5'-P
1	1A	1920	OMC	C2'-C1'-N1-C2

There are no ring outliers.

33 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	1y	8	4SU	1	0
55	2x	8	4SU	2	0
1	2A	1939	5MU	2	0
55	1x	76	31H	1	0
54	1y	55	PSU	1	0
32	1a	967	5MC	1	0
54	2y	37	MIA	1	0
43	2l	92	0TD	1	0
54	1y	46	G7M	1	0
32	1a	1207	2MG	1	0
32	2a	1518	MA6	1	0
32	1a	966	M2G	2	0
32	1a	1519	MA6	1	0
54	2y	46	G7M	2	0
55	1x	8	4SU	2	0
32	2a	967	5MC	2	0
32	2a	966	M2G	1	0
1	1A	1942	5MC	1	0
54	1y	37	MIA	3	0
54	2y	8	4SU	3	0
54	2y	39	PSU	1	0
54	1y	54	5MU	1	0
32	2a	1519	MA6	1	0
54	2y	54	5MU	1	0
32	1a	1518	MA6	1	0
1	2A	1915	5MU	1	0
1	1A	1920	OMC	1	0
32	2a	1207	2MG	1	0
55	2x	76	31H	1	0
32	1a	1402	4OC	1	0
54	2y	55	PSU	7	0
43	1l	92	0TD	1	0
1	1A	1939	5MU	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2763 ligands modelled in this entry, 2759 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
58	WC9	2A	3846	-	34,37,37	1.32	4 (11%)	31,53,53	1.01	2 (6%)
60	SF4	1d	302	35	0,12,12	-	-	-	-	-
58	WC9	1A	4098	1	34,37,37	1.68	6 (17%)	31,53,53	1.10	2 (6%)
60	SF4	2d	303	35	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	WC9	2A	3846	-	-	0/28/71/71	0/3/4/4
60	SF4	1d	302	35	-	-	0/6/5/5
58	WC9	1A	4098	1	-	2/28/71/71	0/3/4/4
60	SF4	2d	303	35	-	-	0/6/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1A	4098	WC9	CAM-CBF	-4.79	1.39	1.51
58	1A	4098	WC9	OAW-CB	4.63	1.47	1.42
58	2A	3846	WC9	CAM-CBF	-4.48	1.40	1.51
58	1A	4098	WC9	OAW-CAX	3.41	1.48	1.43
58	2A	3846	WC9	OAW-CB	3.04	1.45	1.42
58	1A	4098	WC9	CD2-CAZ	-2.46	1.51	1.53
58	1A	4098	WC9	CAK-NAL	2.40	1.49	1.45
58	2A	3846	WC9	CB-CA	-2.15	1.50	1.53
58	1A	4098	WC9	CBF-CBH	2.10	1.40	1.31
58	2A	3846	WC9	CBF-CBH	2.06	1.40	1.31

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	2A	3846	WC9	CBC-CBB-CAZ	-3.13	110.61	116.68
58	1A	4098	WC9	CBC-CBB-CAZ	-2.91	111.02	116.68
58	1A	4098	WC9	CD2-CAZ-CAY	-2.59	109.91	113.78
58	2A	3846	WC9	CAF-OAA-CAB	-2.46	110.94	114.17

There are no chirality outliers.

All (2) torsion outliers are listed below:

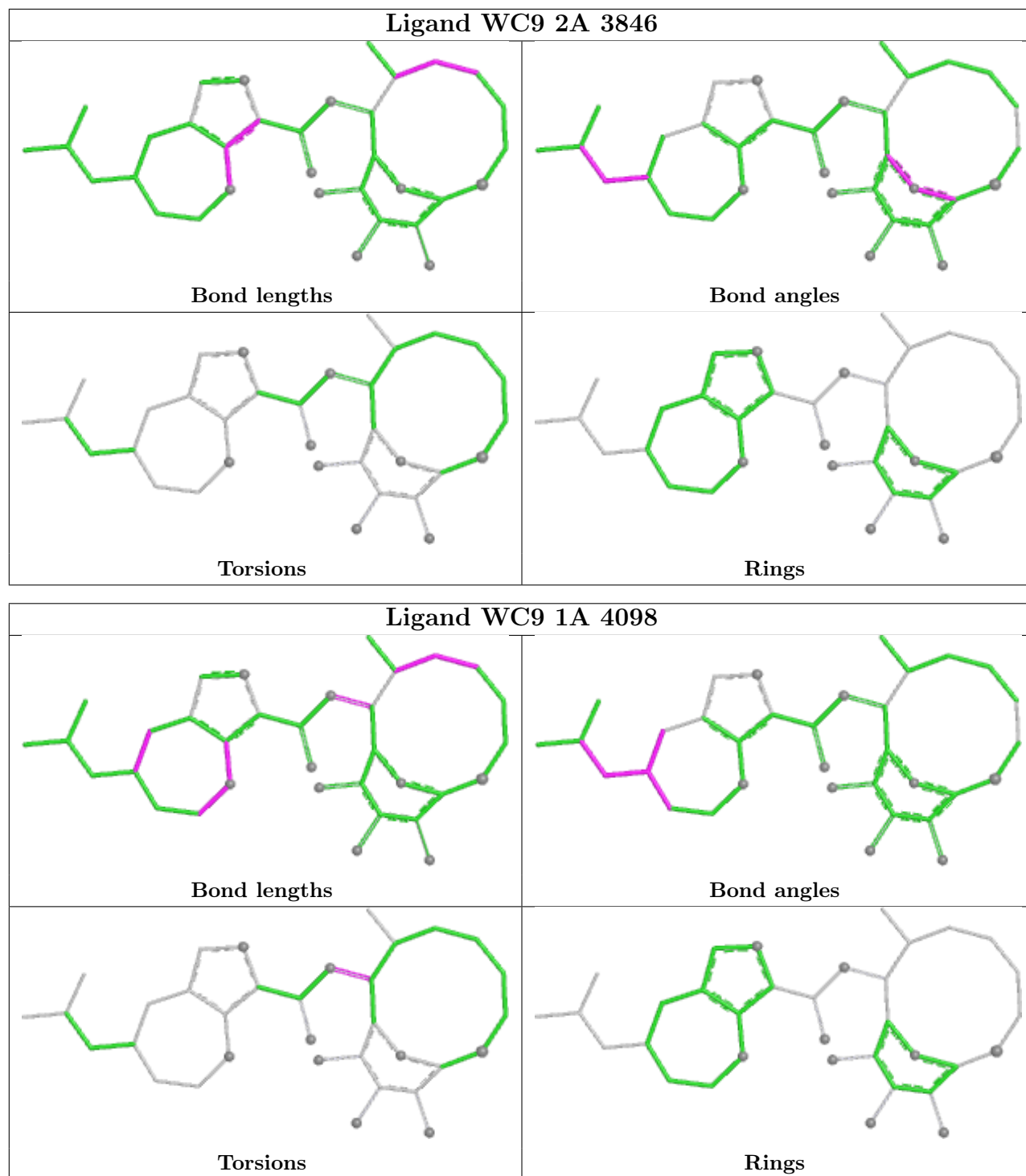
Mol	Chain	Res	Type	Atoms
58	1A	4098	WC9	CAB-CAK-NAL-C
58	1A	4098	WC9	CAM-CAK-NAL-C

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	2A	3846	WC9	1	0
60	1d	302	SF4	2	0
58	1A	4098	WC9	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	-0.52	120 (4%) 40 35	21, 38, 95, 108	0
1	2A	2789/2915 (95%)	-0.05	104 (3%) 45 39	34, 57, 93, 107	0
2	1B	120/121 (99%)	-0.33	0 100 100	33, 52, 67, 88	0
2	2B	120/121 (99%)	0.39	1 (0%) 82 80	61, 73, 82, 93	0
3	1D	275/276 (99%)	-0.25	2 (0%) 84 82	21, 39, 52, 79	0
3	2D	275/276 (99%)	0.10	2 (0%) 84 82	30, 50, 62, 82	0
4	1E	204/206 (99%)	-0.27	0 100 100	21, 39, 61, 72	0
4	2E	204/206 (99%)	0.39	6 (2%) 53 48	39, 60, 72, 83	0
5	1F	203/210 (96%)	-0.07	1 (0%) 87 85	22, 45, 68, 84	0
5	2F	203/210 (96%)	0.38	2 (0%) 79 76	36, 64, 76, 84	0
6	1G	181/182 (99%)	0.30	5 (2%) 55 49	46, 60, 74, 83	0
6	2G	181/182 (99%)	0.73	8 (4%) 39 33	62, 74, 82, 86	0
7	1H	174/180 (96%)	0.08	3 (1%) 69 64	39, 54, 66, 73	0
7	2H	174/180 (96%)	1.31	36 (20%) 2 2	71, 84, 91, 95	0
8	1I	146/148 (98%)	0.67	4 (2%) 56 50	49, 72, 81, 84	0
8	2I	146/148 (98%)	0.81	10 (6%) 23 19	50, 71, 82, 88	0
9	1N	140/140 (100%)	-0.24	1 (0%) 84 82	25, 38, 62, 75	0
9	2N	140/140 (100%)	0.55	5 (3%) 46 40	48, 66, 79, 84	0
10	1O	122/122 (100%)	-0.23	0 100 100	29, 41, 59, 63	0
10	2O	122/122 (100%)	0.35	1 (0%) 82 80	50, 61, 71, 76	0
11	1P	149/150 (99%)	0.02	0 100 100	23, 50, 70, 75	0
11	2P	149/150 (99%)	0.40	2 (1%) 75 71	41, 63, 80, 87	0
12	1Q	141/141 (100%)	-0.06	1 (0%) 84 82	28, 43, 61, 77	0
12	2Q	141/141 (100%)	0.64	5 (3%) 47 41	52, 67, 76, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.33	0 100 100	27, 36, 47, 59	0
13	2R	118/118 (100%)	0.28	1 (0%) 82 80	44, 54, 65, 73	0
14	1S	110/112 (98%)	0.10	0 100 100	41, 52, 64, 70	0
14	2S	110/112 (98%)	0.80	6 (5%) 30 25	58, 68, 77, 80	0
15	1T	131/146 (89%)	0.14	3 (2%) 61 55	36, 48, 73, 81	0
15	2T	131/146 (89%)	0.50	2 (1%) 72 68	53, 65, 75, 81	0
16	1U	116/118 (98%)	-0.47	0 100 100	20, 30, 46, 66	0
16	2U	116/118 (98%)	0.47	3 (2%) 57 51	41, 63, 75, 81	0
17	1V	101/101 (100%)	-0.39	0 100 100	23, 38, 57, 65	0
17	2V	101/101 (100%)	0.44	1 (0%) 79 76	44, 71, 79, 82	0
18	1W	112/113 (99%)	-0.41	1 (0%) 81 78	23, 32, 51, 77	0
18	2W	112/113 (99%)	0.19	0 100 100	42, 51, 67, 83	0
19	1X	95/96 (98%)	-0.23	0 100 100	29, 39, 61, 72	0
19	2X	95/96 (98%)	0.35	3 (3%) 50 44	45, 58, 74, 86	0
20	1Y	107/110 (97%)	0.24	2 (1%) 66 61	37, 52, 69, 78	0
20	2Y	107/110 (97%)	0.96	12 (11%) 10 8	56, 69, 81, 87	0
21	1Z	154/206 (74%)	0.60	6 (3%) 43 38	38, 66, 84, 91	0
21	2Z	160/206 (77%)	1.12	20 (12%) 8 6	69, 80, 89, 92	0
22	10	83/85 (97%)	0.03	3 (3%) 46 40	30, 40, 60, 76	0
22	20	83/85 (97%)	0.79	8 (9%) 13 10	45, 62, 74, 83	0
23	11	97/98 (98%)	0.20	3 (3%) 51 45	31, 46, 72, 77	0
23	21	97/98 (98%)	0.22	1 (1%) 79 76	38, 53, 72, 81	0
24	12	70/72 (97%)	-0.00	2 (2%) 53 48	38, 50, 59, 71	0
24	22	70/72 (97%)	0.50	2 (2%) 53 48	57, 67, 75, 76	0
25	13	59/60 (98%)	-0.24	2 (3%) 48 42	26, 38, 61, 82	0
25	23	59/60 (98%)	0.38	1 (1%) 69 64	54, 65, 78, 81	0
26	14	69/71 (97%)	0.96	10 (14%) 6 4	56, 76, 87, 90	0
26	24	69/71 (97%)	1.06	7 (10%) 12 9	71, 83, 92, 101	0
27	15	59/60 (98%)	-0.48	0 100 100	20, 33, 52, 59	0
27	25	59/60 (98%)	0.32	3 (5%) 33 28	39, 54, 69, 76	0
28	16	53/54 (98%)	-0.24	0 100 100	35, 47, 60, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.40	0 100 100	47, 59, 66, 75	0
29	17	48/49 (97%)	-0.18	3 (6%) 26 20	23, 29, 59, 69	0
29	27	48/49 (97%)	0.04	3 (6%) 26 20	35, 42, 68, 73	0
30	18	64/65 (98%)	-0.25	0 100 100	28, 38, 44, 58	0
30	28	64/65 (98%)	0.26	1 (1%) 70 66	46, 53, 60, 68	0
31	19	37/37 (100%)	-0.19	0 100 100	34, 42, 55, 66	0
31	29	37/37 (100%)	1.04	3 (8%) 18 14	63, 69, 78, 84	0
32	1a	1488/1521 (97%)	0.19	49 (3%) 49 43	36, 66, 93, 109	0
32	2a	1491/1521 (98%)	0.41	65 (4%) 39 33	45, 73, 93, 106	0
33	1b	231/256 (90%)	1.11	41 (17%) 4 3	64, 78, 87, 93	0
33	2b	231/256 (90%)	1.23	41 (17%) 4 3	68, 82, 88, 93	0
34	1c	206/239 (86%)	0.68	8 (3%) 43 38	60, 72, 82, 91	0
34	2c	206/239 (86%)	1.17	24 (11%) 9 7	71, 79, 86, 90	0
35	1d	208/209 (99%)	0.77	13 (6%) 26 20	56, 69, 78, 85	0
35	2d	208/209 (99%)	0.51	3 (1%) 73 69	54, 66, 74, 79	0
36	1e	148/162 (91%)	0.42	3 (2%) 65 60	51, 64, 74, 85	0
36	2e	148/162 (91%)	0.74	4 (2%) 56 50	57, 71, 79, 88	0
37	1f	100/101 (99%)	0.48	0 100 100	56, 68, 74, 77	0
37	2f	100/101 (99%)	0.51	2 (2%) 65 60	55, 67, 75, 77	0
38	1g	155/156 (99%)	0.58	8 (5%) 33 27	59, 70, 80, 88	0
38	2g	155/156 (99%)	0.70	10 (6%) 25 19	67, 74, 81, 88	0
39	1h	137/138 (99%)	0.39	1 (0%) 84 82	55, 67, 73, 78	0
39	2h	137/138 (99%)	0.83	3 (2%) 62 57	65, 73, 78, 82	0
40	1i	127/128 (99%)	1.21	20 (15%) 5 4	56, 77, 83, 88	0
40	2i	127/128 (99%)	1.42	30 (23%) 2 1	64, 81, 87, 90	0
41	1j	97/105 (92%)	1.12	13 (13%) 7 5	58, 77, 87, 92	0
41	2j	96/105 (91%)	1.89	42 (43%) 0 0	71, 82, 90, 91	0
42	1k	114/129 (88%)	0.53	4 (3%) 47 41	43, 64, 76, 81	0
42	2k	114/129 (88%)	0.57	4 (3%) 47 41	53, 70, 79, 81	0
43	1l	121/132 (91%)	0.13	2 (1%) 69 64	44, 53, 67, 74	0
43	2l	121/132 (91%)	0.51	4 (3%) 49 43	55, 63, 74, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.77	8 (6%) 25 19	52, 70, 78, 90	0
44	2m	122/126 (96%)	1.38	21 (17%) 4 3	66, 79, 85, 90	0
45	1n	60/61 (98%)	1.03	7 (11%) 9 7	60, 68, 77, 81	0
45	2n	60/61 (98%)	1.85	21 (35%) 1 1	73, 80, 85, 89	0
46	1o	88/89 (98%)	0.55	1 (1%) 78 74	50, 65, 75, 82	0
46	2o	88/89 (98%)	0.61	2 (2%) 61 55	57, 68, 79, 81	0
47	1p	82/88 (93%)	0.90	2 (2%) 59 54	55, 69, 77, 85	0
47	2p	82/88 (93%)	0.85	5 (6%) 27 22	57, 67, 75, 79	0
48	1q	99/105 (94%)	0.72	3 (3%) 52 47	53, 66, 74, 77	0
48	2q	99/105 (94%)	0.71	5 (5%) 33 28	61, 70, 77, 80	0
49	1r	68/88 (77%)	0.36	1 (1%) 72 68	53, 66, 76, 78	0
49	2r	68/88 (77%)	0.45	1 (1%) 72 68	57, 68, 75, 80	0
50	1s	83/93 (89%)	0.67	3 (3%) 46 40	62, 74, 79, 82	0
50	2s	83/93 (89%)	1.31	14 (16%) 4 3	74, 82, 87, 93	0
51	1t	96/106 (90%)	0.81	7 (7%) 21 17	58, 70, 80, 83	0
51	2t	96/106 (90%)	0.65	2 (2%) 63 58	57, 68, 80, 86	0
52	1u	23/27 (85%)	1.05	4 (17%) 4 3	63, 68, 71, 79	0
52	2u	23/27 (85%)	1.32	4 (17%) 4 3	69, 76, 79, 85	0
53	1v	13/24 (54%)	0.22	1 (7%) 19 15	48, 58, 84, 92	0
53	2v	13/24 (54%)	0.79	3 (23%) 2 1	62, 72, 87, 98	0
54	1w	67/76 (88%)	1.09	13 (19%) 3 2	49, 86, 99, 101	0
54	1y	67/76 (88%)	0.83	2 (2%) 52 47	38, 90, 97, 101	0
54	2w	65/76 (85%)	1.37	14 (21%) 2 2	69, 94, 102, 108	0
54	2y	66/76 (86%)	1.06	9 (13%) 7 5	50, 92, 98, 102	0
55	1x	71/77 (92%)	0.21	2 (2%) 55 49	33, 63, 80, 86	0
55	2x	71/77 (92%)	0.42	3 (4%) 40 35	46, 75, 86, 97	0
All	All	20873/21748 (95%)	0.25	983 (4%) 36 30	20, 63, 88, 109	0

All (983) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	652(V)	C	10.6
1	1A	653	A	10.6

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Mol	Chain	Res	Type	RSRZ
1	2A	652(V)	C	10.5
1	2A	652(U)	G	10.5
1	1A	652(U)	G	9.6
1	2A	652(C)	G	9.5
44	2m	123	ALA	8.5
1	2A	653	A	7.4
1	1A	652(C)	G	6.7
41	2j	32	ALA	6.6
23	2l	2	SER	6.6
44	1m	123	ALA	6.5
1	1A	654	A	6.5
45	1n	2	ALA	6.5
1	1A	652(T)	C	6.2
1	2A	652(T)	C	6.2
23	1l	2	SER	6.2
1	2A	883	G	6.1
45	2n	2	ALA	6.1
1	2A	654	A	6.1
32	1a	1036	G	5.8
1	2A	884	C	5.4
1	2A	2802	G	5.3
44	2m	124	PRO	5.2
1	1A	652(S)	C	5.2
44	2m	122	LYS	5.2
32	2a	1033	G	5.1
20	2Y	54	LYS	5.1
1	1A	652(E)	G	5.1
21	2Z	172	ALA	5.0
1	1A	1058	G	5.0
1	2A	652(D)	C	5.0
22	10	6	GLY	5.0
32	1a	1035	A	5.0
1	1A	652(D)	C	5.0
44	1m	124	PRO	4.9
1	1A	1078	U	4.9
45	2n	25	VAL	4.9
21	2Z	146	ILE	4.8
1	2A	2896	C	4.7
22	10	3	HIS	4.7
1	2A	652(B)	A	4.6
54	1w	1	G	4.6
45	2n	39	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	2A	2794	C	4.4
32	2a	1038	C	4.4
33	2b	237	ALA	4.4
1	1A	1057	A	4.4
21	1Z	141	VAL	4.4
40	2i	9	ARG	4.3
44	2m	121	LYS	4.3
1	2A	2145	C	4.3
21	2Z	149	SER	4.3
34	2c	2	GLY	4.3
41	2j	74	ILE	4.3
1	2A	2893	G	4.2
1	2A	1536	C	4.2
22	20	3	HIS	4.2
38	1g	80	VAL	4.2
1	1A	2793	G	4.2
1	2A	2147	G	4.2
32	2a	1032	G	4.2
32	1a	630	G	4.1
54	2w	71	G	4.1
1	2A	885	C	4.1
15	1T	131	ALA	4.1
33	1b	237	ALA	4.1
1	2A	2751	G	4.1
1	1A	1094	U	4.0
1	2A	1509	C	4.0
51	1t	103	GLY	4.0
1	1A	885	C	4.0
32	1a	1002	G	4.0
1	1A	884	C	4.0
32	2a	1004	A	3.9
21	2Z	174	VAL	3.9
1	1A	1059	G	3.9
1	1A	2114	A	3.9
40	2i	14	VAL	3.9
1	2A	2803	C	3.9
7	2H	60	ARG	3.9
7	2H	175	LYS	3.9
34	1c	2	GLY	3.9
1	1A	2804	C	3.9
32	2a	1030(B)	C	3.9
43	2l	18	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
21	1Z	146	ILE	3.8
32	1a	1286	A	3.8
32	2a	1035	A	3.8
32	1a	204	U	3.8
32	2a	1001(A)	G	3.8
1	2A	2117	A	3.8
1	2A	2111	C	3.8
41	2j	47	PHE	3.8
44	2m	102	ARG	3.8
1	1A	896	A	3.8
1	2A	896	A	3.8
29	17	48	LYS	3.8
32	1a	1003	G	3.8
32	2a	1117	G	3.8
1	1A	2790	A	3.7
26	14	54	GLY	3.7
32	2a	1030	C	3.7
20	2Y	1	MET	3.7
38	2g	156	TRP	3.7
44	2m	7	VAL	3.7
22	10	2	ALA	3.7
50	2s	84	GLY	3.7
41	2j	37	PRO	3.7
41	2j	77	PRO	3.7
1	1A	2792	G	3.7
1	2A	2155	G	3.7
32	2a	1002	G	3.7
32	2a	1034	G	3.7
1	1A	1509	C	3.7
32	2a	1039	C	3.7
1	2A	882	G	3.6
40	2i	20	ARG	3.6
1	2A	894	C	3.6
32	2a	1018	C	3.6
7	1H	2	SER	3.6
1	1A	1096	A	3.6
26	14	56	VAL	3.6
41	2j	100	THR	3.6
32	2a	1005	A	3.6
44	2m	6	GLY	3.6
41	2j	63	PHE	3.6
40	1i	64	THR	3.6

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Mol	Chain	Res	Type	RSRZ
41	2j	76	ASN	3.5
38	1g	81	GLY	3.5
23	11	93	GLU	3.5
1	1A	889	C	3.5
1	1A	1063	G	3.5
7	2H	43	VAL	3.5
33	2b	165	VAL	3.5
42	2k	14	VAL	3.5
31	29	20	HIS	3.5
1	2A	2113	U	3.5
54	1w	73	A	3.5
3	1D	276	LYS	3.5
48	1q	98	LEU	3.5
1	1A	1176	G	3.5
32	2a	1030(A)	G	3.5
44	1m	122	LYS	3.5
41	2j	65	LEU	3.5
7	2H	2	SER	3.4
15	1T	130	ALA	3.4
32	2a	1031	G	3.4
33	1b	11	LEU	3.4
33	2b	70	PHE	3.4
1	1A	1073	A	3.4
11	2P	15	ARG	3.4
26	24	56	VAL	3.4
45	2n	3	ARG	3.4
1	1A	888	C	3.4
1	2A	2804	C	3.4
54	2w	3	C	3.4
33	2b	121	LEU	3.4
1	1A	2110	G	3.4
32	1a	1034	G	3.4
32	1a	1027	C	3.4
32	2a	1037	C	3.4
20	2Y	55	TYR	3.4
32	1a	1023	G	3.4
32	2a	1003	G	3.4
41	2j	31	GLY	3.4
46	2o	89	GLY	3.4
1	1A	1064	C	3.3
1	1A	1081	U	3.3
7	2H	174	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
44	1m	2	ALA	3.3
52	2u	2	GLY	3.3
1	1A	1070	A	3.3
1	2A	2792	G	3.3
12	1Q	32	TYR	3.3
33	1b	44	LEU	3.3
40	1i	19	LEU	3.3
45	2n	38	GLY	3.3
1	1A	1077	A	3.3
1	1A	1087	G	3.3
32	1a	1030(A)	G	3.3
27	25	29	THR	3.3
38	2g	85	TYR	3.3
1	1A	2896	C	3.3
1	2A	897	C	3.3
1	2A	2114	A	3.3
1	2A	2793	G	3.3
41	1j	32	ALA	3.3
7	2H	36	PRO	3.2
25	13	60	GLU	3.2
32	1a	1005	A	3.2
32	2a	1286	A	3.2
54	1w	71	G	3.2
38	2g	80	VAL	3.2
44	2m	53	VAL	3.2
32	1a	1257	U	3.2
1	2A	2137	C	3.2
1	2A	2146	C	3.2
32	1a	1038	C	3.2
20	2Y	58	GLY	3.2
35	1d	87	GLY	3.2
42	1k	25	TYR	3.2
33	2b	163	PHE	3.2
32	1a	1001(A)	G	3.2
35	1d	118	ARG	3.2
1	1A	1065	U	3.2
50	2s	15	LEU	3.2
51	1t	10	LEU	3.2
33	1b	19	HIS	3.2
1	2A	2169	A	3.2
44	2m	120	LYS	3.2
1	2A	1533	G	3.2

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Mol	Chain	Res	Type	RSRZ
1	2A	2157	G	3.2
41	1j	10	GLY	3.2
29	27	45	ALA	3.2
33	2b	123	ALA	3.2
40	2i	106	ALA	3.2
40	1i	14	VAL	3.2
44	1m	121	LYS	3.1
54	2w	73	A	3.1
33	1b	50	GLU	3.1
41	2j	34	VAL	3.1
1	2A	652(E)	G	3.1
1	2A	2125	G	3.1
32	2a	470	C	3.1
32	2a	1149	C	3.1
1	1A	2119	A	3.1
34	2c	207	VAL	3.1
41	2j	59	SER	3.1
33	2b	21	ARG	3.1
33	1b	10	LEU	3.1
34	1c	47	LEU	3.1
1	1A	2151	G	3.1
1	2A	2156	G	3.1
54	2w	72	C	3.1
22	20	2	ALA	3.1
40	1i	15	ALA	3.1
1	1A	1509(A)	A	3.1
32	1a	1001	A	3.1
50	2s	4	SER	3.1
45	2n	34	TYR	3.1
40	1i	2	GLU	3.1
1	1A	652(F)	G	3.1
1	1A	2115	G	3.1
35	2d	23	GLY	3.1
54	1y	18	G	3.1
7	2H	72	ILE	3.1
21	2Z	171	ILE	3.1
54	2w	2	C	3.1
54	2w	13	C	3.1
1	1A	1098	A	3.0
6	2G	52	ILE	3.0
33	2b	201	ILE	3.0
55	2x	70	G	3.0

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Mol	Chain	Res	Type	RSRZ
1	1A	897	C	3.0
1	2A	888	C	3.0
33	1b	31	TYR	3.0
33	2b	132	LYS	3.0
1	2A	895	U	3.0
32	1a	1020	U	3.0
32	1a	1025	U	3.0
41	2j	5	ARG	3.0
20	2Y	48	ALA	3.0
40	2i	82	ALA	3.0
32	2a	1024	G	3.0
47	2p	82	GLN	3.0
54	2w	5	G	3.0
32	1a	1030	C	3.0
1	1A	1088	A	3.0
32	2a	1001	A	3.0
38	2g	2	ALA	3.0
7	2H	136	ILE	3.0
1	2A	2115	G	3.0
32	2a	630	G	3.0
1	1A	886	C	3.0
1	1A	1072	C	3.0
32	1a	1029	C	3.0
1	2A	2150	U	2.9
26	14	63	TYR	2.9
47	2p	45	THR	2.9
7	2H	96	ALA	2.9
33	2b	136	VAL	2.9
32	1a	1030(B)	C	2.9
33	2b	19	HIS	2.9
50	2s	2	PRO	2.9
26	24	32	TYR	2.9
40	1i	106	ALA	2.9
33	1b	17	PHE	2.9
6	1G	26	GLN	2.9
1	1A	655	A	2.9
1	1A	1095	A	2.9
1	2A	2158	A	2.9
54	2w	70	G	2.9
40	1i	8	GLY	2.9
7	2H	79	VAL	2.9
26	14	55	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
50	1s	13	ASP	2.9
1	1A	2150	U	2.9
1	1A	2803	C	2.9
1	2A	2138	C	2.9
32	1a	1503	A	2.9
32	1a	1532	U	2.9
33	1b	18	GLY	2.9
33	2b	236	TYR	2.9
1	2A	1171	G	2.9
8	1I	146	ALA	2.9
22	20	5	LYS	2.9
34	2c	87	LEU	2.9
26	24	49	PHE	2.9
41	1j	66	ARG	2.8
45	2n	12	ARG	2.8
47	1p	82	GLN	2.8
6	2G	132	ASN	2.8
33	1b	22	LYS	2.8
34	1c	13	GLY	2.8
35	1d	194	LEU	2.8
1	2A	2119	A	2.8
1	2A	2170	A	2.8
1	2A	2897	U	2.8
54	1y	47	U	2.8
1	1A	1093	G	2.8
1	2A	2805	G	2.8
32	1a	1033	G	2.8
32	2a	1182	G	2.8
52	1u	24	ARG	2.8
41	2j	75	ILE	2.8
12	2Q	22	LYS	2.8
40	1i	91	ASP	2.8
42	2k	118	GLY	2.8
8	2I	146	ALA	2.8
45	2n	33	VAL	2.8
1	1A	2113	U	2.8
21	2Z	95	PRO	2.8
21	2Z	159	PRO	2.8
54	1w	20	U	2.8
1	1A	1046	A	2.8
1	1A	898	C	2.8
33	2b	41	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
40	1i	126	SER	2.8
1	2A	2148	G	2.8
1	2A	2159	G	2.8
21	2Z	150	LEU	2.8
41	2j	10	GLY	2.8
34	2c	201	TYR	2.8
1	2A	652(A)	A	2.8
45	2n	7	ILE	2.8
54	1w	7	A	2.8
54	2w	4	C	2.8
45	2n	18	VAL	2.8
1	1A	1068	G	2.8
1	1A	1089	G	2.8
1	1A	2802	G	2.8
1	2A	2149	G	2.8
54	1w	65	G	2.8
54	2w	15	G	2.8
20	2Y	53	PRO	2.7
25	13	2	PRO	2.7
33	1b	125	PRO	2.7
41	1j	77	PRO	2.7
48	2q	100	LYS	2.7
1	1A	1175	U	2.7
13	2R	14	SER	2.7
40	2i	102	LEU	2.7
1	2A	2134	A	2.7
32	1a	1531	A	2.7
26	24	50	VAL	2.7
32	2a	1027	C	2.7
45	2n	5	ALA	2.7
7	2H	10	PRO	2.7
40	2i	5	TYR	2.7
41	2j	91	PRO	2.7
45	2n	14	PRO	2.7
41	2j	55	LYS	2.7
1	1A	2159	G	2.7
1	2A	1112	G	2.7
41	2j	36	GLY	2.7
41	2j	78	ASN	2.7
47	1p	48	TRP	2.7
32	2a	1148	U	2.7
33	2b	140	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
7	2H	19	VAL	2.7
7	2H	45	VAL	2.7
9	1N	140	VAL	2.7
38	2g	83	ALA	2.7
40	2i	66	ARG	2.7
45	1n	29	ARG	2.7
1	1A	652(A)	A	2.7
1	1A	1054	A	2.7
25	23	2	PRO	2.7
42	2k	25	TYR	2.7
43	2l	126	LYS	2.7
51	1t	68	LYS	2.7
38	2g	16	LEU	2.7
1	1A	1091	G	2.7
1	1A	2805	G	2.7
1	2A	2894	G	2.7
32	1a	1026	G	2.7
32	2a	485	G	2.7
32	2a	1021	G	2.7
35	1d	23	GLY	2.7
39	2h	130	GLY	2.7
41	2j	35	SER	2.7
44	2m	100	GLY	2.7
45	2n	55	GLY	2.7
54	2y	18	G	2.7
8	1I	107	VAL	2.7
1	1A	2109	U	2.7
1	1A	2897	U	2.7
7	2H	12	PRO	2.7
7	2H	21	PRO	2.7
32	2a	1030(D)	A	2.7
33	1b	172	ILE	2.7
33	2b	185	ILE	2.7
22	20	7	LEU	2.7
4	2E	10	GLY	2.7
22	20	4	LYS	2.7
41	2j	72	VAL	2.7
45	2n	22	THR	2.7
33	1b	232	PRO	2.7
32	2a	1036	G	2.6
41	2j	33	GLN	2.6
1	1A	1060	U	2.6

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Mol	Chain	Res	Type	RSRZ
38	2g	154	TYR	2.6
55	2x	47	U	2.6
36	2e	10	MET	2.6
1	1A	2158	A	2.6
7	2H	7	LEU	2.6
7	2H	64	LEU	2.6
54	2y	36	A	2.6
40	2i	10	ARG	2.6
1	2A	886	C	2.6
55	1x	69	C	2.6
21	1Z	149	SER	2.6
33	2b	186	ALA	2.6
21	2Z	170	THR	2.6
20	2Y	57	GLN	2.6
20	2Y	107	ASP	2.6
33	2b	214	ILE	2.6
34	2c	5	ILE	2.6
41	2j	50	ILE	2.6
1	1A	1071	G	2.6
54	2y	19	G	2.6
40	1i	9	ARG	2.6
40	1i	66	ARG	2.6
33	1b	9	GLU	2.6
35	1d	167	GLY	2.6
1	1A	2117	A	2.6
2	2B	120	A	2.6
7	2H	11	VAL	2.6
26	14	49	PHE	2.6
33	2b	161	ALA	2.6
35	1d	137	SER	2.6
50	2s	9	VAL	2.6
1	2A	2136	C	2.6
38	1g	154	TYR	2.6
3	2D	276	LYS	2.6
32	2a	1219	U	2.6
33	2b	12	GLU	2.6
42	2k	49	GLY	2.6
32	1a	1024	G	2.6
34	2c	55	VAL	2.6
26	14	59	PHE	2.6
1	1A	899	A	2.6
1	2A	1509(A)	A	2.6

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Mol	Chain	Res	Type	RSRZ
1	2A	2135	A	2.6
1	2A	2801(A)	A	2.6
32	2a	965	A	2.6
32	2a	1503	A	2.6
53	2v	24	A	2.6
34	2c	77	ILE	2.6
38	2g	79	ARG	2.6
41	2j	79	ARG	2.6
50	2s	80	TYR	2.6
51	1t	83	ARG	2.6
33	1b	132	LYS	2.6
40	2i	11	LYS	2.6
1	2A	614(A)	U	2.6
6	2G	50	ALA	2.6
31	29	16	VAL	2.6
42	1k	14	VAL	2.6
38	2g	84	ASN	2.6
45	1n	60	SER	2.5
1	1A	1056	G	2.5
1	2A	2112	G	2.5
7	2H	41	MET	2.5
54	1w	70	G	2.5
54	2y	57	G	2.5
41	1j	74	ILE	2.5
1	1A	2170	A	2.5
1	2A	2173	A	2.5
8	2I	75	LEU	2.5
40	2i	19	LEU	2.5
24	12	69	ARG	2.5
41	2j	80	LYS	2.5
41	2j	56	HIS	2.5
6	1G	146	TYR	2.5
1	1A	1075	C	2.5
32	1a	1037	C	2.5
7	1H	174	GLY	2.5
33	2b	71	VAL	2.5
15	2T	131	ALA	2.5
44	2m	28	ALA	2.5
1	2A	271(K)	U	2.5
20	2Y	5	MET	2.5
21	2Z	166	SER	2.5
54	2y	45	U	2.5

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Mol	Chain	Res	Type	RSRZ
8	1I	109	ILE	2.5
19	2X	68	ARG	2.5
44	2m	114	ARG	2.5
8	2I	135	GLU	2.5
44	2m	21	TYR	2.5
54	2w	76	A	2.5
4	2E	186	GLY	2.5
41	1j	93	GLY	2.5
14	2S	46	VAL	2.5
33	1b	188	ALA	2.5
21	1Z	170	THR	2.5
40	2i	105	ASP	2.5
45	2n	4	LYS	2.5
1	2A	1026	U	2.5
32	2a	1257	U	2.5
34	2c	43	LEU	2.5
34	2c	188	LEU	2.5
33	1b	33	TYR	2.5
12	2Q	15	GLY	2.5
31	29	37	GLY	2.5
40	1i	67	GLY	2.5
1	2A	881	G	2.5
1	2A	2126	A	2.5
1	2A	2154	G	2.5
21	2Z	141	VAL	2.5
32	1a	143	A	2.5
54	2w	7	A	2.5
35	1d	195	ALA	2.5
48	1q	7	THR	2.5
14	2S	83	LYS	2.5
33	1b	127	ILE	2.5
1	1A	2138	C	2.5
32	1a	1019	C	2.5
44	2m	64	TRP	2.5
33	1b	40	HIS	2.5
1	1A	1066	U	2.5
26	14	45	GLY	2.5
51	1t	69	GLY	2.5
7	2H	128	PRO	2.5
5	2F	183	VAL	2.5
26	24	59	PHE	2.5
33	2b	77	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
45	2n	36	PHE	2.5
26	14	69	LYS	2.4
51	1t	74	LYS	2.4
1	1A	1045	A	2.4
32	2a	1016	A	2.4
35	2d	5	ILE	2.4
41	1j	4	ILE	2.4
51	1t	13	LEU	2.4
54	2w	19	G	2.4
8	2I	7	GLU	2.4
27	25	59	GLU	2.4
1	1A	1076	C	2.4
1	2A	2139	C	2.4
32	2a	1045	C	2.4
9	2N	44	PRO	2.4
38	1g	85	TYR	2.4
40	2i	125	TYR	2.4
7	2H	125	VAL	2.4
34	2c	135	LYS	2.4
36	1e	69	VAL	2.4
33	2b	122	PHE	2.4
44	2m	33	ALA	2.4
50	2s	81	ARG	2.4
41	2j	82	ILE	2.4
47	2p	68	ASP	2.4
33	2b	134	GLU	2.4
1	1A	2141	G	2.4
1	2A	271(M)	G	2.4
40	2i	8	GLY	2.4
7	2H	26	VAL	2.4
50	1s	9	VAL	2.4
1	1A	1097	U	2.4
21	2Z	164	ALA	2.4
32	2a	1196	U	2.4
33	2b	152	PHE	2.4
33	1b	61	LEU	2.4
33	2b	11	LEU	2.4
33	2b	42	ILE	2.4
40	1i	102	LEU	2.4
49	2r	66	LEU	2.4
41	1j	76	ASN	2.4
40	2i	126	SER	2.4

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Mol	Chain	Res	Type	RSRZ
22	20	68	GLU	2.4
41	2j	73	ASP	2.4
45	2n	8	GLU	2.4
45	2n	61	TRP	2.4
7	1H	175	LYS	2.4
20	2Y	4	LYS	2.4
32	2a	969	A	2.4
41	2j	14	LYS	2.4
51	2t	103	GLY	2.4
29	17	46	VAL	2.4
34	1c	76	VAL	2.4
40	2i	109	VAL	2.4
1	2A	11	G	2.4
1	2A	2166	G	2.4
32	2a	1124	G	2.4
33	2b	34	ALA	2.4
40	2i	16	ARG	2.4
4	2E	63	LEU	2.4
33	2b	200	ILE	2.4
40	1i	47	LEU	2.4
40	2i	79	LEU	2.4
41	2j	88	LEU	2.4
1	1A	1100	C	2.4
1	2A	2118	U	2.4
1	2A	2167	U	2.4
50	2s	14	HIS	2.4
39	2h	4	ASP	2.4
40	1i	105	ASP	2.4
33	1b	48	MET	2.4
29	27	48	LYS	2.4
6	1G	149	VAL	2.4
7	2H	6	ARG	2.4
7	2H	15	VAL	2.4
21	1Z	165	VAL	2.4
33	1b	15	VAL	2.4
34	2c	195	VAL	2.4
41	2j	46	ARG	2.4
1	1A	548	A	2.4
1	1A	1103	A	2.4
1	1A	2173	A	2.4
32	1a	1030(D)	A	2.4
32	2a	1130	A	2.4

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Mol	Chain	Res	Type	RSRZ
54	2y	21	A	2.4
40	1i	13	ALA	2.4
8	2I	38	LEU	2.3
21	2Z	144	LEU	2.3
34	1c	39	ILE	2.3
1	1A	2123	G	2.3
1	1A	2167	U	2.3
1	2A	892	G	2.3
1	2A	2151	G	2.3
1	2A	2318	G	2.3
54	1w	69	G	2.3
9	2N	1	MET	2.3
54	1w	2	C	2.3
54	1w	72	C	2.3
21	2Z	105	VAL	2.3
33	1b	229	VAL	2.3
33	1b	70	PHE	2.3
41	1j	11	PHE	2.3
33	2b	187	LEU	2.3
48	2q	98	LEU	2.3
40	2i	62	TYR	2.3
1	1A	278	A	2.3
1	2A	878	A	2.3
32	1a	344	A	2.3
53	1v	13	A	2.3
33	2b	22	LYS	2.3
40	2i	2	GLU	2.3
32	2a	1159	U	2.3
1	1A	882	G	2.3
32	1a	631	G	2.3
1	1A	2111	C	2.3
32	2a	1029	C	2.3
32	2a	1054	C	2.3
52	1u	9	ARG	2.3
36	1e	21	ALA	2.3
33	1b	201	ILE	2.3
33	1b	54	THR	2.3
44	2m	105	THR	2.3
3	1D	275	LYS	2.3
33	1b	126	GLU	2.3
32	1a	1447	A	2.3
7	2H	39	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
33	2b	137	ARG	2.3
32	1a	1000	U	2.3
32	2a	1126	U	2.3
7	2H	24	VAL	2.3
40	2i	17	VAL	2.3
12	2Q	104	PHE	2.3
41	2j	90	LEU	2.3
35	1d	5	ILE	2.3
40	2i	45	ALA	2.3
40	2i	84	ALA	2.3
1	1A	883	G	2.3
1	1A	2152	G	2.3
1	1A	2162	G	2.3
1	2A	893	C	2.3
1	2A	2110	G	2.3
1	2A	2807	G	2.3
32	2a	1023	G	2.3
32	2a	1118	C	2.3
36	1e	10	MET	2.3
48	2q	95	TYR	2.3
52	1u	18	TYR	2.3
21	2Z	103	ARG	2.3
33	1b	131	PRO	2.3
44	1m	102	ARG	2.3
44	2m	104	ARG	2.3
47	2p	75	ARG	2.3
50	2s	13	ASP	2.3
1	1A	1067	A	2.3
32	1a	162	A	2.3
40	2i	39	GLY	2.3
5	2F	6	VAL	2.3
19	2X	70	LEU	2.3
19	2X	95	LEU	2.3
26	14	50	VAL	2.3
29	27	46	VAL	2.3
39	1h	2	LEU	2.3
32	2a	1040	U	2.2
32	2a	1125	U	2.2
54	2w	45	U	2.2
40	2i	4	TYR	2.2
46	1o	69	TYR	2.2
1	2A	277	C	2.2

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Mol	Chain	Res	Type	RSRZ
32	2a	1043	C	2.2
32	2a	1115	C	2.2
32	2a	1119	C	2.2
1	2A	2133	G	2.2
9	2N	45	ASN	2.2
32	1a	1021	G	2.2
32	2a	993	G	2.2
6	1G	51	ARG	2.2
6	2G	118	ARG	2.2
35	1d	76	ARG	2.2
45	1n	57	ARG	2.2
45	2n	35	ARG	2.2
34	2c	62	ASP	2.2
33	1b	165	VAL	2.2
33	2b	213	LEU	2.2
34	1c	12	LEU	2.2
1	1A	1069	A	2.2
1	1A	1086	A	2.2
1	2A	1508	A	2.2
6	2G	182	LYS	2.2
33	1b	133	LYS	2.2
45	1n	30	ALA	2.2
33	1b	190	THR	2.2
41	2j	61	GLU	2.2
42	1k	75	TYR	2.2
48	2q	75	ARG	2.2
41	2j	39	PRO	2.2
1	1A	2894	G	2.2
1	2A	2153	G	2.2
22	20	6	GLY	2.2
34	1c	17	ASP	2.2
41	1j	31	GLY	2.2
44	1m	100	GLY	2.2
41	2j	40	LEU	2.2
14	2S	11	LYS	2.2
17	2V	14	VAL	2.2
41	2j	49	VAL	2.2
40	2i	18	PHE	2.2
34	2c	53	ALA	2.2
40	1i	76	ALA	2.2
1	1A	1084	A	2.2
1	2A	887	A	2.2

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Mol	Chain	Res	Type	RSRZ
32	2a	1531	A	2.2
1	2A	2895	U	2.2
12	2Q	6	ARG	2.2
21	2Z	79	ARG	2.2
38	2g	5	ARG	2.2
45	1n	3	ARG	2.2
21	2Z	158	PRO	2.2
8	2I	54	GLN	2.2
7	2H	38	SER	2.2
9	2N	118	LYS	2.2
15	2T	28	VAL	2.2
41	2j	86	MET	2.2
41	2j	94	VAL	2.2
1	1A	2794	C	2.2
1	2A	898	C	2.2
10	2O	69	ILE	2.2
21	2Z	136	PHE	2.2
55	1x	67	C	2.2
55	2x	71	C	2.2
33	1b	120	ALA	2.2
34	2c	200	ALA	2.2
38	1g	2	ALA	2.2
49	1r	20	ALA	2.2
1	1A	1055	G	2.2
1	1A	2125	G	2.2
32	2a	1017	G	2.2
41	2j	42	THR	2.2
8	2I	82	ARG	2.2
16	2U	59	ARG	2.2
41	2j	28	ARG	2.2
44	2m	29	ARG	2.2
52	1u	15	ARG	2.2
1	1A	890	A	2.2
1	1A	2801(A)	A	2.2
1	2A	901	A	2.2
16	2U	2	PRO	2.2
38	1g	84	ASN	2.2
43	1l	64	TYR	2.2
50	2s	42	PRO	2.2
53	2v	12	A	2.2
53	2v	13	A	2.2
36	2e	20	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
44	1m	27	LYS	2.2
22	20	84	LEU	2.2
37	2f	21	LEU	2.2
50	2s	71	LEU	2.2
52	2u	5	ASP	2.2
26	24	31	ILE	2.2
33	1b	200	ILE	2.2
33	1b	214	ILE	2.2
33	2b	164	VAL	2.2
40	2i	65	VAL	2.2
46	2o	60	VAL	2.2
12	2Q	40	ALA	2.1
34	2c	137	ALA	2.1
24	22	51	ARG	2.1
32	1a	1132	C	2.1
1	1A	271(M)	G	2.1
1	1A	2116	G	2.1
1	2A	2131	G	2.1
1	2A	2168	G	2.1
32	2a	1131	G	2.1
52	2u	23	PRO	2.1
8	2I	11	ASN	2.1
33	2b	75	LYS	2.1
50	2s	53	ASN	2.1
36	2e	133	TYR	2.1
23	11	97	LEU	2.1
27	25	30	LEU	2.1
34	2c	47	LEU	2.1
18	1W	112	GLY	2.1
32	2a	1256	A	2.1
43	2l	63	GLY	2.1
1	1A	1082	U	2.1
1	1A	2808	U	2.1
7	2H	52	VAL	2.1
7	2H	61	HIS	2.1
32	1a	841	U	2.1
33	2b	93	VAL	2.1
34	2c	182	ILE	2.1
45	2n	37	PHE	2.1
41	2j	27	ALA	2.1
44	2m	18	ALA	2.1
6	1G	48	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
6	2G	54	GLU	2.1
8	2I	64	GLU	2.1
24	22	5	GLU	2.1
26	24	57	GLU	2.1
52	2u	14	TRP	2.1
33	1b	53	ARG	2.1
1	1A	34	C	2.1
1	1A	1092	C	2.1
1	1A	2145	C	2.1
32	1a	1028	C	2.1
32	1a	1039	C	2.1
32	1a	1158	C	2.1
33	1b	187	LEU	2.1
33	2b	33	TYR	2.1
1	1A	2112	G	2.1
7	2H	4	ILE	2.1
7	2H	76	VAL	2.1
32	1a	346	G	2.1
32	2a	1026	G	2.1
32	2a	1220	G	2.1
40	1i	86	VAL	2.1
47	2p	2	VAL	2.1
54	1w	6	G	2.1
54	1w	19	G	2.1
54	2y	15	G	2.1
1	1A	895	U	2.1
1	1A	1090	U	2.1
1	1A	1177	A	2.1
4	2E	204	ALA	2.1
29	17	45	ALA	2.1
32	2a	1150	U	2.1
33	1b	123	ALA	2.1
40	2i	13	ALA	2.1
4	2E	163	GLU	2.1
7	2H	32	GLU	2.1
8	2I	131	LYS	2.1
33	1b	234	PRO	2.1
39	2h	5	PRO	2.1
51	2t	98	PRO	2.1
35	1d	62	GLN	2.1
21	2Z	125	LEU	2.1
33	2b	69	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
35	1d	157	LEU	2.1
45	2n	47	LEU	2.1
50	2s	5	LEU	2.1
41	1j	78	ASN	2.1
3	2D	256	GLY	2.1
4	2E	115	GLY	2.1
11	2P	109	GLY	2.1
1	1A	154(A)	C	2.1
1	2A	645	C	2.1
7	2H	17	VAL	2.1
32	1a	848	C	2.1
41	1j	75	ILE	2.1
26	14	57	GLU	2.1
34	2c	92	ALA	2.1
38	1g	115	ARG	2.1
1	1A	879	G	2.1
1	2A	916	G	2.1
1	2A	2116	G	2.1
1	2A	2206	G	2.1
32	2a	1030(C)	G	2.1
54	2y	44	G	2.1
1	1A	887	A	2.1
1	2A	6	A	2.1
1	2A	229	A	2.1
34	2c	95	THR	2.1
5	1F	14	PRO	2.1
6	2G	142	PRO	2.1
48	1q	28	PRO	2.1
8	1I	68	LEU	2.1
21	1Z	150	LEU	2.1
48	2q	43	LEU	2.1
33	1b	38	GLY	2.1
33	2b	38	GLY	2.1
43	1l	63	GLY	2.1
7	2H	83	TYR	2.1
7	2H	157	TYR	2.1
35	1d	158	ILE	2.1
33	2b	7	VAL	2.1
33	2b	189	ASP	2.0
50	2s	10	PHE	2.1
21	2Z	97	GLU	2.0
33	1b	13	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
45	1n	5	ALA	2.0
20	2Y	94	LYS	2.0
30	28	29	LYS	2.0
32	1a	221	C	2.0
32	2a	1006	C	2.0
54	1w	68	C	2.0
34	2c	167	TRP	2.0
20	1Y	1	MET	2.0
6	2G	133	LEU	2.0
14	2S	110	LEU	2.0
50	1s	15	LEU	2.0
54	2y	59	U	2.0
1	1A	1062	G	2.0
1	1A	2124	G	2.0
1	1A	2135	A	2.0
1	1A	2892	A	2.0
1	2A	528	A	2.0
1	2A	2319	G	2.0
32	1a	197	A	2.0
32	2a	1123	A	2.0
32	2a	1221	G	2.0
20	2Y	61	ILE	2.0
40	1i	69	GLY	2.0
7	2H	35	VAL	2.0
9	2N	9	VAL	2.0
34	2c	138	VAL	2.0
43	2l	69	TYR	2.0
14	2S	3	ARG	2.0
20	1Y	60	PHE	2.0
36	2e	45	PHE	2.0
38	1g	78	ARG	2.0
40	2i	104	ARG	2.0
33	1b	129	GLU	2.0
41	2j	54	PHE	2.0
34	1c	62	ASP	2.0
42	1k	15	ALA	2.0
44	2m	118	ALA	2.0
40	2i	7	THR	2.0
24	12	70	GLN	2.0
32	1a	1006	C	2.0
35	1d	135	LEU	2.0
1	2A	271(L)	U	2.0

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Mol	Chain	Res	Type	RSRZ
32	1a	173	U	2.0
32	1a	1040	U	2.0
16	2U	62	ILE	2.0
34	2c	124	ILE	2.0
34	2c	145	GLY	2.0
34	2c	157	ILE	2.0
15	1T	129	ARG	2.0
32	2a	1251	A	2.0
33	2b	36	ARG	2.0
35	2d	132	ARG	2.0
40	1i	26	VAL	2.0
41	1j	45	ARG	2.0
44	2m	54	VAL	2.0
14	2S	92	TYR	2.0
37	2f	59	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	PSU	2y	55	20/21	0.60	0.15	91,95,108,119	0
54	4SU	2y	8	20/21	0.68	0.16	85,95,101,110	0
54	4SU	2w	8	20/21	0.70	0.15	91,95,111,121	0
54	PSU	1y	55	20/21	0.71	0.13	93,96,110,114	0
54	G7M	2w	46	24/25	0.72	0.15	84,94,106,115	0
54	G7M	2y	46	24/25	0.74	0.15	86,94,102,115	0
54	G7M	1w	46	24/25	0.74	0.15	81,90,102,115	0
54	MIA	2y	37	22/30	0.75	0.14	83,90,101,107	0
54	G7M	1y	46	24/25	0.76	0.16	84,92,106,114	0
54	5MU	1y	54	21/22	0.76	0.16	81,92,102,108	0
54	4SU	1y	8	20/21	0.76	0.12	88,92,100,101	0
54	5MU	2y	54	21/22	0.78	0.15	85,93,105,118	0
54	PSU	2y	32	20/21	0.80	0.12	84,90,96,103	0
54	MIA	1y	37	22/30	0.81	0.12	77,84,90,93	0
54	PSU	2w	55	20/21	0.81	0.10	82,87,96,99	0
54	PSU	1w	55	20/21	0.83	0.11	65,80,88,89	0
54	PSU	1y	39	20/21	0.84	0.11	77,82,86,92	0
54	4SU	1w	8	20/21	0.86	0.12	78,86,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	PSU	1y	32	20/21	0.86	0.10	78,84,89,90	0
54	PSU	2y	39	20/21	0.87	0.10	81,89,98,99	0
55	4SU	2x	8	20/21	0.88	0.12	77,80,85,87	0
54	5MU	2w	54	21/22	0.89	0.10	77,80,85,89	0
55	5MU	2x	54	21/22	0.90	0.11	72,76,81,84	0
54	PSU	2w	32	20/21	0.90	0.13	67,77,87,91	0
54	MIA	2w	37	25/30	0.90	0.13	58,71,83,101	0
43	0TD	2l	92	10/11	0.90	0.11	59,61,67,70	0
32	PSU	2a	516	20/21	0.91	0.10	63,69,75,81	0
55	PSU	2x	55	20/21	0.91	0.09	66,74,79,86	0
32	G7M	2a	527	24/25	0.91	0.12	58,64,70,75	0
54	PSU	1w	32	20/21	0.92	0.12	59,66,73,75	0
55	5MU	1x	54	21/22	0.92	0.09	53,64,77,81	0
55	5MC	2x	32	21/22	0.92	0.12	68,71,74,81	0
55	PSU	1x	55	20/21	0.92	0.09	54,61,75,85	0
1	PSU	2A	1917	20/21	0.92	0.09	53,63,68,69	0
32	2MG	2a	1207	24/25	0.93	0.09	70,79,82,83	0
55	4SU	1x	8	20/21	0.93	0.10	54,66,73,75	0
54	5MU	1w	54	21/22	0.93	0.09	47,66,73,75	0
1	5MU	2A	1915	21/22	0.93	0.09	57,63,68,70	0
32	M2G	2a	966	25/26	0.93	0.15	58,65,77,83	0
32	5MC	2a	967	21/22	0.94	0.12	59,65,73,80	0
43	0TD	1l	92	10/11	0.94	0.09	48,54,56,71	0
32	5MC	2a	1400	21/22	0.94	0.12	65,70,73,83	0
32	5MC	2a	1404	21/22	0.94	0.10	52,56,60,65	0
54	MIA	1w	37	29/30	0.94	0.13	45,57,69,81	0
55	5MC	1x	32	21/22	0.94	0.11	56,59,62,72	0
32	4OC	2a	1402	22/23	0.95	0.10	51,60,64,65	0
32	G7M	1a	527	24/25	0.95	0.09	44,51,57,63	0
32	MA6	2a	1518	24/25	0.95	0.11	51,62,66,70	0
32	M2G	1a	966	25/26	0.95	0.11	46,53,62,64	0
32	5MC	1a	967	21/22	0.95	0.09	46,53,61,62	0
32	2MG	1a	1207	24/25	0.95	0.09	61,70,73,75	0
54	PSU	1w	39	20/21	0.95	0.09	54,64,74,76	0
1	PSU	1A	1917	20/21	0.95	0.08	47,52,56,58	0
54	PSU	2w	39	20/21	0.95	0.09	60,74,83,83	0
1	OMC	2A	1920	21/22	0.95	0.10	48,59,62,68	0
1	5MC	2A	1942	21/22	0.95	0.09	50,56,60,64	0
32	MA6	2a	1519	24/25	0.96	0.11	45,56,65,67	0
55	31H	2x	76	32/33	0.96	0.09	39,51,61,69	0
1	PSU	2A	1911	20/21	0.96	0.07	56,58,63,63	0
1	5MU	1A	1915	21/22	0.96	0.09	46,52,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MA6	1a	1519	24/25	0.96	0.09	36,43,48,52	0
55	31H	1x	76	32/33	0.96	0.10	26,37,45,60	10
32	5MC	2a	1407	21/22	0.96	0.08	48,53,59,61	0
32	UR3	2a	1498	21/22	0.96	0.10	48,53,59,60	0
1	5MC	1A	1942	21/22	0.96	0.08	32,37,41,42	0
32	PSU	1a	516	20/21	0.96	0.08	44,56,61,64	0
1	OMU	2A	2552	21/22	0.96	0.09	43,47,50,62	0
32	4OC	1a	1402	22/23	0.97	0.07	42,46,53,60	0
32	5MC	1a	1404	21/22	0.97	0.07	33,38,42,44	0
32	5MC	1a	1407	21/22	0.97	0.08	36,45,46,49	0
32	UR3	1a	1498	21/22	0.97	0.08	37,40,43,55	0
1	5MU	2A	1939	21/22	0.97	0.07	34,40,46,47	0
1	PSU	1A	1911	20/21	0.97	0.07	36,46,54,54	0
32	MA6	1a	1518	24/25	0.97	0.09	34,43,47,49	0
1	5MC	2A	1962	21/22	0.97	0.08	36,49,53,62	0
1	8AH	2A	2503	24/25	0.97	0.08	35,41,45,50	0
32	5MC	1a	1400	21/22	0.97	0.09	46,53,57,63	0
1	PSU	1A	2605	20/21	0.97	0.06	25,29,32,33	0
1	PSU	2A	2605	20/21	0.97	0.07	33,40,46,47	0
1	OMG	2A	2251	24/25	0.98	0.07	37,43,49,57	0
1	OMC	1A	1920	21/22	0.98	0.06	38,47,50,54	0
1	OMU	1A	2552	21/22	0.98	0.06	27,30,35,37	0
1	5MC	1A	1962	21/22	0.98	0.06	28,36,41,47	0
1	5MU	1A	1939	21/22	0.98	0.06	26,32,34,39	0
1	OMG	1A	2251	24/25	0.98	0.06	22,26,30,32	0
1	8AH	1A	2503	24/25	0.99	0.06	14,24,29,30	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2w	104	1/1	0.63	0.20	79,79,79,79	0
56	MG	2A	3083	1/1	0.64	0.15	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	1A	3985	1/1	0.66	0.18	37,37,37,37	0
56	MG	1A	3992	1/1	0.68	0.16	70,70,70,70	0
56	MG	2v	102	1/1	0.69	0.29	82,82,82,82	0
56	MG	2W	202	1/1	0.69	0.14	76,76,76,76	0
56	MG	1a	1771	1/1	0.70	0.15	78,78,78,78	0
56	MG	2a	1748	1/1	0.70	0.19	96,96,96,96	0
56	MG	2A	3100	1/1	0.70	0.17	78,78,78,78	0
56	MG	2A	3585	1/1	0.70	0.18	73,73,73,73	0
56	MG	2A	3689	1/1	0.71	0.22	66,66,66,66	0
56	MG	1B	207	1/1	0.71	0.25	73,73,73,73	0
56	MG	2A	3217	1/1	0.71	0.18	69,69,69,69	0
56	MG	1Z	302	1/1	0.71	0.13	72,72,72,72	0
56	MG	2A	3593	1/1	0.71	0.18	74,74,74,74	0
56	MG	1A	3587	1/1	0.72	0.36	54,54,54,54	0
56	MG	1A	3674	1/1	0.72	0.14	59,59,59,59	0
56	MG	2a	1720	1/1	0.72	0.28	78,78,78,78	0
56	MG	20	101	1/1	0.73	0.30	64,64,64,64	0
56	MG	1A	3966	1/1	0.73	0.14	70,70,70,70	0
56	MG	2A	3650	1/1	0.73	0.14	72,72,72,72	0
56	MG	2a	1821	1/1	0.73	0.25	81,81,81,81	0
56	MG	2A	3227	1/1	0.73	0.24	69,69,69,69	0
56	MG	1A	3724	1/1	0.73	0.14	63,63,63,63	0
56	MG	2A	3336	1/1	0.74	0.14	78,78,78,78	0
56	MG	2A	3368	1/1	0.74	0.31	83,83,83,83	0
56	MG	1A	4015	1/1	0.74	0.24	51,51,51,51	0
56	MG	1A	3459	1/1	0.74	0.13	63,63,63,63	0
56	MG	1a	1807	1/1	0.74	0.23	85,85,85,85	0
56	MG	1w	105	1/1	0.74	0.26	86,86,86,86	0
56	MG	2A	3699	1/1	0.74	0.14	62,62,62,62	0
56	MG	1A	3761	1/1	0.75	0.09	21,21,21,21	0
56	MG	1A	3823	1/1	0.75	0.14	62,62,62,62	0
56	MG	1A	3585	1/1	0.75	0.26	64,64,64,64	0
56	MG	2A	3442	1/1	0.75	0.19	72,72,72,72	0
56	MG	2A	3815	1/1	0.75	0.14	63,63,63,63	0
56	MG	1A	4087	1/1	0.75	0.21	62,62,62,62	0
56	MG	2a	1672	1/1	0.76	0.12	63,63,63,63	0
56	MG	1A	3596	1/1	0.76	0.13	36,36,36,36	0
56	MG	2A	3712	1/1	0.76	0.18	68,68,68,68	0
56	MG	2A	3006	1/1	0.76	0.14	78,78,78,78	0
56	MG	1a	1711	1/1	0.76	0.28	60,60,60,60	0
56	MG	2w	101	1/1	0.76	0.14	79,79,79,79	0
56	MG	2A	3483	1/1	0.76	0.20	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	2w	106	1/1	0.76	0.22	77,77,77,77	0
56	MG	1A	3738	1/1	0.77	0.18	63,63,63,63	0
56	MG	1a	1797	1/1	0.77	0.17	76,76,76,76	0
56	MG	2a	1794	1/1	0.77	0.30	65,65,65,65	0
56	MG	2a	1796	1/1	0.77	0.16	70,70,70,70	0
56	MG	2a	1814	1/1	0.77	0.38	80,80,80,80	0
56	MG	1A	3715	1/1	0.77	0.21	62,62,62,62	0
56	MG	2B	201	1/1	0.77	0.38	82,82,82,82	0
56	MG	1A	3781	1/1	0.77	0.18	75,75,75,75	0
56	MG	1A	3516	1/1	0.77	0.18	79,79,79,79	0
56	MG	2A	3069	1/1	0.77	0.30	69,69,69,69	0
56	MG	2a	1730	1/1	0.78	0.23	68,68,68,68	0
56	MG	1A	4072	1/1	0.78	0.14	60,60,60,60	0
56	MG	2A	3391	1/1	0.78	0.17	65,65,65,65	0
56	MG	1Z	304	1/1	0.78	0.11	62,62,62,62	0
56	MG	1a	1660	1/1	0.78	0.20	71,71,71,71	0
56	MG	1A	3700	1/1	0.78	0.18	52,52,52,52	0
56	MG	2A	3233	1/1	0.78	0.30	61,61,61,61	0
56	MG	2a	1607	1/1	0.78	0.33	69,69,69,69	0
56	MG	2A	3299	1/1	0.78	0.15	70,70,70,70	0
56	MG	1A	3828	1/1	0.78	0.18	63,63,63,63	0
56	MG	1A	4071	1/1	0.79	0.17	69,69,69,69	0
56	MG	2a	1778	1/1	0.79	0.22	67,67,67,67	0
56	MG	2A	3833	1/1	0.79	0.17	65,65,65,65	0
56	MG	1A	3745	1/1	0.79	0.12	46,46,46,46	0
56	MG	2A	3239	1/1	0.79	0.16	57,57,57,57	0
56	MG	2A	3243	1/1	0.79	0.15	72,72,72,72	0
56	MG	1B	226	1/1	0.79	0.19	65,65,65,65	0
56	MG	1D	312	1/1	0.79	0.17	66,66,66,66	0
56	MG	2A	3184	1/1	0.79	0.22	82,82,82,82	0
56	MG	1w	107	1/1	0.79	0.20	70,70,70,70	0
56	MG	2A	3289	1/1	0.80	0.13	66,66,66,66	0
56	MG	2A	3606	1/1	0.80	0.26	70,70,70,70	0
56	MG	2A	3110	1/1	0.80	0.17	71,71,71,71	0
56	MG	2A	3319	1/1	0.80	0.19	61,61,61,61	0
56	MG	1A	3526	1/1	0.80	0.12	51,51,51,51	0
56	MG	2A	3340	1/1	0.80	0.22	76,76,76,76	0
56	MG	1x	113	1/1	0.80	0.16	71,71,71,71	0
56	MG	2A	3821	1/1	0.80	0.15	45,45,45,45	0
56	MG	1B	221	1/1	0.80	0.16	67,67,67,67	0
56	MG	1A	3532	1/1	0.80	0.24	59,59,59,59	0
56	MG	1B	229	1/1	0.80	0.22	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	3544	1/1	0.80	0.18	40,40,40,40	0
56	MG	1a	1663	1/1	0.80	0.13	57,57,57,57	0
56	MG	2x	106	1/1	0.80	0.29	71,71,71,71	0
56	MG	2A	3724	1/1	0.81	0.17	62,62,62,62	0
56	MG	2A	3043	1/1	0.81	0.19	66,66,66,66	0
56	MG	1A	3978	1/1	0.81	0.13	38,38,38,38	0
56	MG	1A	3075	1/1	0.81	0.30	65,65,65,65	0
56	MG	2A	3835	1/1	0.81	0.13	65,65,65,65	0
56	MG	1A	3529	1/1	0.81	0.28	57,57,57,57	0
56	MG	2A	3365	1/1	0.81	0.18	74,74,74,74	0
56	MG	1a	1712	1/1	0.81	0.36	58,58,58,58	0
56	MG	2a	1603	1/1	0.81	0.17	78,78,78,78	0
56	MG	2A	3112	1/1	0.81	0.26	73,73,73,73	0
56	MG	2a	1653	1/1	0.81	0.31	74,74,74,74	0
56	MG	2A	3182	1/1	0.81	0.20	76,76,76,76	0
56	MG	2A	3473	1/1	0.81	0.17	63,63,63,63	0
56	MG	2A	3480	1/1	0.81	0.14	67,67,67,67	0
56	MG	1A	3705	1/1	0.81	0.22	64,64,64,64	0
56	MG	2A	3215	1/1	0.81	0.12	65,65,65,65	0
56	MG	1A	3873	1/1	0.81	0.12	26,26,26,26	0
56	MG	1E	309	1/1	0.81	0.38	79,79,79,79	0
56	MG	1S	202	1/1	0.81	0.27	62,62,62,62	0
56	MG	2A	3234	1/1	0.81	0.19	63,63,63,63	0
56	MG	2A	3685	1/1	0.81	0.19	70,70,70,70	0
56	MG	1A	3931	1/1	0.81	0.20	37,37,37,37	0
56	MG	2A	3690	1/1	0.81	0.23	72,72,72,72	0
56	MG	1A	3095	1/1	0.81	0.12	71,71,71,71	0
56	MG	1a	1623	1/1	0.81	0.12	68,68,68,68	0
56	MG	1A	3897	1/1	0.82	0.14	52,52,52,52	0
56	MG	2A	3474	1/1	0.82	0.17	71,71,71,71	0
56	MG	2E	302	1/1	0.82	0.08	69,69,69,69	0
56	MG	1a	1714	1/1	0.82	0.23	64,64,64,64	0
56	MG	2A	3013	1/1	0.82	0.13	59,59,59,59	0
56	MG	1a	1739	1/1	0.82	0.16	53,53,53,53	0
56	MG	1a	1740	1/1	0.82	0.24	81,81,81,81	0
56	MG	2a	1641	1/1	0.82	0.22	70,70,70,70	0
56	MG	2a	1646	1/1	0.82	0.17	63,63,63,63	0
56	MG	2a	1650	1/1	0.82	0.34	79,79,79,79	0
56	MG	1A	4008	1/1	0.82	0.19	65,65,65,65	0
56	MG	2A	3600	1/1	0.82	0.13	44,44,44,44	0
56	MG	2a	1701	1/1	0.82	0.16	69,69,69,69	0
56	MG	2a	1703	1/1	0.82	0.30	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	1a	1789	1/1	0.82	0.20	61,61,61,61	0
56	MG	2A	3648	1/1	0.82	0.17	60,60,60,60	0
56	MG	2A	3304	1/1	0.82	0.14	62,62,62,62	0
56	MG	2a	1777	1/1	0.82	0.29	78,78,78,78	0
56	MG	1a	1658	1/1	0.82	0.13	63,63,63,63	0
56	MG	1A	3704	1/1	0.82	0.13	63,63,63,63	0
56	MG	1n	101	1/1	0.82	0.37	73,73,73,73	0
56	MG	2A	3354	1/1	0.82	0.38	66,66,66,66	0
56	MG	1w	104	1/1	0.82	0.16	67,67,67,67	0
56	MG	2a	1825	1/1	0.82	0.30	72,72,72,72	0
56	MG	2l	202	1/1	0.82	0.17	65,65,65,65	0
56	MG	2A	3213	1/1	0.82	0.11	60,60,60,60	0
56	MG	2A	3744	1/1	0.82	0.15	50,50,50,50	0
56	MG	1A	4069	1/1	0.82	0.22	71,71,71,71	0
56	MG	2A	3414	1/1	0.82	0.19	58,58,58,58	0
56	MG	1A	3932	1/1	0.82	0.14	32,32,32,32	0
56	MG	2A	3292	1/1	0.83	0.41	75,75,75,75	0
56	MG	2a	1605	1/1	0.83	0.20	67,67,67,67	0
56	MG	1a	1689	1/1	0.83	0.34	56,56,56,56	0
56	MG	2a	1611	1/1	0.83	0.39	75,75,75,75	0
56	MG	2a	1618	1/1	0.83	0.19	69,69,69,69	0
56	MG	2a	1636	1/1	0.83	0.25	61,61,61,61	0
56	MG	1Y	203	1/1	0.83	0.11	73,73,73,73	0
56	MG	1A	4059	1/1	0.83	0.11	48,48,48,48	0
56	MG	2A	3142	1/1	0.83	0.22	71,71,71,71	0
56	MG	1A	3819	1/1	0.83	0.13	39,39,39,39	0
56	MG	2A	3659	1/1	0.83	0.18	58,58,58,58	0
56	MG	2a	1677	1/1	0.83	0.31	59,59,59,59	0
56	MG	2A	3669	1/1	0.83	0.17	64,64,64,64	0
56	MG	1x	104	1/1	0.83	0.14	60,60,60,60	0
56	MG	2a	1713	1/1	0.83	0.19	67,67,67,67	0
56	MG	1a	1604	1/1	0.83	0.21	64,64,64,64	0
56	MG	2A	3005	1/1	0.83	0.18	69,69,69,69	0
56	MG	1A	3230	1/1	0.83	0.15	54,54,54,54	0
56	MG	2a	1775	1/1	0.83	0.23	73,73,73,73	0
56	MG	1A	3339	1/1	0.83	0.14	48,48,48,48	0
56	MG	1A	3956	1/1	0.83	0.23	64,64,64,64	0
56	MG	2A	3470	1/1	0.83	0.16	66,66,66,66	0
56	MG	2A	3781	1/1	0.83	0.14	77,77,77,77	0
56	MG	2a	1804	1/1	0.83	0.18	60,60,60,60	0
56	MG	2A	3784	1/1	0.83	0.11	52,52,52,52	0
56	MG	2A	3045	1/1	0.83	0.14	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	3358	1/1	0.83	0.12	72,72,72,72	0
56	MG	2j	201	1/1	0.83	0.25	80,80,80,80	0
56	MG	2A	3477	1/1	0.83	0.15	63,63,63,63	0
56	MG	2v	101	1/1	0.83	0.35	73,73,73,73	0
56	MG	2A	3078	1/1	0.83	0.37	62,62,62,62	0
56	MG	1a	1668	1/1	0.83	0.17	62,62,62,62	0
56	MG	2A	3491	1/1	0.83	0.17	66,66,66,66	0
56	MG	2A	3523	1/1	0.83	0.38	76,76,76,76	0
56	MG	2A	3291	1/1	0.83	0.16	68,68,68,68	0
56	MG	2A	3315	1/1	0.84	0.26	78,78,78,78	0
56	MG	1y	4301	1/1	0.84	0.11	63,63,63,63	0
56	MG	1a	1640	1/1	0.84	0.29	72,72,72,72	0
56	MG	2A	3338	1/1	0.84	0.11	67,67,67,67	0
56	MG	2A	3209	1/1	0.84	0.21	74,74,74,74	0
56	MG	1a	1764	1/1	0.84	0.26	58,58,58,58	0
56	MG	2A	3684	1/1	0.84	0.12	79,79,79,79	0
56	MG	1A	3837	1/1	0.84	0.16	67,67,67,67	0
56	MG	1W	207	1/1	0.84	0.26	43,43,43,43	0
56	MG	2A	3371	1/1	0.84	0.19	67,67,67,67	0
56	MG	2A	3697	1/1	0.84	0.17	63,63,63,63	0
56	MG	2A	3225	1/1	0.84	0.24	62,62,62,62	0
56	MG	2A	3701	1/1	0.84	0.14	58,58,58,58	0
56	MG	1A	3435	1/1	0.84	0.10	70,70,70,70	0
56	MG	2A	3718	1/1	0.84	0.17	65,65,65,65	0
56	MG	2A	3719	1/1	0.84	0.11	66,66,66,66	0
56	MG	1A	3649	1/1	0.84	0.17	57,57,57,57	0
56	MG	1a	1673	1/1	0.84	0.15	67,67,67,67	0
56	MG	2A	3778	1/1	0.84	0.28	73,73,73,73	0
56	MG	1A	3971	1/1	0.84	0.11	59,59,59,59	0
56	MG	14	101	1/1	0.84	0.16	70,70,70,70	0
56	MG	2A	3791	1/1	0.84	0.14	48,48,48,48	0
56	MG	2A	3266	1/1	0.84	0.15	72,72,72,72	0
56	MG	2a	1815	1/1	0.84	0.22	58,58,58,58	0
56	MG	2A	3267	1/1	0.84	0.16	58,58,58,58	0
56	MG	2a	1824	1/1	0.84	0.22	65,65,65,65	0
56	MG	2A	3273	1/1	0.84	0.25	72,72,72,72	0
56	MG	1a	1603	1/1	0.84	0.15	66,66,66,66	0
56	MG	2A	3111	1/1	0.84	0.22	68,68,68,68	0
56	MG	2A	3541	1/1	0.84	0.13	70,70,70,70	0
56	MG	2F	304	1/1	0.84	0.17	61,61,61,61	0
56	MG	1A	3245	1/1	0.84	0.18	56,56,56,56	0
56	MG	2A	3547	1/1	0.84	0.19	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	1E	312	1/1	0.84	0.21	61,61,61,61	0
56	MG	2A	3176	1/1	0.84	0.34	74,74,74,74	0
56	MG	2y	102	1/1	0.84	0.18	79,79,79,79	0
56	MG	2A	3524	1/1	0.85	0.18	63,63,63,63	0
56	MG	1A	4070	1/1	0.85	0.15	70,70,70,70	0
56	MG	1A	3518	1/1	0.85	0.15	90,90,90,90	0
56	MG	1A	3313	1/1	0.85	0.21	51,51,51,51	0
56	MG	25	101	1/1	0.85	0.20	63,63,63,63	0
56	MG	1A	3447	1/1	0.85	0.09	64,64,64,64	0
56	MG	1A	3385	1/1	0.85	0.16	64,64,64,64	0
56	MG	1B	215	1/1	0.85	0.13	68,68,68,68	0
56	MG	2a	1609	1/1	0.85	0.21	68,68,68,68	0
56	MG	2A	3602	1/1	0.85	0.18	52,52,52,52	0
56	MG	2a	1617	1/1	0.85	0.21	70,70,70,70	0
56	MG	1A	3494	1/1	0.85	0.21	69,69,69,69	0
56	MG	2A	3120	1/1	0.85	0.18	60,60,60,60	0
56	MG	2a	1638	1/1	0.85	0.38	72,72,72,72	0
56	MG	2A	3124	1/1	0.85	0.29	59,59,59,59	0
56	MG	2A	3331	1/1	0.85	0.14	66,66,66,66	0
56	MG	2a	1648	1/1	0.85	0.28	64,64,64,64	0
56	MG	1B	222	1/1	0.85	0.13	68,68,68,68	0
56	MG	1A	3586	1/1	0.85	0.22	60,60,60,60	0
56	MG	2a	1670	1/1	0.85	0.20	60,60,60,60	0
56	MG	1A	3506	1/1	0.85	0.17	75,75,75,75	0
56	MG	2A	3341	1/1	0.85	0.17	81,81,81,81	0
56	MG	1A	4006	1/1	0.85	0.13	47,47,47,47	0
56	MG	2a	1702	1/1	0.85	0.20	62,62,62,62	0
56	MG	2A	3363	1/1	0.85	0.18	61,61,61,61	0
56	MG	2A	3698	1/1	0.85	0.19	65,65,65,65	0
56	MG	2A	3208	1/1	0.85	0.22	59,59,59,59	0
56	MG	1A	3876	1/1	0.85	0.14	28,28,28,28	0
56	MG	2a	1738	1/1	0.85	0.14	71,71,71,71	0
56	MG	1A	3590	1/1	0.85	0.36	60,60,60,60	0
56	MG	2a	1749	1/1	0.85	0.13	69,69,69,69	0
56	MG	2A	3389	1/1	0.85	0.43	70,70,70,70	0
56	MG	2a	1776	1/1	0.85	0.15	61,61,61,61	0
56	MG	1x	115	1/1	0.85	0.29	71,71,71,71	0
56	MG	1A	4045	1/1	0.85	0.12	44,44,44,44	0
56	MG	2a	1785	1/1	0.85	0.25	62,62,62,62	0
56	MG	2A	3728	1/1	0.85	0.23	60,60,60,60	0
56	MG	2A	3422	1/1	0.85	0.29	64,64,64,64	0
56	MG	2A	3753	1/1	0.85	0.23	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	1807	1/1	0.85	0.32	74,74,74,74	0
56	MG	2A	3756	1/1	0.85	0.12	64,64,64,64	0
56	MG	2A	3222	1/1	0.85	0.39	69,69,69,69	0
56	MG	1A	3899	1/1	0.85	0.11	58,58,58,58	0
56	MG	1A	3428	1/1	0.85	0.24	58,58,58,58	0
56	MG	2A	3231	1/1	0.85	0.25	70,70,70,70	0
56	MG	2A	3805	1/1	0.85	0.13	66,66,66,66	0
56	MG	1a	1720	1/1	0.85	0.29	73,73,73,73	0
56	MG	2A	3030	1/1	0.85	0.24	61,61,61,61	0
56	MG	1a	1722	1/1	0.85	0.27	71,71,71,71	0
56	MG	1a	1737	1/1	0.85	0.14	59,59,59,59	0
56	MG	2A	3058	1/1	0.85	0.12	54,54,54,54	0
56	MG	2B	206	1/1	0.85	0.26	65,65,65,65	0
56	MG	2B	210	1/1	0.85	0.17	72,72,72,72	0
56	MG	2B	211	1/1	0.85	0.22	68,68,68,68	0
56	MG	2A	3510	1/1	0.86	0.14	61,61,61,61	0
56	MG	2A	3230	1/1	0.86	0.13	63,63,63,63	0
56	MG	1A	3410	1/1	0.86	0.24	70,70,70,70	0
56	MG	1B	218	1/1	0.86	0.14	59,59,59,59	0
56	MG	2a	1604	1/1	0.86	0.21	56,56,56,56	0
56	MG	2A	3003	1/1	0.86	0.29	64,64,64,64	0
56	MG	1A	3800	1/1	0.86	0.10	33,33,33,33	0
56	MG	2A	3561	1/1	0.86	0.18	60,60,60,60	0
56	MG	1A	3813	1/1	0.86	0.13	37,37,37,37	0
56	MG	2a	1615	1/1	0.86	0.24	73,73,73,73	0
56	MG	2A	3255	1/1	0.86	0.33	56,56,56,56	0
56	MG	1a	1683	1/1	0.86	0.17	66,66,66,66	0
56	MG	2a	1620	1/1	0.86	0.12	65,65,65,65	0
56	MG	2a	1629	1/1	0.86	0.32	76,76,76,76	0
56	MG	2a	1635	1/1	0.86	0.25	69,69,69,69	0
56	MG	1A	3414	1/1	0.86	0.24	47,47,47,47	0
56	MG	2A	3272	1/1	0.86	0.20	73,73,73,73	0
56	MG	2A	3611	1/1	0.86	0.13	53,53,53,53	0
56	MG	1a	1691	1/1	0.86	0.26	62,62,62,62	0
56	MG	2A	3275	1/1	0.86	0.12	70,70,70,70	0
56	MG	2A	3280	1/1	0.86	0.14	63,63,63,63	0
56	MG	2A	3666	1/1	0.86	0.12	72,72,72,72	0
56	MG	2A	3286	1/1	0.86	0.27	65,65,65,65	0
56	MG	1A	3420	1/1	0.86	0.32	61,61,61,61	0
56	MG	1A	3091	1/1	0.86	0.23	54,54,54,54	0
56	MG	2a	1690	1/1	0.86	0.11	79,79,79,79	0
56	MG	2a	1695	1/1	0.86	0.24	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	1D	313	1/1	0.86	0.18	44,44,44,44	0
56	MG	1A	3195	1/1	0.86	0.23	50,50,50,50	0
56	MG	1A	3360	1/1	0.86	0.33	65,65,65,65	0
56	MG	2A	3084	1/1	0.86	0.15	58,58,58,58	0
56	MG	2A	3097	1/1	0.86	0.17	61,61,61,61	0
56	MG	1a	1729	1/1	0.86	0.20	65,65,65,65	0
56	MG	1G	205	1/1	0.86	0.16	62,62,62,62	0
56	MG	2a	1740	1/1	0.86	0.25	62,62,62,62	0
56	MG	1A	4022	1/1	0.86	0.12	45,45,45,45	0
56	MG	1S	203	1/1	0.86	0.12	73,73,73,73	0
56	MG	1a	1745	1/1	0.86	0.16	62,62,62,62	0
56	MG	1a	1749	1/1	0.86	0.22	68,68,68,68	0
56	MG	1A	4023	1/1	0.86	0.10	40,40,40,40	0
56	MG	2A	3149	1/1	0.86	0.14	67,67,67,67	0
56	MG	2a	1784	1/1	0.86	0.23	71,71,71,71	0
56	MG	1A	4043	1/1	0.86	0.17	39,39,39,39	0
56	MG	2A	3768	1/1	0.86	0.26	80,80,80,80	0
56	MG	2A	3181	1/1	0.86	0.17	67,67,67,67	0
56	MG	2a	1802	1/1	0.86	0.10	62,62,62,62	0
56	MG	1a	1781	1/1	0.86	0.14	59,59,59,59	0
56	MG	1A	3544	1/1	0.86	0.13	64,64,64,64	0
56	MG	2a	1813	1/1	0.86	0.15	71,71,71,71	0
56	MG	1A	3371	1/1	0.86	0.22	50,50,50,50	0
56	MG	1A	3476	1/1	0.86	0.13	61,61,61,61	0
56	MG	2A	3436	1/1	0.86	0.30	58,58,58,58	0
56	MG	2A	3210	1/1	0.86	0.15	53,53,53,53	0
56	MG	1A	3905	1/1	0.86	0.12	23,23,23,23	0
56	MG	1A	3208	1/1	0.86	0.15	63,63,63,63	0
56	MG	1A	3500	1/1	0.86	0.17	63,63,63,63	0
56	MG	2A	3218	1/1	0.86	0.20	64,64,64,64	0
56	MG	1A	3951	1/1	0.86	0.12	56,56,56,56	0
56	MG	1a	1656	1/1	0.86	0.23	57,57,57,57	0
56	MG	2w	103	1/1	0.86	0.16	83,83,83,83	0
56	MG	2B	215	1/1	0.86	0.23	61,61,61,61	0
56	MG	2D	307	1/1	0.86	0.30	49,49,49,49	0
56	MG	2x	102	1/1	0.86	0.24	67,67,67,67	0
56	MG	2A	3485	1/1	0.86	0.23	48,48,48,48	0
56	MG	2x	107	1/1	0.86	0.14	55,55,55,55	0
56	MG	2y	101	1/1	0.86	0.15	74,74,74,74	0
56	MG	1A	3779	1/1	0.86	0.10	46,46,46,46	0
56	MG	2A	3503	1/1	0.87	0.22	59,59,59,59	0
56	MG	2A	3012	1/1	0.87	0.23	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	1A	3187	1/1	0.87	0.12	47,47,47,47	0
56	MG	2A	3253	1/1	0.87	0.24	77,77,77,77	0
56	MG	1F	310	1/1	0.87	0.13	52,52,52,52	0
56	MG	2A	3261	1/1	0.87	0.32	63,63,63,63	0
56	MG	1A	3326	1/1	0.87	0.15	57,57,57,57	0
56	MG	2A	3548	1/1	0.87	0.14	61,61,61,61	0
56	MG	1A	3957	1/1	0.87	0.18	63,63,63,63	0
56	MG	2A	3268	1/1	0.87	0.33	78,78,78,78	0
56	MG	1A	3965	1/1	0.87	0.11	64,64,64,64	0
56	MG	1A	3592	1/1	0.87	0.31	70,70,70,70	0
56	MG	2A	3076	1/1	0.87	0.30	58,58,58,58	0
56	MG	1A	3250	1/1	0.87	0.13	67,67,67,67	0
56	MG	1a	1738	1/1	0.87	0.16	60,60,60,60	0
56	MG	2A	3630	1/1	0.87	0.18	55,55,55,55	0
56	MG	2A	3640	1/1	0.87	0.17	62,62,62,62	0
56	MG	1A	4075	1/1	0.87	0.15	61,61,61,61	0
56	MG	2A	3089	1/1	0.87	0.21	60,60,60,60	0
56	MG	1A	3613	1/1	0.87	0.11	33,33,33,33	0
56	MG	1a	1744	1/1	0.87	0.11	60,60,60,60	0
56	MG	1A	4092	1/1	0.87	0.31	45,45,45,45	0
56	MG	2A	3680	1/1	0.87	0.15	56,56,56,56	0
56	MG	18	104	1/1	0.87	0.19	53,53,53,53	0
56	MG	1A	3625	1/1	0.87	0.08	25,25,25,25	0
56	MG	2A	3320	1/1	0.87	0.17	66,66,66,66	0
56	MG	2A	3325	1/1	0.87	0.18	76,76,76,76	0
56	MG	1a	1770	1/1	0.87	0.09	71,71,71,71	0
56	MG	2A	3122	1/1	0.87	0.24	65,65,65,65	0
56	MG	2a	1707	1/1	0.87	0.19	72,72,72,72	0
56	MG	1A	3991	1/1	0.87	0.12	72,72,72,72	0
56	MG	2a	1717	1/1	0.87	0.14	76,76,76,76	0
56	MG	1a	1605	1/1	0.87	0.11	67,67,67,67	0
56	MG	1a	1788	1/1	0.87	0.13	86,86,86,86	0
56	MG	1A	3887	1/1	0.87	0.21	42,42,42,42	0
56	MG	2A	3361	1/1	0.87	0.11	66,66,66,66	0
56	MG	1A	3556	1/1	0.87	0.29	52,52,52,52	0
56	MG	1a	1798	1/1	0.87	0.18	53,53,53,53	0
56	MG	2a	1763	1/1	0.87	0.13	59,59,59,59	0
56	MG	2A	3739	1/1	0.87	0.13	61,61,61,61	0
56	MG	1a	1800	1/1	0.87	0.10	58,58,58,58	0
56	MG	2A	3206	1/1	0.87	0.25	63,63,63,63	0
56	MG	2A	3372	1/1	0.87	0.17	60,60,60,60	0
56	MG	2a	1781	1/1	0.87	0.25	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	1A	3492	1/1	0.87	0.12	48,48,48,48	0
56	MG	1a	1808	1/1	0.87	0.10	55,55,55,55	0
56	MG	2a	1792	1/1	0.87	0.25	68,68,68,68	0
56	MG	1A	4009	1/1	0.87	0.10	75,75,75,75	0
56	MG	1A	3678	1/1	0.87	0.13	67,67,67,67	0
56	MG	1B	232	1/1	0.87	0.13	59,59,59,59	0
56	MG	2A	3801	1/1	0.87	0.16	69,69,69,69	0
56	MG	2A	3804	1/1	0.87	0.09	53,53,53,53	0
56	MG	1B	233	1/1	0.87	0.15	69,69,69,69	0
56	MG	2A	3806	1/1	0.87	0.10	66,66,66,66	0
56	MG	2A	3811	1/1	0.87	0.13	52,52,52,52	0
56	MG	2A	3444	1/1	0.87	0.24	65,65,65,65	0
56	MG	2A	3448	1/1	0.87	0.27	69,69,69,69	0
56	MG	2A	3458	1/1	0.87	0.12	62,62,62,62	0
56	MG	1w	108	1/1	0.87	0.10	71,71,71,71	0
56	MG	2A	3836	1/1	0.87	0.12	66,66,66,66	0
56	MG	1a	1672	1/1	0.87	0.19	62,62,62,62	0
56	MG	1A	3921	1/1	0.87	0.13	54,54,54,54	0
56	MG	1a	1681	1/1	0.87	0.14	62,62,62,62	0
56	MG	1A	3689	1/1	0.87	0.09	33,33,33,33	0
56	MG	2A	3481	1/1	0.87	0.12	77,77,77,77	0
56	MG	1D	314	1/1	0.87	0.22	44,44,44,44	0
56	MG	1A	3300	1/1	0.87	0.20	56,56,56,56	0
56	MG	2E	309	1/1	0.87	0.11	59,59,59,59	0
56	MG	1a	1698	1/1	0.87	0.23	66,66,66,66	0
56	MG	2V	201	1/1	0.87	0.24	60,60,60,60	0
56	MG	2A	3495	1/1	0.87	0.12	62,62,62,62	0
56	MG	2y	107	1/1	0.87	0.18	72,72,72,72	0
56	MG	28	103	1/1	0.88	0.26	54,54,54,54	0
56	MG	2A	3567	1/1	0.88	0.17	68,68,68,68	0
56	MG	2A	3308	1/1	0.88	0.29	61,61,61,61	0
56	MG	2A	3312	1/1	0.88	0.10	57,57,57,57	0
56	MG	2A	3163	1/1	0.88	0.16	67,67,67,67	0
56	MG	2A	3316	1/1	0.88	0.14	61,61,61,61	0
56	MG	2A	3164	1/1	0.88	0.18	65,65,65,65	0
56	MG	1a	1709	1/1	0.88	0.46	70,70,70,70	0
56	MG	2A	3615	1/1	0.88	0.21	42,42,42,42	0
56	MG	2A	3324	1/1	0.88	0.16	57,57,57,57	0
56	MG	2A	3638	1/1	0.88	0.24	66,66,66,66	0
56	MG	2a	1627	1/1	0.88	0.27	71,71,71,71	0
56	MG	1A	4080	1/1	0.88	0.28	43,43,43,43	0
56	MG	2A	3327	1/1	0.88	0.12	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	1x	111	1/1	0.88	0.09	55,55,55,55	0
56	MG	1A	3732	1/1	0.88	0.11	24,24,24,24	0
56	MG	2A	3661	1/1	0.88	0.16	44,44,44,44	0
56	MG	2a	1643	1/1	0.88	0.16	70,70,70,70	0
56	MG	2A	3665	1/1	0.88	0.28	71,71,71,71	0
56	MG	2A	3189	1/1	0.88	0.20	52,52,52,52	0
56	MG	1A	3455	1/1	0.88	0.16	53,53,53,53	0
56	MG	1A	3182	1/1	0.88	0.15	55,55,55,55	0
56	MG	2A	3352	1/1	0.88	0.24	75,75,75,75	0
56	MG	1A	4004	1/1	0.88	0.12	73,73,73,73	0
56	MG	2A	3355	1/1	0.88	0.23	64,64,64,64	0
56	MG	2a	1686	1/1	0.88	0.29	70,70,70,70	0
56	MG	1A	3676	1/1	0.88	0.12	52,52,52,52	0
56	MG	2a	1692	1/1	0.88	0.27	68,68,68,68	0
56	MG	1A	3289	1/1	0.88	0.19	66,66,66,66	0
56	MG	18	106	1/1	0.88	0.10	74,74,74,74	0
56	MG	1A	3545	1/1	0.88	0.26	61,61,61,61	0
56	MG	2A	3022	1/1	0.88	0.31	62,62,62,62	0
56	MG	2A	3025	1/1	0.88	0.17	57,57,57,57	0
56	MG	2A	3713	1/1	0.88	0.17	69,69,69,69	0
56	MG	2A	3374	1/1	0.88	0.26	65,65,65,65	0
56	MG	2A	3388	1/1	0.88	0.20	55,55,55,55	0
56	MG	1B	225	1/1	0.88	0.11	58,58,58,58	0
56	MG	2a	1733	1/1	0.88	0.35	68,68,68,68	0
56	MG	2A	3042	1/1	0.88	0.33	60,60,60,60	0
56	MG	2A	3738	1/1	0.88	0.15	61,61,61,61	0
56	MG	2A	3400	1/1	0.88	0.13	68,68,68,68	0
56	MG	2A	3403	1/1	0.88	0.11	68,68,68,68	0
56	MG	1A	3788	1/1	0.88	0.09	17,17,17,17	0
56	MG	2a	1769	1/1	0.88	0.14	57,57,57,57	0
56	MG	1A	3054	1/1	0.88	0.15	55,55,55,55	0
56	MG	2A	3764	1/1	0.88	0.18	69,69,69,69	0
56	MG	2A	3767	1/1	0.88	0.17	69,69,69,69	0
56	MG	2A	3425	1/1	0.88	0.15	58,58,58,58	0
56	MG	2A	3433	1/1	0.88	0.26	61,61,61,61	0
56	MG	2A	3050	1/1	0.88	0.25	57,57,57,57	0
56	MG	2A	3053	1/1	0.88	0.18	61,61,61,61	0
56	MG	2a	1786	1/1	0.88	0.15	71,71,71,71	0
56	MG	2a	1789	1/1	0.88	0.20	78,78,78,78	0
56	MG	1A	3579	1/1	0.88	0.14	42,42,42,42	0
56	MG	1a	1641	1/1	0.88	0.24	63,63,63,63	0
56	MG	2A	3450	1/1	0.88	0.18	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	3948	1/1	0.88	0.07	41,41,41,41	0
56	MG	2A	3254	1/1	0.88	0.18	71,71,71,71	0
56	MG	2A	3807	1/1	0.88	0.14	45,45,45,45	0
56	MG	1A	3618	1/1	0.88	0.15	66,66,66,66	0
56	MG	1A	3163	1/1	0.88	0.20	56,56,56,56	0
56	MG	1a	1661	1/1	0.88	0.17	63,63,63,63	0
56	MG	2a	1816	1/1	0.88	0.17	69,69,69,69	0
56	MG	2A	3822	1/1	0.88	0.12	52,52,52,52	0
56	MG	1A	3827	1/1	0.88	0.10	51,51,51,51	0
56	MG	1A	3631	1/1	0.88	0.14	54,54,54,54	0
56	MG	2f	202	1/1	0.88	0.20	71,71,71,71	0
56	MG	2A	3098	1/1	0.88	0.10	53,53,53,53	0
56	MG	1a	1670	1/1	0.88	0.11	59,59,59,59	0
56	MG	2A	3489	1/1	0.88	0.15	56,56,56,56	0
56	MG	1A	3835	1/1	0.88	0.12	54,54,54,54	0
56	MG	1A	3725	1/1	0.88	0.13	60,60,60,60	0
56	MG	2A	3282	1/1	0.88	0.21	63,63,63,63	0
56	MG	1A	3848	1/1	0.88	0.13	51,51,51,51	0
56	MG	1I	201	1/1	0.88	0.10	67,67,67,67	0
56	MG	1w	101	1/1	0.88	0.18	55,55,55,55	0
56	MG	2x	104	1/1	0.88	0.31	66,66,66,66	0
56	MG	1O	201	1/1	0.88	0.09	56,56,56,56	0
56	MG	2A	3296	1/1	0.88	0.10	58,58,58,58	0
56	MG	2A	3297	1/1	0.88	0.16	62,62,62,62	0
56	MG	1Q	206	1/1	0.88	0.13	47,47,47,47	0
56	MG	2y	105	1/1	0.88	0.23	85,85,85,85	0
56	MG	1A	4076	1/1	0.88	0.24	76,76,76,76	0
56	MG	1a	1768	1/1	0.89	0.19	66,66,66,66	0
56	MG	1A	3770	1/1	0.89	0.10	35,35,35,35	0
56	MG	1A	3259	1/1	0.89	0.17	51,51,51,51	0
56	MG	1a	1772	1/1	0.89	0.21	71,71,71,71	0
56	MG	2A	3187	1/1	0.89	0.08	55,55,55,55	0
56	MG	2A	3407	1/1	0.89	0.22	56,56,56,56	0
56	MG	2A	3819	1/1	0.89	0.11	78,78,78,78	0
56	MG	2A	3410	1/1	0.89	0.21	54,54,54,54	0
56	MG	2A	3411	1/1	0.89	0.24	56,56,56,56	0
56	MG	1a	1780	1/1	0.89	0.14	51,51,51,51	0
56	MG	2A	3200	1/1	0.89	0.15	70,70,70,70	0
56	MG	2A	3204	1/1	0.89	0.17	59,59,59,59	0
56	MG	2A	3842	1/1	0.89	0.20	63,63,63,63	0
56	MG	2A	3426	1/1	0.89	0.12	62,62,62,62	0
56	MG	2B	202	1/1	0.89	0.13	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	2A	3430	1/1	0.89	0.34	61,61,61,61	0
56	MG	15	102	1/1	0.89	0.18	33,33,33,33	0
56	MG	1A	3682	1/1	0.89	0.11	24,24,24,24	0
56	MG	1A	3942	1/1	0.89	0.10	46,46,46,46	0
56	MG	2B	219	1/1	0.89	0.21	71,71,71,71	0
56	MG	19	101	1/1	0.89	0.14	45,45,45,45	0
56	MG	1A	3943	1/1	0.89	0.14	70,70,70,70	0
56	MG	1A	3683	1/1	0.89	0.08	19,19,19,19	0
56	MG	2A	3457	1/1	0.89	0.14	53,53,53,53	0
56	MG	1A	4090	1/1	0.89	0.11	59,59,59,59	0
56	MG	2A	3467	1/1	0.89	0.30	68,68,68,68	0
56	MG	2A	3469	1/1	0.89	0.10	68,68,68,68	0
56	MG	1a	1612	1/1	0.89	0.09	63,63,63,63	0
56	MG	1l	201	1/1	0.89	0.15	59,59,59,59	0
56	MG	1a	1622	1/1	0.89	0.25	65,65,65,65	0
56	MG	1n	102	1/1	0.89	0.17	60,60,60,60	0
56	MG	1t	201	1/1	0.89	0.26	58,58,58,58	0
56	MG	1A	3262	1/1	0.89	0.18	60,60,60,60	0
56	MG	1a	1637	1/1	0.89	0.20	65,65,65,65	0
56	MG	1A	4096	1/1	0.89	0.26	59,59,59,59	0
56	MG	2a	1613	1/1	0.89	0.27	72,72,72,72	0
56	MG	2A	3238	1/1	0.89	0.16	53,53,53,53	0
56	MG	1B	202	1/1	0.89	0.16	45,45,45,45	0
56	MG	2A	3242	1/1	0.89	0.21	64,64,64,64	0
56	MG	2A	3502	1/1	0.89	0.13	29,29,29,29	0
56	MG	2a	1622	1/1	0.89	0.16	73,73,73,73	0
56	MG	1a	1642	1/1	0.89	0.15	65,65,65,65	0
56	MG	2A	3250	1/1	0.89	0.11	65,65,65,65	0
56	MG	2a	1633	1/1	0.89	0.26	67,67,67,67	0
56	MG	2a	1634	1/1	0.89	0.32	67,67,67,67	0
56	MG	2A	3517	1/1	0.89	0.08	40,40,40,40	0
56	MG	2A	3252	1/1	0.89	0.34	64,64,64,64	0
56	MG	1a	1649	1/1	0.89	0.21	61,61,61,61	0
56	MG	2A	3529	1/1	0.89	0.14	42,42,42,42	0
56	MG	2A	3534	1/1	0.89	0.14	54,54,54,54	0
56	MG	1A	3807	1/1	0.89	0.18	64,64,64,64	0
56	MG	1A	3811	1/1	0.89	0.10	26,26,26,26	0
56	MG	1A	3959	1/1	0.89	0.16	66,66,66,66	0
56	MG	2A	3264	1/1	0.89	0.28	71,71,71,71	0
56	MG	2a	1655	1/1	0.89	0.25	67,67,67,67	0
56	MG	2a	1657	1/1	0.89	0.17	64,64,64,64	0
56	MG	2a	1659	1/1	0.89	0.17	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	3539	1/1	0.89	0.18	63,63,63,63	0
56	MG	1A	3817	1/1	0.89	0.13	55,55,55,55	0
56	MG	2A	3582	1/1	0.89	0.16	65,65,65,65	0
56	MG	2a	1681	1/1	0.89	0.21	50,50,50,50	0
56	MG	1a	1665	1/1	0.89	0.17	64,64,64,64	0
56	MG	2A	3586	1/1	0.89	0.19	66,66,66,66	0
56	MG	1a	1667	1/1	0.89	0.27	58,58,58,58	0
56	MG	2a	1693	1/1	0.89	0.20	59,59,59,59	0
56	MG	1B	223	1/1	0.89	0.18	63,63,63,63	0
56	MG	1A	3702	1/1	0.89	0.19	55,55,55,55	0
56	MG	2A	3605	1/1	0.89	0.12	42,42,42,42	0
56	MG	2A	3019	1/1	0.89	0.37	66,66,66,66	0
56	MG	2A	3608	1/1	0.89	0.13	74,74,74,74	0
56	MG	2a	1710	1/1	0.89	0.20	76,76,76,76	0
56	MG	1a	1671	1/1	0.89	0.11	56,56,56,56	0
56	MG	2A	3283	1/1	0.89	0.18	57,57,57,57	0
56	MG	1A	3542	1/1	0.89	0.14	63,63,63,63	0
56	MG	2a	1721	1/1	0.89	0.23	55,55,55,55	0
56	MG	1A	3825	1/1	0.89	0.14	47,47,47,47	0
56	MG	1B	231	1/1	0.89	0.13	63,63,63,63	0
56	MG	1A	3498	1/1	0.89	0.14	49,49,49,49	0
56	MG	1A	3707	1/1	0.89	0.14	55,55,55,55	0
56	MG	1A	4001	1/1	0.89	0.11	45,45,45,45	0
56	MG	1a	1693	1/1	0.89	0.25	52,52,52,52	0
56	MG	2a	1754	1/1	0.89	0.17	70,70,70,70	0
56	MG	2a	1761	1/1	0.89	0.13	54,54,54,54	0
56	MG	2A	3663	1/1	0.89	0.15	68,68,68,68	0
56	MG	1a	1697	1/1	0.89	0.27	64,64,64,64	0
56	MG	1A	3171	1/1	0.89	0.10	44,44,44,44	0
56	MG	1a	1700	1/1	0.89	0.16	57,57,57,57	0
56	MG	1A	3716	1/1	0.89	0.12	53,53,53,53	0
56	MG	2A	3681	1/1	0.89	0.16	57,57,57,57	0
56	MG	1A	3041	1/1	0.89	0.23	56,56,56,56	0
56	MG	2A	3318	1/1	0.89	0.29	66,66,66,66	0
56	MG	1A	3573	1/1	0.89	0.18	67,67,67,67	0
56	MG	1A	3634	1/1	0.89	0.13	62,62,62,62	0
56	MG	2A	3695	1/1	0.89	0.17	40,40,40,40	0
56	MG	2A	3322	1/1	0.89	0.11	49,49,49,49	0
56	MG	2A	3323	1/1	0.89	0.23	60,60,60,60	0
56	MG	2A	3092	1/1	0.89	0.12	64,64,64,64	0
56	MG	2a	1798	1/1	0.89	0.16	68,68,68,68	0
56	MG	2a	1801	1/1	0.89	0.11	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3700	1/1	0.89	0.24	60,60,60,60	0
56	MG	2A	3095	1/1	0.89	0.20	60,60,60,60	0
56	MG	1G	202	1/1	0.89	0.18	59,59,59,59	0
56	MG	1G	203	1/1	0.89	0.09	69,69,69,69	0
56	MG	1A	3062	1/1	0.89	0.17	67,67,67,67	0
56	MG	2A	3101	1/1	0.89	0.27	70,70,70,70	0
56	MG	1A	3053	1/1	0.89	0.15	48,48,48,48	0
56	MG	2a	1817	1/1	0.89	0.18	50,50,50,50	0
56	MG	1A	4039	1/1	0.89	0.15	61,61,61,61	0
56	MG	2A	3729	1/1	0.89	0.20	54,54,54,54	0
56	MG	2A	3343	1/1	0.89	0.15	67,67,67,67	0
56	MG	2A	3344	1/1	0.89	0.09	67,67,67,67	0
56	MG	1A	3758	1/1	0.89	0.11	45,45,45,45	0
56	MG	2A	3749	1/1	0.89	0.14	54,54,54,54	0
56	MG	1A	3331	1/1	0.89	0.16	54,54,54,54	0
56	MG	1A	3906	1/1	0.89	0.12	33,33,33,33	0
56	MG	2A	3758	1/1	0.89	0.12	55,55,55,55	0
56	MG	1A	4068	1/1	0.89	0.09	49,49,49,49	0
56	MG	1A	3913	1/1	0.89	0.10	64,64,64,64	0
56	MG	2A	3147	1/1	0.89	0.25	49,49,49,49	0
56	MG	2A	3769	1/1	0.89	0.12	70,70,70,70	0
56	MG	1a	1759	1/1	0.89	0.22	66,66,66,66	0
56	MG	2A	3779	1/1	0.89	0.13	51,51,51,51	0
56	MG	2A	3370	1/1	0.89	0.16	67,67,67,67	0
56	MG	1a	1761	1/1	0.89	0.12	50,50,50,50	0
56	MG	2A	3787	1/1	0.89	0.09	61,61,61,61	0
56	MG	1A	3915	1/1	0.89	0.13	42,42,42,42	0
56	MG	2A	3172	1/1	0.89	0.22	51,51,51,51	0
56	MG	1A	3938	1/1	0.90	0.12	63,63,63,63	0
56	MG	1A	3341	1/1	0.90	0.10	58,58,58,58	0
56	MG	2A	3838	1/1	0.90	0.20	55,55,55,55	0
56	MG	1A	3429	1/1	0.90	0.11	55,55,55,55	0
56	MG	1A	3635	1/1	0.90	0.13	54,54,54,54	0
56	MG	1A	3799	1/1	0.90	0.15	58,58,58,58	0
56	MG	1x	107	1/1	0.90	0.14	55,55,55,55	0
56	MG	1A	3644	1/1	0.90	0.16	46,46,46,46	0
56	MG	2A	3248	1/1	0.90	0.13	57,57,57,57	0
56	MG	2B	213	1/1	0.90	0.16	66,66,66,66	0
56	MG	1A	3536	1/1	0.90	0.10	61,61,61,61	0
56	MG	1A	3656	1/1	0.90	0.09	40,40,40,40	0
56	MG	1A	3431	1/1	0.90	0.09	44,44,44,44	0
56	MG	1A	3342	1/1	0.90	0.14	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2E	307	1/1	0.90	0.17	53,53,53,53	0
56	MG	1B	224	1/1	0.90	0.14	62,62,62,62	0
56	MG	1A	3437	1/1	0.90	0.14	51,51,51,51	0
56	MG	2Q	203	1/1	0.90	0.09	64,64,64,64	0
56	MG	2R	201	1/1	0.90	0.14	62,62,62,62	0
56	MG	2A	3009	1/1	0.90	0.20	46,46,46,46	0
56	MG	1A	3976	1/1	0.90	0.10	26,26,26,26	0
56	MG	1A	3442	1/1	0.90	0.18	36,36,36,36	0
56	MG	2A	3015	1/1	0.90	0.37	69,69,69,69	0
56	MG	25	102	1/1	0.90	0.15	50,50,50,50	0
56	MG	25	104	1/1	0.90	0.23	53,53,53,53	0
56	MG	1A	3354	1/1	0.90	0.16	66,66,66,66	0
56	MG	2a	1602	1/1	0.90	0.18	73,73,73,73	0
56	MG	1A	3987	1/1	0.90	0.26	40,40,40,40	0
56	MG	1a	1678	1/1	0.90	0.16	60,60,60,60	0
56	MG	2A	3528	1/1	0.90	0.16	59,59,59,59	0
56	MG	1A	3299	1/1	0.90	0.18	55,55,55,55	0
56	MG	2A	3032	1/1	0.90	0.12	62,62,62,62	0
56	MG	2A	3037	1/1	0.90	0.26	62,62,62,62	0
56	MG	1A	3699	1/1	0.90	0.14	44,44,44,44	0
56	MG	1a	1684	1/1	0.90	0.39	63,63,63,63	0
56	MG	1A	3831	1/1	0.90	0.27	62,62,62,62	0
56	MG	1A	3246	1/1	0.90	0.22	67,67,67,67	0
56	MG	2A	3566	1/1	0.90	0.16	61,61,61,61	0
56	MG	2A	3294	1/1	0.90	0.24	59,59,59,59	0
56	MG	1A	4005	1/1	0.90	0.11	73,73,73,73	0
56	MG	2A	3584	1/1	0.90	0.15	50,50,50,50	0
56	MG	2a	1630	1/1	0.90	0.25	54,54,54,54	0
56	MG	1A	3583	1/1	0.90	0.27	62,62,62,62	0
56	MG	1A	4007	1/1	0.90	0.10	53,53,53,53	0
56	MG	2A	3070	1/1	0.90	0.22	68,68,68,68	0
56	MG	1A	3584	1/1	0.90	0.17	52,52,52,52	0
56	MG	2A	3309	1/1	0.90	0.10	59,59,59,59	0
56	MG	1a	1706	1/1	0.90	0.10	60,60,60,60	0
56	MG	2A	3313	1/1	0.90	0.14	61,61,61,61	0
56	MG	2A	3314	1/1	0.90	0.13	63,63,63,63	0
56	MG	2a	1647	1/1	0.90	0.27	64,64,64,64	0
56	MG	1A	3850	1/1	0.90	0.19	66,66,66,66	0
56	MG	1A	3858	1/1	0.90	0.09	35,35,35,35	0
56	MG	1A	3866	1/1	0.90	0.13	44,44,44,44	0
56	MG	2A	3632	1/1	0.90	0.11	73,73,73,73	0
56	MG	2A	3635	1/1	0.90	0.23	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	1658	1/1	0.90	0.22	44,44,44,44	0
56	MG	1N	205	1/1	0.90	0.24	62,62,62,62	0
56	MG	2a	1663	1/1	0.90	0.21	54,54,54,54	0
56	MG	2a	1669	1/1	0.90	0.18	61,61,61,61	0
56	MG	1a	1715	1/1	0.90	0.20	62,62,62,62	0
56	MG	2A	3645	1/1	0.90	0.16	57,57,57,57	0
56	MG	2A	3647	1/1	0.90	0.18	64,64,64,64	0
56	MG	1A	3872	1/1	0.90	0.10	35,35,35,35	0
56	MG	1O	205	1/1	0.90	0.20	66,66,66,66	0
56	MG	1A	4035	1/1	0.90	0.10	65,65,65,65	0
56	MG	2a	1691	1/1	0.90	0.49	65,65,65,65	0
56	MG	1S	201	1/1	0.90	0.34	56,56,56,56	0
56	MG	1A	3362	1/1	0.90	0.15	53,53,53,53	0
56	MG	2A	3328	1/1	0.90	0.09	53,53,53,53	0
56	MG	1A	3364	1/1	0.90	0.09	45,45,45,45	0
56	MG	1W	203	1/1	0.90	0.09	48,48,48,48	0
56	MG	2A	3673	1/1	0.90	0.18	58,58,58,58	0
56	MG	2a	1705	1/1	0.90	0.14	72,72,72,72	0
56	MG	2A	3115	1/1	0.90	0.14	73,73,73,73	0
56	MG	2a	1708	1/1	0.90	0.17	60,60,60,60	0
56	MG	1A	3179	1/1	0.90	0.11	44,44,44,44	0
56	MG	2A	3682	1/1	0.90	0.16	66,66,66,66	0
56	MG	2a	1715	1/1	0.90	0.27	59,59,59,59	0
56	MG	1X	106	1/1	0.90	0.07	32,32,32,32	0
56	MG	2A	3342	1/1	0.90	0.09	54,54,54,54	0
56	MG	1A	4046	1/1	0.90	0.12	55,55,55,55	0
56	MG	2a	1726	1/1	0.90	0.22	77,77,77,77	0
56	MG	2a	1727	1/1	0.90	0.20	55,55,55,55	0
56	MG	2A	3137	1/1	0.90	0.22	65,65,65,65	0
56	MG	2A	3351	1/1	0.90	0.20	73,73,73,73	0
56	MG	2a	1734	1/1	0.90	0.35	65,65,65,65	0
56	MG	1a	1755	1/1	0.90	0.12	64,64,64,64	0
56	MG	1Z	301	1/1	0.90	0.16	59,59,59,59	0
56	MG	2a	1743	1/1	0.90	0.09	66,66,66,66	0
56	MG	1A	3588	1/1	0.90	0.15	50,50,50,50	0
56	MG	2A	3357	1/1	0.90	0.23	64,64,64,64	0
56	MG	2a	1751	1/1	0.90	0.10	41,41,41,41	0
56	MG	1A	4060	1/1	0.90	0.14	43,43,43,43	0
56	MG	2A	3709	1/1	0.90	0.09	56,56,56,56	0
56	MG	2a	1762	1/1	0.90	0.11	70,70,70,70	0
56	MG	2A	3711	1/1	0.90	0.19	58,58,58,58	0
56	MG	2a	1764	1/1	0.90	0.14	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	4064	1/1	0.90	0.17	60,60,60,60	0
56	MG	2A	3364	1/1	0.90	0.28	71,71,71,71	0
56	MG	2A	3717	1/1	0.90	0.12	59,59,59,59	0
56	MG	2A	3170	1/1	0.90	0.13	58,58,58,58	0
56	MG	1A	3379	1/1	0.90	0.18	76,76,76,76	0
56	MG	15	105	1/1	0.90	0.23	55,55,55,55	0
56	MG	15	110	1/1	0.90	0.08	55,55,55,55	0
56	MG	1a	1775	1/1	0.90	0.24	50,50,50,50	0
56	MG	1A	3325	1/1	0.90	0.16	51,51,51,51	0
56	MG	2a	1788	1/1	0.90	0.20	63,63,63,63	0
56	MG	1A	3594	1/1	0.90	0.22	51,51,51,51	0
56	MG	2a	1791	1/1	0.90	0.12	69,69,69,69	0
56	MG	1a	1782	1/1	0.90	0.12	57,57,57,57	0
56	MG	2A	3746	1/1	0.90	0.20	59,59,59,59	0
56	MG	1A	3069	1/1	0.90	0.10	49,49,49,49	0
56	MG	2A	3393	1/1	0.90	0.15	73,73,73,73	0
56	MG	2A	3397	1/1	0.90	0.13	63,63,63,63	0
56	MG	2A	3202	1/1	0.90	0.22	68,68,68,68	0
56	MG	1A	3600	1/1	0.90	0.09	29,29,29,29	0
56	MG	2A	3404	1/1	0.90	0.14	60,60,60,60	0
56	MG	1a	1793	1/1	0.90	0.12	77,77,77,77	0
56	MG	1A	3917	1/1	0.90	0.15	52,52,52,52	0
56	MG	2A	3770	1/1	0.90	0.10	64,64,64,64	0
56	MG	2A	3777	1/1	0.90	0.12	68,68,68,68	0
56	MG	1A	3242	1/1	0.90	0.10	48,48,48,48	0
56	MG	1A	4078	1/1	0.90	0.17	51,51,51,51	0
56	MG	2a	1822	1/1	0.90	0.29	68,68,68,68	0
56	MG	2A	3416	1/1	0.90	0.36	54,54,54,54	0
56	MG	2A	3211	1/1	0.90	0.24	67,67,67,67	0
56	MG	2A	3212	1/1	0.90	0.20	64,64,64,64	0
56	MG	2g	201	1/1	0.90	0.23	72,72,72,72	0
56	MG	2A	3788	1/1	0.90	0.10	69,69,69,69	0
56	MG	1A	3417	1/1	0.90	0.20	56,56,56,56	0
56	MG	2q	203	1/1	0.90	0.20	66,66,66,66	0
56	MG	1A	4084	1/1	0.90	0.16	46,46,46,46	0
56	MG	1f	202	1/1	0.90	0.17	63,63,63,63	0
56	MG	1a	1627	1/1	0.90	0.20	46,46,46,46	0
56	MG	2w	102	1/1	0.90	0.16	82,82,82,82	0
56	MG	2A	3437	1/1	0.90	0.20	69,69,69,69	0
56	MG	2A	3440	1/1	0.90	0.27	56,56,56,56	0
56	MG	2w	105	1/1	0.90	0.11	76,76,76,76	0
56	MG	2A	3808	1/1	0.90	0.08	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1632	1/1	0.90	0.18	60,60,60,60	0
56	MG	1a	1635	1/1	0.90	0.24	75,75,75,75	0
56	MG	2A	3446	1/1	0.90	0.27	61,61,61,61	0
56	MG	1A	3207	1/1	0.90	0.09	56,56,56,56	0
56	MG	1a	1638	1/1	0.90	0.34	66,66,66,66	0
56	MG	2A	3824	1/1	0.90	0.08	50,50,50,50	0
56	MG	2A	3454	1/1	0.90	0.20	42,42,42,42	0
56	MG	2y	106	1/1	0.90	0.26	64,64,64,64	0
56	MG	2A	3834	1/1	0.90	0.09	55,55,55,55	0
59	ZN	14	102	1/1	0.90	0.17	134,134,134,134	0
56	MG	1A	4036	1/1	0.91	0.10	75,75,75,75	0
56	MG	1A	4037	1/1	0.91	0.09	23,23,23,23	0
56	MG	2A	3841	1/1	0.91	0.19	61,61,61,61	0
56	MG	2A	3219	1/1	0.91	0.13	58,58,58,58	0
56	MG	2A	3220	1/1	0.91	0.25	64,64,64,64	0
56	MG	10	102	1/1	0.91	0.11	58,58,58,58	0
56	MG	2B	204	1/1	0.91	0.16	66,66,66,66	0
56	MG	10	107	1/1	0.91	0.16	59,59,59,59	0
56	MG	1a	1796	1/1	0.91	0.10	66,66,66,66	0
56	MG	2A	3228	1/1	0.91	0.23	60,60,60,60	0
56	MG	1A	3015	1/1	0.91	0.11	38,38,38,38	0
56	MG	2B	214	1/1	0.91	0.08	74,74,74,74	0
56	MG	2A	3472	1/1	0.91	0.12	46,46,46,46	0
56	MG	2B	217	1/1	0.91	0.16	62,62,62,62	0
56	MG	1A	4041	1/1	0.91	0.12	60,60,60,60	0
56	MG	1A	4042	1/1	0.91	0.14	38,38,38,38	0
56	MG	1A	3462	1/1	0.91	0.12	56,56,56,56	0
56	MG	2E	306	1/1	0.91	0.10	66,66,66,66	0
56	MG	1A	3466	1/1	0.91	0.11	39,39,39,39	0
56	MG	1A	3212	1/1	0.91	0.07	37,37,37,37	0
56	MG	2F	301	1/1	0.91	0.10	54,54,54,54	0
56	MG	1A	4057	1/1	0.91	0.10	50,50,50,50	0
56	MG	2N	201	1/1	0.91	0.15	75,75,75,75	0
56	MG	2O	201	1/1	0.91	0.18	65,65,65,65	0
56	MG	1A	3877	1/1	0.91	0.09	42,42,42,42	0
56	MG	1A	3883	1/1	0.91	0.08	25,25,25,25	0
56	MG	2U	201	1/1	0.91	0.08	60,60,60,60	0
56	MG	1A	4061	1/1	0.91	0.13	50,50,50,50	0
56	MG	1A	3885	1/1	0.91	0.19	70,70,70,70	0
56	MG	2Z	301	1/1	0.91	0.10	77,77,77,77	0
56	MG	1w	102	1/1	0.91	0.24	68,68,68,68	0
56	MG	20	103	1/1	0.91	0.19	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	1A	4066	1/1	0.91	0.14	51,51,51,51	0
56	MG	1A	3102	1/1	0.91	0.12	65,65,65,65	0
56	MG	2A	3513	1/1	0.91	0.12	49,49,49,49	0
56	MG	27	102	1/1	0.91	0.18	58,58,58,58	0
56	MG	28	102	1/1	0.91	0.23	54,54,54,54	0
56	MG	2A	3515	1/1	0.91	0.10	37,37,37,37	0
56	MG	1w	106	1/1	0.91	0.15	62,62,62,62	0
56	MG	2A	3519	1/1	0.91	0.15	64,64,64,64	0
56	MG	1A	3374	1/1	0.91	0.19	47,47,47,47	0
56	MG	1A	3104	1/1	0.91	0.21	42,42,42,42	0
56	MG	2a	1606	1/1	0.91	0.18	56,56,56,56	0
56	MG	2A	3526	1/1	0.91	0.13	53,53,53,53	0
56	MG	1x	101	1/1	0.91	0.28	57,57,57,57	0
56	MG	1A	3324	1/1	0.91	0.09	45,45,45,45	0
56	MG	1A	3730	1/1	0.91	0.14	62,62,62,62	0
56	MG	1A	4073	1/1	0.91	0.09	52,52,52,52	0
56	MG	2A	3543	1/1	0.91	0.14	38,38,38,38	0
56	MG	1a	1639	1/1	0.91	0.13	54,54,54,54	0
56	MG	2A	3277	1/1	0.91	0.10	65,65,65,65	0
56	MG	2A	3279	1/1	0.91	0.16	56,56,56,56	0
56	MG	2a	1624	1/1	0.91	0.12	63,63,63,63	0
56	MG	2A	3554	1/1	0.91	0.10	39,39,39,39	0
56	MG	1A	3595	1/1	0.91	0.07	28,28,28,28	0
56	MG	1A	3115	1/1	0.91	0.22	40,40,40,40	0
56	MG	2a	1632	1/1	0.91	0.33	60,60,60,60	0
56	MG	2A	3001	1/1	0.91	0.11	54,54,54,54	0
56	MG	1A	3508	1/1	0.91	0.21	37,37,37,37	0
56	MG	1a	1643	1/1	0.91	0.22	56,56,56,56	0
56	MG	1a	1646	1/1	0.91	0.15	54,54,54,54	0
56	MG	1a	1648	1/1	0.91	0.37	61,61,61,61	0
56	MG	2a	1640	1/1	0.91	0.15	60,60,60,60	0
56	MG	2A	3590	1/1	0.91	0.17	67,67,67,67	0
56	MG	2A	3592	1/1	0.91	0.17	63,63,63,63	0
56	MG	1A	3749	1/1	0.91	0.08	20,20,20,20	0
56	MG	1A	4082	1/1	0.91	0.10	36,36,36,36	0
56	MG	1A	3750	1/1	0.91	0.13	44,44,44,44	0
56	MG	2a	1649	1/1	0.91	0.24	71,71,71,71	0
56	MG	2A	3298	1/1	0.91	0.16	58,58,58,58	0
56	MG	2a	1652	1/1	0.91	0.27	57,57,57,57	0
56	MG	1A	3752	1/1	0.91	0.10	22,22,22,22	0
56	MG	2A	3607	1/1	0.91	0.11	58,58,58,58	0
56	MG	1A	3601	1/1	0.91	0.14	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	2A	3307	1/1	0.91	0.23	70,70,70,70	0
56	MG	1A	3939	1/1	0.91	0.13	58,58,58,58	0
56	MG	2A	3621	1/1	0.91	0.14	38,38,38,38	0
56	MG	2a	1668	1/1	0.91	0.24	54,54,54,54	0
56	MG	2A	3629	1/1	0.91	0.11	50,50,50,50	0
56	MG	1A	3131	1/1	0.91	0.17	43,43,43,43	0
56	MG	1a	1666	1/1	0.91	0.18	64,64,64,64	0
56	MG	2a	1674	1/1	0.91	0.10	62,62,62,62	0
56	MG	1A	3327	1/1	0.91	0.19	62,62,62,62	0
56	MG	2A	3637	1/1	0.91	0.12	56,56,56,56	0
56	MG	1A	3945	1/1	0.91	0.10	41,41,41,41	0
56	MG	2a	1689	1/1	0.91	0.21	62,62,62,62	0
56	MG	1A	3142	1/1	0.91	0.11	50,50,50,50	0
56	MG	2A	3641	1/1	0.91	0.23	65,65,65,65	0
56	MG	2A	3642	1/1	0.91	0.14	67,67,67,67	0
56	MG	2A	3643	1/1	0.91	0.16	63,63,63,63	0
56	MG	1A	3630	1/1	0.91	0.09	48,48,48,48	0
56	MG	2a	1697	1/1	0.91	0.34	67,67,67,67	0
56	MG	2a	1699	1/1	0.91	0.08	70,70,70,70	0
56	MG	1A	3953	1/1	0.91	0.06	44,44,44,44	0
56	MG	1A	3332	1/1	0.91	0.15	52,52,52,52	0
56	MG	1a	1675	1/1	0.91	0.19	59,59,59,59	0
56	MG	2A	3061	1/1	0.91	0.17	61,61,61,61	0
56	MG	2A	3660	1/1	0.91	0.17	68,68,68,68	0
56	MG	2A	3063	1/1	0.91	0.23	66,66,66,66	0
56	MG	2A	3067	1/1	0.91	0.13	60,60,60,60	0
56	MG	2A	3664	1/1	0.91	0.19	66,66,66,66	0
56	MG	1A	3632	1/1	0.91	0.10	22,22,22,22	0
56	MG	1A	3531	1/1	0.91	0.14	51,51,51,51	0
56	MG	2A	3074	1/1	0.91	0.11	61,61,61,61	0
56	MG	2A	3670	1/1	0.91	0.18	49,49,49,49	0
56	MG	1A	3960	1/1	0.91	0.13	66,66,66,66	0
56	MG	2A	3674	1/1	0.91	0.14	59,59,59,59	0
56	MG	1A	3962	1/1	0.91	0.10	73,73,73,73	0
56	MG	2a	1731	1/1	0.91	0.33	67,67,67,67	0
56	MG	2A	3337	1/1	0.91	0.22	61,61,61,61	0
56	MG	1A	3254	1/1	0.91	0.12	58,58,58,58	0
56	MG	2A	3339	1/1	0.91	0.20	71,71,71,71	0
56	MG	2a	1739	1/1	0.91	0.22	71,71,71,71	0
56	MG	1a	1690	1/1	0.91	0.25	46,46,46,46	0
56	MG	2a	1742	1/1	0.91	0.07	74,74,74,74	0
56	MG	1A	3641	1/1	0.91	0.09	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	1A	3968	1/1	0.91	0.12	71,71,71,71	0
56	MG	2A	3691	1/1	0.91	0.23	65,65,65,65	0
56	MG	1A	3340	1/1	0.91	0.26	62,62,62,62	0
56	MG	1A	3648	1/1	0.91	0.11	48,48,48,48	0
56	MG	1A	3537	1/1	0.91	0.23	60,60,60,60	0
56	MG	1a	1705	1/1	0.91	0.10	59,59,59,59	0
56	MG	1A	3981	1/1	0.91	0.10	54,54,54,54	0
56	MG	1a	1708	1/1	0.91	0.14	70,70,70,70	0
56	MG	2a	1767	1/1	0.91	0.12	59,59,59,59	0
56	MG	1A	3198	1/1	0.91	0.08	43,43,43,43	0
56	MG	2a	1773	1/1	0.91	0.14	59,59,59,59	0
56	MG	1A	3824	1/1	0.91	0.10	58,58,58,58	0
56	MG	1A	3658	1/1	0.91	0.09	25,25,25,25	0
56	MG	1F	313	1/1	0.91	0.15	35,35,35,35	0
56	MG	1A	3151	1/1	0.91	0.13	41,41,41,41	0
56	MG	2a	1779	1/1	0.91	0.11	82,82,82,82	0
56	MG	2A	3366	1/1	0.91	0.10	70,70,70,70	0
56	MG	2A	3367	1/1	0.91	0.12	56,56,56,56	0
56	MG	1a	1719	1/1	0.91	0.17	58,58,58,58	0
56	MG	2A	3369	1/1	0.91	0.13	69,69,69,69	0
56	MG	2A	3132	1/1	0.91	0.14	46,46,46,46	0
56	MG	1A	3993	1/1	0.91	0.10	54,54,54,54	0
56	MG	1a	1721	1/1	0.91	0.12	62,62,62,62	0
56	MG	2A	3740	1/1	0.91	0.10	58,58,58,58	0
56	MG	2A	3741	1/1	0.91	0.17	59,59,59,59	0
56	MG	1G	204	1/1	0.91	0.10	50,50,50,50	0
56	MG	2A	3376	1/1	0.91	0.13	60,60,60,60	0
56	MG	2A	3386	1/1	0.91	0.22	62,62,62,62	0
56	MG	1A	3264	1/1	0.91	0.11	48,48,48,48	0
56	MG	1A	3829	1/1	0.91	0.15	59,59,59,59	0
56	MG	1A	3443	1/1	0.91	0.11	50,50,50,50	0
56	MG	2a	1808	1/1	0.91	0.24	56,56,56,56	0
56	MG	2a	1810	1/1	0.91	0.12	64,64,64,64	0
56	MG	2A	3392	1/1	0.91	0.18	57,57,57,57	0
56	MG	1A	3270	1/1	0.91	0.10	44,44,44,44	0
56	MG	2A	3395	1/1	0.91	0.10	62,62,62,62	0
56	MG	2A	3396	1/1	0.91	0.18	74,74,74,74	0
56	MG	1A	3836	1/1	0.91	0.11	64,64,64,64	0
56	MG	2A	3774	1/1	0.91	0.09	62,62,62,62	0
56	MG	2A	3398	1/1	0.91	0.12	61,61,61,61	0
56	MG	1Q	205	1/1	0.91	0.12	51,51,51,51	0
56	MG	2A	3178	1/1	0.91	0.13	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	2A	3780	1/1	0.91	0.11	70,70,70,70	0
56	MG	1A	3450	1/1	0.91	0.14	53,53,53,53	0
56	MG	2A	3783	1/1	0.91	0.10	55,55,55,55	0
56	MG	1R	201	1/1	0.91	0.10	45,45,45,45	0
56	MG	2I	205	1/1	0.91	0.15	67,67,67,67	0
56	MG	2A	3408	1/1	0.91	0.27	47,47,47,47	0
56	MG	2A	3409	1/1	0.91	0.24	47,47,47,47	0
56	MG	1a	1752	1/1	0.91	0.11	56,56,56,56	0
56	MG	2A	3794	1/1	0.91	0.20	60,60,60,60	0
56	MG	1A	3839	1/1	0.91	0.15	58,58,58,58	0
56	MG	2A	3412	1/1	0.91	0.25	45,45,45,45	0
56	MG	1A	4012	1/1	0.91	0.12	55,55,55,55	0
56	MG	1A	3288	1/1	0.91	0.17	48,48,48,48	0
56	MG	1T	201	1/1	0.91	0.10	73,73,73,73	0
56	MG	1V	201	1/1	0.91	0.17	37,37,37,37	0
56	MG	1V	206	1/1	0.91	0.09	56,56,56,56	0
56	MG	1A	3580	1/1	0.91	0.09	37,37,37,37	0
56	MG	2A	3432	1/1	0.91	0.28	62,62,62,62	0
56	MG	1A	3855	1/1	0.91	0.15	68,68,68,68	0
56	MG	1A	4024	1/1	0.91	0.08	31,31,31,31	0
56	MG	2y	104	1/1	0.91	0.13	81,81,81,81	0
56	MG	1a	1778	1/1	0.91	0.11	46,46,46,46	0
56	MG	1a	1779	1/1	0.91	0.09	54,54,54,54	0
56	MG	1A	4030	1/1	0.91	0.14	34,34,34,34	0
56	MG	1A	3456	1/1	0.91	0.14	61,61,61,61	0
56	MG	2A	3497	1/1	0.92	0.11	41,41,41,41	0
56	MG	1A	3432	1/1	0.92	0.17	51,51,51,51	0
56	MG	2D	308	1/1	0.92	0.09	60,60,60,60	0
56	MG	1x	112	1/1	0.92	0.20	59,59,59,59	0
56	MG	2A	3265	1/1	0.92	0.25	59,59,59,59	0
56	MG	1A	4011	1/1	0.92	0.17	61,61,61,61	0
56	MG	2E	308	1/1	0.92	0.11	42,42,42,42	0
56	MG	1E	306	1/1	0.92	0.11	55,55,55,55	0
56	MG	1A	3741	1/1	0.92	0.10	59,59,59,59	0
56	MG	2F	303	1/1	0.92	0.17	74,74,74,74	0
56	MG	1A	3880	1/1	0.92	0.11	22,22,22,22	0
56	MG	1F	303	1/1	0.92	0.15	55,55,55,55	0
56	MG	1F	304	1/1	0.92	0.29	71,71,71,71	0
56	MG	2Q	201	1/1	0.92	0.11	57,57,57,57	0
56	MG	1A	4016	1/1	0.92	0.11	45,45,45,45	0
56	MG	1A	4019	1/1	0.92	0.14	54,54,54,54	0
56	MG	2R	202	1/1	0.92	0.19	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	1680	1/1	0.92	0.18	67,67,67,67	0
56	MG	1F	314	1/1	0.92	0.10	65,65,65,65	0
56	MG	2W	201	1/1	0.92	0.18	60,60,60,60	0
56	MG	2A	3014	1/1	0.92	0.20	66,66,66,66	0
56	MG	1a	1682	1/1	0.92	0.19	63,63,63,63	0
56	MG	1A	3335	1/1	0.92	0.15	55,55,55,55	0
56	MG	1A	3368	1/1	0.92	0.14	47,47,47,47	0
56	MG	2I	101	1/1	0.92	0.17	55,55,55,55	0
56	MG	1A	3107	1/1	0.92	0.25	50,50,50,50	0
56	MG	1A	4026	1/1	0.92	0.08	55,55,55,55	0
56	MG	2A	3558	1/1	0.92	0.15	62,62,62,62	0
56	MG	25	106	1/1	0.92	0.27	69,69,69,69	0
56	MG	1A	3890	1/1	0.92	0.09	48,48,48,48	0
56	MG	1A	3372	1/1	0.92	0.10	46,46,46,46	0
56	MG	1a	1694	1/1	0.92	0.27	53,53,53,53	0
56	MG	2A	3578	1/1	0.92	0.11	75,75,75,75	0
56	MG	2A	3579	1/1	0.92	0.18	61,61,61,61	0
56	MG	1a	1695	1/1	0.92	0.26	54,54,54,54	0
56	MG	2A	3301	1/1	0.92	0.12	48,48,48,48	0
56	MG	1N	206	1/1	0.92	0.07	53,53,53,53	0
56	MG	2A	3046	1/1	0.92	0.10	43,43,43,43	0
56	MG	1A	3757	1/1	0.92	0.11	24,24,24,24	0
56	MG	2A	3591	1/1	0.92	0.21	61,61,61,61	0
56	MG	1A	3028	1/1	0.92	0.12	63,63,63,63	0
56	MG	1a	1702	1/1	0.92	0.21	51,51,51,51	0
56	MG	2A	3598	1/1	0.92	0.14	63,63,63,63	0
56	MG	1a	1703	1/1	0.92	0.06	43,43,43,43	0
56	MG	1P	205	1/1	0.92	0.16	42,42,42,42	0
56	MG	2A	3064	1/1	0.92	0.11	51,51,51,51	0
56	MG	2A	3065	1/1	0.92	0.17	67,67,67,67	0
56	MG	2a	1626	1/1	0.92	0.09	68,68,68,68	0
56	MG	2A	3317	1/1	0.92	0.11	52,52,52,52	0
56	MG	1A	3376	1/1	0.92	0.24	39,39,39,39	0
56	MG	1A	3766	1/1	0.92	0.11	68,68,68,68	0
56	MG	1A	3640	1/1	0.92	0.06	25,25,25,25	0
56	MG	1A	3453	1/1	0.92	0.13	51,51,51,51	0
56	MG	2A	3627	1/1	0.92	0.15	60,60,60,60	0
56	MG	2A	3628	1/1	0.92	0.10	38,38,38,38	0
56	MG	1A	3543	1/1	0.92	0.07	63,63,63,63	0
56	MG	2a	1637	1/1	0.92	0.22	55,55,55,55	0
56	MG	1a	1713	1/1	0.92	0.24	49,49,49,49	0
56	MG	1A	3290	1/1	0.92	0.18	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	1A	3791	1/1	0.92	0.09	56,56,56,56	0
56	MG	1a	1718	1/1	0.92	0.11	58,58,58,58	0
56	MG	2a	1645	1/1	0.92	0.24	62,62,62,62	0
56	MG	1A	3793	1/1	0.92	0.14	47,47,47,47	0
56	MG	1A	3297	1/1	0.92	0.10	43,43,43,43	0
56	MG	1A	3655	1/1	0.92	0.09	56,56,56,56	0
56	MG	1A	3395	1/1	0.92	0.32	40,40,40,40	0
56	MG	1a	1727	1/1	0.92	0.19	58,58,58,58	0
56	MG	1A	3944	1/1	0.92	0.13	69,69,69,69	0
56	MG	2A	3107	1/1	0.92	0.19	70,70,70,70	0
56	MG	1a	1731	1/1	0.92	0.12	59,59,59,59	0
56	MG	1A	3558	1/1	0.92	0.11	49,49,49,49	0
56	MG	2A	3654	1/1	0.92	0.10	59,59,59,59	0
56	MG	1A	3946	1/1	0.92	0.11	45,45,45,45	0
56	MG	2a	1660	1/1	0.92	0.07	59,59,59,59	0
56	MG	2A	3346	1/1	0.92	0.13	54,54,54,54	0
56	MG	2A	3350	1/1	0.92	0.15	63,63,63,63	0
56	MG	1A	3947	1/1	0.92	0.08	48,48,48,48	0
56	MG	2A	3118	1/1	0.92	0.13	45,45,45,45	0
56	MG	1A	3662	1/1	0.92	0.08	39,39,39,39	0
56	MG	1A	3816	1/1	0.92	0.11	32,32,32,32	0
56	MG	2A	3123	1/1	0.92	0.26	57,57,57,57	0
56	MG	2a	1679	1/1	0.92	0.11	64,64,64,64	0
56	MG	2A	3360	1/1	0.92	0.10	57,57,57,57	0
56	MG	2A	3671	1/1	0.92	0.17	50,50,50,50	0
56	MG	10	103	1/1	0.92	0.11	40,40,40,40	0
56	MG	2A	3125	1/1	0.92	0.36	67,67,67,67	0
56	MG	2A	3675	1/1	0.92	0.13	50,50,50,50	0
56	MG	2A	3130	1/1	0.92	0.11	45,45,45,45	0
56	MG	2A	3131	1/1	0.92	0.27	82,82,82,82	0
56	MG	1a	1748	1/1	0.92	0.10	51,51,51,51	0
56	MG	2A	3683	1/1	0.92	0.10	56,56,56,56	0
56	MG	2a	1698	1/1	0.92	0.16	60,60,60,60	0
56	MG	10	104	1/1	0.92	0.16	58,58,58,58	0
56	MG	10	106	1/1	0.92	0.11	50,50,50,50	0
56	MG	2A	3145	1/1	0.92	0.17	54,54,54,54	0
56	MG	2A	3146	1/1	0.92	0.19	61,61,61,61	0
56	MG	1A	3461	1/1	0.92	0.16	50,50,50,50	0
56	MG	1A	3399	1/1	0.92	0.14	43,43,43,43	0
56	MG	2A	3155	1/1	0.92	0.10	61,61,61,61	0
56	MG	2A	3156	1/1	0.92	0.21	59,59,59,59	0
56	MG	2A	3379	1/1	0.92	0.15	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	2A	3384	1/1	0.92	0.18	66,66,66,66	0
56	MG	2A	3161	1/1	0.92	0.19	57,57,57,57	0
56	MG	2A	3706	1/1	0.92	0.11	58,58,58,58	0
56	MG	1A	3821	1/1	0.92	0.25	60,60,60,60	0
56	MG	2a	1722	1/1	0.92	0.21	55,55,55,55	0
56	MG	1a	1762	1/1	0.92	0.12	60,60,60,60	0
56	MG	1A	4077	1/1	0.92	0.07	53,53,53,53	0
56	MG	2a	1728	1/1	0.92	0.29	50,50,50,50	0
56	MG	1a	1766	1/1	0.92	0.14	58,58,58,58	0
56	MG	2A	3175	1/1	0.92	0.12	48,48,48,48	0
56	MG	2a	1732	1/1	0.92	0.18	62,62,62,62	0
56	MG	1A	3406	1/1	0.92	0.23	65,65,65,65	0
56	MG	2A	3177	1/1	0.92	0.40	56,56,56,56	0
56	MG	1a	1769	1/1	0.92	0.10	68,68,68,68	0
56	MG	16	101	1/1	0.92	0.11	51,51,51,51	0
56	MG	1A	3472	1/1	0.92	0.12	50,50,50,50	0
56	MG	2A	3733	1/1	0.92	0.10	53,53,53,53	0
56	MG	1A	3348	1/1	0.92	0.14	41,41,41,41	0
56	MG	2A	3185	1/1	0.92	0.23	62,62,62,62	0
56	MG	2A	3405	1/1	0.92	0.24	63,63,63,63	0
56	MG	2a	1750	1/1	0.92	0.13	58,58,58,58	0
56	MG	1a	1773	1/1	0.92	0.12	58,58,58,58	0
56	MG	2A	3743	1/1	0.92	0.16	43,43,43,43	0
56	MG	2a	1758	1/1	0.92	0.18	69,69,69,69	0
56	MG	1A	3684	1/1	0.92	0.09	26,26,26,26	0
56	MG	2A	3190	1/1	0.92	0.14	65,65,65,65	0
56	MG	2A	3747	1/1	0.92	0.08	71,71,71,71	0
56	MG	1a	1776	1/1	0.92	0.17	57,57,57,57	0
56	MG	1A	4086	1/1	0.92	0.08	44,44,44,44	0
56	MG	1A	3485	1/1	0.92	0.09	49,49,49,49	0
56	MG	2a	1771	1/1	0.92	0.19	69,69,69,69	0
56	MG	2a	1772	1/1	0.92	0.11	68,68,68,68	0
56	MG	2A	3413	1/1	0.92	0.17	36,36,36,36	0
56	MG	2A	3763	1/1	0.92	0.16	64,64,64,64	0
56	MG	2A	3205	1/1	0.92	0.25	67,67,67,67	0
56	MG	1A	4088	1/1	0.92	0.15	59,59,59,59	0
56	MG	2A	3419	1/1	0.92	0.25	62,62,62,62	0
56	MG	1a	1610	1/1	0.92	0.19	65,65,65,65	0
56	MG	2A	3423	1/1	0.92	0.28	63,63,63,63	0
56	MG	2A	3772	1/1	0.92	0.10	52,52,52,52	0
56	MG	2A	3773	1/1	0.92	0.08	55,55,55,55	0
56	MG	1A	4089	1/1	0.92	0.13	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	1614	1/1	0.92	0.09	68,68,68,68	0
56	MG	2A	3427	1/1	0.92	0.29	60,60,60,60	0
56	MG	2A	3429	1/1	0.92	0.21	59,59,59,59	0
56	MG	1A	3412	1/1	0.92	0.17	69,69,69,69	0
56	MG	2A	3431	1/1	0.92	0.18	63,63,63,63	0
56	MG	2A	3782	1/1	0.92	0.16	65,65,65,65	0
56	MG	2a	1797	1/1	0.92	0.25	58,58,58,58	0
56	MG	1A	3349	1/1	0.92	0.15	46,46,46,46	0
56	MG	2a	1799	1/1	0.92	0.16	73,73,73,73	0
56	MG	1A	3972	1/1	0.92	0.15	54,54,54,54	0
56	MG	1a	1629	1/1	0.92	0.27	63,63,63,63	0
56	MG	2a	1803	1/1	0.92	0.12	61,61,61,61	0
56	MG	1A	3252	1/1	0.92	0.17	57,57,57,57	0
56	MG	2a	1806	1/1	0.92	0.18	80,80,80,80	0
56	MG	1A	3328	1/1	0.92	0.16	49,49,49,49	0
56	MG	1a	1802	1/1	0.92	0.07	60,60,60,60	0
56	MG	2A	3443	1/1	0.92	0.30	54,54,54,54	0
56	MG	1a	1636	1/1	0.92	0.11	51,51,51,51	0
56	MG	1B	210	1/1	0.92	0.17	41,41,41,41	0
56	MG	1e	202	1/1	0.92	0.09	64,64,64,64	0
56	MG	1A	3501	1/1	0.92	0.12	51,51,51,51	0
56	MG	1A	3426	1/1	0.92	0.11	44,44,44,44	0
56	MG	2A	3456	1/1	0.92	0.27	67,67,67,67	0
56	MG	2A	3229	1/1	0.92	0.30	55,55,55,55	0
56	MG	1A	3844	1/1	0.92	0.08	53,53,53,53	0
56	MG	2A	3461	1/1	0.92	0.20	72,72,72,72	0
56	MG	2A	3463	1/1	0.92	0.14	54,54,54,54	0
56	MG	2A	3823	1/1	0.92	0.07	47,47,47,47	0
56	MG	2A	3466	1/1	0.92	0.13	62,62,62,62	0
56	MG	1A	3205	1/1	0.92	0.12	55,55,55,55	0
56	MG	1A	3309	1/1	0.92	0.32	57,57,57,57	0
56	MG	2q	201	1/1	0.92	0.27	69,69,69,69	0
56	MG	1A	3598	1/1	0.92	0.10	30,30,30,30	0
56	MG	2t	201	1/1	0.92	0.21	60,60,60,60	0
56	MG	1A	3997	1/1	0.92	0.10	36,36,36,36	0
56	MG	1A	3517	1/1	0.92	0.10	67,67,67,67	0
56	MG	2A	3840	1/1	0.92	0.12	70,70,70,70	0
56	MG	2A	3241	1/1	0.92	0.17	62,62,62,62	0
56	MG	1A	3363	1/1	0.92	0.14	51,51,51,51	0
56	MG	2A	3845	1/1	0.92	0.12	66,66,66,66	0
56	MG	1A	3867	1/1	0.92	0.16	36,36,36,36	0
56	MG	1A	3869	1/1	0.92	0.15	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	2x	101	1/1	0.92	0.18	60,60,60,60	0
56	MG	2B	203	1/1	0.92	0.25	63,63,63,63	0
56	MG	1A	3520	1/1	0.92	0.10	53,53,53,53	0
56	MG	1B	234	1/1	0.92	0.09	70,70,70,70	0
56	MG	2B	208	1/1	0.92	0.20	56,56,56,56	0
56	MG	2A	3487	1/1	0.92	0.13	61,61,61,61	0
56	MG	1D	310	1/1	0.92	0.18	47,47,47,47	0
56	MG	2B	212	1/1	0.92	0.18	76,76,76,76	0
56	MG	1A	3734	1/1	0.92	0.06	41,41,41,41	0
56	MG	2A	3492	1/1	0.92	0.13	56,56,56,56	0
56	MG	1x	109	1/1	0.92	0.20	65,65,65,65	0
58	WC9	1A	4098	34/34	0.92	0.12	27,38,47,50	0
56	MG	2A	3496	1/1	0.92	0.08	52,52,52,52	0
59	ZN	24	501	1/1	0.92	0.19	142,142,142,142	0
56	MG	2A	3500	1/1	0.93	0.11	35,35,35,35	0
56	MG	1A	3926	1/1	0.93	0.13	63,63,63,63	0
56	MG	1A	3036	1/1	0.93	0.06	49,49,49,49	0
56	MG	1A	3387	1/1	0.93	0.16	26,26,26,26	0
56	MG	1a	1647	1/1	0.93	0.12	52,52,52,52	0
56	MG	2A	3259	1/1	0.93	0.15	55,55,55,55	0
56	MG	2F	305	1/1	0.93	0.08	42,42,42,42	0
56	MG	2G	201	1/1	0.93	0.17	67,67,67,67	0
56	MG	1x	103	1/1	0.93	0.22	63,63,63,63	0
56	MG	2A	3262	1/1	0.93	0.14	56,56,56,56	0
56	MG	2P	202	1/1	0.93	0.09	61,61,61,61	0
56	MG	1A	3934	1/1	0.93	0.08	65,65,65,65	0
56	MG	2Q	202	1/1	0.93	0.15	50,50,50,50	0
56	MG	1A	3747	1/1	0.93	0.17	49,49,49,49	0
56	MG	1a	1651	1/1	0.93	0.10	50,50,50,50	0
56	MG	1A	3112	1/1	0.93	0.14	35,35,35,35	0
56	MG	2T	202	1/1	0.93	0.12	64,64,64,64	0
56	MG	1A	3481	1/1	0.93	0.14	57,57,57,57	0
56	MG	2A	3270	1/1	0.93	0.15	59,59,59,59	0
56	MG	1a	1659	1/1	0.93	0.08	54,54,54,54	0
56	MG	1A	3016	1/1	0.93	0.30	57,57,57,57	0
56	MG	1B	214	1/1	0.93	0.23	56,56,56,56	0
56	MG	1A	3597	1/1	0.93	0.08	50,50,50,50	0
56	MG	1A	3488	1/1	0.93	0.08	62,62,62,62	0
56	MG	1A	3400	1/1	0.93	0.13	55,55,55,55	0
56	MG	23	102	1/1	0.93	0.15	54,54,54,54	0
56	MG	1A	3763	1/1	0.93	0.08	22,22,22,22	0
56	MG	1A	3402	1/1	0.93	0.13	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	2A	3562	1/1	0.93	0.11	49,49,49,49	0
56	MG	2A	3284	1/1	0.93	0.10	52,52,52,52	0
56	MG	2A	3285	1/1	0.93	0.22	64,64,64,64	0
56	MG	28	101	1/1	0.93	0.25	58,58,58,58	0
56	MG	2A	3573	1/1	0.93	0.12	61,61,61,61	0
56	MG	1a	1669	1/1	0.93	0.15	65,65,65,65	0
56	MG	2A	3287	1/1	0.93	0.08	69,69,69,69	0
56	MG	2A	3288	1/1	0.93	0.11	66,66,66,66	0
56	MG	1A	3949	1/1	0.93	0.13	46,46,46,46	0
56	MG	1A	3607	1/1	0.93	0.07	24,24,24,24	0
56	MG	1A	3776	1/1	0.93	0.06	30,30,30,30	0
56	MG	2A	3589	1/1	0.93	0.13	54,54,54,54	0
56	MG	2A	3293	1/1	0.93	0.24	55,55,55,55	0
56	MG	1B	227	1/1	0.93	0.09	41,41,41,41	0
56	MG	2a	1612	1/1	0.93	0.34	69,69,69,69	0
56	MG	1a	1674	1/1	0.93	0.21	62,62,62,62	0
56	MG	1A	3955	1/1	0.93	0.12	43,43,43,43	0
56	MG	2a	1616	1/1	0.93	0.14	67,67,67,67	0
56	MG	1A	3088	1/1	0.93	0.17	50,50,50,50	0
56	MG	2A	3599	1/1	0.93	0.07	35,35,35,35	0
56	MG	1A	3408	1/1	0.93	0.13	54,54,54,54	0
56	MG	2A	3034	1/1	0.93	0.14	60,60,60,60	0
56	MG	2a	1623	1/1	0.93	0.18	64,64,64,64	0
56	MG	2A	3603	1/1	0.93	0.16	46,46,46,46	0
56	MG	2a	1625	1/1	0.93	0.19	58,58,58,58	0
56	MG	1A	3783	1/1	0.93	0.12	60,60,60,60	0
56	MG	2A	3306	1/1	0.93	0.12	50,50,50,50	0
56	MG	1A	3409	1/1	0.93	0.11	40,40,40,40	0
56	MG	1A	3503	1/1	0.93	0.11	55,55,55,55	0
56	MG	2a	1631	1/1	0.93	0.27	54,54,54,54	0
56	MG	1A	3963	1/1	0.93	0.10	64,64,64,64	0
56	MG	2A	3614	1/1	0.93	0.11	49,49,49,49	0
56	MG	1a	1685	1/1	0.93	0.21	62,62,62,62	0
56	MG	1a	1686	1/1	0.93	0.29	66,66,66,66	0
56	MG	1A	3964	1/1	0.93	0.08	29,29,29,29	0
56	MG	1A	3505	1/1	0.93	0.11	63,63,63,63	0
56	MG	1E	302	1/1	0.93	0.17	50,50,50,50	0
56	MG	1A	3794	1/1	0.93	0.06	22,22,22,22	0
56	MG	1A	3141	1/1	0.93	0.09	43,43,43,43	0
56	MG	1A	3344	1/1	0.93	0.14	48,48,48,48	0
56	MG	2A	3066	1/1	0.93	0.09	49,49,49,49	0
56	MG	1E	314	1/1	0.93	0.09	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	1A	3804	1/1	0.93	0.17	57,57,57,57	0
56	MG	1a	1699	1/1	0.93	0.41	60,60,60,60	0
56	MG	2A	3072	1/1	0.93	0.18	49,49,49,49	0
56	MG	2A	3326	1/1	0.93	0.36	51,51,51,51	0
56	MG	2A	3644	1/1	0.93	0.12	59,59,59,59	0
56	MG	1A	3974	1/1	0.93	0.09	34,34,34,34	0
56	MG	1A	3805	1/1	0.93	0.17	60,60,60,60	0
56	MG	2A	3329	1/1	0.93	0.23	72,72,72,72	0
56	MG	1A	3511	1/1	0.93	0.37	46,46,46,46	0
56	MG	2A	3333	1/1	0.93	0.10	54,54,54,54	0
56	MG	2A	3079	1/1	0.93	0.07	41,41,41,41	0
56	MG	2A	3081	1/1	0.93	0.14	57,57,57,57	0
56	MG	1a	1704	1/1	0.93	0.10	59,59,59,59	0
56	MG	1A	3980	1/1	0.93	0.11	52,52,52,52	0
56	MG	1A	3809	1/1	0.93	0.08	54,54,54,54	0
56	MG	1A	3025	1/1	0.93	0.22	53,53,53,53	0
56	MG	1A	3415	1/1	0.93	0.25	56,56,56,56	0
56	MG	2a	1675	1/1	0.93	0.20	56,56,56,56	0
56	MG	1A	3814	1/1	0.93	0.07	38,38,38,38	0
56	MG	1A	3001	1/1	0.93	0.11	37,37,37,37	0
56	MG	2A	3345	1/1	0.93	0.13	60,60,60,60	0
56	MG	2a	1683	1/1	0.93	0.13	58,58,58,58	0
56	MG	2A	3099	1/1	0.93	0.15	57,57,57,57	0
56	MG	2a	1687	1/1	0.93	0.17	43,43,43,43	0
56	MG	1A	3647	1/1	0.93	0.10	51,51,51,51	0
56	MG	1A	3351	1/1	0.93	0.14	58,58,58,58	0
56	MG	2A	3106	1/1	0.93	0.19	68,68,68,68	0
56	MG	1A	3820	1/1	0.93	0.18	43,43,43,43	0
56	MG	1A	4003	1/1	0.93	0.13	46,46,46,46	0
56	MG	1A	3424	1/1	0.93	0.11	41,41,41,41	0
56	MG	1Q	203	1/1	0.93	0.09	55,55,55,55	0
56	MG	1A	3652	1/1	0.93	0.07	29,29,29,29	0
56	MG	2A	3687	1/1	0.93	0.17	53,53,53,53	0
56	MG	1A	3527	1/1	0.93	0.25	47,47,47,47	0
56	MG	2A	3119	1/1	0.93	0.24	62,62,62,62	0
56	MG	1a	1725	1/1	0.93	0.18	53,53,53,53	0
56	MG	2a	1704	1/1	0.93	0.09	59,59,59,59	0
56	MG	1a	1726	1/1	0.93	0.15	45,45,45,45	0
56	MG	1A	3217	1/1	0.93	0.13	53,53,53,53	0
56	MG	1A	3826	1/1	0.93	0.07	39,39,39,39	0
56	MG	1A	3157	1/1	0.93	0.19	58,58,58,58	0
56	MG	2a	1711	1/1	0.93	0.31	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	3101	1/1	0.93	0.14	68,68,68,68	0
56	MG	2a	1714	1/1	0.93	0.10	54,54,54,54	0
56	MG	1A	3243	1/1	0.93	0.07	47,47,47,47	0
56	MG	1A	3055	1/1	0.93	0.10	54,54,54,54	0
56	MG	2A	3135	1/1	0.93	0.07	45,45,45,45	0
56	MG	1A	3035	1/1	0.93	0.35	31,31,31,31	0
56	MG	1A	3541	1/1	0.93	0.09	45,45,45,45	0
56	MG	2A	3380	1/1	0.93	0.10	56,56,56,56	0
56	MG	2A	3715	1/1	0.93	0.25	52,52,52,52	0
56	MG	2A	3144	1/1	0.93	0.28	49,49,49,49	0
56	MG	1A	3365	1/1	0.93	0.16	46,46,46,46	0
56	MG	1A	3249	1/1	0.93	0.13	43,43,43,43	0
56	MG	1A	3843	1/1	0.93	0.14	62,62,62,62	0
56	MG	2A	3390	1/1	0.93	0.11	69,69,69,69	0
56	MG	1a	1750	1/1	0.93	0.22	51,51,51,51	0
56	MG	2a	1735	1/1	0.93	0.27	59,59,59,59	0
56	MG	2A	3731	1/1	0.93	0.13	50,50,50,50	0
56	MG	2A	3151	1/1	0.93	0.22	58,58,58,58	0
56	MG	1A	3180	1/1	0.93	0.19	50,50,50,50	0
56	MG	2A	3394	1/1	0.93	0.06	62,62,62,62	0
56	MG	1a	1753	1/1	0.93	0.08	73,73,73,73	0
56	MG	2a	1745	1/1	0.93	0.12	64,64,64,64	0
56	MG	2a	1747	1/1	0.93	0.13	70,70,70,70	0
56	MG	1A	3691	1/1	0.93	0.06	50,50,50,50	0
56	MG	2A	3162	1/1	0.93	0.24	55,55,55,55	0
56	MG	1A	3693	1/1	0.93	0.06	26,26,26,26	0
56	MG	2A	3399	1/1	0.93	0.08	65,65,65,65	0
56	MG	2a	1753	1/1	0.93	0.10	65,65,65,65	0
56	MG	1A	3853	1/1	0.93	0.12	45,45,45,45	0
56	MG	2a	1757	1/1	0.93	0.19	68,68,68,68	0
56	MG	2A	3166	1/1	0.93	0.13	44,44,44,44	0
56	MG	2A	3751	1/1	0.93	0.13	57,57,57,57	0
56	MG	2A	3168	1/1	0.93	0.11	54,54,54,54	0
56	MG	1A	3854	1/1	0.93	0.17	56,56,56,56	0
56	MG	1A	3697	1/1	0.93	0.10	28,28,28,28	0
56	MG	1A	3444	1/1	0.93	0.11	50,50,50,50	0
56	MG	1A	3860	1/1	0.93	0.15	33,33,33,33	0
56	MG	2a	1770	1/1	0.93	0.24	63,63,63,63	0
56	MG	2A	3766	1/1	0.93	0.08	51,51,51,51	0
56	MG	1A	3552	1/1	0.93	0.33	42,42,42,42	0
56	MG	1A	3251	1/1	0.93	0.16	47,47,47,47	0
56	MG	1A	3703	1/1	0.93	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	1A	4052	1/1	0.93	0.08	23,23,23,23	0
56	MG	2A	3183	1/1	0.93	0.17	65,65,65,65	0
56	MG	1A	3448	1/1	0.93	0.09	47,47,47,47	0
56	MG	2A	3418	1/1	0.93	0.17	39,39,39,39	0
56	MG	17	106	1/1	0.93	0.08	49,49,49,49	0
56	MG	2A	3421	1/1	0.93	0.14	47,47,47,47	0
56	MG	2A	3186	1/1	0.93	0.10	52,52,52,52	0
56	MG	1A	3571	1/1	0.93	0.19	31,31,31,31	0
56	MG	1a	1777	1/1	0.93	0.09	68,68,68,68	0
56	MG	1A	3105	1/1	0.93	0.10	32,32,32,32	0
56	MG	2A	3193	1/1	0.93	0.29	65,65,65,65	0
56	MG	2A	3196	1/1	0.93	0.20	54,54,54,54	0
56	MG	2A	3786	1/1	0.93	0.12	66,66,66,66	0
56	MG	2A	3198	1/1	0.93	0.17	54,54,54,54	0
56	MG	1A	3709	1/1	0.93	0.11	55,55,55,55	0
56	MG	1A	3183	1/1	0.93	0.19	72,72,72,72	0
56	MG	1A	3881	1/1	0.93	0.09	30,30,30,30	0
56	MG	2A	3434	1/1	0.93	0.23	53,53,53,53	0
56	MG	1A	3377	1/1	0.93	0.08	44,44,44,44	0
56	MG	1a	1607	1/1	0.93	0.17	60,60,60,60	0
56	MG	2A	3438	1/1	0.93	0.22	56,56,56,56	0
56	MG	2a	1805	1/1	0.93	0.12	68,68,68,68	0
56	MG	2A	3439	1/1	0.93	0.19	40,40,40,40	0
56	MG	1A	3884	1/1	0.93	0.08	23,23,23,23	0
56	MG	1A	3717	1/1	0.93	0.11	49,49,49,49	0
56	MG	2a	1809	1/1	0.93	0.14	64,64,64,64	0
56	MG	2A	3814	1/1	0.93	0.14	58,58,58,58	0
56	MG	2a	1812	1/1	0.93	0.12	60,60,60,60	0
56	MG	1a	1795	1/1	0.93	0.17	54,54,54,54	0
56	MG	1a	1613	1/1	0.93	0.18	58,58,58,58	0
56	MG	1A	3720	1/1	0.93	0.07	37,37,37,37	0
56	MG	1a	1616	1/1	0.93	0.14	50,50,50,50	0
56	MG	1A	3257	1/1	0.93	0.10	44,44,44,44	0
56	MG	2a	1820	1/1	0.93	0.08	66,66,66,66	0
56	MG	1A	3457	1/1	0.93	0.17	65,65,65,65	0
56	MG	2A	3829	1/1	0.93	0.15	63,63,63,63	0
56	MG	1a	1804	1/1	0.93	0.16	59,59,59,59	0
56	MG	1a	1805	1/1	0.93	0.20	51,51,51,51	0
56	MG	2e	201	1/1	0.93	0.07	70,70,70,70	0
56	MG	1a	1806	1/1	0.93	0.19	65,65,65,65	0
56	MG	1a	1624	1/1	0.93	0.22	49,49,49,49	0
56	MG	2A	3837	1/1	0.93	0.14	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	2l	201	1/1	0.93	0.14	62,62,62,62	0
56	MG	2A	3224	1/1	0.93	0.15	55,55,55,55	0
56	MG	2l	203	1/1	0.93	0.11	64,64,64,64	0
56	MG	1a	1626	1/1	0.93	0.16	52,52,52,52	0
56	MG	2m	201	1/1	0.93	0.24	68,68,68,68	0
56	MG	2A	3226	1/1	0.93	0.10	65,65,65,65	0
56	MG	1b	301	1/1	0.93	0.14	66,66,66,66	0
56	MG	2A	3843	1/1	0.93	0.07	62,62,62,62	0
56	MG	1d	301	1/1	0.93	0.43	68,68,68,68	0
56	MG	2A	3471	1/1	0.93	0.14	62,62,62,62	0
56	MG	1A	3728	1/1	0.93	0.08	60,60,60,60	0
56	MG	1A	3729	1/1	0.93	0.09	43,43,43,43	0
56	MG	1A	3382	1/1	0.93	0.11	43,43,43,43	0
56	MG	2B	205	1/1	0.93	0.20	59,59,59,59	0
56	MG	2A	3475	1/1	0.93	0.08	51,51,51,51	0
56	MG	1A	3908	1/1	0.93	0.21	61,61,61,61	0
56	MG	1A	3383	1/1	0.93	0.10	50,50,50,50	0
56	MG	2A	3236	1/1	0.93	0.08	46,46,46,46	0
56	MG	2x	103	1/1	0.93	0.08	69,69,69,69	0
56	MG	2A	3482	1/1	0.93	0.25	50,50,50,50	0
56	MG	1p	101	1/1	0.93	0.23	49,49,49,49	0
56	MG	1A	3384	1/1	0.93	0.12	53,53,53,53	0
56	MG	2A	3240	1/1	0.93	0.16	56,56,56,56	0
56	MG	2B	216	1/1	0.93	0.20	61,61,61,61	0
56	MG	1A	3916	1/1	0.93	0.08	45,45,45,45	0
56	MG	1A	4085	1/1	0.93	0.13	42,42,42,42	0
56	MG	2D	301	1/1	0.93	0.14	49,49,49,49	0
56	MG	1w	103	1/1	0.93	0.11	64,64,64,64	0
56	MG	2A	3247	1/1	0.93	0.09	62,62,62,62	0
58	WC9	2A	3846	34/34	0.93	0.12	43,52,58,60	0
56	MG	1A	3736	1/1	0.93	0.20	52,52,52,52	0
56	MG	1A	3463	1/1	0.93	0.23	57,57,57,57	0
56	MG	1A	3565	1/1	0.94	0.21	50,50,50,50	0
56	MG	1x	102	1/1	0.94	0.16	60,60,60,60	0
56	MG	2A	3488	1/1	0.94	0.10	53,53,53,53	0
56	MG	1A	3361	1/1	0.94	0.18	55,55,55,55	0
56	MG	1A	3902	1/1	0.94	0.14	34,34,34,34	0
56	MG	1x	105	1/1	0.94	0.20	66,66,66,66	0
56	MG	2D	306	1/1	0.94	0.22	42,42,42,42	0
56	MG	1A	3084	1/1	0.94	0.19	39,39,39,39	0
56	MG	1A	3577	1/1	0.94	0.13	42,42,42,42	0
56	MG	1A	3446	1/1	0.94	0.28	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3498	1/1	0.94	0.19	48,48,48,48	0
56	MG	1A	3909	1/1	0.94	0.06	34,34,34,34	0
56	MG	1A	3735	1/1	0.94	0.05	16,16,16,16	0
56	MG	1A	3293	1/1	0.94	0.08	38,38,38,38	0
56	MG	2A	3504	1/1	0.94	0.24	46,46,46,46	0
56	MG	2F	302	1/1	0.94	0.15	43,43,43,43	0
56	MG	1A	3581	1/1	0.94	0.09	45,45,45,45	0
56	MG	1a	1655	1/1	0.94	0.18	52,52,52,52	0
56	MG	1A	3740	1/1	0.94	0.06	32,32,32,32	0
56	MG	2A	3516	1/1	0.94	0.07	37,37,37,37	0
56	MG	1a	1657	1/1	0.94	0.13	64,64,64,64	0
56	MG	2A	3274	1/1	0.94	0.12	62,62,62,62	0
56	MG	1A	3919	1/1	0.94	0.08	46,46,46,46	0
56	MG	1B	201	1/1	0.94	0.15	54,54,54,54	0
56	MG	2A	3525	1/1	0.94	0.19	53,53,53,53	0
56	MG	1A	3296	1/1	0.94	0.12	62,62,62,62	0
56	MG	1B	206	1/1	0.94	0.10	53,53,53,53	0
56	MG	2A	3281	1/1	0.94	0.26	67,67,67,67	0
56	MG	1A	3449	1/1	0.94	0.13	48,48,48,48	0
56	MG	1a	1664	1/1	0.94	0.12	60,60,60,60	0
56	MG	2U	202	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	3221	1/1	0.94	0.06	49,49,49,49	0
56	MG	1B	211	1/1	0.94	0.09	46,46,46,46	0
56	MG	2A	3546	1/1	0.94	0.10	40,40,40,40	0
56	MG	1A	3748	1/1	0.94	0.11	50,50,50,50	0
56	MG	2A	3027	1/1	0.94	0.09	51,51,51,51	0
56	MG	2A	3028	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3555	1/1	0.94	0.09	38,38,38,38	0
56	MG	1A	3366	1/1	0.94	0.12	63,63,63,63	0
56	MG	2A	3290	1/1	0.94	0.13	68,68,68,68	0
56	MG	1A	3367	1/1	0.94	0.14	45,45,45,45	0
56	MG	2A	3564	1/1	0.94	0.08	36,36,36,36	0
56	MG	25	105	1/1	0.94	0.15	52,52,52,52	0
56	MG	2A	3033	1/1	0.94	0.09	35,35,35,35	0
56	MG	1A	3060	1/1	0.94	0.18	57,57,57,57	0
56	MG	27	103	1/1	0.94	0.32	52,52,52,52	0
56	MG	2A	3570	1/1	0.94	0.18	51,51,51,51	0
56	MG	2A	3571	1/1	0.94	0.14	47,47,47,47	0
56	MG	1A	3941	1/1	0.94	0.09	56,56,56,56	0
56	MG	2A	3038	1/1	0.94	0.18	62,62,62,62	0
56	MG	1A	3753	1/1	0.94	0.12	36,36,36,36	0
56	MG	1A	3756	1/1	0.94	0.09	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3583	1/1	0.94	0.16	61,61,61,61	0
56	MG	1A	3589	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	3233	1/1	0.94	0.09	55,55,55,55	0
56	MG	2A	3303	1/1	0.94	0.08	48,48,48,48	0
56	MG	2a	1610	1/1	0.94	0.27	64,64,64,64	0
56	MG	2A	3587	1/1	0.94	0.10	37,37,37,37	0
56	MG	1A	3304	1/1	0.94	0.17	51,51,51,51	0
56	MG	2A	3305	1/1	0.94	0.13	58,58,58,58	0
56	MG	2a	1614	1/1	0.94	0.21	54,54,54,54	0
56	MG	1A	3305	1/1	0.94	0.32	60,60,60,60	0
56	MG	2A	3055	1/1	0.94	0.19	65,65,65,65	0
56	MG	1B	230	1/1	0.94	0.08	71,71,71,71	0
56	MG	1A	3764	1/1	0.94	0.12	26,26,26,26	0
56	MG	2A	3310	1/1	0.94	0.15	46,46,46,46	0
56	MG	2A	3311	1/1	0.94	0.13	54,54,54,54	0
56	MG	2A	3601	1/1	0.94	0.09	37,37,37,37	0
56	MG	1A	3375	1/1	0.94	0.13	51,51,51,51	0
56	MG	1A	3950	1/1	0.94	0.06	24,24,24,24	0
56	MG	2A	3604	1/1	0.94	0.16	40,40,40,40	0
56	MG	1A	3768	1/1	0.94	0.07	35,35,35,35	0
56	MG	1B	235	1/1	0.94	0.08	49,49,49,49	0
56	MG	1A	3952	1/1	0.94	0.07	49,49,49,49	0
56	MG	2A	3068	1/1	0.94	0.14	63,63,63,63	0
56	MG	2A	3609	1/1	0.94	0.09	43,43,43,43	0
56	MG	1A	3167	1/1	0.94	0.09	38,38,38,38	0
56	MG	2A	3612	1/1	0.94	0.11	50,50,50,50	0
56	MG	1A	3774	1/1	0.94	0.06	69,69,69,69	0
56	MG	1A	3775	1/1	0.94	0.09	39,39,39,39	0
56	MG	2A	3617	1/1	0.94	0.10	42,42,42,42	0
56	MG	2A	3619	1/1	0.94	0.10	61,61,61,61	0
56	MG	2a	1639	1/1	0.94	0.10	58,58,58,58	0
56	MG	2A	3073	1/1	0.94	0.08	55,55,55,55	0
56	MG	2A	3626	1/1	0.94	0.12	58,58,58,58	0
56	MG	2a	1642	1/1	0.94	0.20	54,54,54,54	0
56	MG	1A	3464	1/1	0.94	0.15	65,65,65,65	0
56	MG	1E	303	1/1	0.94	0.23	45,45,45,45	0
56	MG	1a	1696	1/1	0.94	0.13	49,49,49,49	0
56	MG	1A	3170	1/1	0.94	0.18	41,41,41,41	0
56	MG	2A	3631	1/1	0.94	0.12	37,37,37,37	0
56	MG	1A	3468	1/1	0.94	0.08	64,64,64,64	0
56	MG	2A	3634	1/1	0.94	0.09	51,51,51,51	0
56	MG	2a	1651	1/1	0.94	0.13	63,63,63,63	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	0.94	0.10	50,50,50,50	0
56	MG	1E	310	1/1	0.94	0.07	17,17,17,17	0
56	MG	1A	3961	1/1	0.94	0.09	60,60,60,60	0
56	MG	2a	1656	1/1	0.94	0.15	76,76,76,76	0
56	MG	2A	3639	1/1	0.94	0.18	49,49,49,49	0
56	MG	2A	3332	1/1	0.94	0.19	63,63,63,63	0
56	MG	1a	1701	1/1	0.94	0.22	61,61,61,61	0
56	MG	2A	3334	1/1	0.94	0.09	51,51,51,51	0
56	MG	2a	1662	1/1	0.94	0.14	56,56,56,56	0
56	MG	2A	3335	1/1	0.94	0.11	57,57,57,57	0
56	MG	1A	3314	1/1	0.94	0.11	46,46,46,46	0
56	MG	1A	3784	1/1	0.94	0.09	47,47,47,47	0
56	MG	1A	3315	1/1	0.94	0.13	52,52,52,52	0
56	MG	1A	3609	1/1	0.94	0.10	10,10,10,10	0
56	MG	1F	312	1/1	0.94	0.13	57,57,57,57	0
56	MG	1a	1707	1/1	0.94	0.18	60,60,60,60	0
56	MG	2A	3657	1/1	0.94	0.11	63,63,63,63	0
56	MG	2A	3658	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3479	1/1	0.94	0.18	45,45,45,45	0
56	MG	2A	3104	1/1	0.94	0.12	48,48,48,48	0
56	MG	2a	1685	1/1	0.94	0.30	54,54,54,54	0
56	MG	1A	3480	1/1	0.94	0.09	41,41,41,41	0
56	MG	1F	315	1/1	0.94	0.09	41,41,41,41	0
56	MG	2a	1688	1/1	0.94	0.11	53,53,53,53	0
56	MG	2A	3109	1/1	0.94	0.11	61,61,61,61	0
56	MG	2A	3348	1/1	0.94	0.09	60,60,60,60	0
56	MG	1A	3970	1/1	0.94	0.12	62,62,62,62	0
56	MG	1A	3622	1/1	0.94	0.07	35,35,35,35	0
56	MG	1A	3318	1/1	0.94	0.19	51,51,51,51	0
56	MG	2A	3353	1/1	0.94	0.22	56,56,56,56	0
56	MG	2a	1696	1/1	0.94	0.07	63,63,63,63	0
56	MG	2A	3672	1/1	0.94	0.14	53,53,53,53	0
56	MG	1A	3803	1/1	0.94	0.09	62,62,62,62	0
56	MG	1A	3628	1/1	0.94	0.08	23,23,23,23	0
56	MG	1A	3629	1/1	0.94	0.10	43,43,43,43	0
56	MG	2A	3676	1/1	0.94	0.08	74,74,74,74	0
56	MG	2A	3358	1/1	0.94	0.10	54,54,54,54	0
56	MG	2A	3359	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3806	1/1	0.94	0.10	30,30,30,30	0
56	MG	2a	1706	1/1	0.94	0.24	57,57,57,57	0
56	MG	1A	3482	1/1	0.94	0.11	56,56,56,56	0
56	MG	1O	202	1/1	0.94	0.10	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	1724	1/1	0.94	0.23	57,57,57,57	0
56	MG	1O	204	1/1	0.94	0.07	61,61,61,61	0
56	MG	1A	3244	1/1	0.94	0.19	48,48,48,48	0
56	MG	1A	3486	1/1	0.94	0.07	49,49,49,49	0
56	MG	1A	3017	1/1	0.94	0.13	54,54,54,54	0
56	MG	2A	3133	1/1	0.94	0.22	61,61,61,61	0
56	MG	2a	1719	1/1	0.94	0.19	48,48,48,48	0
56	MG	2A	3134	1/1	0.94	0.16	54,54,54,54	0
56	MG	1A	3490	1/1	0.94	0.13	33,33,33,33	0
56	MG	2A	3136	1/1	0.94	0.07	62,62,62,62	0
56	MG	2a	1724	1/1	0.94	0.23	53,53,53,53	0
56	MG	1a	1736	1/1	0.94	0.14	58,58,58,58	0
56	MG	2A	3375	1/1	0.94	0.18	52,52,52,52	0
56	MG	2A	3703	1/1	0.94	0.07	43,43,43,43	0
56	MG	2A	3704	1/1	0.94	0.07	63,63,63,63	0
56	MG	2A	3138	1/1	0.94	0.11	55,55,55,55	0
56	MG	2A	3378	1/1	0.94	0.29	55,55,55,55	0
56	MG	1A	3638	1/1	0.94	0.08	38,38,38,38	0
56	MG	1A	3068	1/1	0.94	0.06	33,33,33,33	0
56	MG	1A	3388	1/1	0.94	0.16	27,27,27,27	0
56	MG	2a	1737	1/1	0.94	0.22	59,59,59,59	0
56	MG	2A	3385	1/1	0.94	0.13	55,55,55,55	0
56	MG	1A	3389	1/1	0.94	0.12	45,45,45,45	0
56	MG	1A	3499	1/1	0.94	0.09	38,38,38,38	0
56	MG	1A	3393	1/1	0.94	0.29	61,61,61,61	0
56	MG	1U	209	1/1	0.94	0.14	54,54,54,54	0
56	MG	2a	1744	1/1	0.94	0.11	71,71,71,71	0
56	MG	2A	3725	1/1	0.94	0.16	59,59,59,59	0
56	MG	2A	3726	1/1	0.94	0.11	74,74,74,74	0
56	MG	2A	3152	1/1	0.94	0.09	44,44,44,44	0
56	MG	1A	3116	1/1	0.94	0.17	33,33,33,33	0
56	MG	1A	3122	1/1	0.94	0.07	42,42,42,42	0
56	MG	2A	3732	1/1	0.94	0.13	38,38,38,38	0
56	MG	2A	3158	1/1	0.94	0.20	39,39,39,39	0
56	MG	2A	3734	1/1	0.94	0.17	45,45,45,45	0
56	MG	2A	3736	1/1	0.94	0.15	53,53,53,53	0
56	MG	1a	1751	1/1	0.94	0.17	53,53,53,53	0
56	MG	2a	1760	1/1	0.94	0.24	59,59,59,59	0
56	MG	1A	3329	1/1	0.94	0.09	38,38,38,38	0
56	MG	1W	206	1/1	0.94	0.13	27,27,27,27	0
56	MG	1a	1754	1/1	0.94	0.13	59,59,59,59	0
56	MG	2A	3742	1/1	0.94	0.08	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	3129	1/1	0.94	0.10	66,66,66,66	0
56	MG	1a	1758	1/1	0.94	0.12	59,59,59,59	0
56	MG	2A	3401	1/1	0.94	0.06	59,59,59,59	0
56	MG	1X	104	1/1	0.94	0.25	43,43,43,43	0
56	MG	1a	1760	1/1	0.94	0.11	62,62,62,62	0
56	MG	1A	3405	1/1	0.94	0.08	51,51,51,51	0
56	MG	2A	3752	1/1	0.94	0.16	68,68,68,68	0
56	MG	1Y	202	1/1	0.94	0.10	53,53,53,53	0
56	MG	2A	3754	1/1	0.94	0.11	81,81,81,81	0
56	MG	2A	3755	1/1	0.94	0.10	62,62,62,62	0
56	MG	1A	3661	1/1	0.94	0.09	29,29,29,29	0
56	MG	1Y	205	1/1	0.94	0.15	61,61,61,61	0
56	MG	2a	1782	1/1	0.94	0.17	61,61,61,61	0
56	MG	2a	1783	1/1	0.94	0.07	62,62,62,62	0
56	MG	2A	3759	1/1	0.94	0.11	69,69,69,69	0
56	MG	2A	3180	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	3007	1/1	0.94	0.08	39,39,39,39	0
56	MG	2A	3765	1/1	0.94	0.07	48,48,48,48	0
56	MG	1A	3673	1/1	0.94	0.06	27,27,27,27	0
56	MG	2a	1790	1/1	0.94	0.22	60,60,60,60	0
56	MG	1A	3333	1/1	0.94	0.21	52,52,52,52	0
56	MG	1A	3334	1/1	0.94	0.23	56,56,56,56	0
56	MG	2A	3415	1/1	0.94	0.26	49,49,49,49	0
56	MG	1A	3194	1/1	0.94	0.14	36,36,36,36	0
56	MG	1A	3338	1/1	0.94	0.07	54,54,54,54	0
56	MG	1A	4025	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3420	1/1	0.94	0.14	50,50,50,50	0
56	MG	2A	3775	1/1	0.94	0.13	64,64,64,64	0
56	MG	1A	3051	1/1	0.94	0.09	24,24,24,24	0
56	MG	11	103	1/1	0.94	0.17	62,62,62,62	0
56	MG	11	105	1/1	0.94	0.10	62,62,62,62	0
56	MG	12	101	1/1	0.94	0.11	59,59,59,59	0
56	MG	1A	4029	1/1	0.94	0.11	32,32,32,32	0
56	MG	1A	3845	1/1	0.94	0.12	24,24,24,24	0
56	MG	1A	3846	1/1	0.94	0.09	30,30,30,30	0
56	MG	1a	1784	1/1	0.94	0.11	49,49,49,49	0
56	MG	15	109	1/1	0.94	0.10	39,39,39,39	0
56	MG	2a	1811	1/1	0.94	0.19	60,60,60,60	0
56	MG	1A	3103	1/1	0.94	0.06	25,25,25,25	0
56	MG	1A	3849	1/1	0.94	0.21	36,36,36,36	0
56	MG	2A	3789	1/1	0.94	0.08	44,44,44,44	0
56	MG	17	105	1/1	0.94	0.11	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	1A	3261	1/1	0.94	0.12	60,60,60,60	0
56	MG	2A	3795	1/1	0.94	0.12	59,59,59,59	0
56	MG	2a	1819	1/1	0.94	0.22	66,66,66,66	0
56	MG	1A	3851	1/1	0.94	0.06	47,47,47,47	0
56	MG	1A	3419	1/1	0.94	0.13	50,50,50,50	0
56	MG	1a	1799	1/1	0.94	0.21	59,59,59,59	0
56	MG	1A	3146	1/1	0.94	0.09	34,34,34,34	0
56	MG	2A	3441	1/1	0.94	0.27	53,53,53,53	0
56	MG	2d	301	1/1	0.94	0.30	59,59,59,59	0
56	MG	2A	3216	1/1	0.94	0.16	52,52,52,52	0
56	MG	2A	3809	1/1	0.94	0.07	43,43,43,43	0
56	MG	1A	3694	1/1	0.94	0.06	11,11,11,11	0
56	MG	1A	3263	1/1	0.94	0.11	61,61,61,61	0
56	MG	2A	3445	1/1	0.94	0.25	49,49,49,49	0
56	MG	2A	3817	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	4051	1/1	0.94	0.10	56,56,56,56	0
56	MG	1A	3345	1/1	0.94	0.16	60,60,60,60	0
56	MG	2A	3449	1/1	0.94	0.34	53,53,53,53	0
56	MG	1A	3538	1/1	0.94	0.13	47,47,47,47	0
56	MG	2A	3451	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3452	1/1	0.94	0.09	38,38,38,38	0
56	MG	1A	3701	1/1	0.94	0.07	47,47,47,47	0
56	MG	2A	3455	1/1	0.94	0.10	69,69,69,69	0
56	MG	1a	1809	1/1	0.94	0.15	57,57,57,57	0
56	MG	1A	3147	1/1	0.94	0.24	44,44,44,44	0
56	MG	1A	3540	1/1	0.94	0.14	50,50,50,50	0
56	MG	1A	3268	1/1	0.94	0.21	56,56,56,56	0
56	MG	1f	201	1/1	0.94	0.11	59,59,59,59	0
56	MG	1a	1618	1/1	0.94	0.06	55,55,55,55	0
56	MG	1A	3081	1/1	0.94	0.08	51,51,51,51	0
56	MG	1A	4067	1/1	0.94	0.09	46,46,46,46	0
56	MG	2A	3844	1/1	0.94	0.11	63,63,63,63	0
56	MG	1A	3353	1/1	0.94	0.06	50,50,50,50	0
56	MG	1a	1625	1/1	0.94	0.22	58,58,58,58	0
56	MG	1A	3287	1/1	0.94	0.05	45,45,45,45	0
56	MG	1A	3156	1/1	0.94	0.16	38,38,38,38	0
56	MG	1A	3438	1/1	0.94	0.22	45,45,45,45	0
56	MG	1a	1631	1/1	0.94	0.27	57,57,57,57	0
56	MG	1A	3554	1/1	0.94	0.20	49,49,49,49	0
56	MG	2B	207	1/1	0.94	0.12	68,68,68,68	0
56	MG	1A	3439	1/1	0.94	0.31	44,44,44,44	0
56	MG	1A	3213	1/1	0.94	0.15	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	1A	3562	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	3894	1/1	0.94	0.14	41,41,41,41	0
56	MG	2A	3484	1/1	0.94	0.10	68,68,68,68	0
56	MG	1A	3355	1/1	0.95	0.19	47,47,47,47	0
56	MG	1A	3706	1/1	0.95	0.06	26,26,26,26	0
56	MG	1A	3879	1/1	0.95	0.05	43,43,43,43	0
56	MG	2A	3007	1/1	0.95	0.32	58,58,58,58	0
56	MG	1a	1644	1/1	0.95	0.13	56,56,56,56	0
56	MG	1A	3357	1/1	0.95	0.09	60,60,60,60	0
56	MG	2F	306	1/1	0.95	0.11	53,53,53,53	0
56	MG	2A	3560	1/1	0.95	0.12	63,63,63,63	0
56	MG	1A	3708	1/1	0.95	0.12	32,32,32,32	0
56	MG	1A	3548	1/1	0.95	0.11	57,57,57,57	0
56	MG	2P	201	1/1	0.95	0.10	63,63,63,63	0
56	MG	1A	4083	1/1	0.95	0.12	56,56,56,56	0
56	MG	2A	3565	1/1	0.95	0.12	52,52,52,52	0
56	MG	2A	3017	1/1	0.95	0.23	50,50,50,50	0
56	MG	2A	3018	1/1	0.95	0.24	49,49,49,49	0
56	MG	2A	3569	1/1	0.95	0.08	49,49,49,49	0
56	MG	1A	3127	1/1	0.95	0.15	56,56,56,56	0
56	MG	1a	1654	1/1	0.95	0.06	48,48,48,48	0
56	MG	2T	203	1/1	0.95	0.09	59,59,59,59	0
56	MG	1A	3553	1/1	0.95	0.15	40,40,40,40	0
56	MG	1A	3886	1/1	0.95	0.07	35,35,35,35	0
56	MG	1A	3271	1/1	0.95	0.08	38,38,38,38	0
56	MG	2V	202	1/1	0.95	0.05	56,56,56,56	0
56	MG	1A	3718	1/1	0.95	0.07	54,54,54,54	0
56	MG	2A	3300	1/1	0.95	0.08	54,54,54,54	0
56	MG	1A	3719	1/1	0.95	0.09	39,39,39,39	0
56	MG	2A	3302	1/1	0.95	0.28	45,45,45,45	0
56	MG	1A	3895	1/1	0.95	0.21	24,24,24,24	0
56	MG	20	104	1/1	0.95	0.11	61,61,61,61	0
56	MG	1A	3896	1/1	0.95	0.12	53,53,53,53	0
56	MG	2A	3588	1/1	0.95	0.27	67,67,67,67	0
56	MG	2A	3036	1/1	0.95	0.12	44,44,44,44	0
56	MG	1a	1662	1/1	0.95	0.13	65,65,65,65	0
56	MG	25	103	1/1	0.95	0.18	50,50,50,50	0
56	MG	1A	3555	1/1	0.95	0.28	47,47,47,47	0
56	MG	1A	3898	1/1	0.95	0.18	49,49,49,49	0
56	MG	1A	3723	1/1	0.95	0.09	64,64,64,64	0
56	MG	26	101	1/1	0.95	0.10	49,49,49,49	0
56	MG	2A	3595	1/1	0.95	0.10	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	3596	1/1	0.95	0.09	50,50,50,50	0
56	MG	1B	204	1/1	0.95	0.20	56,56,56,56	0
56	MG	1A	3901	1/1	0.95	0.10	30,30,30,30	0
56	MG	2A	3047	1/1	0.95	0.14	39,39,39,39	0
56	MG	2a	1601	1/1	0.95	0.07	58,58,58,58	0
56	MG	1A	3281	1/1	0.95	0.13	29,29,29,29	0
56	MG	2A	3052	1/1	0.95	0.12	30,30,30,30	0
56	MG	1A	3203	1/1	0.95	0.10	22,22,22,22	0
56	MG	1A	3727	1/1	0.95	0.06	36,36,36,36	0
56	MG	1B	212	1/1	0.95	0.17	56,56,56,56	0
56	MG	1B	213	1/1	0.95	0.13	56,56,56,56	0
56	MG	2a	1608	1/1	0.95	0.26	58,58,58,58	0
56	MG	1A	3907	1/1	0.95	0.10	39,39,39,39	0
56	MG	1A	3559	1/1	0.95	0.12	34,34,34,34	0
56	MG	1A	3560	1/1	0.95	0.08	36,36,36,36	0
56	MG	2A	3610	1/1	0.95	0.06	35,35,35,35	0
56	MG	1A	3047	1/1	0.95	0.04	27,27,27,27	0
56	MG	1A	3206	1/1	0.95	0.10	41,41,41,41	0
56	MG	2A	3613	1/1	0.95	0.07	41,41,41,41	0
56	MG	1A	3569	1/1	0.95	0.08	39,39,39,39	0
56	MG	1A	3451	1/1	0.95	0.08	56,56,56,56	0
56	MG	1A	3918	1/1	0.95	0.07	42,42,42,42	0
56	MG	1A	3013	1/1	0.95	0.14	29,29,29,29	0
56	MG	1A	3454	1/1	0.95	0.18	43,43,43,43	0
56	MG	2A	3623	1/1	0.95	0.07	39,39,39,39	0
56	MG	2A	3330	1/1	0.95	0.07	51,51,51,51	0
56	MG	1A	3136	1/1	0.95	0.27	39,39,39,39	0
56	MG	1a	1687	1/1	0.95	0.06	57,57,57,57	0
56	MG	2A	3077	1/1	0.95	0.15	59,59,59,59	0
56	MG	1a	1688	1/1	0.95	0.23	52,52,52,52	0
56	MG	1A	3929	1/1	0.95	0.09	62,62,62,62	0
56	MG	2A	3080	1/1	0.95	0.09	36,36,36,36	0
56	MG	1A	3294	1/1	0.95	0.18	43,43,43,43	0
56	MG	1A	3743	1/1	0.95	0.07	35,35,35,35	0
56	MG	2A	3636	1/1	0.95	0.17	39,39,39,39	0
56	MG	1a	1692	1/1	0.95	0.23	47,47,47,47	0
56	MG	1A	3295	1/1	0.95	0.18	54,54,54,54	0
56	MG	2A	3085	1/1	0.95	0.09	46,46,46,46	0
56	MG	2A	3086	1/1	0.95	0.30	45,45,45,45	0
56	MG	1A	3935	1/1	0.95	0.06	66,66,66,66	0
56	MG	1A	3936	1/1	0.95	0.08	48,48,48,48	0
56	MG	2A	3093	1/1	0.95	0.14	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	1D	306	1/1	0.95	0.07	38,38,38,38	0
56	MG	2A	3347	1/1	0.95	0.31	77,77,77,77	0
56	MG	2A	3646	1/1	0.95	0.18	59,59,59,59	0
56	MG	2A	3096	1/1	0.95	0.07	56,56,56,56	0
56	MG	1A	3027	1/1	0.95	0.09	47,47,47,47	0
56	MG	2A	3649	1/1	0.95	0.15	62,62,62,62	0
56	MG	1A	3089	1/1	0.95	0.07	44,44,44,44	0
56	MG	2A	3652	1/1	0.95	0.06	57,57,57,57	0
56	MG	2A	3653	1/1	0.95	0.10	56,56,56,56	0
56	MG	1A	3940	1/1	0.95	0.08	54,54,54,54	0
56	MG	2A	3656	1/1	0.95	0.09	54,54,54,54	0
56	MG	1A	3373	1/1	0.95	0.15	47,47,47,47	0
56	MG	1A	3214	1/1	0.95	0.11	50,50,50,50	0
56	MG	1A	3216	1/1	0.95	0.10	35,35,35,35	0
56	MG	2A	3105	1/1	0.95	0.07	39,39,39,39	0
56	MG	1A	3302	1/1	0.95	0.09	29,29,29,29	0
56	MG	2A	3662	1/1	0.95	0.07	47,47,47,47	0
56	MG	1E	308	1/1	0.95	0.11	53,53,53,53	0
56	MG	1A	3754	1/1	0.95	0.08	28,28,28,28	0
56	MG	2a	1666	1/1	0.95	0.24	61,61,61,61	0
56	MG	1A	3467	1/1	0.95	0.12	52,52,52,52	0
56	MG	1A	3143	1/1	0.95	0.09	38,38,38,38	0
56	MG	2A	3668	1/1	0.95	0.19	49,49,49,49	0
56	MG	2a	1671	1/1	0.95	0.22	55,55,55,55	0
56	MG	1A	3591	1/1	0.95	0.15	44,44,44,44	0
56	MG	2A	3114	1/1	0.95	0.13	60,60,60,60	0
56	MG	1A	3471	1/1	0.95	0.10	52,52,52,52	0
56	MG	2a	1676	1/1	0.95	0.23	56,56,56,56	0
56	MG	1A	3219	1/1	0.95	0.14	47,47,47,47	0
56	MG	2a	1678	1/1	0.95	0.10	55,55,55,55	0
56	MG	1F	307	1/1	0.95	0.11	45,45,45,45	0
56	MG	1F	308	1/1	0.95	0.18	31,31,31,31	0
56	MG	1A	3308	1/1	0.95	0.05	43,43,43,43	0
56	MG	1A	3477	1/1	0.95	0.17	59,59,59,59	0
56	MG	2A	3678	1/1	0.95	0.12	60,60,60,60	0
56	MG	1A	3090	1/1	0.95	0.15	38,38,38,38	0
56	MG	1A	3954	1/1	0.95	0.07	34,34,34,34	0
56	MG	2A	3127	1/1	0.95	0.12	46,46,46,46	0
56	MG	1A	3312	1/1	0.95	0.16	44,44,44,44	0
56	MG	1A	3771	1/1	0.95	0.06	49,49,49,49	0
56	MG	1A	3223	1/1	0.95	0.09	44,44,44,44	0
56	MG	1a	1723	1/1	0.95	0.24	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	1694	1/1	0.95	0.07	51,51,51,51	0
56	MG	2A	3383	1/1	0.95	0.07	64,64,64,64	0
56	MG	1A	3224	1/1	0.95	0.16	40,40,40,40	0
56	MG	1A	3602	1/1	0.95	0.07	28,28,28,28	0
56	MG	1A	3604	1/1	0.95	0.09	36,36,36,36	0
56	MG	1A	3605	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	3782	1/1	0.95	0.11	64,64,64,64	0
56	MG	1A	3225	1/1	0.95	0.12	56,56,56,56	0
56	MG	1a	1734	1/1	0.95	0.14	38,38,38,38	0
56	MG	1A	3004	1/1	0.95	0.05	27,27,27,27	0
56	MG	1O	203	1/1	0.95	0.08	53,53,53,53	0
56	MG	1A	3487	1/1	0.95	0.08	60,60,60,60	0
56	MG	1A	3967	1/1	0.95	0.08	54,54,54,54	0
56	MG	1A	3789	1/1	0.95	0.07	37,37,37,37	0
56	MG	2a	1709	1/1	0.95	0.12	69,69,69,69	0
56	MG	1a	1743	1/1	0.95	0.08	42,42,42,42	0
56	MG	1A	3320	1/1	0.95	0.18	36,36,36,36	0
56	MG	1A	3619	1/1	0.95	0.07	27,27,27,27	0
56	MG	2A	3157	1/1	0.95	0.20	64,64,64,64	0
56	MG	1A	3621	1/1	0.95	0.04	33,33,33,33	0
56	MG	2A	3402	1/1	0.95	0.06	56,56,56,56	0
56	MG	1A	3795	1/1	0.95	0.04	19,19,19,19	0
56	MG	2A	3720	1/1	0.95	0.05	71,71,71,71	0
56	MG	1A	3798	1/1	0.95	0.28	27,27,27,27	0
56	MG	1A	3232	1/1	0.95	0.25	42,42,42,42	0
56	MG	1A	3397	1/1	0.95	0.21	41,41,41,41	0
56	MG	2a	1725	1/1	0.95	0.17	62,62,62,62	0
56	MG	2A	3727	1/1	0.95	0.08	69,69,69,69	0
56	MG	1A	3493	1/1	0.95	0.23	40,40,40,40	0
56	MG	2A	3167	1/1	0.95	0.09	41,41,41,41	0
56	MG	1T	202	1/1	0.95	0.15	50,50,50,50	0
56	MG	2A	3169	1/1	0.95	0.11	59,59,59,59	0
56	MG	1U	202	1/1	0.95	0.16	35,35,35,35	0
56	MG	1U	204	1/1	0.95	0.18	37,37,37,37	0
56	MG	2A	3173	1/1	0.95	0.20	65,65,65,65	0
56	MG	2A	3174	1/1	0.95	0.10	61,61,61,61	0
56	MG	1A	3984	1/1	0.95	0.08	44,44,44,44	0
56	MG	1A	3031	1/1	0.95	0.20	26,26,26,26	0
56	MG	1V	205	1/1	0.95	0.11	31,31,31,31	0
56	MG	1A	3496	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	3497	1/1	0.95	0.10	47,47,47,47	0
56	MG	1A	3236	1/1	0.95	0.10	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	1A	3401	1/1	0.95	0.10	49,49,49,49	0
56	MG	1X	102	1/1	0.95	0.15	39,39,39,39	0
56	MG	1A	3096	1/1	0.95	0.15	41,41,41,41	0
56	MG	1A	3998	1/1	0.95	0.07	25,25,25,25	0
56	MG	1A	3100	1/1	0.95	0.07	62,62,62,62	0
56	MG	1A	3160	1/1	0.95	0.17	36,36,36,36	0
56	MG	1A	3407	1/1	0.95	0.08	48,48,48,48	0
56	MG	1A	3642	1/1	0.95	0.13	49,49,49,49	0
56	MG	1A	3059	1/1	0.95	0.10	45,45,45,45	0
56	MG	2A	3194	1/1	0.95	0.15	51,51,51,51	0
56	MG	1A	3164	1/1	0.95	0.21	36,36,36,36	0
56	MG	2A	3761	1/1	0.95	0.09	37,37,37,37	0
56	MG	1A	3509	1/1	0.95	0.34	44,44,44,44	0
56	MG	1A	3002	1/1	0.95	0.08	46,46,46,46	0
56	MG	1A	3512	1/1	0.95	0.12	37,37,37,37	0
56	MG	1A	3654	1/1	0.95	0.07	21,21,21,21	0
56	MG	2a	1765	1/1	0.95	0.07	52,52,52,52	0
56	MG	1a	1783	1/1	0.95	0.11	51,51,51,51	0
56	MG	1A	3513	1/1	0.95	0.14	54,54,54,54	0
56	MG	2A	3207	1/1	0.95	0.16	52,52,52,52	0
56	MG	1a	1786	1/1	0.95	0.17	67,67,67,67	0
56	MG	1A	3514	1/1	0.95	0.12	60,60,60,60	0
56	MG	1A	3061	1/1	0.95	0.10	27,27,27,27	0
56	MG	2A	3447	1/1	0.95	0.21	55,55,55,55	0
56	MG	1a	1790	1/1	0.95	0.05	54,54,54,54	0
56	MG	1a	1791	1/1	0.95	0.12	66,66,66,66	0
56	MG	1A	3413	1/1	0.95	0.09	50,50,50,50	0
56	MG	2A	3214	1/1	0.95	0.11	53,53,53,53	0
56	MG	2a	1780	1/1	0.95	0.18	66,66,66,66	0
56	MG	13	103	1/1	0.95	0.09	52,52,52,52	0
56	MG	2A	3453	1/1	0.95	0.08	63,63,63,63	0
56	MG	1A	3011	1/1	0.95	0.20	46,46,46,46	0
56	MG	1A	3666	1/1	0.95	0.04	22,22,22,22	0
56	MG	15	103	1/1	0.95	0.17	38,38,38,38	0
56	MG	2A	3785	1/1	0.95	0.06	51,51,51,51	0
56	MG	1A	3671	1/1	0.95	0.12	38,38,38,38	0
56	MG	15	106	1/1	0.95	0.13	43,43,43,43	0
56	MG	2A	3221	1/1	0.95	0.09	69,69,69,69	0
56	MG	2A	3462	1/1	0.95	0.11	54,54,54,54	0
56	MG	2A	3790	1/1	0.95	0.09	44,44,44,44	0
56	MG	2a	1793	1/1	0.95	0.07	59,59,59,59	0
56	MG	15	108	1/1	0.95	0.07	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	1795	1/1	0.95	0.20	76,76,76,76	0
56	MG	2A	3793	1/1	0.95	0.08	34,34,34,34	0
56	MG	2A	3465	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	3067	1/1	0.95	0.08	30,30,30,30	0
56	MG	1A	4027	1/1	0.95	0.09	38,38,38,38	0
56	MG	1A	3838	1/1	0.95	0.13	43,43,43,43	0
56	MG	1A	3524	1/1	0.95	0.24	32,32,32,32	0
56	MG	1A	4031	1/1	0.95	0.06	38,38,38,38	0
56	MG	1A	4033	1/1	0.95	0.08	41,41,41,41	0
56	MG	1a	1810	1/1	0.95	0.23	56,56,56,56	0
56	MG	1A	3840	1/1	0.95	0.14	47,47,47,47	0
56	MG	2A	3810	1/1	0.95	0.07	58,58,58,58	0
56	MG	1A	3841	1/1	0.95	0.08	20,20,20,20	0
56	MG	2A	3813	1/1	0.95	0.13	80,80,80,80	0
56	MG	2A	3476	1/1	0.95	0.08	39,39,39,39	0
56	MG	1e	201	1/1	0.95	0.30	59,59,59,59	0
56	MG	2A	3478	1/1	0.95	0.22	63,63,63,63	0
56	MG	2A	3818	1/1	0.95	0.05	31,31,31,31	0
56	MG	2A	3235	1/1	0.95	0.09	50,50,50,50	0
56	MG	1a	1601	1/1	0.95	0.20	52,52,52,52	0
56	MG	1a	1602	1/1	0.95	0.13	64,64,64,64	0
56	MG	1A	3525	1/1	0.95	0.09	36,36,36,36	0
56	MG	2a	1818	1/1	0.95	0.16	62,62,62,62	0
56	MG	1A	3037	1/1	0.95	0.12	37,37,37,37	0
56	MG	2A	3826	1/1	0.95	0.16	59,59,59,59	0
56	MG	1m	3001	1/1	0.95	0.12	52,52,52,52	0
56	MG	2A	3832	1/1	0.95	0.13	58,58,58,58	0
56	MG	2a	1823	1/1	0.95	0.12	56,56,56,56	0
56	MG	1A	4040	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	3681	1/1	0.95	0.09	33,33,33,33	0
56	MG	1A	3255	1/1	0.95	0.14	65,65,65,65	0
56	MG	1A	3847	1/1	0.95	0.07	32,32,32,32	0
56	MG	1A	3528	1/1	0.95	0.10	44,44,44,44	0
56	MG	2A	3251	1/1	0.95	0.15	59,59,59,59	0
56	MG	1A	3181	1/1	0.95	0.20	53,53,53,53	0
56	MG	1A	4048	1/1	0.95	0.10	45,45,45,45	0
56	MG	1a	1617	1/1	0.95	0.05	54,54,54,54	0
56	MG	2A	3499	1/1	0.95	0.22	71,71,71,71	0
56	MG	2l	204	1/1	0.95	0.07	68,68,68,68	0
56	MG	1A	3686	1/1	0.95	0.11	27,27,27,27	0
56	MG	2A	3257	1/1	0.95	0.13	54,54,54,54	0
56	MG	1a	1621	1/1	0.95	0.26	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	1A	3111	1/1	0.95	0.13	37,37,37,37	0
56	MG	2A	3506	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	3018	1/1	0.95	0.08	36,36,36,36	0
56	MG	1A	3533	1/1	0.95	0.21	47,47,47,47	0
56	MG	2A	3514	1/1	0.95	0.10	56,56,56,56	0
56	MG	1A	3072	1/1	0.95	0.12	28,28,28,28	0
56	MG	1A	3857	1/1	0.95	0.10	40,40,40,40	0
56	MG	2B	209	1/1	0.95	0.14	48,48,48,48	0
56	MG	1A	4063	1/1	0.95	0.14	40,40,40,40	0
56	MG	1A	3347	1/1	0.95	0.19	38,38,38,38	0
56	MG	2A	3522	1/1	0.95	0.12	63,63,63,63	0
56	MG	2A	3269	1/1	0.95	0.16	60,60,60,60	0
56	MG	1A	3859	1/1	0.95	0.15	51,51,51,51	0
56	MG	1A	3042	1/1	0.95	0.06	32,32,32,32	0
56	MG	1x	110	1/1	0.95	0.31	67,67,67,67	0
56	MG	1A	3862	1/1	0.95	0.12	39,39,39,39	0
56	MG	1A	3078	1/1	0.95	0.25	54,54,54,54	0
56	MG	2A	3530	1/1	0.95	0.14	42,42,42,42	0
56	MG	2D	303	1/1	0.95	0.28	55,55,55,55	0
56	MG	2A	3531	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3533	1/1	0.95	0.11	48,48,48,48	0
56	MG	1A	3350	1/1	0.95	0.16	30,30,30,30	0
57	K	2A	3459	1/1	0.95	0.10	73,73,73,73	0
56	MG	1A	3265	1/1	0.95	0.07	52,52,52,52	0
56	MG	1A	3267	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3197	1/1	0.95	0.21	41,41,41,41	0
56	MG	2A	3545	1/1	0.95	0.11	59,59,59,59	0
56	MG	1A	3491	1/1	0.96	0.13	37,37,37,37	0
56	MG	2A	3020	1/1	0.96	0.20	44,44,44,44	0
56	MG	2F	307	1/1	0.96	0.14	39,39,39,39	0
56	MG	1A	3910	1/1	0.96	0.06	65,65,65,65	0
56	MG	2A	3572	1/1	0.96	0.09	46,46,46,46	0
56	MG	2A	3024	1/1	0.96	0.06	47,47,47,47	0
56	MG	2A	3575	1/1	0.96	0.14	60,60,60,60	0
56	MG	2A	3577	1/1	0.96	0.08	70,70,70,70	0
56	MG	1B	203	1/1	0.96	0.12	50,50,50,50	0
56	MG	2A	3026	1/1	0.96	0.11	45,45,45,45	0
56	MG	1A	3404	1/1	0.96	0.12	51,51,51,51	0
56	MG	2Q	204	1/1	0.96	0.10	57,57,57,57	0
56	MG	1a	1650	1/1	0.96	0.11	53,53,53,53	0
56	MG	1A	3914	1/1	0.96	0.06	54,54,54,54	0
56	MG	2R	203	1/1	0.96	0.16	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	1a	1652	1/1	0.96	0.08	50,50,50,50	0
56	MG	1a	1653	1/1	0.96	0.08	47,47,47,47	0
56	MG	1A	3603	1/1	0.96	0.09	48,48,48,48	0
56	MG	1A	3063	1/1	0.96	0.29	63,63,63,63	0
56	MG	1A	3337	1/1	0.96	0.22	44,44,44,44	0
56	MG	1A	3755	1/1	0.96	0.09	39,39,39,39	0
56	MG	2A	3040	1/1	0.96	0.10	47,47,47,47	0
56	MG	1A	3066	1/1	0.96	0.17	51,51,51,51	0
56	MG	1A	3052	1/1	0.96	0.15	29,29,29,29	0
56	MG	2A	3594	1/1	0.96	0.14	56,56,56,56	0
56	MG	1A	3269	1/1	0.96	0.23	49,49,49,49	0
56	MG	1A	3759	1/1	0.96	0.07	23,23,23,23	0
56	MG	1B	219	1/1	0.96	0.24	53,53,53,53	0
56	MG	23	101	1/1	0.96	0.06	50,50,50,50	0
56	MG	2A	3048	1/1	0.96	0.06	40,40,40,40	0
56	MG	2A	3049	1/1	0.96	0.11	32,32,32,32	0
56	MG	1B	220	1/1	0.96	0.09	41,41,41,41	0
56	MG	1A	3760	1/1	0.96	0.05	26,26,26,26	0
56	MG	1A	3614	1/1	0.96	0.08	38,38,38,38	0
56	MG	2A	3054	1/1	0.96	0.08	44,44,44,44	0
56	MG	1A	3762	1/1	0.96	0.09	47,47,47,47	0
56	MG	2A	3056	1/1	0.96	0.27	56,56,56,56	0
56	MG	1A	3616	1/1	0.96	0.14	43,43,43,43	0
56	MG	2A	3059	1/1	0.96	0.10	56,56,56,56	0
56	MG	2A	3060	1/1	0.96	0.21	52,52,52,52	0
56	MG	1A	3617	1/1	0.96	0.09	54,54,54,54	0
56	MG	1A	3158	1/1	0.96	0.14	24,24,24,24	0
56	MG	1A	3411	1/1	0.96	0.15	49,49,49,49	0
56	MG	1A	3159	1/1	0.96	0.13	32,32,32,32	0
56	MG	1A	3343	1/1	0.96	0.13	39,39,39,39	0
56	MG	1A	3272	1/1	0.96	0.19	57,57,57,57	0
56	MG	2A	3616	1/1	0.96	0.13	52,52,52,52	0
56	MG	1A	3627	1/1	0.96	0.07	28,28,28,28	0
56	MG	2A	3618	1/1	0.96	0.09	55,55,55,55	0
56	MG	1A	3275	1/1	0.96	0.16	48,48,48,48	0
56	MG	1A	3276	1/1	0.96	0.07	48,48,48,48	0
56	MG	2A	3622	1/1	0.96	0.14	51,51,51,51	0
56	MG	1a	1679	1/1	0.96	0.14	54,54,54,54	0
56	MG	1A	3780	1/1	0.96	0.08	21,21,21,21	0
56	MG	1B	236	1/1	0.96	0.06	39,39,39,39	0
56	MG	1D	302	1/1	0.96	0.09	26,26,26,26	0
56	MG	1D	304	1/1	0.96	0.16	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	3418	1/1	0.96	0.06	40,40,40,40	0
56	MG	1D	309	1/1	0.96	0.10	53,53,53,53	0
56	MG	1A	3093	1/1	0.96	0.10	27,27,27,27	0
56	MG	2a	1619	1/1	0.96	0.07	74,74,74,74	0
56	MG	2A	3633	1/1	0.96	0.08	52,52,52,52	0
56	MG	2a	1621	1/1	0.96	0.17	82,82,82,82	0
56	MG	1A	3285	1/1	0.96	0.17	54,54,54,54	0
56	MG	1A	3422	1/1	0.96	0.10	35,35,35,35	0
56	MG	1A	3423	1/1	0.96	0.16	42,42,42,42	0
56	MG	1A	3636	1/1	0.96	0.10	24,24,24,24	0
56	MG	1A	3790	1/1	0.96	0.06	41,41,41,41	0
56	MG	1A	3118	1/1	0.96	0.16	50,50,50,50	0
56	MG	2a	1628	1/1	0.96	0.31	61,61,61,61	0
56	MG	1A	3639	1/1	0.96	0.05	28,28,28,28	0
56	MG	2A	3349	1/1	0.96	0.06	67,67,67,67	0
56	MG	2A	3090	1/1	0.96	0.32	58,58,58,58	0
56	MG	1A	3425	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	3121	1/1	0.96	0.14	48,48,48,48	0
56	MG	1A	3797	1/1	0.96	0.05	23,23,23,23	0
56	MG	1E	313	1/1	0.96	0.11	40,40,40,40	0
56	MG	1A	3427	1/1	0.96	0.16	50,50,50,50	0
56	MG	2A	3356	1/1	0.96	0.09	58,58,58,58	0
56	MG	1A	3522	1/1	0.96	0.07	40,40,40,40	0
56	MG	1A	3645	1/1	0.96	0.08	43,43,43,43	0
56	MG	2A	3651	1/1	0.96	0.08	34,34,34,34	0
56	MG	1F	305	1/1	0.96	0.17	35,35,35,35	0
56	MG	1A	3801	1/1	0.96	0.04	38,38,38,38	0
56	MG	1A	3523	1/1	0.96	0.14	43,43,43,43	0
56	MG	2a	1644	1/1	0.96	0.08	76,76,76,76	0
56	MG	2A	3655	1/1	0.96	0.08	56,56,56,56	0
56	MG	1A	3165	1/1	0.96	0.17	35,35,35,35	0
56	MG	1F	311	1/1	0.96	0.16	48,48,48,48	0
56	MG	1A	3094	1/1	0.96	0.17	52,52,52,52	0
56	MG	1A	3650	1/1	0.96	0.10	34,34,34,34	0
56	MG	1A	3291	1/1	0.96	0.08	49,49,49,49	0
56	MG	1A	3969	1/1	0.96	0.10	63,63,63,63	0
56	MG	1G	201	1/1	0.96	0.11	42,42,42,42	0
56	MG	1A	3653	1/1	0.96	0.07	22,22,22,22	0
56	MG	2a	1654	1/1	0.96	0.08	60,60,60,60	0
56	MG	1A	3810	1/1	0.96	0.06	37,37,37,37	0
56	MG	2A	3117	1/1	0.96	0.14	54,54,54,54	0
56	MG	1A	3356	1/1	0.96	0.08	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3433	1/1	0.96	0.24	51,51,51,51	0
56	MG	1A	3975	1/1	0.96	0.09	38,38,38,38	0
56	MG	2A	3377	1/1	0.96	0.20	41,41,41,41	0
56	MG	2a	1661	1/1	0.96	0.16	61,61,61,61	0
56	MG	1N	204	1/1	0.96	0.20	43,43,43,43	0
56	MG	1A	3228	1/1	0.96	0.14	37,37,37,37	0
56	MG	2a	1665	1/1	0.96	0.16	44,44,44,44	0
56	MG	1A	3530	1/1	0.96	0.15	39,39,39,39	0
56	MG	2A	3381	1/1	0.96	0.17	58,58,58,58	0
56	MG	1A	3979	1/1	0.96	0.08	53,53,53,53	0
56	MG	1A	3436	1/1	0.96	0.23	46,46,46,46	0
56	MG	2A	3128	1/1	0.96	0.10	62,62,62,62	0
56	MG	2A	3679	1/1	0.96	0.06	65,65,65,65	0
56	MG	2a	1673	1/1	0.96	0.10	56,56,56,56	0
56	MG	1A	3818	1/1	0.96	0.08	46,46,46,46	0
56	MG	2A	3387	1/1	0.96	0.12	64,64,64,64	0
56	MG	1A	3982	1/1	0.96	0.08	46,46,46,46	0
56	MG	1A	3124	1/1	0.96	0.23	41,41,41,41	0
56	MG	1A	3664	1/1	0.96	0.06	23,23,23,23	0
56	MG	1Q	201	1/1	0.96	0.12	33,33,33,33	0
56	MG	2a	1680	1/1	0.96	0.26	65,65,65,65	0
56	MG	1a	1730	1/1	0.96	0.10	51,51,51,51	0
56	MG	2a	1682	1/1	0.96	0.25	54,54,54,54	0
56	MG	2A	3688	1/1	0.96	0.07	30,30,30,30	0
56	MG	2a	1684	1/1	0.96	0.14	50,50,50,50	0
56	MG	1A	3231	1/1	0.96	0.10	57,57,57,57	0
56	MG	1Q	204	1/1	0.96	0.11	56,56,56,56	0
56	MG	1A	3125	1/1	0.96	0.21	33,33,33,33	0
56	MG	2A	3693	1/1	0.96	0.14	55,55,55,55	0
56	MG	2A	3140	1/1	0.96	0.13	52,52,52,52	0
56	MG	2A	3696	1/1	0.96	0.10	44,44,44,44	0
56	MG	2A	3141	1/1	0.96	0.06	55,55,55,55	0
56	MG	1A	3672	1/1	0.96	0.07	48,48,48,48	0
56	MG	2A	3143	1/1	0.96	0.11	47,47,47,47	0
56	MG	1A	3178	1/1	0.96	0.11	36,36,36,36	0
56	MG	1R	205	1/1	0.96	0.16	33,33,33,33	0
56	MG	1A	3298	1/1	0.96	0.13	39,39,39,39	0
56	MG	1a	1742	1/1	0.96	0.09	42,42,42,42	0
56	MG	2A	3148	1/1	0.96	0.21	35,35,35,35	0
56	MG	1A	3235	1/1	0.96	0.09	31,31,31,31	0
56	MG	2A	3406	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3126	1/1	0.96	0.23	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3679	1/1	0.96	0.05	29,29,29,29	0
56	MG	2A	3153	1/1	0.96	0.10	40,40,40,40	0
56	MG	2A	3154	1/1	0.96	0.26	48,48,48,48	0
56	MG	1a	1746	1/1	0.96	0.05	59,59,59,59	0
56	MG	1a	1747	1/1	0.96	0.08	48,48,48,48	0
56	MG	1A	3830	1/1	0.96	0.05	33,33,33,33	0
56	MG	2A	3722	1/1	0.96	0.08	65,65,65,65	0
56	MG	1A	3237	1/1	0.96	0.17	34,34,34,34	0
56	MG	1U	203	1/1	0.96	0.09	38,38,38,38	0
56	MG	2a	1712	1/1	0.96	0.28	59,59,59,59	0
56	MG	1A	3833	1/1	0.96	0.06	58,58,58,58	0
56	MG	1U	207	1/1	0.96	0.10	31,31,31,31	0
56	MG	1A	3241	1/1	0.96	0.23	47,47,47,47	0
56	MG	1A	3026	1/1	0.96	0.13	41,41,41,41	0
56	MG	2a	1718	1/1	0.96	0.11	45,45,45,45	0
56	MG	2A	3730	1/1	0.96	0.06	51,51,51,51	0
56	MG	1A	3369	1/1	0.96	0.12	41,41,41,41	0
56	MG	1A	3685	1/1	0.96	0.06	63,63,63,63	0
56	MG	1W	202	1/1	0.96	0.16	41,41,41,41	0
56	MG	1A	3005	1/1	0.96	0.06	45,45,45,45	0
56	MG	1A	4014	1/1	0.96	0.06	42,42,42,42	0
56	MG	2A	3737	1/1	0.96	0.06	50,50,50,50	0
56	MG	1A	3687	1/1	0.96	0.07	38,38,38,38	0
56	MG	1X	101	1/1	0.96	0.27	44,44,44,44	0
56	MG	1A	3688	1/1	0.96	0.09	41,41,41,41	0
56	MG	1a	1767	1/1	0.96	0.07	50,50,50,50	0
56	MG	1A	3019	1/1	0.96	0.14	46,46,46,46	0
56	MG	1A	4020	1/1	0.96	0.09	51,51,51,51	0
56	MG	1X	107	1/1	0.96	0.06	52,52,52,52	0
56	MG	2A	3745	1/1	0.96	0.14	66,66,66,66	0
56	MG	1Y	201	1/1	0.96	0.12	52,52,52,52	0
56	MG	1A	3310	1/1	0.96	0.24	63,63,63,63	0
56	MG	2A	3748	1/1	0.96	0.10	67,67,67,67	0
56	MG	1A	3692	1/1	0.96	0.09	29,29,29,29	0
56	MG	2a	1741	1/1	0.96	0.06	72,72,72,72	0
56	MG	2A	3750	1/1	0.96	0.08	42,42,42,42	0
56	MG	1A	3132	1/1	0.96	0.06	42,42,42,42	0
56	MG	1A	3184	1/1	0.96	0.08	39,39,39,39	0
56	MG	1A	3695	1/1	0.96	0.10	54,54,54,54	0
56	MG	2a	1746	1/1	0.96	0.12	58,58,58,58	0
56	MG	1Z	303	1/1	0.96	0.06	49,49,49,49	0
56	MG	1A	3248	1/1	0.96	0.26	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	10	101	1/1	0.96	0.10	44,44,44,44	0
56	MG	1A	3698	1/1	0.96	0.06	35,35,35,35	0
56	MG	1A	3134	1/1	0.96	0.09	42,42,42,42	0
56	MG	2a	1752	1/1	0.96	0.16	48,48,48,48	0
56	MG	2A	3195	1/1	0.96	0.10	34,34,34,34	0
56	MG	2A	3762	1/1	0.96	0.08	54,54,54,54	0
56	MG	2a	1755	1/1	0.96	0.15	56,56,56,56	0
56	MG	1A	3852	1/1	0.96	0.07	50,50,50,50	0
56	MG	10	105	1/1	0.96	0.10	62,62,62,62	0
56	MG	1A	4032	1/1	0.96	0.05	44,44,44,44	0
56	MG	2A	3201	1/1	0.96	0.21	70,70,70,70	0
56	MG	1A	3460	1/1	0.96	0.26	36,36,36,36	0
56	MG	10	108	1/1	0.96	0.07	44,44,44,44	0
56	MG	11	102	1/1	0.96	0.11	45,45,45,45	0
56	MG	1A	3378	1/1	0.96	0.10	44,44,44,44	0
56	MG	1A	3316	1/1	0.96	0.06	38,38,38,38	0
56	MG	1A	3381	1/1	0.96	0.15	29,29,29,29	0
56	MG	13	102	1/1	0.96	0.08	45,45,45,45	0
56	MG	1A	3563	1/1	0.96	0.10	52,52,52,52	0
56	MG	2A	3776	1/1	0.96	0.18	62,62,62,62	0
56	MG	1A	3193	1/1	0.96	0.26	30,30,30,30	0
56	MG	2a	1774	1/1	0.96	0.16	50,50,50,50	0
56	MG	1A	3465	1/1	0.96	0.09	60,60,60,60	0
56	MG	1A	3570	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3863	1/1	0.96	0.15	31,31,31,31	0
56	MG	1a	1803	1/1	0.96	0.06	58,58,58,58	0
56	MG	2A	3468	1/1	0.96	0.06	55,55,55,55	0
56	MG	1A	3864	1/1	0.96	0.21	38,38,38,38	0
56	MG	15	107	1/1	0.96	0.19	39,39,39,39	0
56	MG	1A	3135	1/1	0.96	0.21	30,30,30,30	0
56	MG	1A	3321	1/1	0.96	0.10	53,53,53,53	0
56	MG	1A	3712	1/1	0.96	0.10	31,31,31,31	0
56	MG	1A	3870	1/1	0.96	0.06	40,40,40,40	0
56	MG	17	102	1/1	0.96	0.16	34,34,34,34	0
56	MG	2a	1787	1/1	0.96	0.10	51,51,51,51	0
56	MG	2A	3223	1/1	0.96	0.35	42,42,42,42	0
56	MG	1A	4053	1/1	0.96	0.07	50,50,50,50	0
56	MG	1A	4054	1/1	0.96	0.06	42,42,42,42	0
56	MG	18	101	1/1	0.96	0.18	57,57,57,57	0
56	MG	1A	4056	1/1	0.96	0.05	44,44,44,44	0
56	MG	2A	3797	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	3575	1/1	0.96	0.11	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	1A	4058	1/1	0.96	0.07	52,52,52,52	0
56	MG	1k	201	1/1	0.96	0.13	47,47,47,47	0
56	MG	1A	3576	1/1	0.96	0.17	53,53,53,53	0
56	MG	1l	202	1/1	0.96	0.07	57,57,57,57	0
56	MG	1A	3874	1/1	0.96	0.07	29,29,29,29	0
56	MG	2a	1800	1/1	0.96	0.17	57,57,57,57	0
56	MG	1A	3875	1/1	0.96	0.09	28,28,28,28	0
56	MG	1A	3323	1/1	0.96	0.11	47,47,47,47	0
56	MG	1A	3578	1/1	0.96	0.08	48,48,48,48	0
56	MG	1a	1606	1/1	0.96	0.08	54,54,54,54	0
56	MG	1A	3469	1/1	0.96	0.14	51,51,51,51	0
56	MG	1a	1608	1/1	0.96	0.06	55,55,55,55	0
56	MG	1A	3057	1/1	0.96	0.17	45,45,45,45	0
56	MG	1a	1611	1/1	0.96	0.14	27,27,27,27	0
56	MG	2A	3244	1/1	0.96	0.09	58,58,58,58	0
56	MG	1A	3029	1/1	0.96	0.32	29,29,29,29	0
56	MG	1A	3882	1/1	0.96	0.11	21,21,21,21	0
56	MG	1A	3473	1/1	0.96	0.07	42,42,42,42	0
56	MG	1A	3475	1/1	0.96	0.12	37,37,37,37	0
56	MG	2A	3825	1/1	0.96	0.10	47,47,47,47	0
56	MG	2A	3507	1/1	0.96	0.07	48,48,48,48	0
56	MG	2A	3508	1/1	0.96	0.12	44,44,44,44	0
56	MG	2A	3830	1/1	0.96	0.07	66,66,66,66	0
56	MG	1A	3043	1/1	0.96	0.21	27,27,27,27	0
56	MG	2A	3512	1/1	0.96	0.09	71,71,71,71	0
56	MG	1A	3392	1/1	0.96	0.07	50,50,50,50	0
56	MG	1a	1619	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	3478	1/1	0.96	0.10	49,49,49,49	0
56	MG	2A	3256	1/1	0.96	0.13	56,56,56,56	0
56	MG	1A	3201	1/1	0.96	0.09	32,32,32,32	0
56	MG	1x	106	1/1	0.96	0.08	41,41,41,41	0
56	MG	2A	3520	1/1	0.96	0.08	31,31,31,31	0
56	MG	1A	3892	1/1	0.96	0.18	48,48,48,48	0
56	MG	1x	108	1/1	0.96	0.16	58,58,58,58	0
56	MG	1A	3893	1/1	0.96	0.08	45,45,45,45	0
56	MG	1A	3394	1/1	0.96	0.12	66,66,66,66	0
56	MG	1A	3258	1/1	0.96	0.04	39,39,39,39	0
56	MG	1A	3024	1/1	0.96	0.08	29,29,29,29	0
56	MG	1a	1628	1/1	0.96	0.08	51,51,51,51	0
56	MG	1x	114	1/1	0.96	0.12	62,62,62,62	0
56	MG	1A	3483	1/1	0.96	0.18	48,48,48,48	0
56	MG	2A	3271	1/1	0.96	0.06	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	3737	1/1	0.96	0.10	52,52,52,52	0
56	MG	2A	3535	1/1	0.96	0.10	39,39,39,39	0
56	MG	2A	3536	1/1	0.96	0.07	35,35,35,35	0
56	MG	2A	3537	1/1	0.96	0.07	50,50,50,50	0
56	MG	2A	3538	1/1	0.96	0.09	40,40,40,40	0
56	MG	2v	103	1/1	0.96	0.15	50,50,50,50	0
56	MG	1A	3593	1/1	0.96	0.07	39,39,39,39	0
56	MG	2A	3542	1/1	0.96	0.09	39,39,39,39	0
56	MG	2A	3002	1/1	0.96	0.15	43,43,43,43	0
56	MG	1a	1634	1/1	0.96	0.26	58,58,58,58	0
56	MG	2A	3004	1/1	0.96	0.10	48,48,48,48	0
56	MG	2A	3278	1/1	0.96	0.07	55,55,55,55	0
56	MG	2B	218	1/1	0.96	0.19	68,68,68,68	0
56	MG	1A	3087	1/1	0.96	0.31	38,38,38,38	0
56	MG	1A	3006	1/1	0.96	0.21	54,54,54,54	0
56	MG	2A	3552	1/1	0.96	0.07	37,37,37,37	0
56	MG	2x	105	1/1	0.96	0.07	61,61,61,61	0
56	MG	2D	304	1/1	0.96	0.10	49,49,49,49	0
56	MG	1A	3149	1/1	0.96	0.18	39,39,39,39	0
56	MG	2A	3008	1/1	0.96	0.09	41,41,41,41	0
56	MG	2A	3557	1/1	0.96	0.10	57,57,57,57	0
56	MG	2y	103	1/1	0.96	0.05	66,66,66,66	0
56	MG	1A	3150	1/1	0.96	0.08	35,35,35,35	0
56	MG	2A	3559	1/1	0.96	0.06	40,40,40,40	0
56	MG	2A	3010	1/1	0.96	0.28	57,57,57,57	0
56	MG	1A	4091	1/1	0.96	0.20	65,65,65,65	0
56	MG	1A	3489	1/1	0.96	0.13	50,50,50,50	0
56	MG	1A	4094	1/1	0.96	0.09	47,47,47,47	0
56	MG	1A	4095	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	3403	1/1	0.96	0.17	48,48,48,48	0
56	MG	1A	4097	1/1	0.96	0.16	42,42,42,42	0
56	MG	2A	3087	1/1	0.97	0.06	48,48,48,48	0
56	MG	2W	203	1/1	0.97	0.11	58,58,58,58	0
56	MG	2X	101	1/1	0.97	0.06	59,59,59,59	0
56	MG	1P	202	1/1	0.97	0.19	32,32,32,32	0
56	MG	1A	3322	1/1	0.97	0.13	35,35,35,35	0
56	MG	2A	3091	1/1	0.97	0.09	51,51,51,51	0
56	MG	1A	3396	1/1	0.97	0.04	28,28,28,28	0
56	MG	1a	1710	1/1	0.97	0.14	45,45,45,45	0
56	MG	1A	4010	1/1	0.97	0.05	49,49,49,49	0
56	MG	1A	3020	1/1	0.97	0.11	54,54,54,54	0
56	MG	1A	3398	1/1	0.97	0.10	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4013	1/1	0.97	0.07	50,50,50,50	0
56	MG	1A	3044	1/1	0.97	0.17	30,30,30,30	0
56	MG	2A	3625	1/1	0.97	0.05	43,43,43,43	0
56	MG	1a	1716	1/1	0.97	0.13	44,44,44,44	0
56	MG	1R	202	1/1	0.97	0.08	43,43,43,43	0
56	MG	2A	3102	1/1	0.97	0.10	39,39,39,39	0
56	MG	27	101	1/1	0.97	0.04	44,44,44,44	0
56	MG	2A	3103	1/1	0.97	0.11	44,44,44,44	0
56	MG	1R	203	1/1	0.97	0.14	28,28,28,28	0
56	MG	1R	204	1/1	0.97	0.25	37,37,37,37	0
56	MG	1A	3711	1/1	0.97	0.15	48,48,48,48	0
56	MG	1R	206	1/1	0.97	0.17	28,28,28,28	0
56	MG	1A	3253	1/1	0.97	0.12	45,45,45,45	0
56	MG	1A	3714	1/1	0.97	0.08	48,48,48,48	0
56	MG	1A	3196	1/1	0.97	0.06	38,38,38,38	0
56	MG	1A	4021	1/1	0.97	0.06	43,43,43,43	0
56	MG	2A	3113	1/1	0.97	0.06	32,32,32,32	0
56	MG	1A	3148	1/1	0.97	0.11	27,27,27,27	0
56	MG	2A	3362	1/1	0.97	0.05	59,59,59,59	0
56	MG	1a	1728	1/1	0.97	0.15	54,54,54,54	0
56	MG	2A	3116	1/1	0.97	0.17	53,53,53,53	0
56	MG	1U	201	1/1	0.97	0.14	34,34,34,34	0
56	MG	1A	3856	1/1	0.97	0.09	27,27,27,27	0
56	MG	1A	3256	1/1	0.97	0.13	39,39,39,39	0
56	MG	1a	1732	1/1	0.97	0.08	48,48,48,48	0
56	MG	2A	3121	1/1	0.97	0.15	40,40,40,40	0
56	MG	1a	1733	1/1	0.97	0.09	47,47,47,47	0
56	MG	1A	3030	1/1	0.97	0.08	29,29,29,29	0
56	MG	1U	205	1/1	0.97	0.16	37,37,37,37	0
56	MG	2A	3373	1/1	0.97	0.07	52,52,52,52	0
56	MG	1A	3330	1/1	0.97	0.06	36,36,36,36	0
56	MG	2A	3126	1/1	0.97	0.07	46,46,46,46	0
56	MG	1U	208	1/1	0.97	0.22	30,30,30,30	0
56	MG	1A	3199	1/1	0.97	0.20	25,25,25,25	0
56	MG	1A	4028	1/1	0.97	0.11	31,31,31,31	0
56	MG	1A	3861	1/1	0.97	0.04	37,37,37,37	0
56	MG	1A	3722	1/1	0.97	0.08	27,27,27,27	0
56	MG	1W	201	1/1	0.97	0.12	41,41,41,41	0
56	MG	2A	3382	1/1	0.97	0.10	54,54,54,54	0
56	MG	1A	3200	1/1	0.97	0.06	36,36,36,36	0
56	MG	1A	3260	1/1	0.97	0.08	50,50,50,50	0
56	MG	1W	205	1/1	0.97	0.08	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	3865	1/1	0.97	0.22	31,31,31,31	0
56	MG	1A	4034	1/1	0.97	0.08	23,23,23,23	0
56	MG	2A	3139	1/1	0.97	0.12	49,49,49,49	0
56	MG	2A	3667	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3119	1/1	0.97	0.10	36,36,36,36	0
56	MG	1A	3120	1/1	0.97	0.30	42,42,42,42	0
56	MG	1X	103	1/1	0.97	0.05	38,38,38,38	0
56	MG	1A	3868	1/1	0.97	0.20	41,41,41,41	0
56	MG	1X	105	1/1	0.97	0.09	44,44,44,44	0
56	MG	1A	4038	1/1	0.97	0.17	63,63,63,63	0
56	MG	1a	1757	1/1	0.97	0.05	46,46,46,46	0
56	MG	1A	3495	1/1	0.97	0.10	59,59,59,59	0
56	MG	1A	3599	1/1	0.97	0.08	42,42,42,42	0
56	MG	1A	3336	1/1	0.97	0.10	37,37,37,37	0
56	MG	1A	3731	1/1	0.97	0.04	54,54,54,54	0
56	MG	1Y	204	1/1	0.97	0.21	52,52,52,52	0
56	MG	1a	1763	1/1	0.97	0.10	55,55,55,55	0
56	MG	1A	3154	1/1	0.97	0.09	46,46,46,46	0
56	MG	1A	3155	1/1	0.97	0.27	36,36,36,36	0
56	MG	1A	3073	1/1	0.97	0.12	30,30,30,30	0
56	MG	1A	3049	1/1	0.97	0.10	33,33,33,33	0
56	MG	1A	3416	1/1	0.97	0.06	50,50,50,50	0
56	MG	2A	3159	1/1	0.97	0.06	38,38,38,38	0
56	MG	2A	3160	1/1	0.97	0.11	47,47,47,47	0
56	MG	1A	3606	1/1	0.97	0.06	40,40,40,40	0
56	MG	1A	3209	1/1	0.97	0.08	45,45,45,45	0
56	MG	2A	3692	1/1	0.97	0.05	53,53,53,53	0
56	MG	1A	3608	1/1	0.97	0.04	33,33,33,33	0
56	MG	1A	3504	1/1	0.97	0.16	45,45,45,45	0
56	MG	2A	3165	1/1	0.97	0.06	58,58,58,58	0
56	MG	1a	1774	1/1	0.97	0.10	60,60,60,60	0
56	MG	1A	3210	1/1	0.97	0.07	43,43,43,43	0
56	MG	1A	3746	1/1	0.97	0.10	48,48,48,48	0
56	MG	2a	1664	1/1	0.97	0.15	44,44,44,44	0
56	MG	1A	3076	1/1	0.97	0.06	32,32,32,32	0
56	MG	1A	3507	1/1	0.97	0.26	32,32,32,32	0
56	MG	2a	1667	1/1	0.97	0.05	43,43,43,43	0
56	MG	2A	3702	1/1	0.97	0.04	49,49,49,49	0
56	MG	2A	3171	1/1	0.97	0.08	59,59,59,59	0
56	MG	11	101	1/1	0.97	0.29	43,43,43,43	0
56	MG	1A	3888	1/1	0.97	0.07	54,54,54,54	0
56	MG	2A	3708	1/1	0.97	0.06	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	1A	3889	1/1	0.97	0.09	25,25,25,25	0
56	MG	2A	3424	1/1	0.97	0.23	51,51,51,51	0
56	MG	1A	3050	1/1	0.97	0.06	22,22,22,22	0
56	MG	11	106	1/1	0.97	0.07	54,54,54,54	0
56	MG	2A	3714	1/1	0.97	0.06	56,56,56,56	0
56	MG	1A	3079	1/1	0.97	0.19	45,45,45,45	0
56	MG	2A	3428	1/1	0.97	0.29	62,62,62,62	0
56	MG	12	102	1/1	0.97	0.11	44,44,44,44	0
56	MG	2A	3179	1/1	0.97	0.11	53,53,53,53	0
56	MG	1A	3346	1/1	0.97	0.16	32,32,32,32	0
56	MG	2A	3721	1/1	0.97	0.14	48,48,48,48	0
56	MG	1A	3620	1/1	0.97	0.05	44,44,44,44	0
56	MG	2A	3723	1/1	0.97	0.12	49,49,49,49	0
56	MG	1A	3274	1/1	0.97	0.06	39,39,39,39	0
56	MG	15	101	1/1	0.97	0.16	35,35,35,35	0
56	MG	2A	3435	1/1	0.97	0.20	49,49,49,49	0
56	MG	1A	3161	1/1	0.97	0.36	34,34,34,34	0
56	MG	1A	3624	1/1	0.97	0.08	27,27,27,27	0
56	MG	1A	3039	1/1	0.97	0.31	43,43,43,43	0
56	MG	1A	3218	1/1	0.97	0.16	40,40,40,40	0
56	MG	1A	3900	1/1	0.97	0.06	38,38,38,38	0
56	MG	1A	3283	1/1	0.97	0.39	32,32,32,32	0
56	MG	2A	3191	1/1	0.97	0.13	56,56,56,56	0
56	MG	2A	3192	1/1	0.97	0.12	49,49,49,49	0
56	MG	1A	3352	1/1	0.97	0.13	49,49,49,49	0
56	MG	1a	1801	1/1	0.97	0.05	58,58,58,58	0
56	MG	1A	3519	1/1	0.97	0.04	49,49,49,49	0
56	MG	2a	1700	1/1	0.97	0.06	48,48,48,48	0
56	MG	1A	3284	1/1	0.97	0.08	48,48,48,48	0
56	MG	17	101	1/1	0.97	0.15	40,40,40,40	0
56	MG	2A	3199	1/1	0.97	0.07	40,40,40,40	0
56	MG	1A	3521	1/1	0.97	0.08	52,52,52,52	0
56	MG	17	103	1/1	0.97	0.11	53,53,53,53	0
56	MG	1A	3633	1/1	0.97	0.04	15,15,15,15	0
56	MG	1A	3128	1/1	0.97	0.07	31,31,31,31	0
56	MG	1A	3767	1/1	0.97	0.07	47,47,47,47	0
56	MG	18	102	1/1	0.97	0.09	47,47,47,47	0
56	MG	18	103	1/1	0.97	0.13	43,43,43,43	0
56	MG	1A	3912	1/1	0.97	0.06	47,47,47,47	0
56	MG	18	105	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3286	1/1	0.97	0.06	31,31,31,31	0
56	MG	1A	3434	1/1	0.97	0.07	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	3637	1/1	0.97	0.05	30,30,30,30	0
56	MG	2a	1716	1/1	0.97	0.11	64,64,64,64	0
56	MG	2A	3464	1/1	0.97	0.20	40,40,40,40	0
56	MG	1A	3772	1/1	0.97	0.11	65,65,65,65	0
56	MG	1A	3773	1/1	0.97	0.11	25,25,25,25	0
56	MG	2A	3757	1/1	0.97	0.07	59,59,59,59	0
56	MG	1A	3220	1/1	0.97	0.06	39,39,39,39	0
56	MG	1A	4093	1/1	0.97	0.06	43,43,43,43	0
56	MG	2a	1723	1/1	0.97	0.26	52,52,52,52	0
56	MG	2A	3760	1/1	0.97	0.06	66,66,66,66	0
56	MG	1A	3083	1/1	0.97	0.15	28,28,28,28	0
56	MG	1A	3166	1/1	0.97	0.08	32,32,32,32	0
56	MG	1A	3922	1/1	0.97	0.05	65,65,65,65	0
56	MG	1a	1609	1/1	0.97	0.15	48,48,48,48	0
56	MG	2a	1729	1/1	0.97	0.17	66,66,66,66	0
56	MG	1A	3777	1/1	0.97	0.05	42,42,42,42	0
56	MG	1A	3927	1/1	0.97	0.06	33,33,33,33	0
56	MG	1A	3778	1/1	0.97	0.04	29,29,29,29	0
56	MG	1A	3359	1/1	0.97	0.19	59,59,59,59	0
56	MG	1A	3130	1/1	0.97	0.10	38,38,38,38	0
56	MG	1a	1615	1/1	0.97	0.08	53,53,53,53	0
56	MG	2a	1736	1/1	0.97	0.23	57,57,57,57	0
56	MG	2A	3479	1/1	0.97	0.08	47,47,47,47	0
56	MG	1B	205	1/1	0.97	0.10	53,53,53,53	0
56	MG	1A	3933	1/1	0.97	0.11	59,59,59,59	0
56	MG	1A	3643	1/1	0.97	0.06	28,28,28,28	0
56	MG	1B	208	1/1	0.97	0.11	54,54,54,54	0
56	MG	1a	1620	1/1	0.97	0.05	47,47,47,47	0
56	MG	2A	3232	1/1	0.97	0.50	47,47,47,47	0
56	MG	2A	3486	1/1	0.97	0.15	43,43,43,43	0
56	MG	1B	209	1/1	0.97	0.08	52,52,52,52	0
56	MG	1A	3441	1/1	0.97	0.15	40,40,40,40	0
56	MG	1A	3168	1/1	0.97	0.14	59,59,59,59	0
56	MG	1A	3937	1/1	0.97	0.04	43,43,43,43	0
56	MG	2A	3237	1/1	0.97	0.16	47,47,47,47	0
56	MG	2A	3493	1/1	0.97	0.12	43,43,43,43	0
56	MG	1A	3646	1/1	0.97	0.08	33,33,33,33	0
56	MG	1A	3787	1/1	0.97	0.09	24,24,24,24	0
56	MG	1A	3292	1/1	0.97	0.13	25,25,25,25	0
56	MG	1B	216	1/1	0.97	0.06	58,58,58,58	0
56	MG	1B	217	1/1	0.97	0.09	45,45,45,45	0
56	MG	2a	1756	1/1	0.97	0.09	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	3226	1/1	0.97	0.07	28,28,28,28	0
56	MG	2A	3501	1/1	0.97	0.09	34,34,34,34	0
56	MG	2a	1759	1/1	0.97	0.10	66,66,66,66	0
56	MG	1A	3534	1/1	0.97	0.04	22,22,22,22	0
56	MG	2A	3245	1/1	0.97	0.11	44,44,44,44	0
56	MG	2A	3796	1/1	0.97	0.07	32,32,32,32	0
56	MG	2A	3246	1/1	0.97	0.13	47,47,47,47	0
56	MG	2A	3799	1/1	0.97	0.16	36,36,36,36	0
56	MG	1a	1633	1/1	0.97	0.12	35,35,35,35	0
56	MG	2a	1766	1/1	0.97	0.17	55,55,55,55	0
56	MG	2A	3803	1/1	0.97	0.06	55,55,55,55	0
56	MG	1A	3535	1/1	0.97	0.15	43,43,43,43	0
56	MG	2A	3249	1/1	0.97	0.08	55,55,55,55	0
56	MG	1A	3792	1/1	0.97	0.05	41,41,41,41	0
56	MG	1A	3445	1/1	0.97	0.06	59,59,59,59	0
56	MG	1A	3227	1/1	0.97	0.08	23,23,23,23	0
56	MG	1A	3169	1/1	0.97	0.04	39,39,39,39	0
56	MG	1A	3229	1/1	0.97	0.11	47,47,47,47	0
56	MG	1A	3040	1/1	0.97	0.21	28,28,28,28	0
56	MG	1A	3085	1/1	0.97	0.09	34,34,34,34	0
56	MG	2A	3518	1/1	0.97	0.09	54,54,54,54	0
56	MG	1B	228	1/1	0.97	0.07	37,37,37,37	0
56	MG	1A	3659	1/1	0.97	0.07	29,29,29,29	0
56	MG	1A	3172	1/1	0.97	0.07	36,36,36,36	0
56	MG	2A	3011	1/1	0.97	0.17	42,42,42,42	0
56	MG	2A	3820	1/1	0.97	0.06	54,54,54,54	0
56	MG	1a	1645	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3370	1/1	0.97	0.16	47,47,47,47	0
56	MG	1A	3177	1/1	0.97	0.09	18,18,18,18	0
56	MG	1A	3301	1/1	0.97	0.10	35,35,35,35	0
56	MG	2A	3016	1/1	0.97	0.20	50,50,50,50	0
56	MG	1A	3667	1/1	0.97	0.08	22,22,22,22	0
56	MG	1A	3669	1/1	0.97	0.06	28,28,28,28	0
56	MG	2A	3532	1/1	0.97	0.13	45,45,45,45	0
56	MG	2A	3831	1/1	0.97	0.13	57,57,57,57	0
56	MG	1A	3958	1/1	0.97	0.10	55,55,55,55	0
56	MG	1D	301	1/1	0.97	0.08	32,32,32,32	0
56	MG	2A	3021	1/1	0.97	0.13	46,46,46,46	0
56	MG	1A	3808	1/1	0.97	0.15	24,24,24,24	0
56	MG	1D	303	1/1	0.97	0.14	44,44,44,44	0
56	MG	2A	3276	1/1	0.97	0.24	47,47,47,47	0
56	MG	1A	3546	1/1	0.97	0.11	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	3547	1/1	0.97	0.14	38,38,38,38	0
56	MG	1A	3234	1/1	0.97	0.21	34,34,34,34	0
56	MG	1A	3812	1/1	0.97	0.08	34,34,34,34	0
56	MG	1D	311	1/1	0.97	0.21	33,33,33,33	0
56	MG	1A	3549	1/1	0.97	0.19	35,35,35,35	0
56	MG	1A	3550	1/1	0.97	0.05	29,29,29,29	0
56	MG	1A	3815	1/1	0.97	0.06	42,42,42,42	0
56	MG	2A	3550	1/1	0.97	0.07	30,30,30,30	0
56	MG	1E	301	1/1	0.97	0.17	41,41,41,41	0
56	MG	1A	3551	1/1	0.97	0.09	44,44,44,44	0
56	MG	1A	3133	1/1	0.97	0.07	43,43,43,43	0
56	MG	2A	3556	1/1	0.97	0.06	33,33,33,33	0
56	MG	2A	3039	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3458	1/1	0.97	0.09	35,35,35,35	0
56	MG	2A	3041	1/1	0.97	0.11	37,37,37,37	0
56	MG	1A	3064	1/1	0.97	0.13	46,46,46,46	0
56	MG	1A	3306	1/1	0.97	0.12	45,45,45,45	0
56	MG	2A	3044	1/1	0.97	0.21	50,50,50,50	0
56	MG	1A	3108	1/1	0.97	0.28	27,27,27,27	0
56	MG	1A	3822	1/1	0.97	0.05	43,43,43,43	0
56	MG	1A	3240	1/1	0.97	0.18	32,32,32,32	0
56	MG	1A	3109	1/1	0.97	0.05	36,36,36,36	0
56	MG	1E	315	1/1	0.97	0.04	36,36,36,36	0
56	MG	1F	301	1/1	0.97	0.07	44,44,44,44	0
56	MG	1A	3977	1/1	0.97	0.07	30,30,30,30	0
56	MG	1a	1677	1/1	0.97	0.06	38,38,38,38	0
56	MG	2D	302	1/1	0.97	0.21	51,51,51,51	0
56	MG	2d	302	1/1	0.97	0.06	58,58,58,58	0
56	MG	1A	3311	1/1	0.97	0.05	51,51,51,51	0
56	MG	2f	201	1/1	0.97	0.07	43,43,43,43	0
56	MG	2A	3574	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3561	1/1	0.97	0.06	17,17,17,17	0
56	MG	2A	3576	1/1	0.97	0.08	74,74,74,74	0
56	MG	1F	306	1/1	0.97	0.07	37,37,37,37	0
56	MG	2A	3057	1/1	0.97	0.09	55,55,55,55	0
56	MG	2E	303	1/1	0.97	0.15	49,49,49,49	0
56	MG	2E	304	1/1	0.97	0.18	49,49,49,49	0
56	MG	2E	305	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3138	1/1	0.97	0.12	45,45,45,45	0
56	MG	1A	3690	1/1	0.97	0.09	28,28,28,28	0
56	MG	2q	202	1/1	0.97	0.05	77,77,77,77	0
56	MG	1A	3010	1/1	0.97	0.06	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	3009	1/1	0.97	0.08	24,24,24,24	0
56	MG	2A	3062	1/1	0.97	0.10	27,27,27,27	0
56	MG	1A	3567	1/1	0.97	0.08	25,25,25,25	0
56	MG	1A	3185	1/1	0.97	0.03	32,32,32,32	0
56	MG	1A	3990	1/1	0.97	0.09	50,50,50,50	0
56	MG	1A	3386	1/1	0.97	0.21	26,26,26,26	0
56	MG	1A	3696	1/1	0.97	0.09	28,28,28,28	0
56	MG	1A	3470	1/1	0.97	0.13	42,42,42,42	0
56	MG	2F	308	1/1	0.97	0.17	36,36,36,36	0
56	MG	1A	3994	1/1	0.97	0.05	31,31,31,31	0
56	MG	1A	3995	1/1	0.97	0.07	28,28,28,28	0
56	MG	2A	3071	1/1	0.97	0.17	51,51,51,51	0
56	MG	2A	3321	1/1	0.97	0.07	62,62,62,62	0
56	MG	1A	3996	1/1	0.97	0.04	25,25,25,25	0
56	MG	1A	3114	1/1	0.97	0.09	36,36,36,36	0
56	MG	1N	201	1/1	0.97	0.14	36,36,36,36	0
56	MG	2A	3075	1/1	0.97	0.12	54,54,54,54	0
56	MG	1N	202	1/1	0.97	0.07	38,38,38,38	0
56	MG	1N	203	1/1	0.97	0.07	43,43,43,43	0
56	MG	1A	3317	1/1	0.97	0.16	46,46,46,46	0
56	MG	1A	4000	1/1	0.97	0.06	38,38,38,38	0
56	MG	2T	201	1/1	0.97	0.07	61,61,61,61	0
56	MG	1A	3188	1/1	0.97	0.11	40,40,40,40	0
56	MG	1A	3474	1/1	0.97	0.07	42,42,42,42	0
57	K	1A	3557	1/1	0.97	0.10	64,64,64,64	0
56	MG	1A	3842	1/1	0.97	0.11	40,40,40,40	0
56	MG	1A	3319	1/1	0.97	0.14	39,39,39,39	0
56	MG	1A	3192	1/1	0.97	0.28	39,39,39,39	0
56	MG	1A	3145	1/1	0.97	0.09	30,30,30,30	0
56	MG	1P	201	1/1	0.97	0.17	31,31,31,31	0
56	MG	2D	305	1/1	0.98	0.08	25,25,25,25	0
56	MG	1A	3502	1/1	0.98	0.12	32,32,32,32	0
56	MG	17	104	1/1	0.98	0.06	39,39,39,39	0
56	MG	1A	4062	1/1	0.98	0.06	31,31,31,31	0
56	MG	2E	301	1/1	0.98	0.05	52,52,52,52	0
56	MG	2A	3258	1/1	0.98	0.07	56,56,56,56	0
56	MG	1A	3391	1/1	0.98	0.08	60,60,60,60	0
56	MG	2A	3260	1/1	0.98	0.05	65,65,65,65	0
56	MG	2A	3549	1/1	0.98	0.07	55,55,55,55	0
56	MG	1A	3082	1/1	0.98	0.10	35,35,35,35	0
56	MG	2A	3551	1/1	0.98	0.05	57,57,57,57	0
56	MG	1A	4065	1/1	0.98	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	2A	3263	1/1	0.98	0.04	57,57,57,57	0
56	MG	1A	3239	1/1	0.98	0.21	29,29,29,29	0
56	MG	2A	3716	1/1	0.98	0.13	39,39,39,39	0
56	MG	1A	3046	1/1	0.98	0.05	28,28,28,28	0
56	MG	1A	3710	1/1	0.98	0.15	45,45,45,45	0
56	MG	1a	1717	1/1	0.98	0.11	35,35,35,35	0
56	MG	1A	3568	1/1	0.98	0.32	33,33,33,33	0
56	MG	1A	3056	1/1	0.98	0.03	24,24,24,24	0
56	MG	1A	3033	1/1	0.98	0.17	26,26,26,26	0
56	MG	1A	3452	1/1	0.98	0.15	38,38,38,38	0
56	MG	1H	201	1/1	0.98	0.15	60,60,60,60	0
56	MG	1A	3878	1/1	0.98	0.09	51,51,51,51	0
56	MG	1A	4074	1/1	0.98	0.05	53,53,53,53	0
56	MG	1A	3796	1/1	0.98	0.04	50,50,50,50	0
56	MG	2A	3568	1/1	0.98	0.07	33,33,33,33	0
56	MG	1A	3572	1/1	0.98	0.05	29,29,29,29	0
56	MG	1A	3510	1/1	0.98	0.19	40,40,40,40	0
56	MG	1A	3574	1/1	0.98	0.03	41,41,41,41	0
56	MG	2A	3417	1/1	0.98	0.23	50,50,50,50	0
56	MG	1A	4079	1/1	0.98	0.05	48,48,48,48	0
56	MG	1A	3162	1/1	0.98	0.21	51,51,51,51	0
56	MG	2R	204	1/1	0.98	0.12	48,48,48,48	0
56	MG	2A	3735	1/1	0.98	0.17	64,64,64,64	0
56	MG	1A	4081	1/1	0.98	0.05	60,60,60,60	0
56	MG	1A	3106	1/1	0.98	0.04	24,24,24,24	0
56	MG	1A	3802	1/1	0.98	0.05	48,48,48,48	0
56	MG	1A	3721	1/1	0.98	0.05	26,26,26,26	0
56	MG	1a	1735	1/1	0.98	0.09	39,39,39,39	0
56	MG	2A	3580	1/1	0.98	0.06	32,32,32,32	0
56	MG	1A	3202	1/1	0.98	0.04	40,40,40,40	0
56	MG	1A	3086	1/1	0.98	0.18	31,31,31,31	0
56	MG	2A	3150	1/1	0.98	0.14	39,39,39,39	0
56	MG	1P	203	1/1	0.98	0.21	24,24,24,24	0
56	MG	1A	3515	1/1	0.98	0.04	40,40,40,40	0
56	MG	1A	3247	1/1	0.98	0.15	37,37,37,37	0
56	MG	20	102	1/1	0.98	0.09	52,52,52,52	0
56	MG	1a	1741	1/1	0.98	0.11	53,53,53,53	0
56	MG	1A	3891	1/1	0.98	0.05	45,45,45,45	0
56	MG	1A	3986	1/1	0.98	0.05	11,11,11,11	0
56	MG	2A	3295	1/1	0.98	0.07	52,52,52,52	0
56	MG	1A	3726	1/1	0.98	0.04	44,44,44,44	0
56	MG	1A	3204	1/1	0.98	0.05	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3058	1/1	0.98	0.04	25,25,25,25	0
56	MG	1A	3651	1/1	0.98	0.03	26,26,26,26	0
56	MG	1A	3071	1/1	0.98	0.04	11,11,11,11	0
56	MG	1A	3110	1/1	0.98	0.18	29,29,29,29	0
56	MG	2A	3029	1/1	0.98	0.05	46,46,46,46	0
56	MG	1A	3034	1/1	0.98	0.21	29,29,29,29	0
56	MG	1A	3733	1/1	0.98	0.07	31,31,31,31	0
56	MG	1A	3137	1/1	0.98	0.05	40,40,40,40	0
56	MG	1A	3303	1/1	0.98	0.16	24,24,24,24	0
56	MG	2A	3035	1/1	0.98	0.10	34,34,34,34	0
56	MG	1A	3999	1/1	0.98	0.04	39,39,39,39	0
56	MG	2a	1768	1/1	0.98	0.09	60,60,60,60	0
56	MG	1A	3657	1/1	0.98	0.06	38,38,38,38	0
56	MG	1A	3022	1/1	0.98	0.10	37,37,37,37	0
56	MG	1A	4002	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3211	1/1	0.98	0.10	31,31,31,31	0
56	MG	1A	3739	1/1	0.98	0.05	37,37,37,37	0
56	MG	1A	3660	1/1	0.98	0.05	22,22,22,22	0
56	MG	2A	3771	1/1	0.98	0.09	41,41,41,41	0
56	MG	1A	3139	1/1	0.98	0.12	36,36,36,36	0
56	MG	1U	206	1/1	0.98	0.25	35,35,35,35	0
56	MG	1A	3742	1/1	0.98	0.05	41,41,41,41	0
56	MG	1a	1765	1/1	0.98	0.07	53,53,53,53	0
56	MG	1A	3911	1/1	0.98	0.08	48,48,48,48	0
56	MG	2A	3460	1/1	0.98	0.14	25,25,25,25	0
56	MG	1A	3307	1/1	0.98	0.08	39,39,39,39	0
56	MG	1A	3744	1/1	0.98	0.03	20,20,20,20	0
56	MG	2A	3620	1/1	0.98	0.05	37,37,37,37	0
56	MG	1V	202	1/1	0.98	0.19	31,31,31,31	0
56	MG	2A	3051	1/1	0.98	0.17	49,49,49,49	0
56	MG	1V	203	1/1	0.98	0.08	28,28,28,28	0
56	MG	2A	3624	1/1	0.98	0.04	49,49,49,49	0
56	MG	1V	204	1/1	0.98	0.11	39,39,39,39	0
56	MG	1A	3113	1/1	0.98	0.04	31,31,31,31	0
56	MG	1A	3173	1/1	0.98	0.31	33,33,33,33	0
56	MG	1A	3215	1/1	0.98	0.14	38,38,38,38	0
56	MG	1A	3668	1/1	0.98	0.04	25,25,25,25	0
56	MG	1A	3174	1/1	0.98	0.14	25,25,25,25	0
56	MG	1W	204	1/1	0.98	0.14	37,37,37,37	0
56	MG	2A	3792	1/1	0.98	0.07	30,30,30,30	0
56	MG	1A	3832	1/1	0.98	0.08	38,38,38,38	0
56	MG	1A	4017	1/1	0.98	0.03	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	4018	1/1	0.98	0.05	53,53,53,53	0
56	MG	2A	3197	1/1	0.98	0.08	51,51,51,51	0
56	MG	1A	3175	1/1	0.98	0.04	30,30,30,30	0
56	MG	1A	3834	1/1	0.98	0.04	59,59,59,59	0
56	MG	2A	3800	1/1	0.98	0.07	40,40,40,40	0
56	MG	1A	3925	1/1	0.98	0.06	35,35,35,35	0
56	MG	2A	3802	1/1	0.98	0.06	53,53,53,53	0
56	MG	1A	3751	1/1	0.98	0.06	40,40,40,40	0
56	MG	1a	1785	1/1	0.98	0.05	52,52,52,52	0
56	MG	2A	3203	1/1	0.98	0.04	52,52,52,52	0
56	MG	1A	3008	1/1	0.98	0.08	25,25,25,25	0
56	MG	1a	1787	1/1	0.98	0.08	45,45,45,45	0
56	MG	1A	3928	1/1	0.98	0.04	57,57,57,57	0
56	MG	1A	3092	1/1	0.98	0.08	51,51,51,51	0
56	MG	1A	3930	1/1	0.98	0.04	45,45,45,45	0
56	MG	1A	3021	1/1	0.98	0.06	30,30,30,30	0
56	MG	2A	3812	1/1	0.98	0.05	34,34,34,34	0
56	MG	1a	1792	1/1	0.98	0.05	60,60,60,60	0
56	MG	2A	3490	1/1	0.98	0.08	61,61,61,61	0
56	MG	1A	3421	1/1	0.98	0.13	44,44,44,44	0
56	MG	2A	3816	1/1	0.98	0.08	64,64,64,64	0
56	MG	1a	1794	1/1	0.98	0.07	58,58,58,58	0
56	MG	1A	3117	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3266	1/1	0.98	0.07	44,44,44,44	0
56	MG	1A	3077	1/1	0.98	0.03	27,27,27,27	0
56	MG	1A	3038	1/1	0.98	0.10	24,24,24,24	0
56	MG	1A	3045	1/1	0.98	0.07	37,37,37,37	0
56	MG	1A	3097	1/1	0.98	0.10	32,32,32,32	0
56	MG	1A	3098	1/1	0.98	0.10	19,19,19,19	0
56	MG	1a	1676	1/1	0.98	0.14	52,52,52,52	0
56	MG	1D	305	1/1	0.98	0.07	18,18,18,18	0
56	MG	2A	3827	1/1	0.98	0.12	55,55,55,55	0
56	MG	2A	3828	1/1	0.98	0.04	40,40,40,40	0
56	MG	1A	3186	1/1	0.98	0.14	38,38,38,38	0
56	MG	1D	307	1/1	0.98	0.14	28,28,28,28	0
56	MG	2A	3088	1/1	0.98	0.13	32,32,32,32	0
56	MG	1A	3611	1/1	0.98	0.09	28,28,28,28	0
56	MG	1A	3612	1/1	0.98	0.06	53,53,53,53	0
56	MG	2A	3509	1/1	0.98	0.06	37,37,37,37	0
56	MG	1A	3273	1/1	0.98	0.07	29,29,29,29	0
56	MG	2A	3511	1/1	0.98	0.05	47,47,47,47	0
56	MG	1A	3152	1/1	0.98	0.09	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	3769	1/1	0.98	0.06	25,25,25,25	0
56	MG	2A	3839	1/1	0.98	0.15	42,42,42,42	0
56	MG	2A	3094	1/1	0.98	0.06	49,49,49,49	0
56	MG	1A	3153	1/1	0.98	0.09	36,36,36,36	0
56	MG	1A	3189	1/1	0.98	0.07	37,37,37,37	0
56	MG	1I	104	1/1	0.98	0.04	43,43,43,43	0
56	MG	1A	4044	1/1	0.98	0.03	22,22,22,22	0
56	MG	1A	3277	1/1	0.98	0.06	33,33,33,33	0
56	MG	2A	3677	1/1	0.98	0.04	33,33,33,33	0
56	MG	1E	304	1/1	0.98	0.11	27,27,27,27	0
56	MG	1E	305	1/1	0.98	0.17	33,33,33,33	0
56	MG	13	101	1/1	0.98	0.04	31,31,31,31	0
56	MG	1A	3278	1/1	0.98	0.14	24,24,24,24	0
56	MG	1A	4047	1/1	0.98	0.04	49,49,49,49	0
56	MG	1A	3279	1/1	0.98	0.10	34,34,34,34	0
56	MG	2A	3527	1/1	0.98	0.07	44,44,44,44	0
56	MG	1A	4049	1/1	0.98	0.05	10,10,10,10	0
56	MG	1E	311	1/1	0.98	0.12	22,22,22,22	0
56	MG	2A	3108	1/1	0.98	0.12	58,58,58,58	0
56	MG	1A	3280	1/1	0.98	0.14	38,38,38,38	0
56	MG	1A	3190	1/1	0.98	0.21	42,42,42,42	0
56	MG	1A	3623	1/1	0.98	0.05	18,18,18,18	0
56	MG	1A	3440	1/1	0.98	0.14	43,43,43,43	0
56	MG	1A	4055	1/1	0.98	0.05	28,28,28,28	0
56	MG	2A	3694	1/1	0.98	0.06	35,35,35,35	0
56	MG	1A	3282	1/1	0.98	0.17	30,30,30,30	0
56	MG	1A	3123	1/1	0.98	0.14	35,35,35,35	0
56	MG	1A	3099	1/1	0.98	0.06	42,42,42,42	0
56	MG	2A	3540	1/1	0.98	0.11	40,40,40,40	0
56	MG	1A	3080	1/1	0.98	0.04	23,23,23,23	0
59	ZN	2Y	501	1/1	0.98	0.04	95,95,95,95	0
56	MG	1A	3065	1/1	0.98	0.08	37,37,37,37	0
56	MG	2A	3553	1/1	0.99	0.06	41,41,41,41	0
56	MG	1A	3074	1/1	0.99	0.04	16,16,16,16	0
56	MG	1A	3191	1/1	0.99	0.08	42,42,42,42	0
56	MG	1A	3484	1/1	0.99	0.18	38,38,38,38	0
56	MG	1F	309	1/1	0.99	0.12	31,31,31,31	0
56	MG	1A	3923	1/1	0.99	0.07	32,32,32,32	0
56	MG	1A	3924	1/1	0.99	0.04	40,40,40,40	0
56	MG	1A	3670	1/1	0.99	0.04	27,27,27,27	0
56	MG	1A	3014	1/1	0.99	0.04	28,28,28,28	0
56	MG	1A	3140	1/1	0.99	0.04	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3686	1/1	0.99	0.03	64,64,64,64	0
56	MG	2A	3563	1/1	0.99	0.08	39,39,39,39	0
56	MG	1A	3012	1/1	0.99	0.04	30,30,30,30	0
56	MG	2A	3505	1/1	0.99	0.04	40,40,40,40	0
56	MG	1A	3003	1/1	0.99	0.06	23,23,23,23	0
56	MG	2A	3023	1/1	0.99	0.04	38,38,38,38	0
56	MG	1A	3675	1/1	0.99	0.08	20,20,20,20	0
56	MG	2A	3129	1/1	0.99	0.06	37,37,37,37	0
56	MG	1A	4050	1/1	0.99	0.08	24,24,24,24	0
56	MG	1A	3626	1/1	0.99	0.04	44,44,44,44	0
56	MG	1A	3765	1/1	0.99	0.03	38,38,38,38	0
56	MG	1A	3677	1/1	0.99	0.03	28,28,28,28	0
56	MG	15	104	1/1	0.99	0.28	29,29,29,29	0
56	MG	2A	3188	1/1	0.99	0.04	30,30,30,30	0
56	MG	1A	3582	1/1	0.99	0.13	33,33,33,33	0
56	MG	2A	3031	1/1	0.99	0.11	34,34,34,34	0
56	MG	1a	1630	1/1	0.99	0.20	45,45,45,45	0
56	MG	1A	3070	1/1	0.99	0.10	17,17,17,17	0
56	MG	1A	3973	1/1	0.99	0.09	19,19,19,19	0
56	MG	2A	3705	1/1	0.99	0.10	33,33,33,33	0
56	MG	2A	3521	1/1	0.99	0.08	41,41,41,41	0
56	MG	2A	3707	1/1	0.99	0.07	39,39,39,39	0
56	MG	1D	308	1/1	0.99	0.08	32,32,32,32	0
56	MG	1A	3680	1/1	0.99	0.06	27,27,27,27	0
56	MG	2A	3710	1/1	0.99	0.05	37,37,37,37	0
56	MG	1A	3144	1/1	0.99	0.13	24,24,24,24	0
56	MG	1A	3564	1/1	0.99	0.18	39,39,39,39	0
56	MG	1A	3390	1/1	0.99	0.13	30,30,30,30	0
56	MG	1A	3566	1/1	0.99	0.11	36,36,36,36	0
56	MG	1A	3903	1/1	0.99	0.04	23,23,23,23	0
56	MG	1A	3904	1/1	0.99	0.04	35,35,35,35	0
56	MG	2X	102	1/1	0.99	0.08	51,51,51,51	0
56	MG	1A	3222	1/1	0.99	0.10	32,32,32,32	0
56	MG	1A	3871	1/1	0.99	0.03	26,26,26,26	0
56	MG	1A	3983	1/1	0.99	0.04	39,39,39,39	0
56	MG	1A	3023	1/1	0.99	0.03	12,12,12,12	0
56	MG	1P	204	1/1	0.99	0.03	40,40,40,40	0
56	MG	1A	3176	1/1	0.99	0.10	27,27,27,27	0
56	MG	2A	3597	1/1	0.99	0.14	66,66,66,66	0
56	MG	1E	307	1/1	0.99	0.06	25,25,25,25	0
56	MG	1A	3238	1/1	0.99	0.08	32,32,32,32	0
56	MG	1A	3032	1/1	0.99	0.12	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3539	1/1	0.99	0.08	31,31,31,31	0
56	MG	1A	3988	1/1	0.99	0.08	23,23,23,23	0
56	MG	1A	3989	1/1	0.99	0.05	38,38,38,38	0
56	MG	1A	3615	1/1	0.99	0.10	29,29,29,29	0
56	MG	1A	3380	1/1	0.99	0.22	29,29,29,29	0
56	MG	1A	3663	1/1	0.99	0.02	34,34,34,34	0
56	MG	2A	3798	1/1	0.99	0.03	45,45,45,45	0
56	MG	1A	3048	1/1	0.99	0.09	37,37,37,37	0
56	MG	1A	3665	1/1	0.99	0.06	22,22,22,22	0
56	MG	1F	302	1/1	0.99	0.15	26,26,26,26	0
56	MG	1a	1756	1/1	0.99	0.06	55,55,55,55	0
56	MG	1A	3430	1/1	0.99	0.07	43,43,43,43	0
59	ZN	1Y	206	1/1	0.99	0.03	75,75,75,75	0
56	MG	1A	3785	1/1	0.99	0.03	17,17,17,17	0
59	ZN	1n	103	1/1	0.99	0.03	66,66,66,66	0
56	MG	1A	3786	1/1	0.99	0.04	17,17,17,17	0
56	MG	2A	3494	1/1	0.99	0.07	48,48,48,48	0
59	ZN	29	501	1/1	0.99	0.03	72,72,72,72	0
59	ZN	2n	501	1/1	0.99	0.03	84,84,84,84	0
60	SF4	1d	302	8/8	0.99	0.04	60,64,69,72	0
60	SF4	2d	303	8/8	0.99	0.04	52,65,72,78	0
59	ZN	19	102	1/1	1.00	0.03	42,42,42,42	0
56	MG	1A	3920	1/1	1.00	0.02	13,13,13,13	0
56	MG	1A	3610	1/1	1.00	0.05	32,32,32,32	0
56	MG	1A	3713	1/1	1.00	0.05	17,17,17,17	0
59	ZN	25	107	1/1	1.00	0.05	55,55,55,55	0
59	ZN	26	102	1/1	1.00	0.03	61,61,61,61	0
56	MG	1Q	202	1/1	1.00	0.02	31,31,31,31	0
56	MG	2A	3581	1/1	1.00	0.02	39,39,39,39	0
59	ZN	15	111	1/1	1.00	0.07	47,47,47,47	0
59	ZN	16	102	1/1	1.00	0.02	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.