



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:14 PM UTC

PDB ID : 8UD7 / pdb_00008ud7
Title : Crystal structure of the A2058-N6-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.; Dittmore, 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 : 2.55 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ 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	: 9.0.010 (Gargrove)
Density-Fitness	: 1.0.12

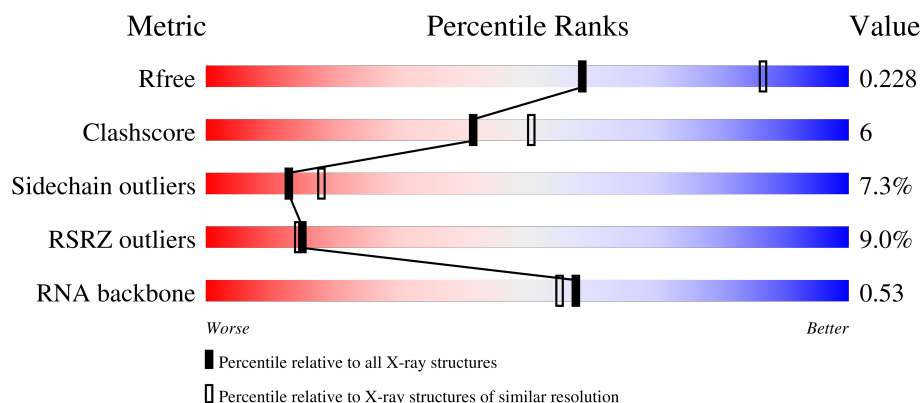
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)
RNA backbone	3983	1112 (2.80-2.28)

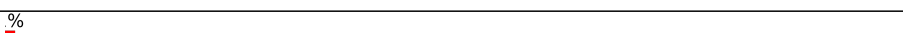
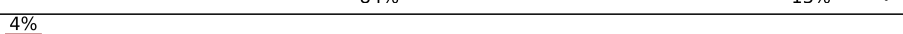
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	6% 71% 22% 6%
1	2A	2915	5% 64% 27% 5%

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	1B	121	
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	
14	1S	112	

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

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Mol	Chain	Length	Quality of chain
27	15	60	
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	
39	1h	138	

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	PSU	2y	55	-	-	X	-
56	MG	1A	3293	-	-	-	X
56	MG	1A	3553	-	-	-	X
56	MG	2A	3130	-	-	-	X
56	MG	2A	3336	-	-	-	X
56	MG	2a	1634	-	-	-	X
56	MG	2a	1647	-	-	-	X
56	MG	2a	1686	-	-	-	X
56	MG	2a	1722	-	-	-	X
56	MG	2a	1814	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 299373 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
			61854	27533	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60324	26850	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	77	Total	C	N	O	S	0	0	0
			608	375	129	103	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	72	Total	C	N	O	P	S	0	0	0
			1550	694	277	505	72	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	69	Total	C	N	O	P	S	0	0	0
			1482	662	267	482	69	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	1097	Total	Mg	0	0
			1097	1097		
56	1B	36	Total	Mg	0	0
			36	36		
56	1D	11	Total	Mg	0	0
			11	11		
56	1E	18	Total	Mg	0	0
			18	18		
56	1F	13	Total	Mg	0	0
			13	13		
56	1G	4	Total	Mg	0	0
			4	4		
56	1I	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1N	6	Total 6	Mg 6	0	0
56	1O	6	Total 6	Mg 6	0	0
56	1P	5	Total 5	Mg 5	0	0
56	1Q	7	Total 7	Mg 7	0	0
56	1R	8	Total 8	Mg 8	0	0
56	1S	3	Total 3	Mg 3	0	0
56	1T	2	Total 2	Mg 2	0	0
56	1U	10	Total 10	Mg 10	0	0
56	1V	7	Total 7	Mg 7	0	0
56	1W	4	Total 4	Mg 4	0	0
56	1X	7	Total 7	Mg 7	0	0
56	1Y	3	Total 3	Mg 3	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	10	9	Total 9	Mg 9	0	0
56	11	5	Total 5	Mg 5	0	0
56	12	2	Total 2	Mg 2	0	0
56	13	4	Total 4	Mg 4	0	0
56	14	1	Total 1	Mg 1	0	0
56	15	8	Total 8	Mg 8	0	0
56	16	1	Total 1	Mg 1	0	0
56	17	5	Total 5	Mg 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	18	6	Total 6	Mg 6	0	0
56	19	1	Total 1	Mg 1	0	0
56	1a	196	Total 196	Mg 196	0	0
56	1b	1	Total 1	Mg 1	0	0
56	1d	1	Total 1	Mg 1	0	0
56	1e	1	Total 1	Mg 1	0	0
56	1f	1	Total 1	Mg 1	0	0
56	1l	2	Total 2	Mg 2	0	0
56	1m	2	Total 2	Mg 2	0	0
56	1n	2	Total 2	Mg 2	0	0
56	1r	1	Total 1	Mg 1	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1w	5	Total 5	Mg 5	0	0
56	1x	14	Total 14	Mg 14	0	0
56	1y	1	Total 1	Mg 1	0	0
56	2A	808	Total 808	Mg 808	0	0
56	2B	15	Total 15	Mg 15	0	0
56	2D	6	Total 6	Mg 6	0	0
56	2E	8	Total 8	Mg 8	0	0
56	2F	7	Total 7	Mg 7	0	0
56	2G	1	Total 1	Mg 1	0	0

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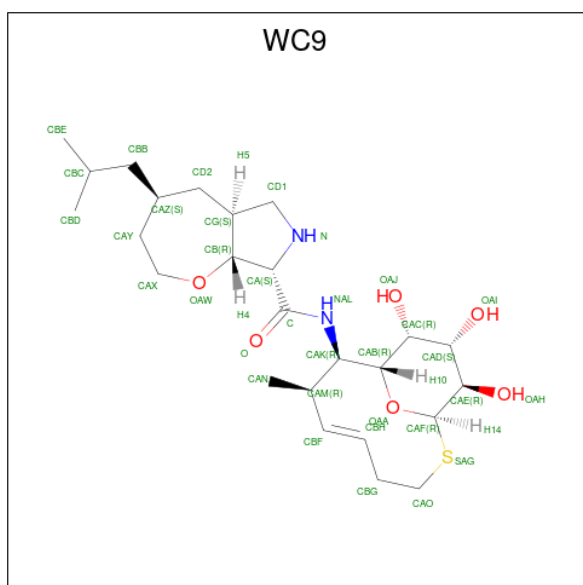
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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56	2O	1	Total 1	Mg 1	0	0
56	2P	1	Total 1	Mg 1	0	0
56	2Q	3	Total 3	Mg 3	0	0
56	2R	3	Total 3	Mg 3	0	0
56	2T	4	Total 4	Mg 4	0	0
56	2U	1	Total 1	Mg 1	0	0
56	2V	2	Total 2	Mg 2	0	0
56	2W	5	Total 5	Mg 5	0	0
56	2X	2	Total 2	Mg 2	0	0
56	20	4	Total 4	Mg 4	0	0
56	21	1	Total 1	Mg 1	0	0
56	23	1	Total 1	Mg 1	0	0
56	25	4	Total 4	Mg 4	0	0
56	27	3	Total 3	Mg 3	0	0
56	28	3	Total 3	Mg 3	0	0
56	2a	230	Total 230	Mg 230	0	0
56	2d	2	Total 2	Mg 2	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	2	Total 2	Mg 2	0	0
56	2j	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2l	4	Total	Mg	0	0
			4	4		
56	2q	2	Total	Mg	0	0
			2	2		
56	2r	1	Total	Mg	0	0
			1	1		
56	2t	1	Total	Mg	0	0
			1	1		
56	2v	3	Total	Mg	0	0
			3	3		
56	2w	4	Total	Mg	0	0
			4	4		
56	2x	5	Total	Mg	0	0
			5	5		
56	2y	3	Total	Mg	0	0
			3	3		

- Molecule 57 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).

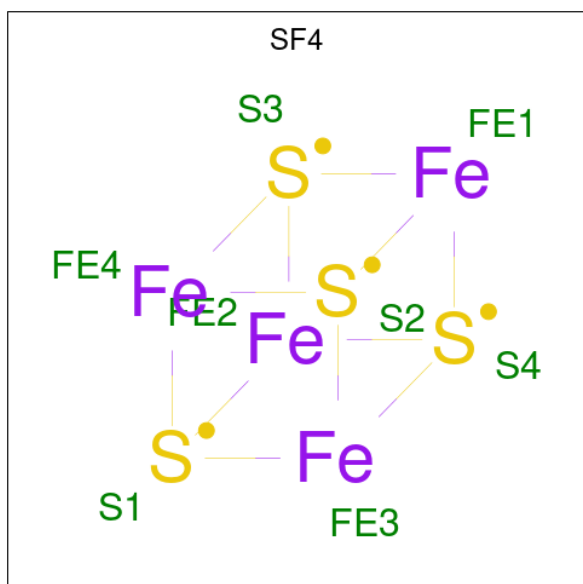


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
57	1A	1	Total	C	N	O	S	0	0
			34	25	2	6	1		
57	2A	1	Total	C	N	O	S	0	0
			34	25	2	6	1		

- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1Y	1	Total Zn 1 1	0	0
58	14	1	Total Zn 1 1	0	0
58	15	1	Total Zn 1 1	0	0
58	16	1	Total Zn 1 1	0	0
58	19	1	Total Zn 1 1	0	0
58	1n	1	Total Zn 1 1	0	0
58	2Y	1	Total Zn 1 1	0	0
58	24	1	Total Zn 1 1	0	0
58	25	1	Total Zn 1 1	0	0
58	26	1	Total Zn 1 1	0	0
58	29	1	Total Zn 1 1	0	0
58	2n	1	Total Zn 1 1	0	0

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	1d	1	Total	Fe	S	0	0
			8	4	4		
59	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1x	1	Total	K	0	0
			1	1		
60	2x	1	Total	K	0	0
			1	1		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1899	Total	O	0	0
			1899	1899		
61	1B	59	Total	O	0	0
			59	59		
61	1D	27	Total	O	0	0
			27	27		
61	1E	26	Total	O	0	0
			26	26		
61	1F	16	Total	O	0	0
			16	16		
61	1G	1	Total	O	0	0
			1	1		
61	1H	2	Total	O	0	0
			2	2		
61	1N	6	Total	O	0	0
			6	6		
61	1O	5	Total	O	0	0
			5	5		
61	1P	22	Total	O	0	0
			22	22		
61	1Q	8	Total	O	0	0
			8	8		
61	1R	9	Total	O	0	0
			9	9		
61	1S	3	Total	O	0	0
			3	3		
61	1T	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1U	14	Total 14	O 14	0	0
61	1V	8	Total 8	O 8	0	0
61	1W	8	Total 8	O 8	0	0
61	1X	4	Total 4	O 4	0	0
61	1Y	3	Total 3	O 3	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	9	Total 9	O 9	0	0
61	11	8	Total 8	O 8	0	0
61	12	3	Total 3	O 3	0	0
61	13	3	Total 3	O 3	0	0
61	14	1	Total 1	O 1	0	0
61	15	4	Total 4	O 4	0	0
61	16	2	Total 2	O 2	0	0
61	17	12	Total 12	O 12	0	0
61	18	9	Total 9	O 9	0	0
61	1a	263	Total 263	O 263	0	0
61	1b	1	Total 1	O 1	0	0
61	1d	2	Total 2	O 2	0	0
61	1f	1	Total 1	O 1	0	0
61	1g	1	Total 1	O 1	0	0
61	1l	3	Total 3	O 3	0	0

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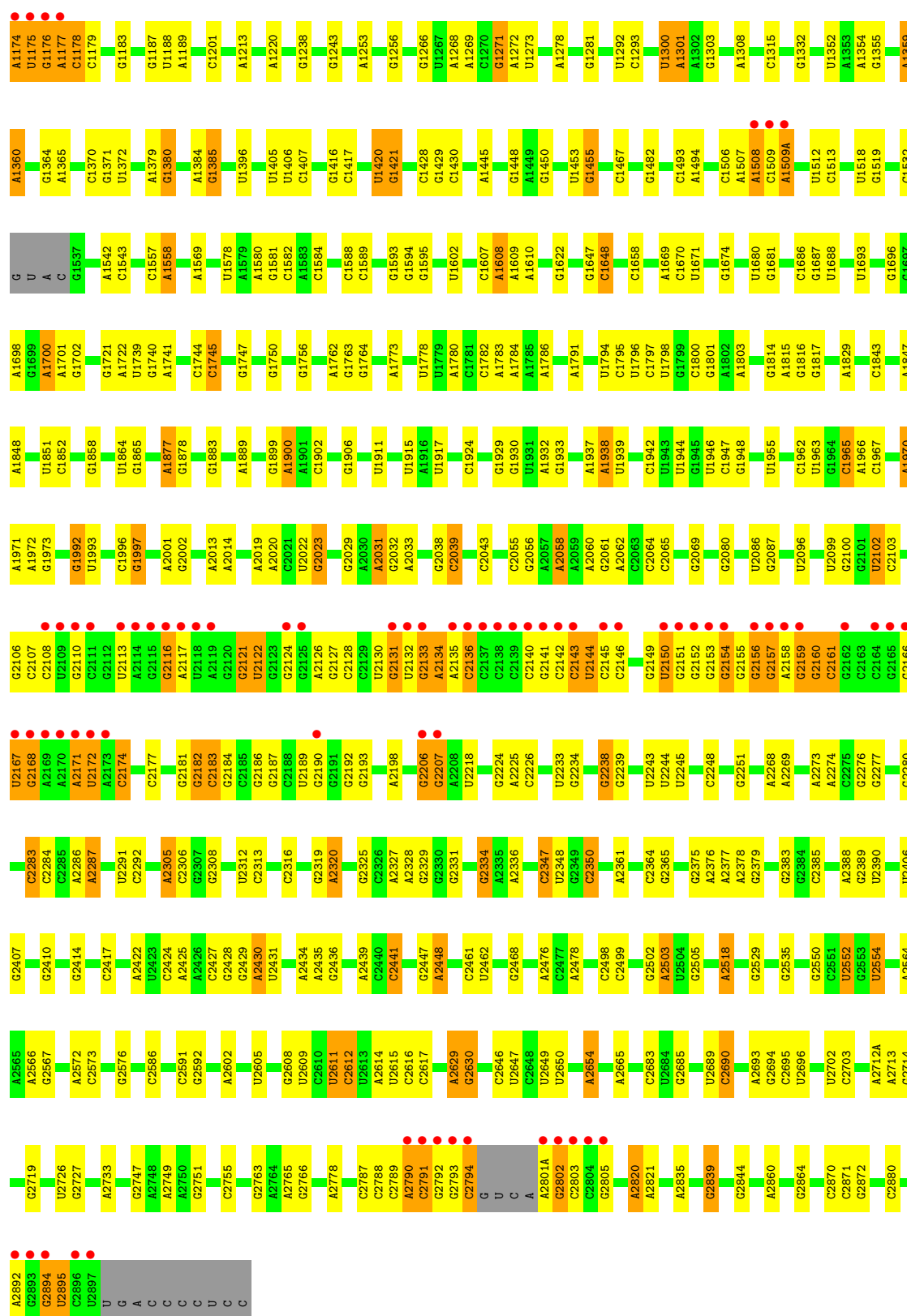
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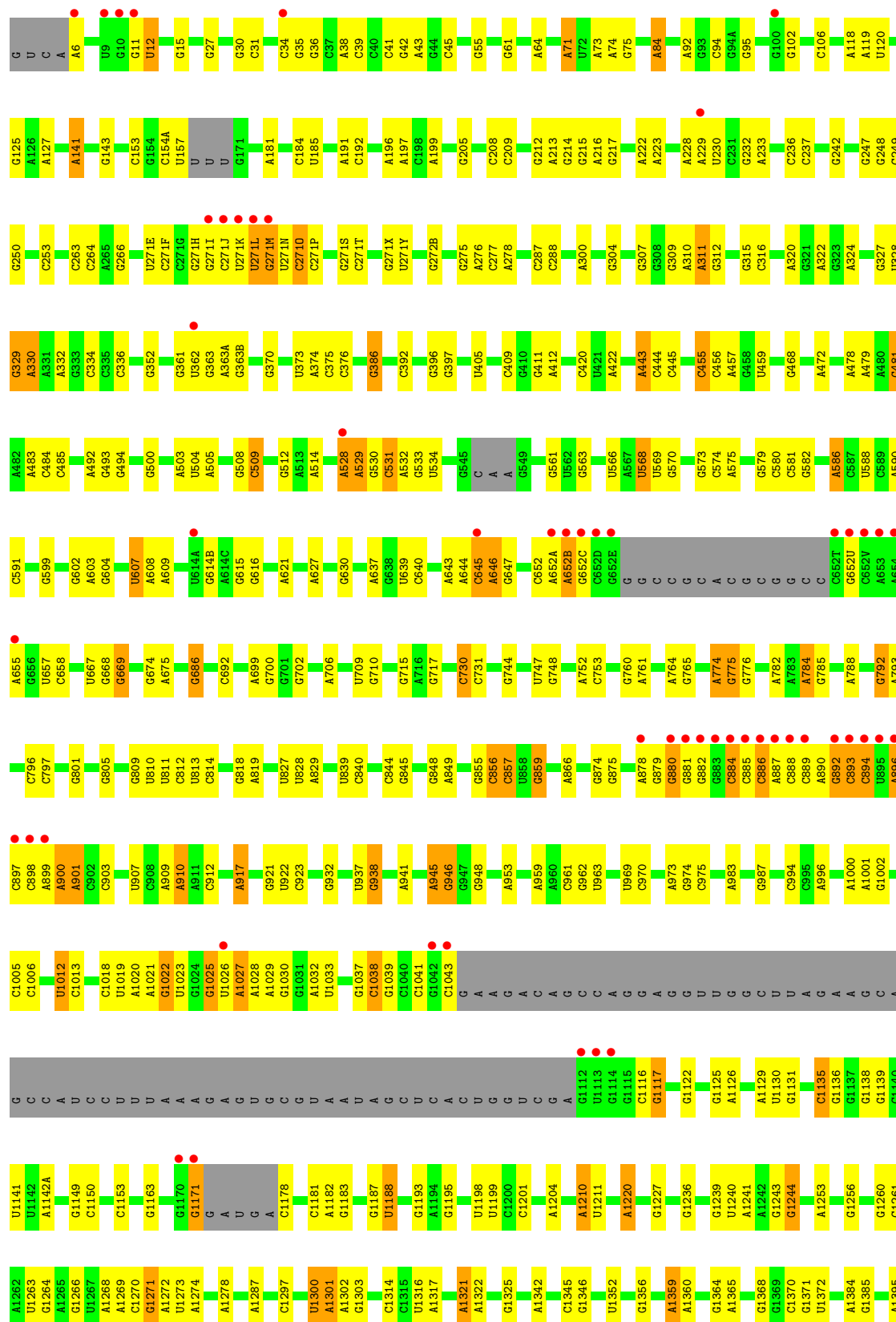
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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61	1q	2	Total 2	O 2	0	0
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61	1w	7	Total 7	O 7	0	0
61	1x	10	Total 10	O 10	0	0
61	1y	1	Total 1	O 1	0	0
61	2A	974	Total 974	O 974	0	0
61	2B	14	Total 14	O 14	0	0
61	2D	19	Total 19	O 19	0	0
61	2E	11	Total 11	O 11	0	0
61	2F	10	Total 10	O 10	0	0
61	2N	1	Total 1	O 1	0	0
61	2O	2	Total 2	O 2	0	0
61	2P	9	Total 9	O 9	0	0
61	2Q	1	Total 1	O 1	0	0
61	2R	4	Total 4	O 4	0	0
61	2T	4	Total 4	O 4	0	0
61	2U	2	Total 2	O 2	0	0
61	2X	2	Total 2	O 2	0	0
61	20	4	Total 4	O 4	0	0
61	21	7	Total 7	O 7	0	0

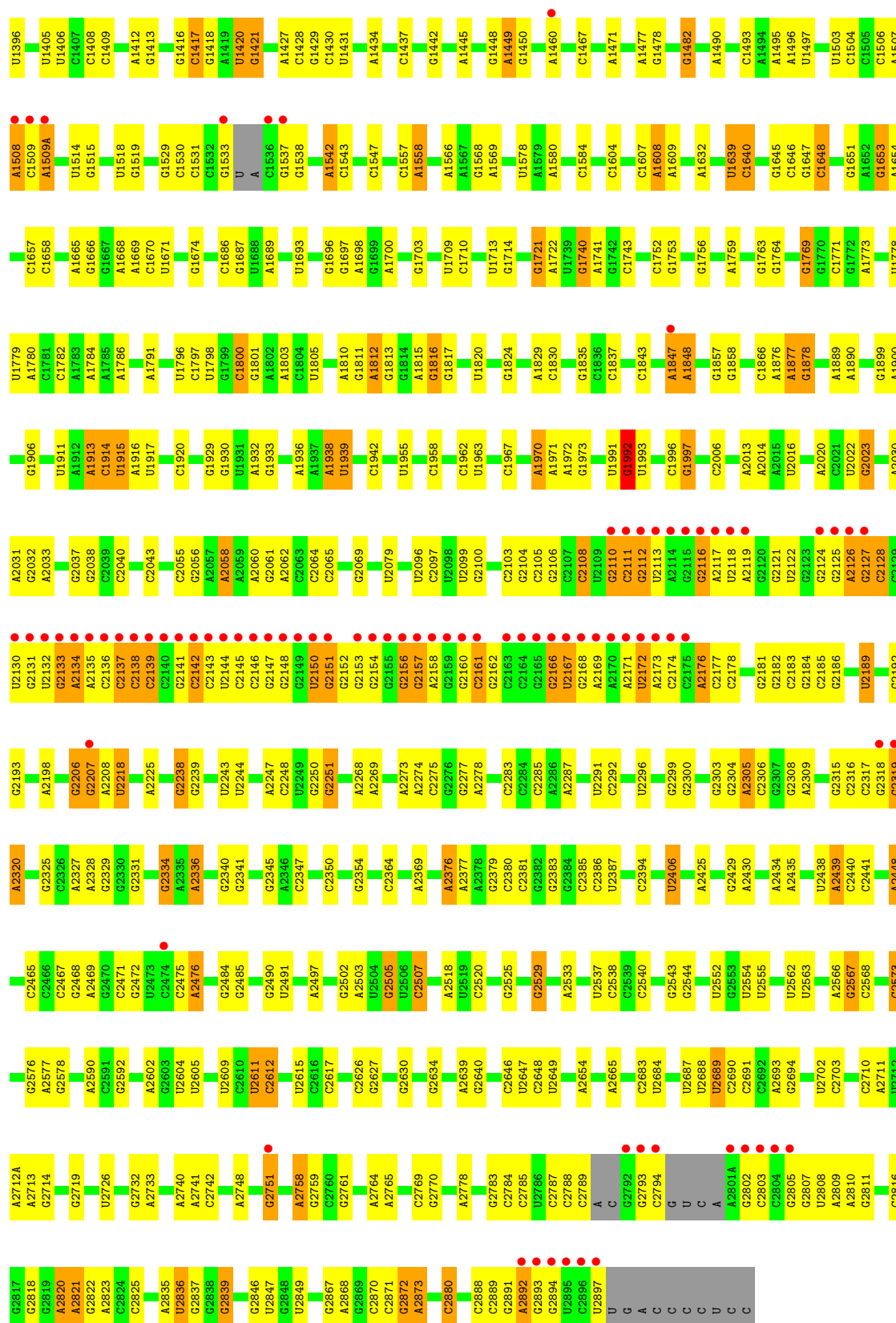
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	23	2	Total 2	O 2	0	0
61	27	4	Total 4	O 4	0	0
61	28	3	Total 3	O 3	0	0
61	29	1	Total 1	O 1	0	0
61	2a	184	Total 184	O 184	0	0
61	2e	1	Total 1	O 1	0	0
61	2g	1	Total 1	O 1	0	0
61	2j	3	Total 3	O 3	0	0
61	2l	3	Total 3	O 3	0	0
61	2t	1	Total 1	O 1	0	0
61	2v	1	Total 1	O 1	0	0
61	2x	4	Total 4	O 4	0	0
61	2y	2	Total 2	O 2	0	0







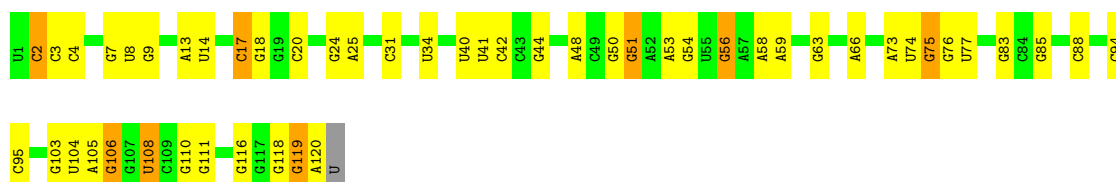
- Molecule 2: 5S Ribosomal RNA

Chain 1B:  76% 20% ..



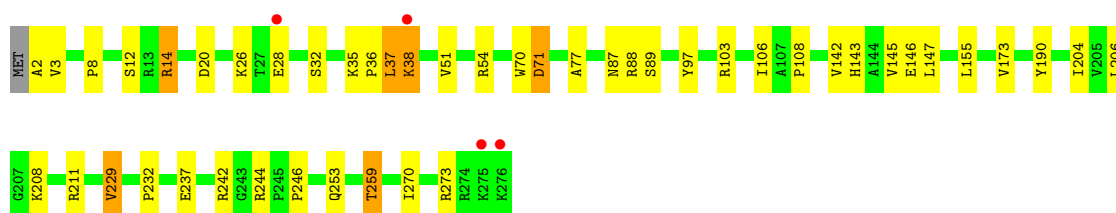
- Molecule 2: 5S Ribosomal RNA

Chain 2B:  58% 35% 7% .



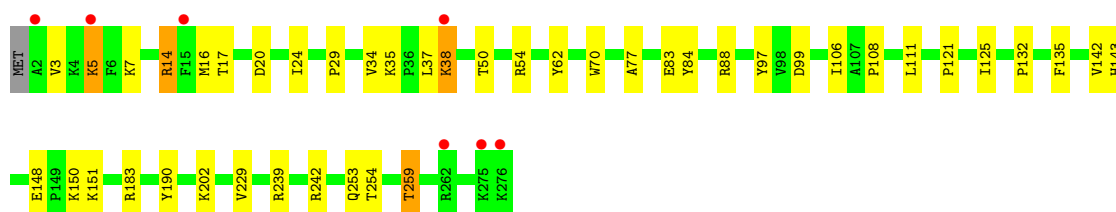
- Molecule 3: 50S ribosomal protein L2

Chain 1D:  83% 15% .



- Molecule 3: 50S ribosomal protein L2

Chain 2D:  84% 14% 3% .



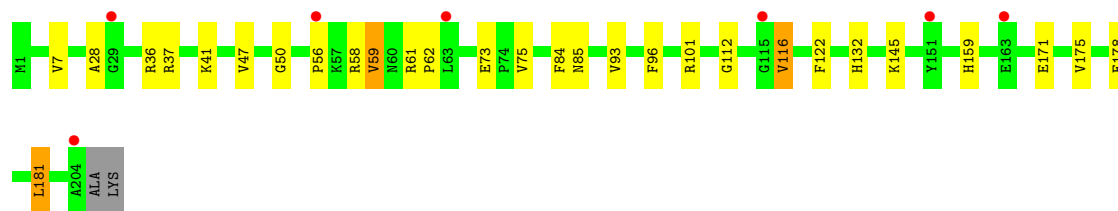
- Molecule 4: 50S ribosomal protein L3

Chain 1E:  86% 12% ..

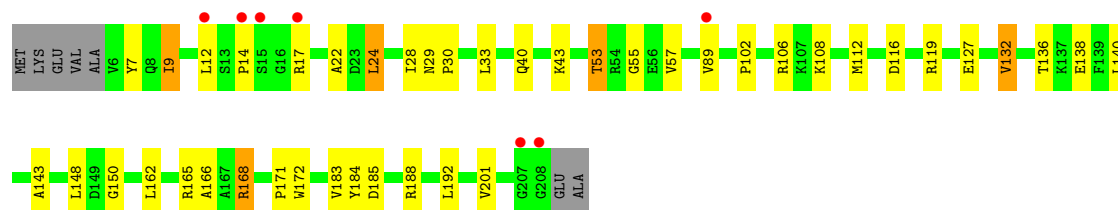
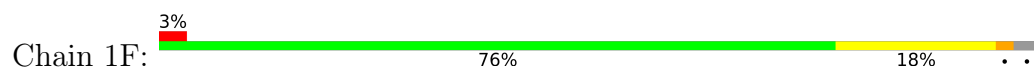


- Molecule 4: 50S ribosomal protein L3

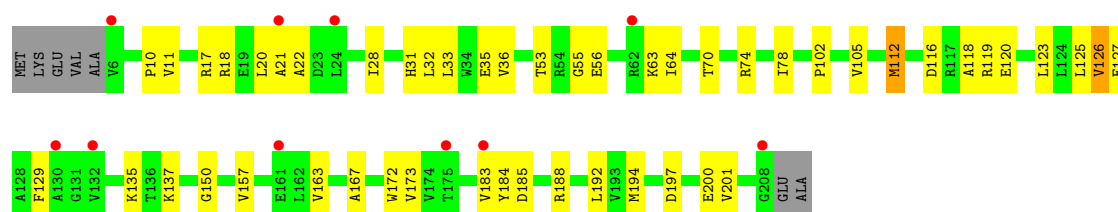
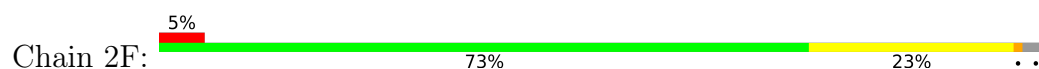
Chain 2E:  85% 13% ..



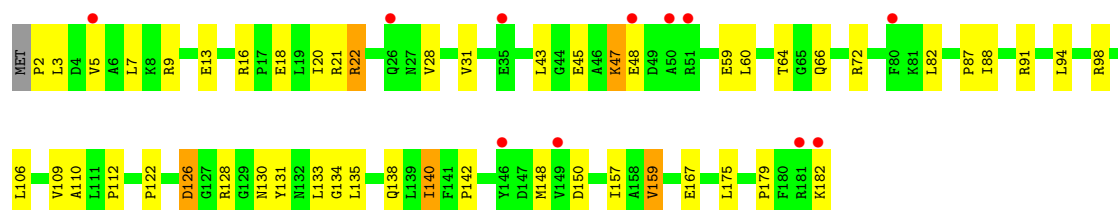
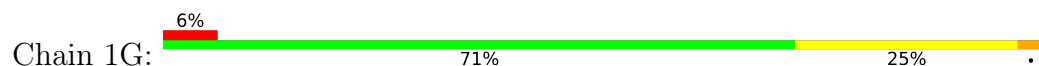
• Molecule 5: 50S ribosomal protein L4



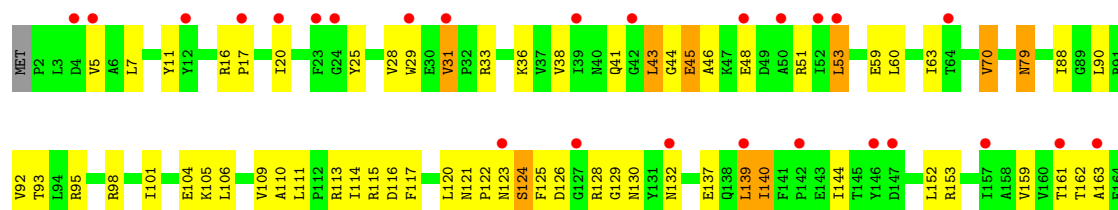
• Molecule 5: 50S ribosomal protein L4



• Molecule 6: 50S ribosomal protein L5

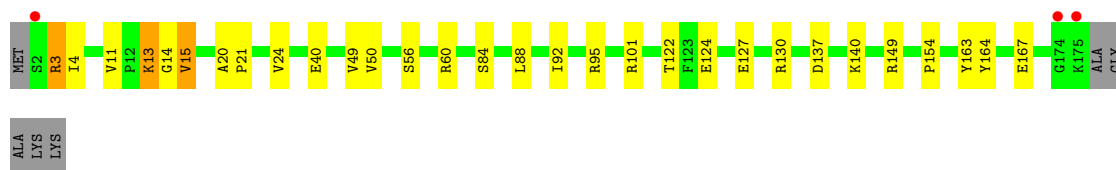
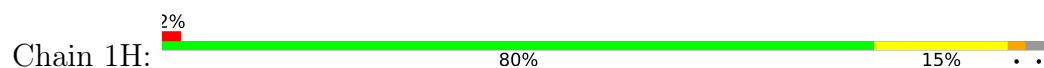


• Molecule 6: 50S ribosomal protein L5

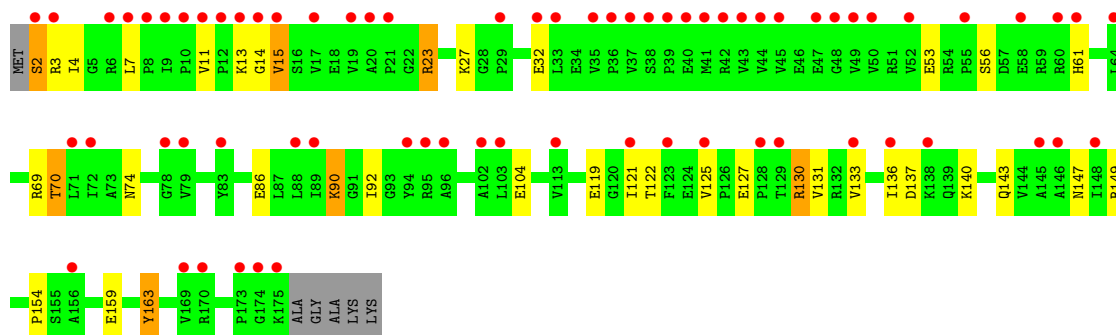
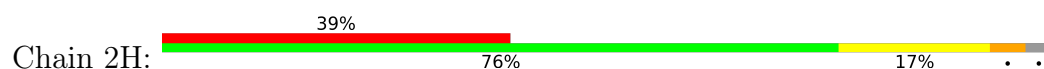




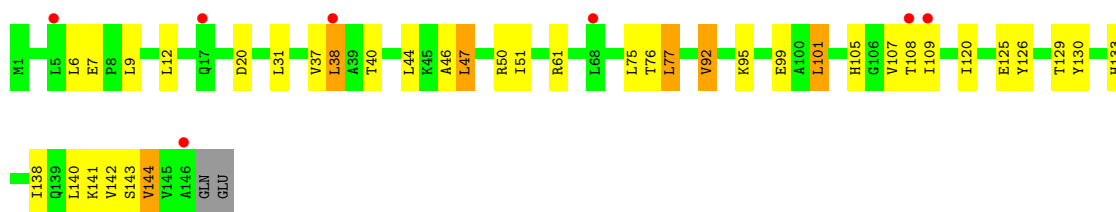
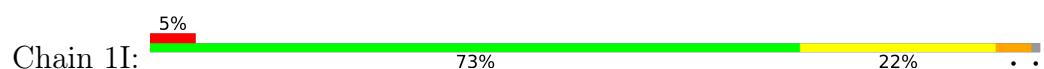
- Molecule 7: 50S ribosomal protein L6



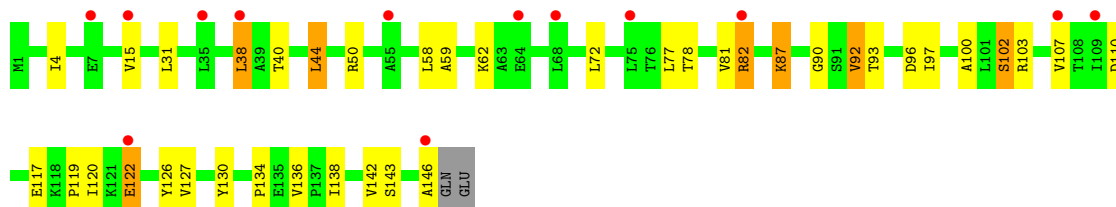
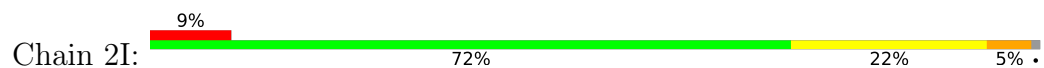
- Molecule 7: 50S ribosomal protein L6



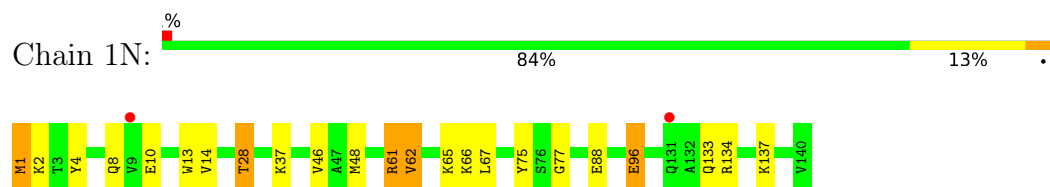
- Molecule 8: 50S ribosomal protein L9



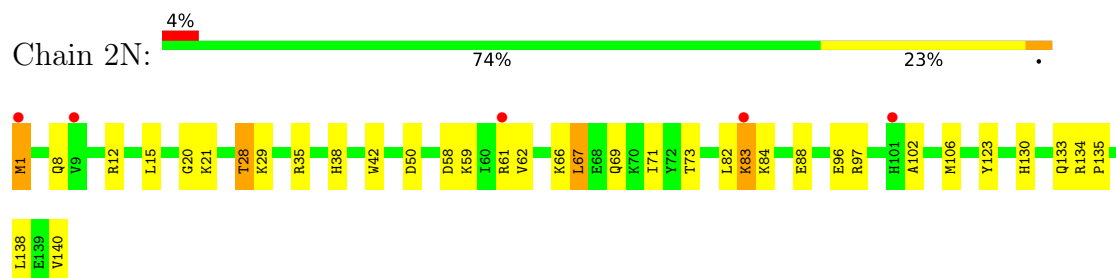
- Molecule 8: 50S ribosomal protein L9



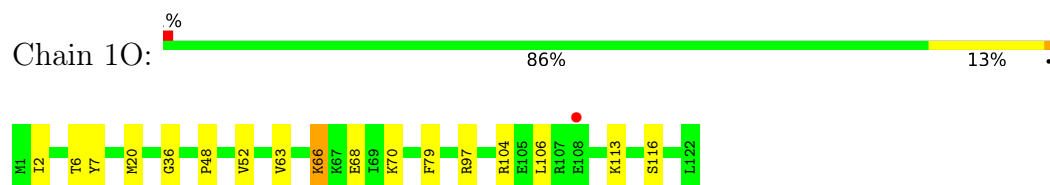
- Molecule 9: 50S ribosomal protein L13



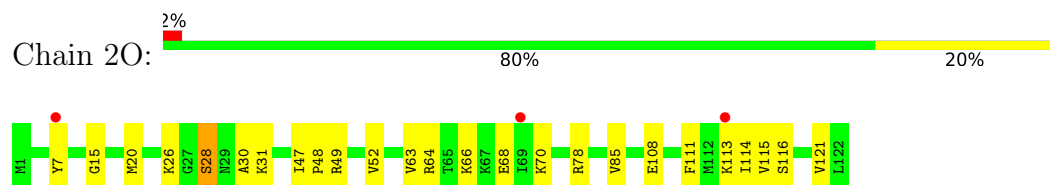
- Molecule 9: 50S ribosomal protein L13



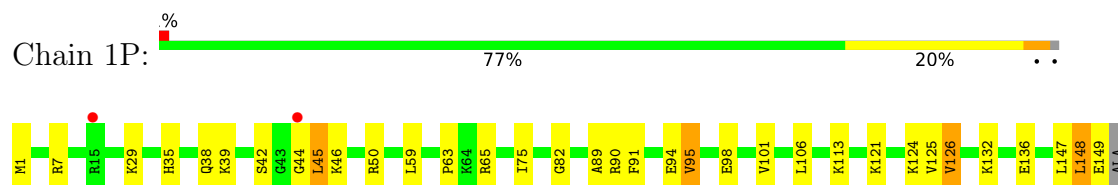
- Molecule 10: 50S ribosomal protein L14



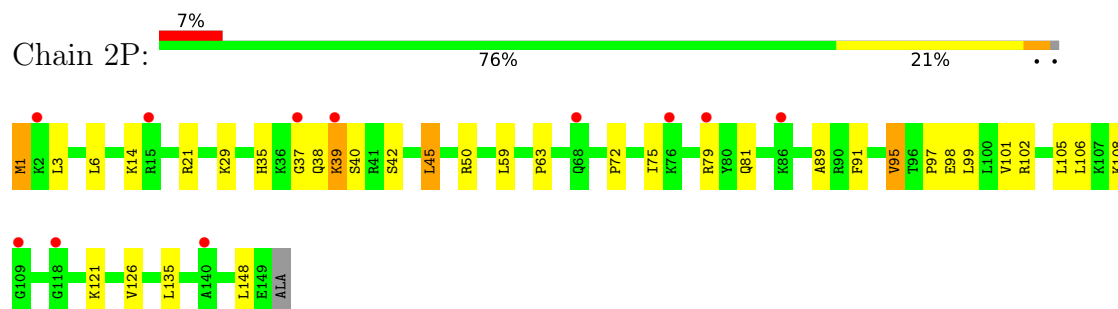
- Molecule 10: 50S ribosomal protein L14



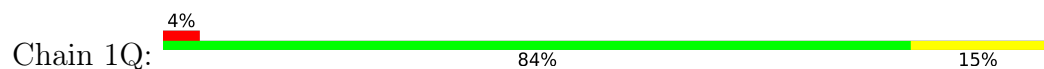
- Molecule 11: 50S ribosomal protein L15



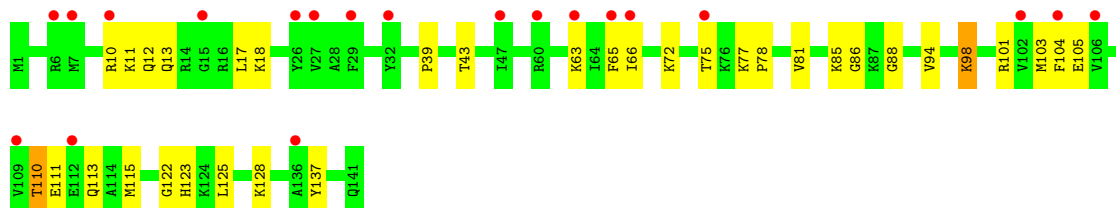
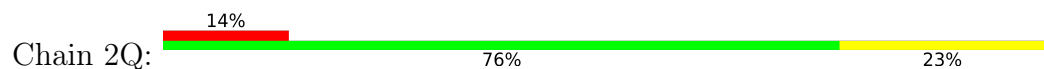
- Molecule 11: 50S ribosomal protein L15



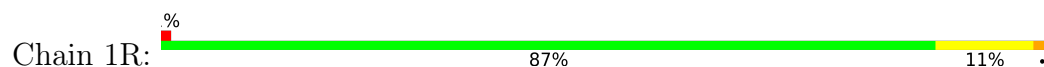
- Molecule 12: 50S ribosomal protein L16



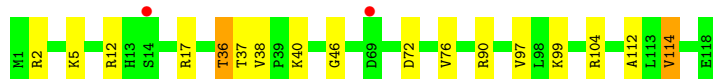
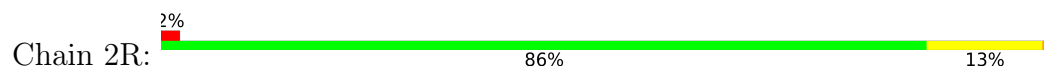
- Molecule 12: 50S ribosomal protein L16



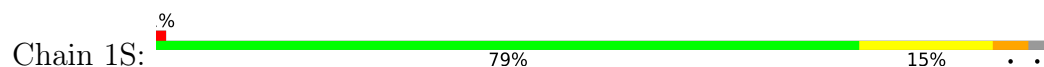
- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17

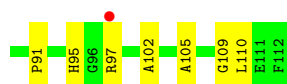


- Molecule 14: 50S ribosomal protein L18

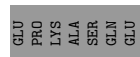
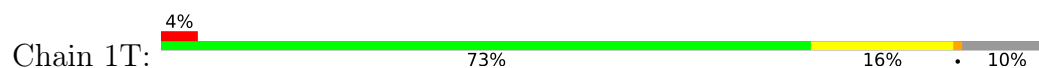


- Molecule 14: 50S ribosomal protein L18

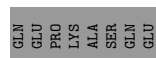
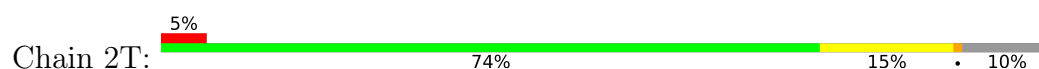




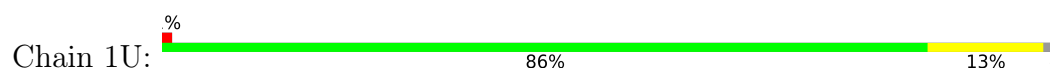
- Molecule 15: 50S ribosomal protein L19



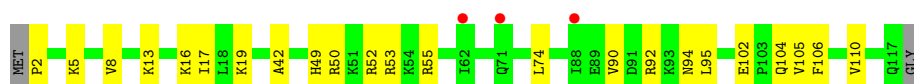
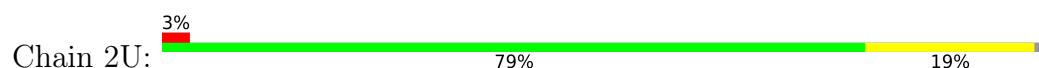
- Molecule 15: 50S ribosomal protein L19



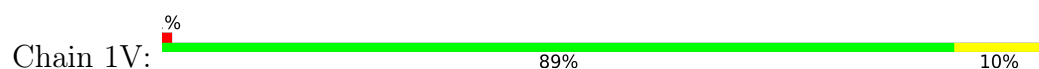
- Molecule 16: 50S ribosomal protein L20



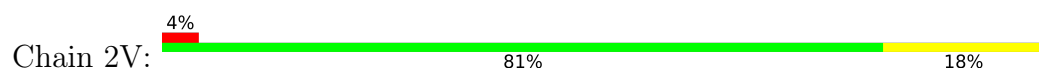
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21



- Molecule 17: 50S ribosomal protein L21

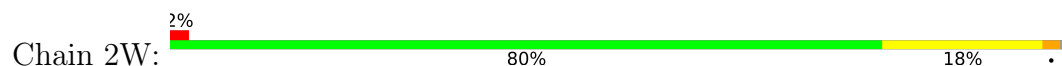




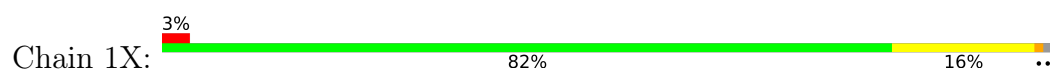
- Molecule 18: 50S ribosomal protein L22



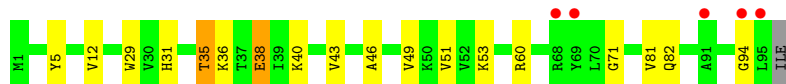
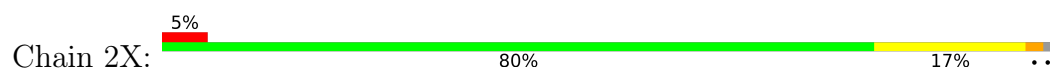
- Molecule 18: 50S ribosomal protein L22



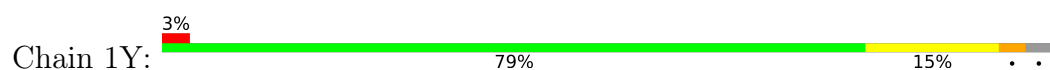
- Molecule 19: 50S ribosomal protein L23



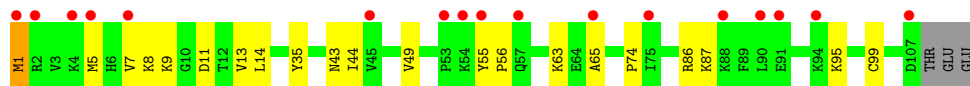
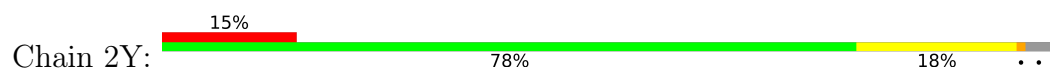
- Molecule 19: 50S ribosomal protein L23



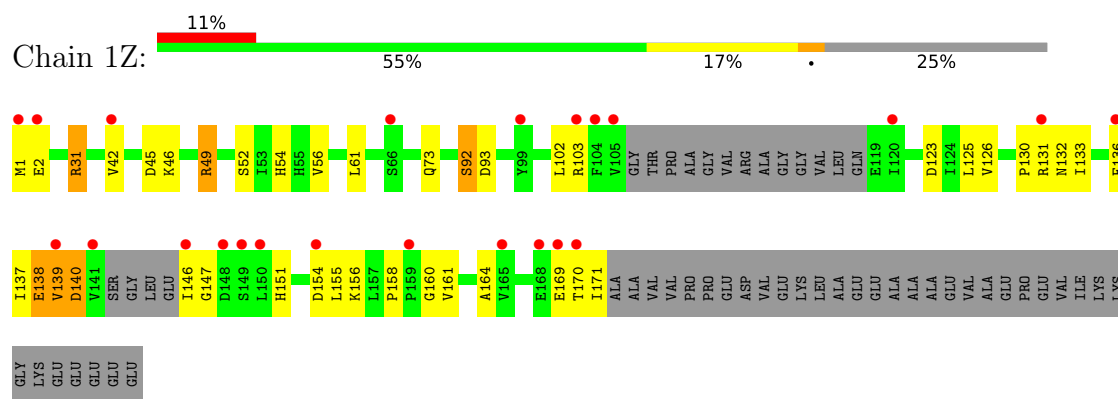
- Molecule 20: 50S ribosomal protein L24



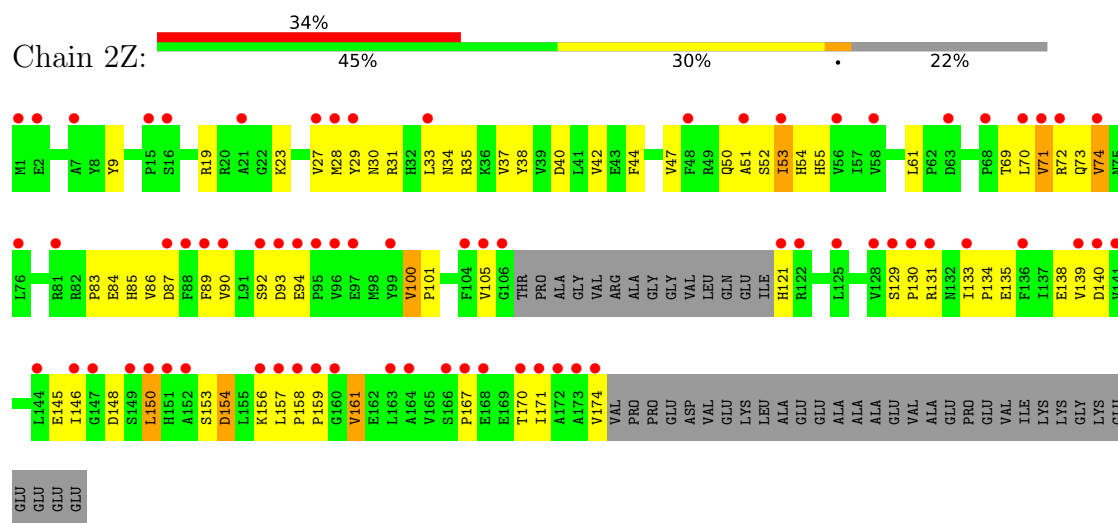
- Molecule 20: 50S ribosomal protein L24



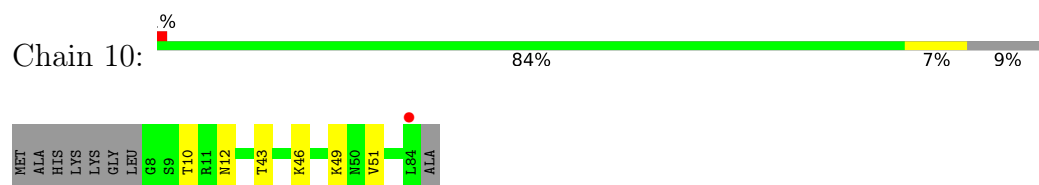
- Molecule 21: 50S ribosomal protein L25



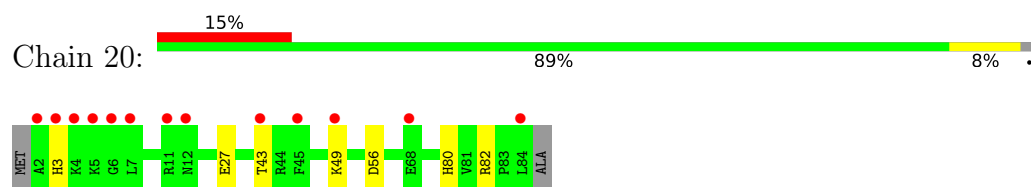
• Molecule 21: 50S ribosomal protein L25



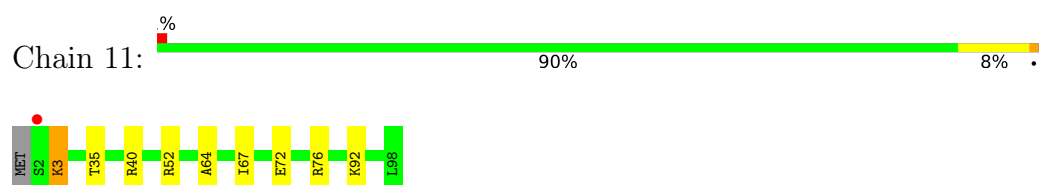
• Molecule 22: 50S ribosomal protein L27



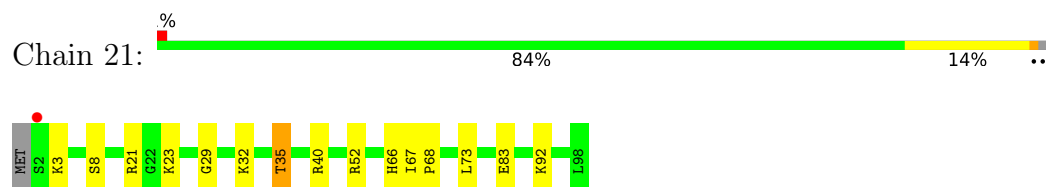
• Molecule 22: 50S ribosomal protein L27



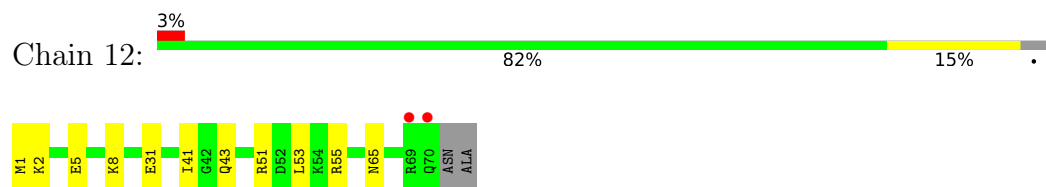
• Molecule 23: 50S ribosomal protein L28



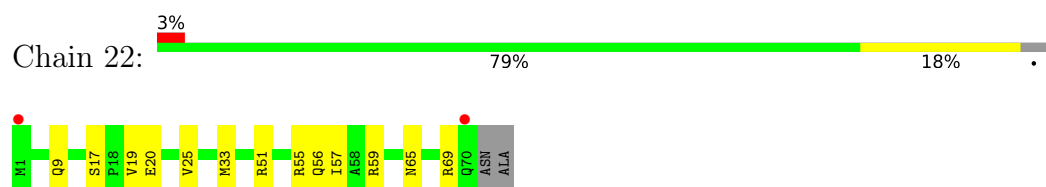
- Molecule 23: 50S ribosomal protein L28



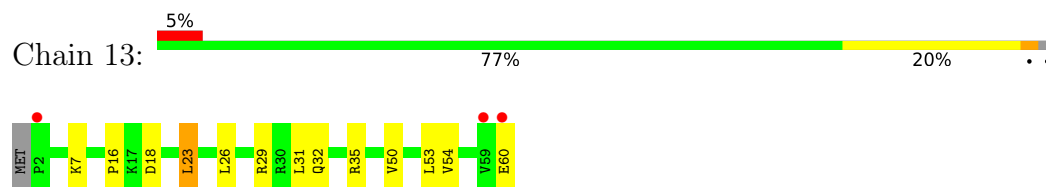
- Molecule 24: 50S ribosomal protein L29



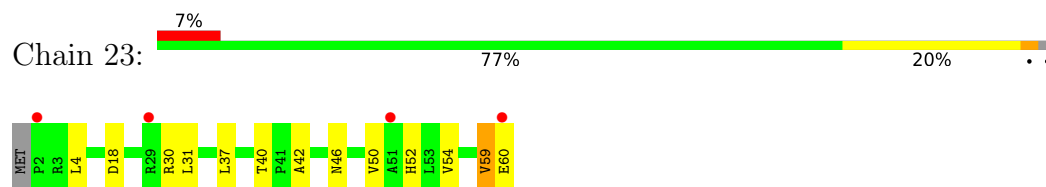
- Molecule 24: 50S ribosomal protein L29



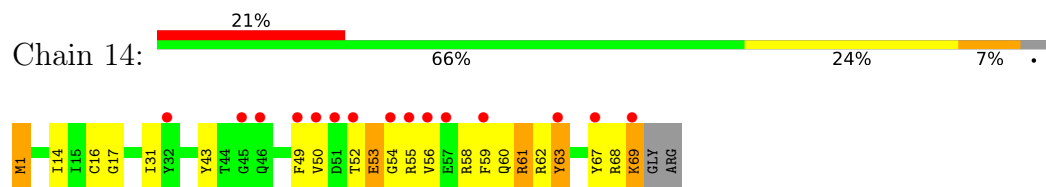
- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30

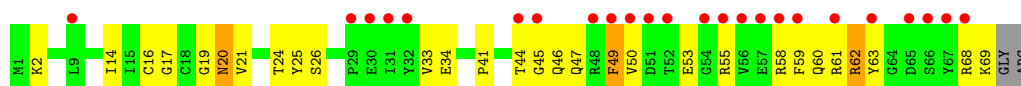


- Molecule 26: 50S ribosomal protein L31

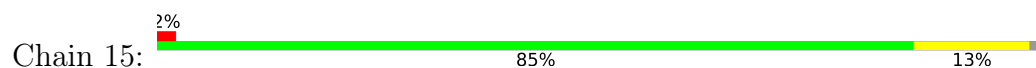


- Molecule 26: 50S ribosomal protein L31





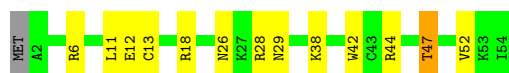
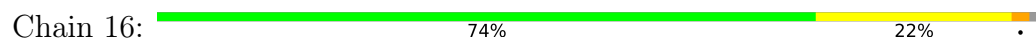
- Molecule 27: 50S ribosomal protein L32



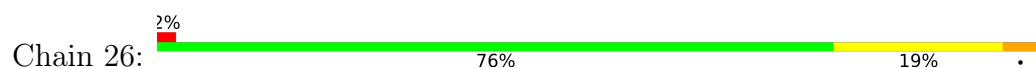
- Molecule 27: 50S ribosomal protein L32



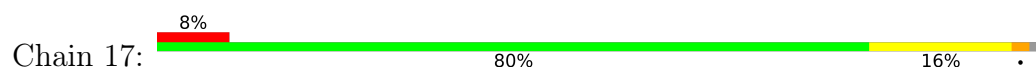
- Molecule 28: 50S ribosomal protein L33



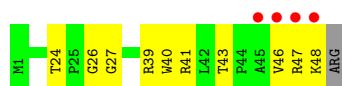
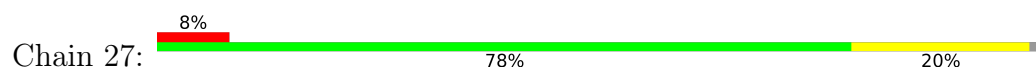
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35

Chain 18:  85% 14%



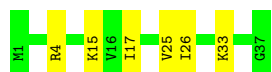
- Molecule 30: 50S ribosomal protein L35

Chain 28:  80% 18%



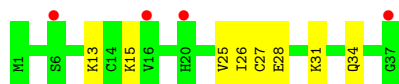
- Molecule 31: 50S ribosomal protein L36

Chain 19:  84% 16%



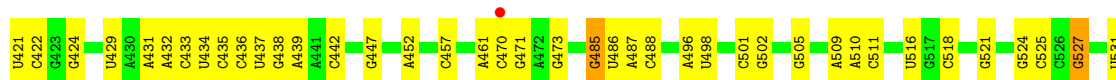
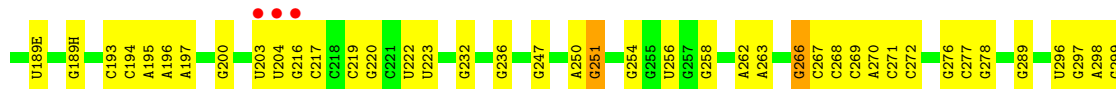
- Molecule 31: 50S ribosomal protein L36

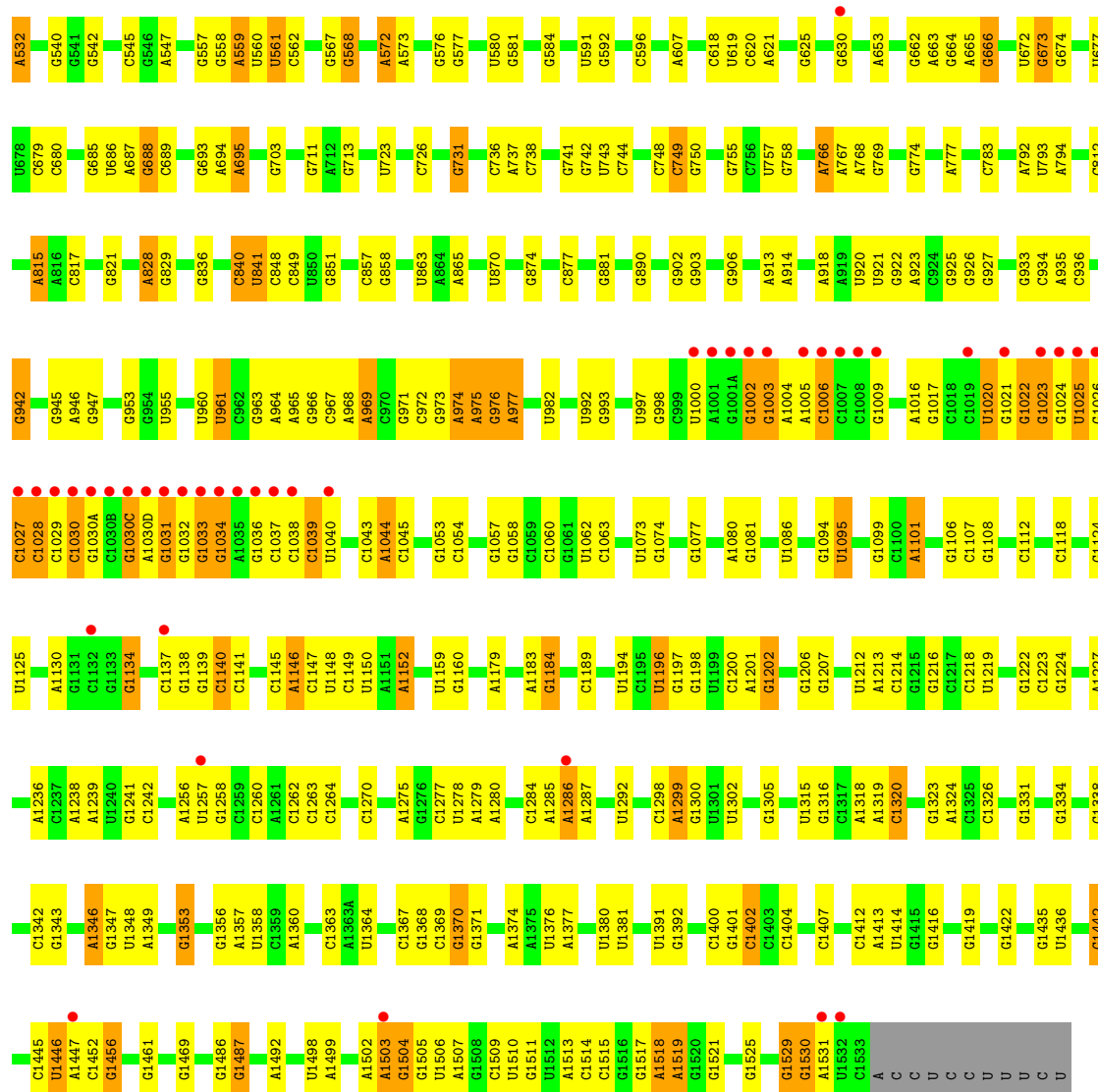
Chain 29:  11% 78% 22%

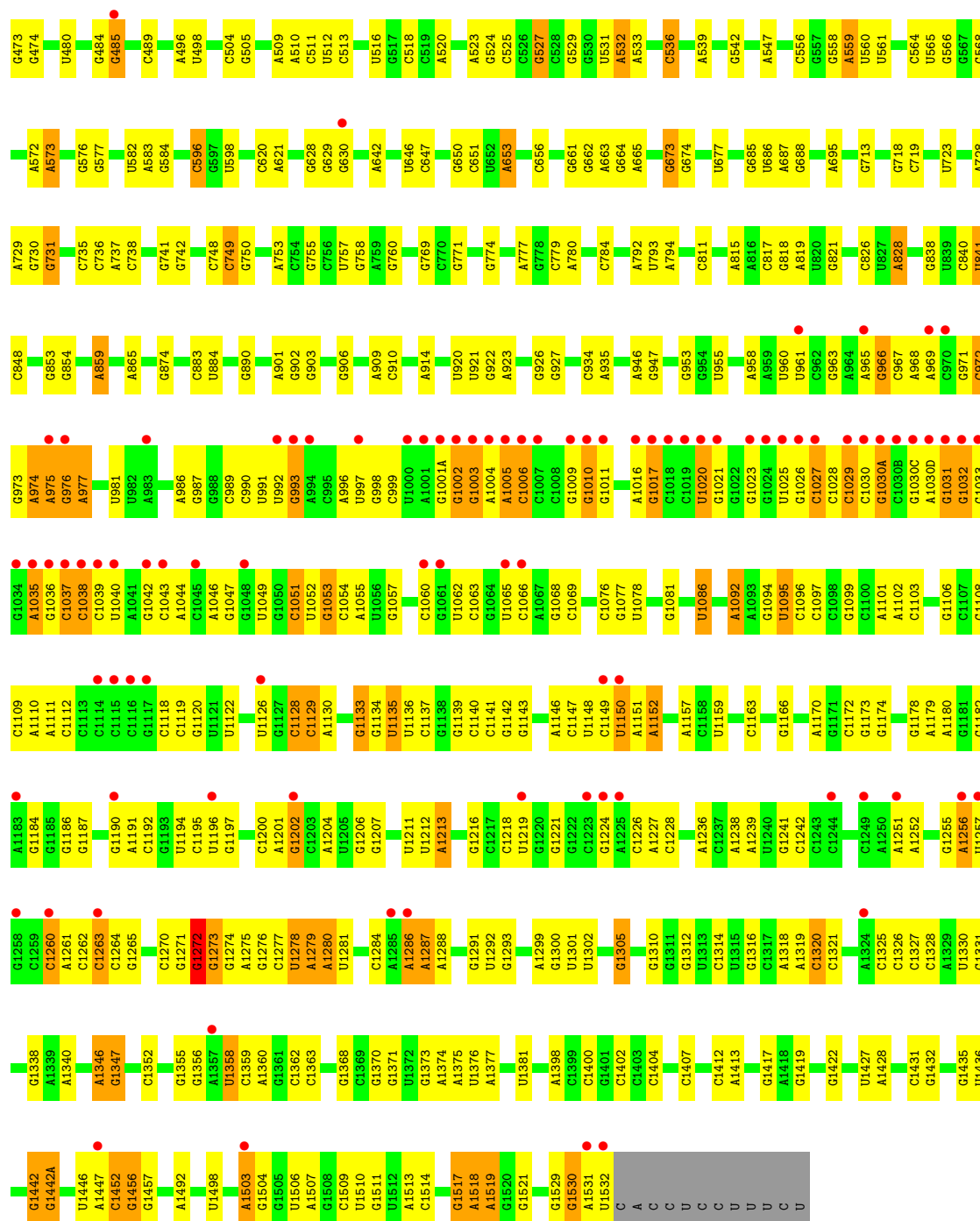


- Molecule 32: 16S Ribosomal RNA

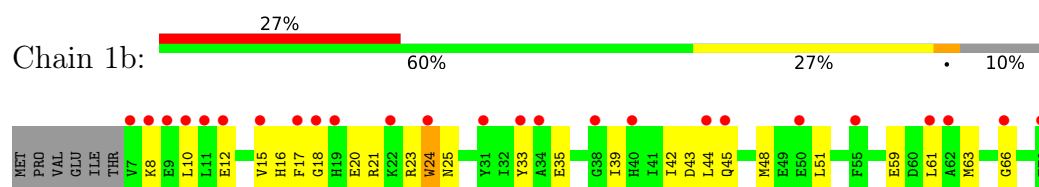
Chain 1a:  4% 63% 31% 5%

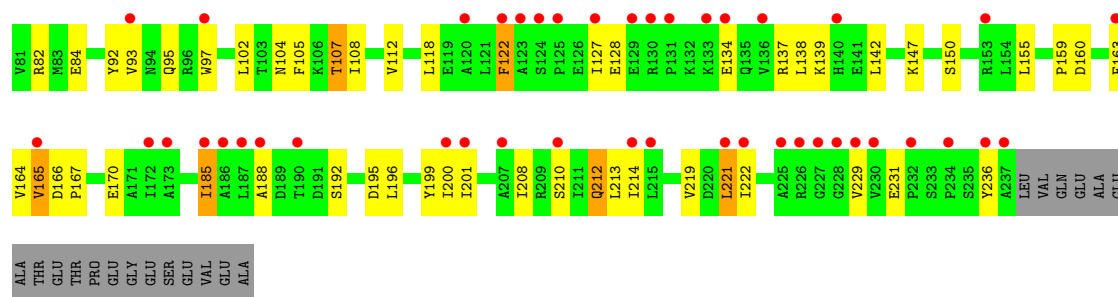




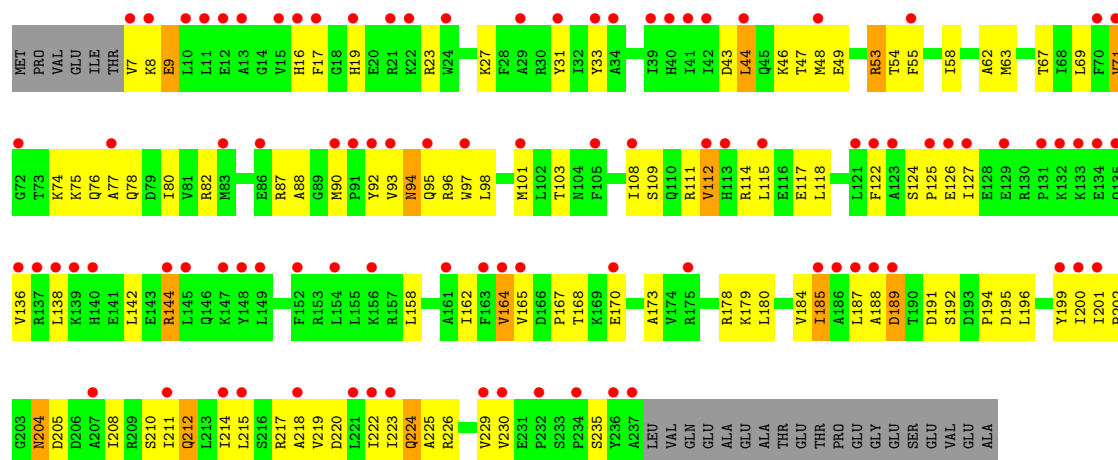


- Molecule 33: 30S ribosomal protein S2

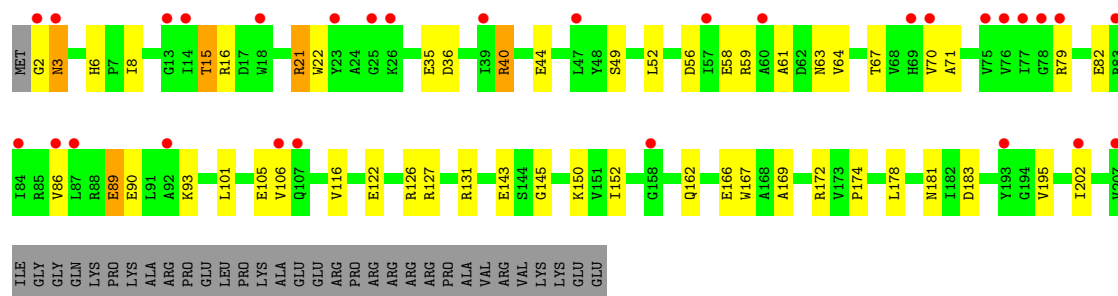




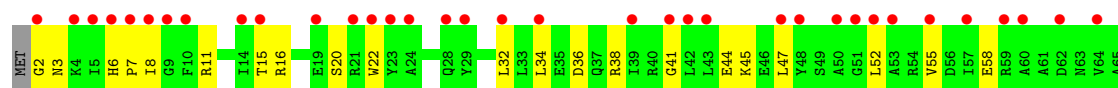
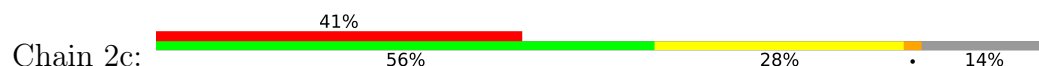
• Molecule 33: 30S ribosomal protein S2

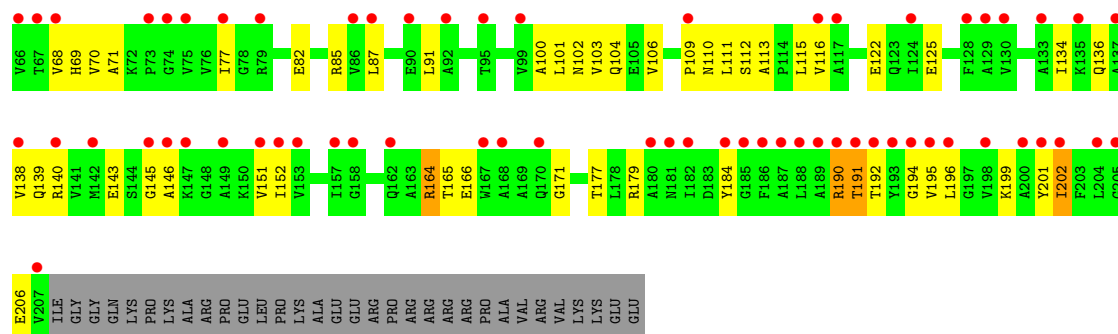


• Molecule 34: 30S ribosomal protein S3

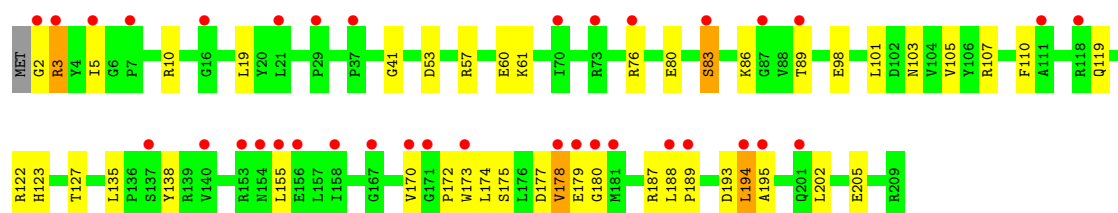
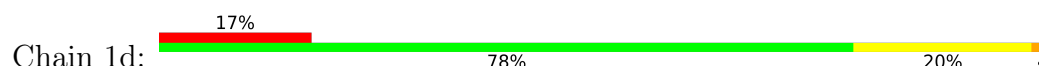


• Molecule 34: 30S ribosomal protein S3

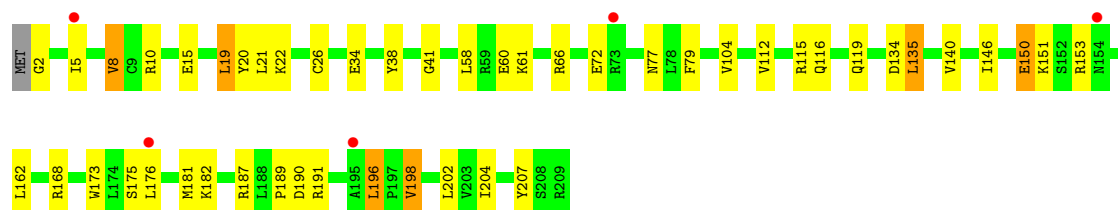
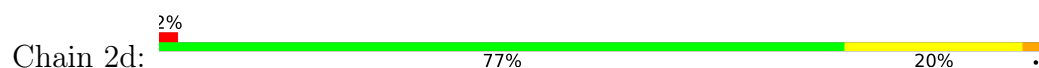




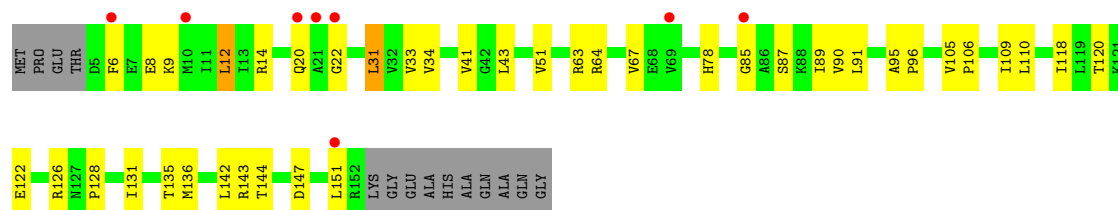
• Molecule 35: 30S ribosomal protein S4



• Molecule 35: 30S ribosomal protein S4



• Molecule 36: 30S ribosomal protein S5

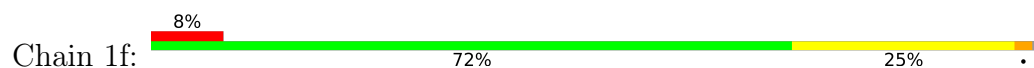


• Molecule 36: 30S ribosomal protein S5

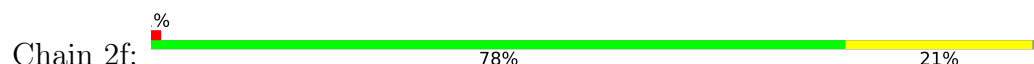




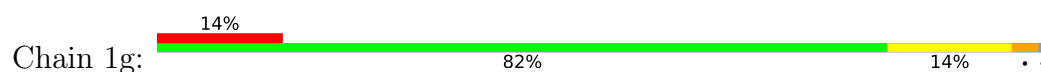
- Molecule 37: 30S ribosomal protein S6



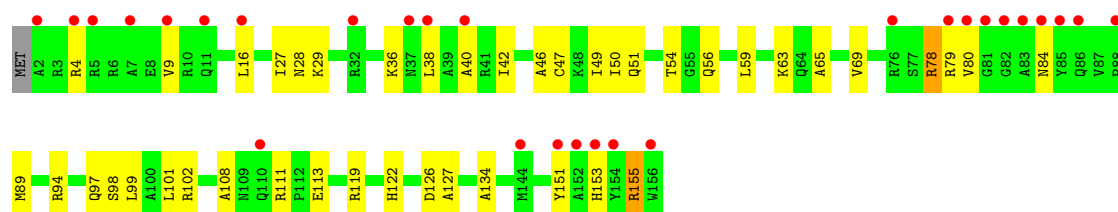
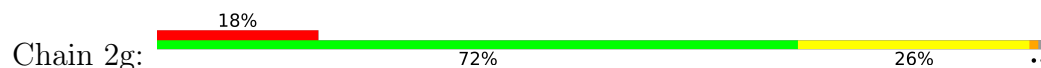
- Molecule 37: 30S ribosomal protein S6



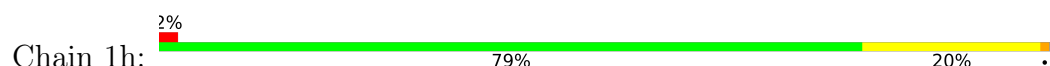
- Molecule 38: 30S ribosomal protein S7



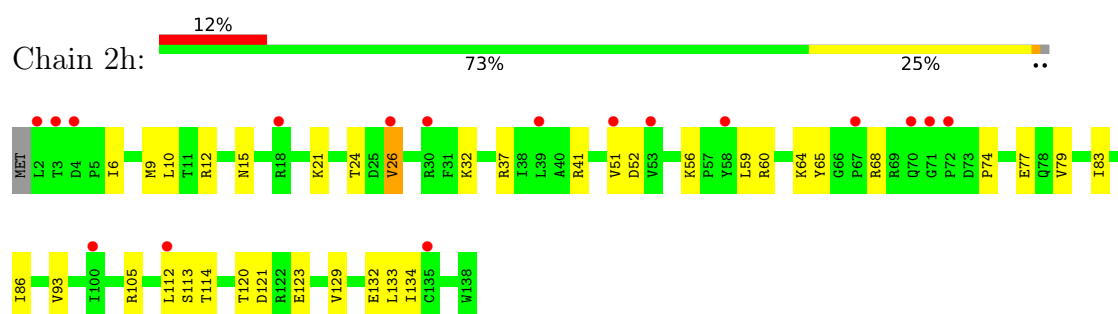
- Molecule 38: 30S ribosomal protein S7



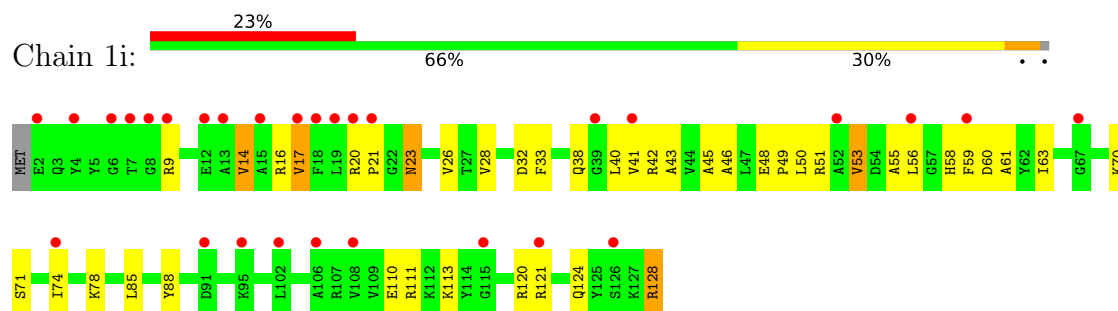
- Molecule 39: 30S ribosomal protein S8



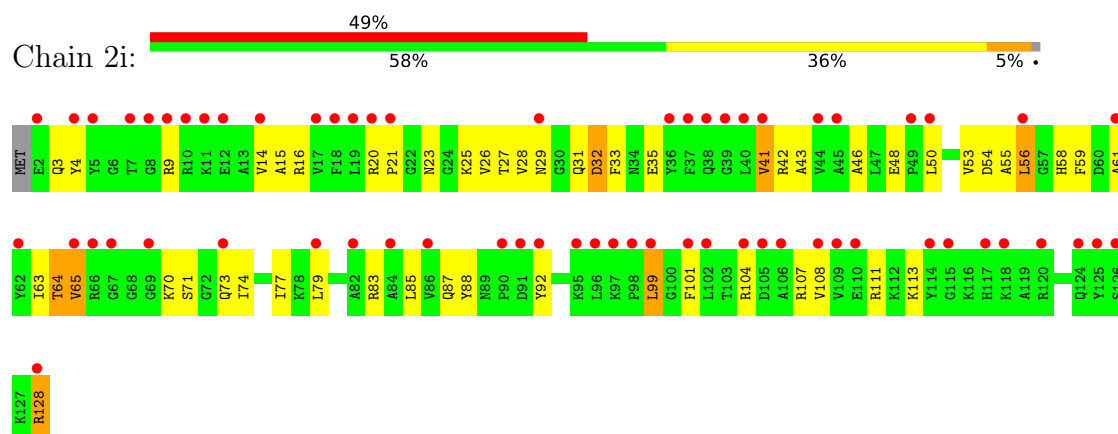
- Molecule 39: 30S ribosomal protein S8



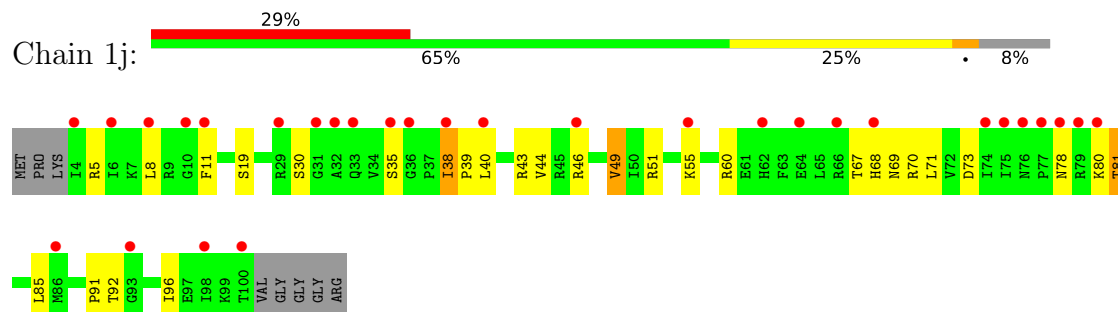
- Molecule 40: 30S ribosomal protein S9



- Molecule 40: 30S ribosomal protein S9

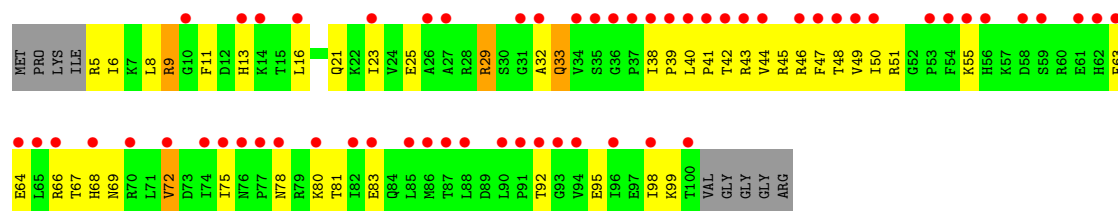


- Molecule 41: 30S ribosomal protein S10

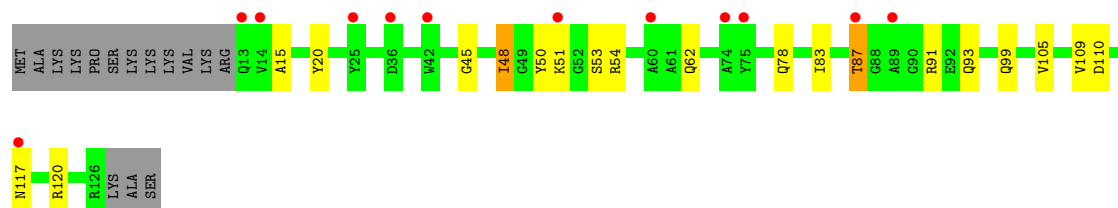
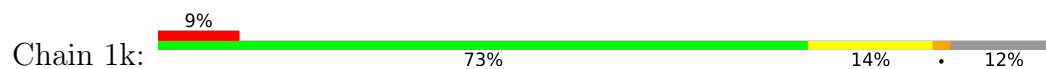


- Molecule 41: 30S ribosomal protein S10

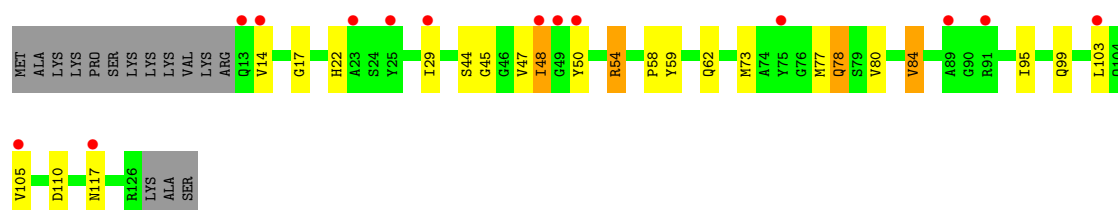
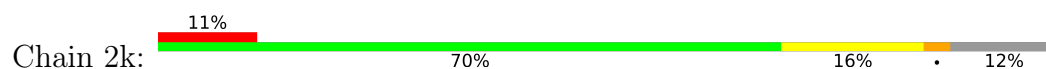




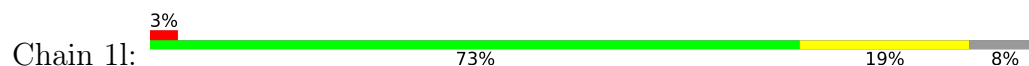
• Molecule 42: 30S ribosomal protein S11



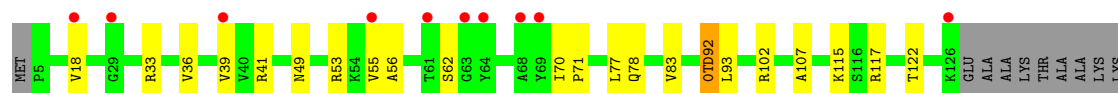
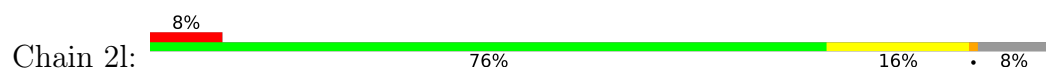
• Molecule 42: 30S ribosomal protein S11



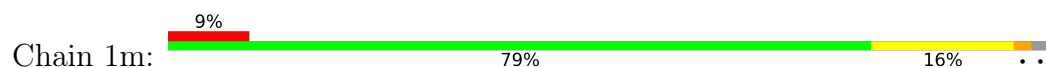
• Molecule 43: 30S ribosomal protein S12

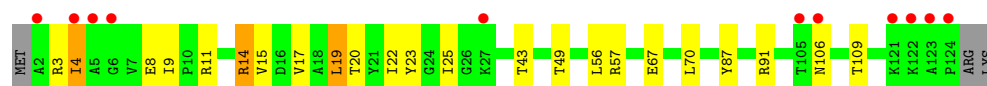


• Molecule 43: 30S ribosomal protein S12

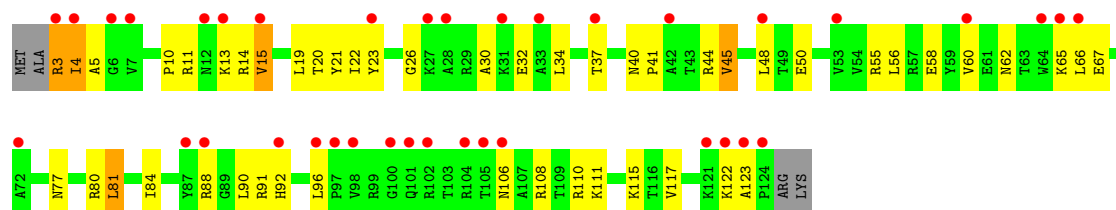


• Molecule 44: 30S ribosomal protein S13

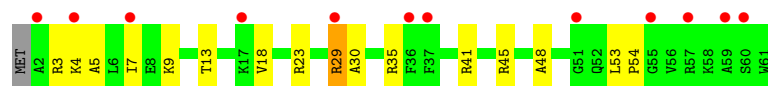
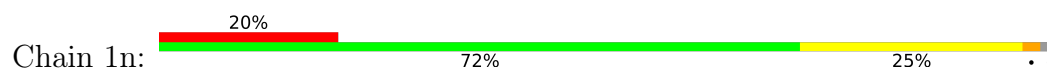




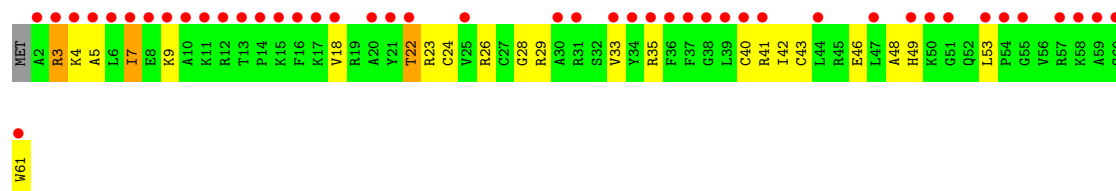
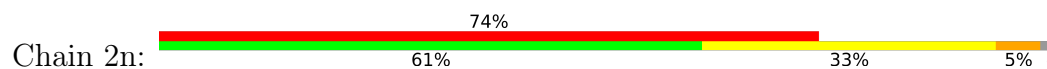
- Molecule 44: 30S ribosomal protein S13



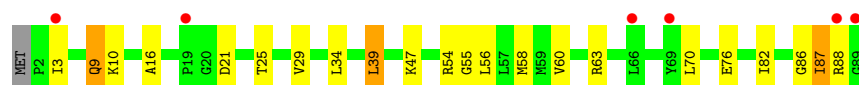
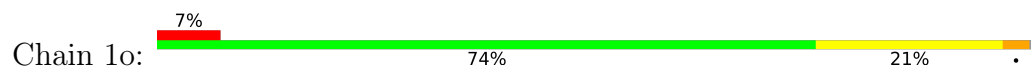
- Molecule 45: 30S ribosomal protein S14 type Z



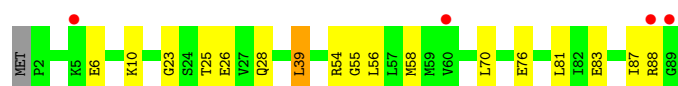
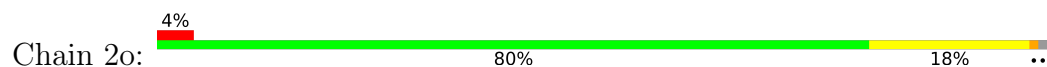
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15

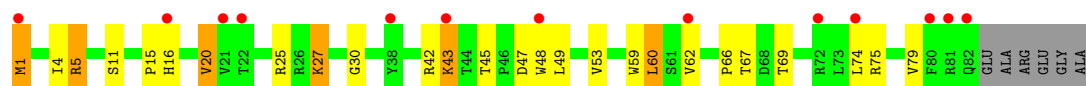


- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16

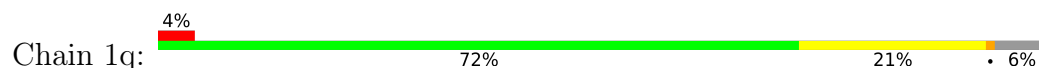




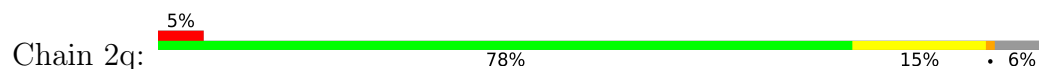
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S18

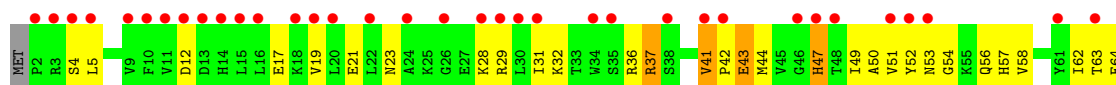


- Molecule 50: 30S ribosomal protein S19

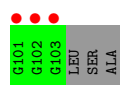
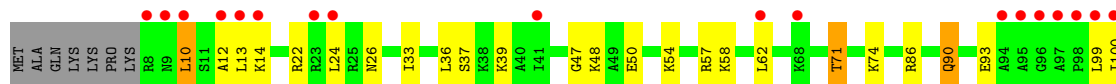




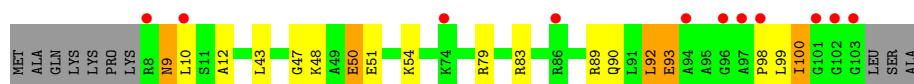
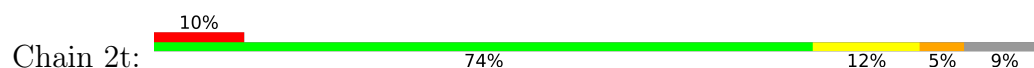
- Molecule 50: 30S ribosomal protein S19



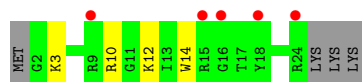
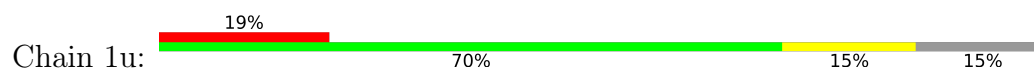
- Molecule 51: 30S ribosomal protein S20



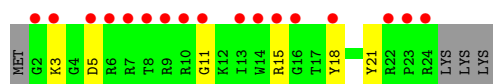
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx

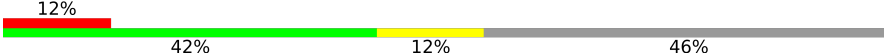


- Molecule 53: MF-mRNA

Chain 1v: 



• Molecule 53: MF-mRNA

Chain 2v: 



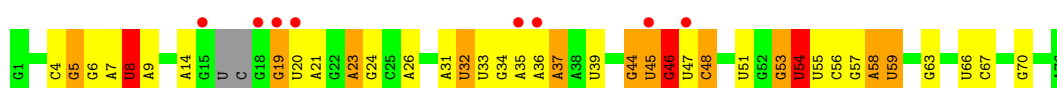
• Molecule 54: A- and E-site Deacylated tRNAphe

Chain 1w: 



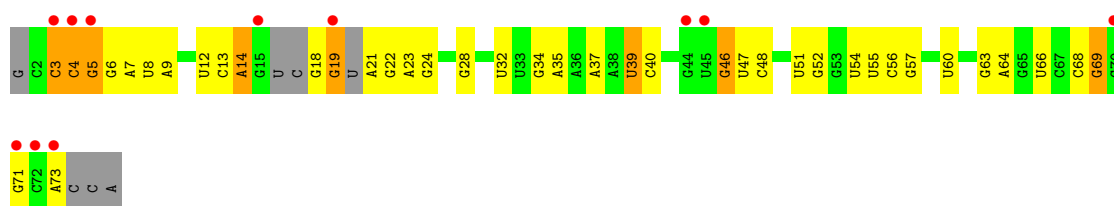
• Molecule 54: A- and E-site Deacylated tRNAphe

Chain 1y: 



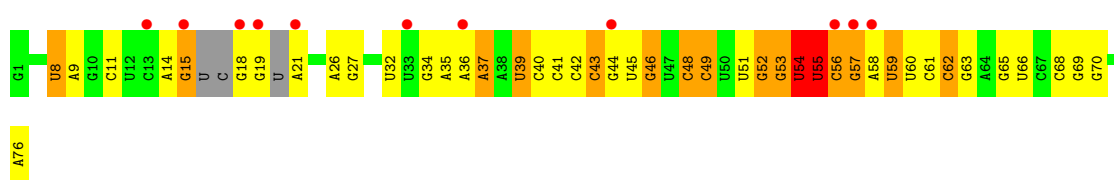
• Molecule 54: A- and E-site Deacylated tRNAphe

Chain 2w: 

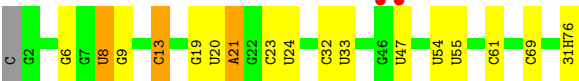
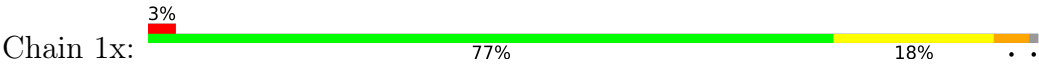


• Molecule 54: A- and E-site Deacylated tRNAphe

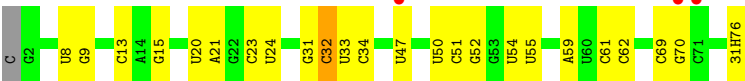
Chain 2y: 



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.03Å 450.06Å 623.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	182.49 – 2.55 182.49 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (182.49-2.55) 100.0 (182.49-2.55)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.205 , 0.242 (Not available) , 0.228	Depositor DCC
R_{free} test set	95005 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	299373	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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: 4SU, MG, 2MG, ZN, SF4, MIA, OMC, OMU, G7M, 5MC, UR3, 5MU, WC9, 2MA, 0TD, 4OC, OMG, M2G, K, 31H, PSU, MA6

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	1/68985 (0.0%)	0.47	3/107677 (0.0%)
1	2A	0.21	0/67269	0.40	1/104999 (0.0%)
2	1B	0.21	0/2882	0.40	0/4494
2	2B	0.18	0/2879	0.36	0/4487
3	1D	0.27	0/2186	0.49	0/2944
3	2D	0.23	0/2186	0.45	0/2944
4	1E	0.26	0/1592	0.50	0/2149
4	2E	0.20	0/1592	0.42	0/2149
5	1F	0.25	0/1619	0.50	0/2193
5	2F	0.19	0/1615	0.45	0/2188
6	1G	0.22	0/1448	0.45	0/1957
6	2G	0.19	0/1453	0.40	0/1963
7	1H	0.21	0/1356	0.40	0/1834
7	2H	0.18	0/1356	0.35	0/1834
8	1I	0.19	0/1112	0.39	0/1514
8	2I	0.18	0/1079	0.40	0/1475
9	1N	0.24	0/1144	0.47	0/1543
9	2N	0.18	0/1144	0.40	0/1543
10	1O	0.25	0/943	0.45	0/1269
10	2O	0.19	0/943	0.42	0/1269
11	1P	0.25	0/1152	0.54	0/1533
11	2P	0.21	0/1152	0.51	0/1533
12	1Q	0.27	0/1143	0.49	0/1527
12	2Q	0.20	0/1143	0.42	0/1527
13	1R	0.27	0/982	0.50	0/1312
13	2R	0.20	0/982	0.44	0/1312
14	1S	0.21	0/883	0.46	0/1176
14	2S	0.20	0/880	0.43	0/1172
15	1T	0.23	0/1105	0.47	0/1477
15	2T	0.19	0/1097	0.42	0/1468
16	1U	0.28	0/977	0.46	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	0.24	0/782	0.49	0/1049
17	2V	0.18	0/782	0.40	0/1049
18	1W	0.27	0/897	0.45	0/1205
18	2W	0.21	0/897	0.40	0/1205
19	1X	0.25	0/764	0.53	0/1025
19	2X	0.21	0/764	0.46	2/1025 (0.2%)
20	1Y	0.23	0/819	0.49	0/1095
20	2Y	0.19	0/819	0.45	0/1095
21	1Z	0.21	0/1267	0.47	0/1717
21	2Z	0.22	0/1299	0.46	0/1763
22	10	0.25	0/616	0.55	0/821
22	20	0.20	0/662	0.46	0/881
23	11	0.23	0/762	0.41	0/1014
23	21	0.21	0/762	0.40	0/1014
24	12	0.24	0/590	0.41	0/781
24	22	0.18	0/590	0.38	0/781
25	13	0.27	0/474	0.48	0/635
25	23	0.17	0/469	0.40	0/630
26	14	0.24	0/565	0.56	0/761
26	24	0.22	0/545	0.47	0/737
27	15	0.28	0/469	0.54	0/635
27	25	0.21	0/469	0.40	0/635
28	16	0.26	0/460	0.47	0/613
28	26	0.20	0/456	0.41	0/608
29	17	0.30	0/426	0.50	0/561
29	27	0.26	0/426	0.50	0/561
30	18	0.25	0/525	0.45	0/691
30	28	0.20	0/525	0.39	0/691
31	19	0.28	0/310	0.52	0/407
31	29	0.18	0/310	0.41	0/407
32	1a	0.20	0/35795	0.38	0/55864
32	2a	0.19	0/35886	0.37	3/56005 (0.0%)
33	1b	0.21	0/1881	0.48	0/2542
33	2b	0.21	0/1860	0.48	0/2518
34	1c	0.19	0/1572	0.40	1/2126 (0.0%)
34	2c	0.21	0/1566	0.42	0/2119
35	1d	0.19	0/1685	0.40	0/2262
35	2d	0.19	0/1704	0.43	0/2284
36	1e	0.20	0/1145	0.44	0/1543
36	2e	0.20	0/1149	0.43	0/1548
37	1f	0.18	0/823	0.40	0/1115
37	2f	0.18	0/829	0.37	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.18	0/1250	0.40	1/1679 (0.1%)
38	2g	0.18	0/1254	0.38	0/1683
39	1h	0.18	0/1108	0.41	0/1494
39	2h	0.18	0/1108	0.42	0/1494
40	1i	0.21	0/1002	0.46	0/1346
40	2i	0.22	0/997	0.47	0/1343
41	1j	0.21	0/722	0.47	0/982
41	2j	0.22	0/727	0.50	0/988
42	1k	0.18	0/844	0.39	0/1145
42	2k	0.18	0/848	0.37	0/1149
43	1l	0.21	0/937	0.41	0/1260
43	2l	0.18	0/937	0.40	0/1260
44	1m	0.19	0/969	0.50	0/1302
44	2m	0.21	0/961	0.45	0/1291
45	1n	0.19	0/501	0.43	0/664
45	2n	0.20	0/501	0.47	0/664
46	1o	0.19	0/739	0.36	0/985
46	2o	0.17	0/739	0.40	0/985
47	1p	0.21	0/697	0.47	0/939
47	2p	0.20	0/693	0.45	0/935
48	1q	0.18	0/836	0.42	0/1117
48	2q	0.17	0/836	0.42	0/1117
49	1r	0.20	0/560	0.42	0/746
49	2r	0.19	0/560	0.38	0/746
50	1s	0.20	0/667	0.46	0/900
50	2s	0.24	0/661	0.57	0/893
51	1t	0.19	0/730	0.49	0/965
51	2t	0.21	0/729	0.45	0/965
52	1u	0.18	0/203	0.44	0/266
52	2u	0.26	0/203	0.46	0/266
53	1v	0.19	0/310	0.33	0/480
53	2v	0.18	0/310	0.34	0/480
54	1w	0.27	1/1559 (0.1%)	0.38	0/2424
54	1y	0.28	2/1606 (0.1%)	0.39	0/2497
54	2w	0.31	1/1487 (0.1%)	0.40	0/2311
54	2y	0.27	0/1583	0.38	0/2459
55	1x	0.28	1/1700 (0.1%)	0.41	0/2650
55	2x	0.26	1/1700 (0.1%)	0.38	0/2650
All	All	0.23	7/316426 (0.0%)	0.42	11/473725 (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
11	1P	0	1
11	2P	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	8	4SU	O3'-P	5.42	1.61	1.56
54	2w	46	G7M	O3'-P	5.27	1.61	1.56
54	1y	46	G7M	O3'-P	5.13	1.61	1.56
55	2x	8	4SU	O3'-P	5.07	1.61	1.56
1	1A	2552	OMU	O3'-P	5.06	1.61	1.56
54	1w	46	G7M	O3'-P	5.04	1.61	1.56
55	1x	8	4SU	O3'-P	5.02	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'	7.65	120.98	109.50
1	2A	1992	G	C2'-C3'-O3'	6.66	119.49	109.50
34	1c	86	VAL	N-CA-C	-5.77	105.77	112.98
1	1A	1992	G	P-O3'-C3'	5.72	128.78	120.20
32	2a	1272	G	N1-C2-N2	-5.56	99.53	116.20
38	1g	69	VAL	N-CA-C	-5.35	107.26	112.29
19	2X	94	GLY	CA-C-N	5.18	131.02	121.70
19	2X	94	GLY	C-N-CA	5.18	131.02	121.70
32	2a	1263	C	N1-C2-O2	5.16	134.38	118.90
1	1A	512	G	O4'-C1'-N9	5.13	115.90	108.20
32	2a	1272	G	N3-C2-N2	5.01	134.93	119.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
11	2P	35	HIS	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	61854	0	31201	432	0
1	2A	60324	0	30432	517	0
2	1B	2577	0	1305	17	0
2	2B	2575	0	1303	37	0
3	1D	2136	0	2218	29	0
3	2D	2136	0	2218	33	0
4	1E	1559	0	1618	16	0
4	2E	1559	0	1618	20	0
5	1F	1584	0	1625	23	0
5	2F	1580	0	1619	35	0
6	1G	1423	0	1436	33	0
6	2G	1428	0	1438	49	0
7	1H	1330	0	1407	14	0
7	2H	1330	0	1407	20	0
8	1I	1097	0	1140	23	0
8	2I	1064	0	1082	28	0
9	1N	1117	0	1184	13	0
9	2N	1117	0	1184	26	0
10	1O	933	0	996	10	0
10	2O	933	0	996	14	0
11	1P	1135	0	1212	23	0
11	2P	1135	0	1212	26	0
12	1Q	1122	0	1179	15	0
12	2Q	1122	0	1179	21	0
13	1R	968	0	1033	12	0
13	2R	968	0	1033	14	0
14	1S	873	0	927	18	0
14	2S	870	0	923	34	0
15	1T	1091	0	1151	12	0
15	2T	1083	0	1136	10	0
16	1U	959	0	1019	11	0
16	2U	959	0	1019	15	0
17	1V	771	0	830	7	0
17	2V	771	0	830	14	0
18	1W	886	0	940	6	0
18	2W	886	0	940	12	0
19	1X	750	0	814	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2X	750	0	813	12	0
20	1Y	806	0	881	13	0
20	2Y	806	0	881	12	0
21	1Z	1240	0	1240	25	0
21	2Z	1271	0	1273	55	0
22	10	608	0	622	7	0
22	20	653	0	674	6	0
23	11	755	0	826	7	0
23	21	755	0	826	12	0
24	12	588	0	643	6	0
24	22	588	0	643	7	0
25	13	469	0	518	7	0
25	23	464	0	514	7	0
26	14	552	0	533	19	0
26	24	532	0	503	20	0
27	15	455	0	465	4	0
27	25	455	0	465	8	0
28	16	453	0	473	7	0
28	26	449	0	469	6	0
29	17	418	0	467	5	0
29	27	418	0	467	6	0
30	18	517	0	582	6	0
30	28	517	0	582	9	0
31	19	307	0	335	3	0
31	29	307	0	335	6	0
32	1a	32246	0	16295	309	0
32	2a	32327	0	16338	357	0
33	1b	1846	0	1867	42	0
33	2b	1825	0	1828	69	0
34	1c	1548	0	1535	31	0
34	2c	1542	0	1517	45	0
35	1d	1655	0	1672	29	0
35	2d	1674	0	1714	34	0
36	1e	1129	0	1185	28	0
36	2e	1133	0	1191	35	0
37	1f	810	0	804	15	0
37	2f	816	0	808	17	0
38	1g	1231	0	1238	15	0
38	2g	1235	0	1249	30	0
39	1h	1088	0	1126	19	0
39	2h	1088	0	1126	25	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	41	0
41	1j	709	0	650	22	0
41	2j	714	0	672	33	0
42	1k	829	0	825	13	0
42	2k	833	0	836	16	0
43	1l	932	0	981	13	0
43	2l	932	0	980	10	0
44	1m	958	0	1002	12	0
44	2m	950	0	988	34	0
45	1n	492	0	529	12	0
45	2n	492	0	529	20	0
46	1o	728	0	760	12	0
46	2o	728	0	760	13	0
47	1p	681	0	697	18	0
47	2p	677	0	686	16	0
48	1q	823	0	891	14	0
48	2q	823	0	891	9	0
49	1r	555	0	618	9	0
49	2r	555	0	618	19	0
50	1s	652	0	662	20	0
50	2s	646	0	644	36	0
51	1t	728	0	798	19	0
51	2t	727	0	796	11	0
52	1u	199	0	208	3	0
52	2u	199	0	208	5	0
53	1v	277	0	140	4	0
53	2v	277	0	140	1	0
54	1w	1550	0	796	36	0
54	1y	1585	0	803	16	0
54	2w	1482	0	754	15	0
54	2y	1565	0	794	35	0
55	1x	1635	0	839	5	0
55	2x	1635	0	839	8	0
56	10	9	0	0	0	0
56	11	5	0	0	0	0
56	12	2	0	0	0	0
56	13	4	0	0	0	0
56	14	1	0	0	0	0
56	15	8	0	0	0	0
56	16	1	0	0	0	0
56	17	5	0	0	0	0
56	18	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	19	1	0	0	0	0
56	1A	1097	0	0	0	0
56	1B	36	0	0	0	0
56	1D	11	0	0	0	0
56	1E	18	0	0	0	0
56	1F	13	0	0	0	0
56	1G	4	0	0	0	0
56	1I	1	0	0	0	0
56	1N	6	0	0	0	0
56	1O	6	0	0	0	0
56	1P	5	0	0	0	0
56	1Q	7	0	0	0	0
56	1R	8	0	0	0	0
56	1S	3	0	0	0	0
56	1T	2	0	0	0	0
56	1U	10	0	0	0	0
56	1V	7	0	0	0	0
56	1W	4	0	0	0	0
56	1X	7	0	0	0	0
56	1Y	3	0	0	0	0
56	1Z	3	0	0	0	0
56	1a	196	0	0	0	0
56	1b	1	0	0	0	0
56	1d	1	0	0	0	0
56	1e	1	0	0	0	0
56	1f	1	0	0	0	0
56	1l	2	0	0	0	0
56	1m	2	0	0	0	0
56	1n	2	0	0	0	0
56	1r	1	0	0	0	0
56	1t	1	0	0	0	0
56	1w	5	0	0	0	0
56	1x	14	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	1	0	0	0	0
56	25	4	0	0	0	0
56	27	3	0	0	0	0
56	28	3	0	0	0	0
56	2A	808	0	0	0	0
56	2B	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2D	6	0	0	0	0
56	2E	8	0	0	0	0
56	2F	7	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	1	0	0	0	0
56	2Q	3	0	0	0	0
56	2R	3	0	0	0	0
56	2T	4	0	0	0	0
56	2U	1	0	0	0	0
56	2V	2	0	0	0	0
56	2W	5	0	0	0	0
56	2X	2	0	0	0	0
56	2a	230	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	2j	1	0	0	0	0
56	2l	4	0	0	0	0
56	2q	2	0	0	0	0
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	3	0	0	0	0
56	2w	4	0	0	0	0
56	2x	5	0	0	0	0
56	2y	3	0	0	0	0
57	1A	34	0	0	1	0
57	2A	34	0	0	4	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	2d	8	0	0	0	0
60	1x	1	0	0	0	0
60	2x	1	0	0	0	0
61	10	9	0	0	0	0
61	11	8	0	0	0	0
61	12	3	0	0	0	0
61	13	3	0	0	0	0
61	14	1	0	0	0	0
61	15	4	0	0	0	0
61	16	2	0	0	0	0
61	17	12	0	0	2	0
61	18	9	0	0	0	0
61	1A	1899	0	0	55	0
61	1B	59	0	0	3	0
61	1D	27	0	0	1	0
61	1E	26	0	0	1	0
61	1F	16	0	0	1	0
61	1G	1	0	0	0	0
61	1H	2	0	0	0	0
61	1N	6	0	0	0	0
61	1O	5	0	0	0	0
61	1P	22	0	0	1	0
61	1Q	8	0	0	0	0
61	1R	9	0	0	0	0
61	1S	3	0	0	1	0
61	1T	8	0	0	0	0
61	1U	14	0	0	0	0
61	1V	8	0	0	0	0
61	1W	8	0	0	2	0
61	1X	4	0	0	0	0
61	1Y	3	0	0	1	0
61	1Z	1	0	0	0	0
61	1a	263	0	0	20	0
61	1b	1	0	0	0	0
61	1d	2	0	0	0	0
61	1f	1	0	0	0	0
61	1g	1	0	0	0	0
61	1l	3	0	0	0	0
61	1n	1	0	0	0	0
61	1q	2	0	0	0	0
61	1v	5	0	0	0	0
61	1w	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1x	10	0	0	0	0
61	1y	1	0	0	0	0
61	20	4	0	0	0	0
61	21	7	0	0	1	0
61	23	2	0	0	0	0
61	27	4	0	0	0	0
61	28	3	0	0	0	0
61	29	1	0	0	0	0
61	2A	974	0	0	49	0
61	2B	14	0	0	2	0
61	2D	19	0	0	0	0
61	2E	11	0	0	0	0
61	2F	10	0	0	0	0
61	2N	1	0	0	0	0
61	2O	2	0	0	0	0
61	2P	9	0	0	1	0
61	2Q	1	0	0	0	0
61	2R	4	0	0	0	0
61	2T	4	0	0	0	0
61	2U	2	0	0	0	0
61	2X	2	0	0	0	0
61	2a	184	0	0	16	0
61	2e	1	0	0	0	0
61	2g	1	0	0	0	0
61	2j	3	0	0	0	0
61	2l	3	0	0	0	0
61	2t	1	0	0	0	0
61	2v	1	0	0	0	0
61	2x	4	0	0	0	0
61	2y	2	0	0	0	0
All	All	299373	0	196613	3107	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (3107) 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	1.24
1:1A:1054:A:H61	1:1A:1105:U:H3	1.15	0.93
1:1A:2136:C:H42	1:1A:2155:G:H1	1.01	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.49	0.93
54:1w:2:C:H42	54:1w:71:G:H1	1.15	0.93
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.53	0.91
29:17:24:THR:HG22	29:17:27:GLY:H	1.35	0.91
1:1A:2427:C:OP1	61:1A:4101:HOH:O	1.89	0.90
1:1A:2554:U:H3	54:1w:74:C:H42	1.19	0.90
1:1A:1082:U:O4	1:1A:1086:A:N1	2.05	0.89
1:1A:1062:G:H1	1:1A:1077:A:H61	1.22	0.87
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.22	0.87
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.41	0.86
1:1A:2136:C:N4	1:1A:2155:G:H1	1.73	0.86
1:2A:2319:G:H22	14:2S:3:ARG:HH11	1.25	0.85
32:2a:406:G:H21	35:2d:119:GLN:HE22	1.23	0.85
34:1c:71:ALA:HA	34:1c:106:VAL:HG21	1.59	0.84
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.59	0.84
9:2N:123:TYR:HH	9:2N:130:HIS:HE2	1.20	0.84
54:2y:18:G:N2	54:2y:55:PSU:N3	2.24	0.84
1:2A:1204:A:H2	1:2A:1241:A:H62	1.23	0.84
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.60	0.84
40:2i:16:ARG:HB2	40:2i:64:THR:HG22	1.57	0.83
32:2a:1316:G:H22	32:2a:1319:A:H5''	1.42	0.83
1:2A:2125:G:N3	1:2A:2173:A:N6	2.27	0.83
32:1a:664:G:H22	32:1a:741:G:H1	1.27	0.83
1:2A:1689:A:H62	1:2A:1698:A:H2	1.22	0.82
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	1.60	0.82
1:1A:1669:A:OP2	61:1A:4102:HOH:O	1.98	0.81
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.28	0.81
32:2a:1029:C:C4	32:2a:1032:G:N1	2.48	0.81
32:2a:953:G:H5'	32:2a:965:A:H61	1.45	0.81
1:1A:1082:U:N3	1:1A:1086:A:N6	2.04	0.80
34:2c:47:LEU:HD22	34:2c:68:VAL:HG11	1.62	0.80
21:2Z:138:GLU:H	21:2Z:156:LYS:HE2	1.45	0.79
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.64	0.79
42:2k:99:GLN:HG2	42:2k:105:VAL:HG21	1.64	0.79
40:2i:28:VAL:HG12	40:2i:63:ILE:HB	1.65	0.79
54:2y:18:G:N2	54:2y:55:PSU:HN3	1.81	0.79
32:1a:975:A:H4'	32:1a:976:G:H5''	1.65	0.79
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.30	0.79
1:1A:2447:G:OP2	61:1A:4103:HOH:O	1.99	0.78
32:1a:1505:G:OP2	61:1a:1801:HOH:O	2.00	0.78
32:1a:1086:U:H3	32:1a:1099:G:H22	1.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:6:ILE:HB	41:2j:72:VAL:HG13	1.66	0.78
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.16	0.78
1:2A:948:G:OP1	61:2A:3902:HOH:O	2.02	0.78
32:2a:975:A:H4'	32:2a:976:G:H5''	1.64	0.78
44:2m:3:ARG:HH22	44:2m:11:ARG:HG3	1.49	0.78
1:1A:884:C:H42	1:1A:892:G:H1	1.32	0.78
10:1O:48:PRO:HB3	32:1a:1422:G:H5''	1.64	0.78
1:2A:2592:G:OP1	61:2A:3901:HOH:O	2.01	0.78
54:2y:18:G:H22	54:2y:55:PSU:HN3	1.32	0.78
32:2a:504:C:OP1	61:2a:1901:HOH:O	2.02	0.77
22:10:10:THR:HG22	22:10:12:ASN:H	1.48	0.77
1:1A:2550:G:OP1	61:1A:4102:HOH:O	2.01	0.77
2:2B:75:G:H22	21:2Z:73:GLN:HE21	1.33	0.77
32:1a:559:A:OP1	36:1e:126:ARG:NH2	2.19	0.76
10:1O:63:VAL:HG12	10:1O:106:LEU:HD11	1.66	0.76
32:2a:1224:G:OP1	61:2a:1903:HOH:O	2.03	0.76
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.49	0.76
26:24:53:GLU:HG2	26:24:55:ARG:H	1.51	0.76
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.19	0.76
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.19	0.76
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.51	0.76
32:1a:1009:G:O6	32:1a:1020:U:O2	2.04	0.76
5:2F:18:ARG:NH1	5:2F:127:GLU:OE2	2.18	0.76
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.66	0.76
6:1G:126:ASP:HB3	6:1G:128:ARG:H	1.51	0.75
54:1w:2:C:N4	54:1w:71:G:H1	1.83	0.75
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.19	0.75
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.20	0.75
32:2a:596:C:OP2	61:2a:1902:HOH:O	2.03	0.75
1:1A:826:U:OP1	61:1A:4101:HOH:O	2.03	0.75
1:1A:1332:G:OP1	61:1A:4104:HOH:O	2.02	0.75
1:2A:962:G:OP1	61:2A:3902:HOH:O	2.05	0.75
32:1a:165:C:H2'	32:1a:166:G:H8	1.51	0.75
11:2P:91:PHE:O	11:2P:121:LYS:NZ	2.19	0.75
1:1A:2136:C:N3	1:1A:2155:G:N2	2.34	0.75
1:1A:1054:A:N6	1:1A:1105:U:H3	1.83	0.75
32:2a:266:G:H5''	32:2a:268:C:H41	1.52	0.74
1:1A:1014:U:OP2	61:1A:4107:HOH:O	2.06	0.74
44:1m:3:ARG:HD2	44:1m:9:ILE:HG12	1.69	0.74
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.21	0.74
1:2A:1021:A:H62	1:2A:1141:U:H3	1.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.19	0.74
32:2a:117:G:OP2	61:2a:1905:HOH:O	2.05	0.74
1:1A:387:U:O4	61:1A:4105:HOH:O	2.04	0.74
39:1h:113:SER:HB2	39:1h:134:ILE:HD11	1.68	0.74
1:2A:1812:A:OP2	61:2A:3903:HOH:O	2.05	0.74
1:1A:1670:C:OP2	61:1A:4102:HOH:O	2.05	0.74
44:2m:23:TYR:HB3	44:2m:67:GLU:HA	1.69	0.74
26:24:16:CYS:SG	26:24:17:GLY:N	2.60	0.73
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.22	0.73
3:2D:125:ILE:HB	37:2f:81:ILE:HD11	1.69	0.73
32:2a:558:G:OP1	61:2a:1904:HOH:O	2.06	0.73
50:2s:41:VAL:HG13	50:2s:43:GLU:H	1.53	0.73
1:1A:1702:G:N7	61:1A:4130:HOH:O	2.20	0.73
1:2A:397:G:N7	61:2A:3937:HOH:O	2.21	0.73
32:2a:299:G:O6	61:2a:1904:HOH:O	2.05	0.73
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.70	0.73
1:1A:2058:MA6:H8	1:1A:2058:MA6:O5'	1.89	0.73
32:1a:953:G:H5'	32:1a:965:A:H61	1.52	0.73
1:2A:1508:A:H4'	1:2A:1509(A):A:C5	2.24	0.73
40:2i:128:ARG:NH2	55:2x:33:U:OP2	2.21	0.73
32:2a:598:U:O4	61:2a:1902:HOH:O	2.07	0.73
32:2a:1272:G:N2	32:2a:1273:G:N7	2.36	0.73
54:1w:1:G:C6	54:1w:72:C:C4	2.76	0.72
1:1A:1647:G:OP1	61:1A:4108:HOH:O	2.06	0.72
34:1c:15:THR:HG22	34:1c:16:ARG:HG2	1.71	0.72
1:1A:1602:U:O4	61:1A:4106:HOH:O	2.06	0.72
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.23	0.72
32:2a:289:G:OP2	61:2a:1905:HOH:O	2.07	0.72
32:2a:1314:C:OP2	50:2s:4:SER:OG	2.05	0.72
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.71	0.72
33:2b:19:HIS:HB2	33:2b:204:ASN:HB2	1.72	0.72
1:1A:2629:A:O2'	1:1A:2630:G:OP2	2.08	0.72
19:1X:88:LYS:NZ	19:1X:90:GLU:OE2	2.22	0.72
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.72	0.72
24:12:41:ILE:HG13	24:12:43:GLN:HG3	1.71	0.72
6:2G:114:ILE:HA	6:2G:140:ILE:HD11	1.71	0.72
1:1A:135:G:N7	61:1A:4139:HOH:O	2.23	0.72
2:1B:58:A:OP2	61:1B:301:HOH:O	2.08	0.72
2:2B:106:G:H5'	21:2Z:31:ARG:HG2	1.72	0.71
1:2A:1647:G:OP1	61:2A:3907:HOH:O	2.08	0.71
1:2A:570:G:O6	61:2A:3906:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.23	0.71
32:2a:1239:A:H62	32:2a:1299:A:H62	1.38	0.71
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.73	0.71
54:1y:8:4SU:H4'	54:1y:48:C:H4'	1.71	0.71
1:2A:730:C:OP2	61:2A:3909:HOH:O	2.09	0.71
32:2a:1521:G:N3	61:2a:1911:HOH:O	2.24	0.71
1:2A:2138:C:H42	1:2A:2153:G:H1	1.36	0.71
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.22	0.71
5:1F:89:VAL:O	61:1F:401:HOH:O	2.09	0.71
14:1S:3:ARG:NH1	61:1S:301:HOH:O	2.24	0.71
26:14:16:CYS:SG	26:14:17:GLY:N	2.64	0.71
32:1a:1224:G:OP1	61:1a:1803:HOH:O	2.08	0.70
1:2A:963:U:OP2	61:2A:3902:HOH:O	2.08	0.70
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.73	0.70
1:1A:2763:G:OP2	61:1A:4110:HOH:O	2.08	0.70
1:2A:1346:G:OP2	61:2A:3905:HOH:O	2.07	0.70
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.72	0.70
1:1A:123:G:OP2	61:1A:4111:HOH:O	2.09	0.70
32:1a:812:C:O2	61:1a:1802:HOH:O	2.05	0.70
33:1b:118:LEU:HB3	33:1b:142:LEU:HD12	1.73	0.70
32:1a:1381:U:H1'	38:1g:79:ARG:HG2	1.74	0.70
36:1e:8:GLU:OE2	36:1e:63:ARG:NH2	2.25	0.70
1:2A:1670:C:OP1	61:2A:3904:HOH:O	2.07	0.70
32:2a:1228:C:OP1	44:2m:115:LYS:NZ	2.23	0.70
1:2A:1973:G:OP1	61:2A:3908:HOH:O	2.09	0.70
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.74	0.70
11:1P:39:LYS:HB2	11:1P:45:LEU:HD13	1.73	0.70
1:1A:602:G:N1	1:1A:655:A:OP2	2.24	0.69
32:1a:677:U:H3	32:1a:713:G:H22	1.40	0.69
38:1g:78:ARG:HD3	38:1g:79:ARG:H	1.57	0.69
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.25	0.69
33:2b:178:ARG:HH22	39:2h:68:ARG:HH12	1.40	0.69
1:1A:2499:C:OP1	61:1A:4113:HOH:O	2.10	0.69
54:1w:1:G:C2	54:1w:72:C:C2	2.80	0.69
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.40	0.69
2:2B:76:G:N7	61:2B:302:HOH:O	2.26	0.69
1:1A:392:C:OP1	61:1A:4112:HOH:O	2.09	0.69
1:1A:1693:U:O2'	3:1D:14:ARG:NH2	2.25	0.69
1:1A:2306:C:O2	61:1A:4109:HOH:O	2.07	0.69
54:1w:26:A:H61	54:1w:44:G:H1	1.40	0.69
1:2A:1693:U:O2'	3:2D:14:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.27	0.69
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.73	0.69
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.25	0.69
40:2i:50:LEU:HD13	40:2i:56:LEU:HA	1.75	0.69
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.73	0.69
1:1A:1058:G:N2	1:1A:1081:U:O2	2.24	0.69
32:2a:1133:G:H1	32:2a:1141:C:H42	1.41	0.69
1:1A:1055:G:H1	1:1A:1104:C:H42	1.41	0.69
54:1w:1:G:C6	54:1w:72:C:N3	2.60	0.69
1:2A:2058:MA6:H91	57:2A:3809:WC9:OAH	1.93	0.69
33:2b:74:LYS:NZ	33:2b:205:ASP:O	2.26	0.69
34:2c:58:GLU:HB3	41:2j:92:THR:HG21	1.74	0.69
40:2i:27:THR:HA	40:2i:32:ASP:HA	1.74	0.69
1:1A:2552:OMU:OP2	61:1A:4114:HOH:O	2.10	0.69
32:2a:1417:G:O6	61:2a:1906:HOH:O	2.09	0.69
32:1a:1025:U:O2	32:1a:1036:G:O6	2.11	0.69
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.75	0.69
61:1A:4109:HOH:O	6:1G:45:GLU:OE2	2.10	0.68
33:1b:24:TRP:CD1	33:1b:24:TRP:H	2.11	0.68
35:1d:76:ARG:NH1	35:1d:80:GLU:OE2	2.25	0.68
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.26	0.68
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.75	0.68
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.75	0.68
1:1A:1243:G:O2'	11:1P:7:ARG:NH2	2.25	0.68
3:1D:8:PRO:HB3	3:1D:14:ARG:HG2	1.75	0.68
32:1a:148:G:H2'	32:1a:149:A:H8	1.58	0.68
1:2A:271(M):G:H21	8:2I:50:ARG:HD3	1.57	0.68
37:2f:97:PHE:HD2	49:2r:31:LEU:HD11	1.59	0.68
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.27	0.68
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.28	0.68
50:2s:28:LYS:HB3	50:2s:29:ARG:HA	1.74	0.68
36:1e:78:HIS:HD2	39:1h:104:ARG:HD2	1.57	0.68
7:2H:121:ILE:HD11	7:2H:140:LYS:HG2	1.74	0.68
26:24:44:THR:O	26:24:46:GLN:N	2.25	0.68
32:2a:664:G:H22	32:2a:741:G:H1	1.40	0.68
32:2a:771:G:N7	61:2a:1915:HOH:O	2.26	0.68
33:2b:54:THR:HG22	33:2b:199:TYR:HB3	1.73	0.68
28:16:13:CYS:SG	28:16:47:THR:HG21	2.33	0.68
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.75	0.68
1:2A:2467:C:H4'	12:2Q:123:HIS:CD2	2.29	0.68
1:1A:668:G:OP2	61:1A:4115:HOH:O	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2O:7:TYR:HE2	10:2O:20:MET:HE3	1.59	0.68
32:2a:1518:MA6:H93	32:2a:1519:MA6:H92	1.76	0.68
1:2A:2058:MA6:OP1	61:2A:3910:HOH:O	2.12	0.68
1:2A:2079:U:OP1	23:21:21:ARG:NH2	2.20	0.68
21:2Z:150:LEU:H	21:2Z:171:ILE:HD11	1.59	0.68
38:2g:97:GLN:HG3	38:2g:101:LEU:HD13	1.74	0.68
1:2A:2250:G:OP1	12:2Q:85:LYS:NZ	2.27	0.68
1:2A:818:G:OP2	61:2A:3912:HOH:O	2.13	0.67
34:2c:34:LEU:HD11	34:2c:38:ARG:HH21	1.59	0.67
32:1a:974:A:OP2	45:1n:29:ARG:NH2	2.27	0.67
8:2I:4:ILE:HD11	8:2I:44:LEU:HD12	1.76	0.67
46:1o:87:ILE:HG22	46:1o:88:ARG:H	1.59	0.67
1:2A:896:A:H1'	54:2w:56:C:H5'	1.76	0.67
1:2A:2143:C:H42	1:2A:2148:G:H1	1.42	0.67
32:2a:1310:G:H5'	44:2m:77:ASN:HD21	1.60	0.67
32:1a:299:G:O6	61:1a:1804:HOH:O	2.10	0.67
1:2A:2218:U:O2	23:21:52:ARG:NH1	2.28	0.67
11:2P:39:LYS:HB2	11:2P:45:LEU:HD22	1.77	0.67
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.07	0.67
54:2y:18:G:O6	54:2y:56:C:N4	2.28	0.67
11:1P:91:PHE:O	11:1P:121:LYS:NZ	2.26	0.67
35:2d:140:VAL:HG11	35:2d:146:ILE:HD11	1.76	0.67
1:1A:1024:G:OP2	61:1A:4117:HOH:O	2.12	0.67
24:12:31:GLU:HB2	24:12:53:LEU:HD21	1.77	0.67
44:1m:3:ARG:HG2	44:1m:8:GLU:HA	1.76	0.67
32:2a:390:C:O3'	47:2p:28:ARG:NH2	2.28	0.67
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.12	0.67
50:2s:77:THR:HG23	50:2s:78:ARG:HG3	1.75	0.67
32:1a:1198:G:OP1	61:1a:1805:HOH:O	2.13	0.66
1:2A:2448:A:OP1	61:2A:3906:HOH:O	2.13	0.66
1:1A:731:C:OP1	61:1A:4116:HOH:O	2.12	0.66
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.76	0.66
32:1a:1521:G:N3	61:1a:1817:HOH:O	2.28	0.66
33:1b:24:TRP:CG	33:1b:25:ASN:H	2.12	0.66
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.59	0.66
33:2b:78:GLN:HE22	33:2b:95:GLN:HE22	1.42	0.66
32:1a:1006:C:H42	32:1a:1023:G:H1	1.42	0.66
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.29	0.66
35:2d:8:VAL:HG22	35:2d:21:LEU:HD13	1.77	0.66
32:1a:558:G:OP1	61:1a:1804:HOH:O	2.12	0.66
16:2U:50:ARG:HH22	17:2V:72:VAL:HG22	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1255:G:OP1	41:2j:45:ARG:NH2	2.28	0.66
2:1B:7:G:N7	61:1B:304:HOH:O	2.28	0.66
1:2A:946:G:OP1	61:2A:3914:HOH:O	2.13	0.66
33:2b:87:ARG:NH2	33:2b:220:ASP:OD1	2.26	0.66
50:2s:32:LYS:HA	50:2s:50:ALA:HB3	1.77	0.66
1:1A:1076:C:O2'	1:1A:1077:A:N7	2.28	0.66
33:1b:17:PHE:HB3	33:1b:44:LEU:HD11	1.78	0.66
11:1P:42:SER:O	61:1P:301:HOH:O	2.14	0.66
1:2A:652(A):A:H3'	1:2A:652(B):A:H5''	1.78	0.66
1:2A:1648:C:OP1	61:2A:3907:HOH:O	2.12	0.66
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.30	0.66
7:2H:70:THR:O	7:2H:74:ASN:ND2	2.28	0.66
32:2a:972:C:O2'	41:2j:55:LYS:O	2.13	0.66
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.43	0.66
54:2y:62:C:H2'	54:2y:63:G:H8	1.60	0.66
1:1A:1023:U:OP2	61:1A:4117:HOH:O	2.14	0.66
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.29	0.66
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	1.78	0.66
11:2P:89:ALA:HA	11:2P:121:LYS:HD3	1.78	0.66
32:2a:1263:C:N3	32:2a:1272:G:O6	2.30	0.65
46:1o:16:ALA:HB1	46:1o:21:ASP:HB3	1.78	0.65
1:2A:330:A:H2	1:2A:1210:A:HO2'	1.42	0.65
1:1A:2428:G:OP1	61:1A:4101:HOH:O	2.14	0.65
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.30	0.65
21:2Z:159:PRO:HA	21:2Z:161:VAL:H	1.62	0.65
40:2i:29:ASN:HD21	40:2i:65:VAL:H	1.45	0.65
1:1A:847:U:OP2	61:1A:4120:HOH:O	2.14	0.65
1:2A:1271:G:OP2	61:2A:3907:HOH:O	2.13	0.65
32:2a:148:G:H2'	32:2a:149:A:H8	1.61	0.65
1:1A:2218:U:O4'	23:11:52:ARG:NH2	2.30	0.65
32:1a:1346:A:OP1	40:1i:120:ARG:NH1	2.20	0.65
1:2A:1970:A:OP1	61:2A:3918:HOH:O	2.15	0.65
32:2a:1278:U:H5'	32:2a:1279:A:H5'	1.79	0.65
1:1A:1648:C:OP1	61:1A:4108:HOH:O	2.15	0.65
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.30	0.65
33:2b:219:VAL:HA	33:2b:222:ILE:HG12	1.79	0.65
1:1A:1075:C:H2'	1:1A:1076:C:H5'	1.79	0.65
1:1A:1271:G:OP2	61:1A:4108:HOH:O	2.14	0.65
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.79	0.65
18:1W:31:GLU:OE1	61:1W:301:HOH:O	2.14	0.64
1:2A:106:C:H1'	20:2Y:1:MET:HE2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:134:ILE:HG23	34:2c:151:VAL:HG13	1.78	0.64
34:2c:138:VAL:HG23	34:2c:151:VAL:HG12	1.78	0.64
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	1.97	0.64
11:2P:126:VAL:HG12	11:2P:148:LEU:HD22	1.79	0.64
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.78	0.64
54:1w:1:G:N1	54:1w:72:C:C2	2.65	0.64
32:2a:1119:C:OP2	40:2i:9:ARG:NH2	2.31	0.64
45:2n:26:ARG:HD3	45:2n:43:CYS:HB3	1.79	0.64
32:1a:903:G:OP1	61:1a:1807:HOH:O	2.15	0.64
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.78	0.64
1:2A:36:G:OP1	61:2A:3916:HOH:O	2.14	0.64
1:2A:307:G:H21	1:2A:330:A:H62	1.44	0.64
1:2A:84:A:H5''	20:2Y:8:LYS:HE3	1.80	0.64
1:1A:409:C:OP1	61:1A:4112:HOH:O	2.15	0.64
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.31	0.64
32:1a:693:G:OP2	61:1a:1806:HOH:O	2.15	0.64
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.31	0.64
32:2a:157:G:H1	32:2a:164:U:H3	1.46	0.64
38:2g:113:GLU:HB2	38:2g:119:ARG:HG2	1.80	0.64
1:1A:1059:G:H1	1:1A:1079:C:H42	1.46	0.63
41:2j:44:VAL:HG13	41:2j:66:ARG:HG2	1.81	0.63
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.79	0.63
33:1b:61:LEU:HG	33:1b:66:GLY:HA3	1.81	0.63
33:2b:126:GLU:CD	33:2b:126:GLU:H	2.06	0.63
1:2A:692:C:O2'	3:2D:38:LYS:NZ	2.31	0.63
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.17	0.63
38:2g:79:ARG:HD2	38:2g:80:VAL:N	2.13	0.63
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.31	0.63
1:1A:2751:G:H4'	7:1H:4:ILE:HD11	1.79	0.63
37:1f:97:PHE:HD2	49:1r:31:LEU:HD11	1.63	0.63
1:2A:2576:G:OP1	61:2A:3917:HOH:O	2.15	0.63
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.33	0.63
34:2c:8:ILE:HG23	34:2c:16:ARG:HG2	1.79	0.63
32:1a:405:U:O4	35:1d:2:GLY:N	2.31	0.63
1:1A:11:G:H2'	1:1A:12:U:H5'	1.80	0.63
33:1b:24:TRP:H	33:1b:24:TRP:HD1	1.44	0.63
1:2A:2438:U:O2'	1:2A:2440:C:OP1	2.17	0.63
1:1A:2719:G:O6	61:1A:4119:HOH:O	2.14	0.63
32:1a:1360:A:OP2	45:1n:35:ARG:NH2	2.32	0.63
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.25	0.63
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:1y:51:U:H3	54:1y:63:G:H1	1.47	0.63
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.14	0.63
4:1E:29:GLY:HA3	61:1E:401:HOH:O	1.97	0.63
7:1H:40:GLU:OE2	7:1H:60:ARG:NH1	2.32	0.63
32:1a:200:G:H1	32:1a:217:C:H42	1.47	0.63
36:1e:78:HIS:HE1	36:1e:143:ARG:H	1.45	0.63
41:1j:49:VAL:HG22	45:1n:41:ARG:HB2	1.80	0.63
1:2A:921:G:O6	61:2A:3915:HOH:O	2.13	0.63
42:2k:78:GLN:HE21	42:2k:78:GLN:HA	1.63	0.62
2:1B:48:A:H4'	14:1S:95:HIS:HD2	1.63	0.62
33:1b:201:ILE:HG21	33:1b:214:ILE:HG21	1.81	0.62
33:2b:185:ILE:HG22	33:2b:199:TYR:HB2	1.80	0.62
1:2A:2145:C:O2'	1:2A:2147:G:N7	2.33	0.62
32:2a:1060:C:C5	34:2c:2:GLY:HA3	2.34	0.62
1:1A:1721:G:H1'	1:1A:1741:A:H61	1.64	0.62
37:1f:89:MET:HE1	49:1r:72:ARG:HB3	1.81	0.62
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	1.81	0.62
18:2W:4:LYS:HD3	18:2W:6:ILE:HD11	1.81	0.62
1:1A:603:A:O4'	1:1A:655:A:N6	2.32	0.62
42:2k:48:ILE:O	42:2k:50:TYR:N	2.32	0.62
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.81	0.62
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.34	0.62
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.63	0.62
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.82	0.62
32:2a:1029:C:N3	32:2a:1032:G:N2	2.48	0.62
32:1a:134:A:H61	47:1p:25:ARG:HH12	1.47	0.62
11:2P:38:GLN:O	11:2P:39:LYS:HB3	2.00	0.62
12:2Q:18:LYS:O	12:2Q:98:LYS:NZ	2.21	0.62
32:1a:53:A:OP2	61:1a:1808:HOH:O	2.16	0.62
1:2A:568:U:O4	61:2A:3913:HOH:O	2.13	0.62
3:1D:237:GLU:OE2	61:1D:401:HOH:O	2.16	0.62
34:1c:162:GLN:NE2	53:1v:24:A:O2'	2.32	0.62
36:1e:142:LEU:O	36:1e:143:ARG:NH1	2.30	0.62
1:2A:890:A:H2'	1:2A:892:G:C8	2.35	0.62
21:2Z:54:HIS:HD2	21:2Z:101:PRO:HG3	1.65	0.62
42:2k:73:MET:HG2	42:2k:103:LEU:HD21	1.82	0.62
3:1D:147:LEU:HD13	3:1D:155:LEU:HD11	1.82	0.61
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.82	0.61
33:1b:80:ILE:HD12	33:1b:212:GLN:HA	1.81	0.61
32:1a:1353:G:OP1	52:1u:10:ARG:NH1	2.33	0.61
15:2T:65:LYS:HE3	15:2T:67:SER:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.35	0.61
1:2A:775:G:O3'	61:2A:3920:HOH:O	2.16	0.61
32:2a:677:U:H3	32:2a:713:G:H22	1.48	0.61
32:2a:1118:C:OP1	40:2i:104:ARG:NH1	2.33	0.61
40:2i:55:ALA:HA	40:2i:58:HIS:HD2	1.64	0.61
49:2r:52:PRO:HB2	49:2r:54:ARG:HG3	1.82	0.61
6:2G:79:ASN:N	6:2G:79:ASN:OD1	2.30	0.61
32:2a:976:G:H5'	32:2a:1358:U:O2'	2.01	0.61
32:1a:1036:G:H5''	32:1a:1037:C:C5	2.34	0.61
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.35	0.61
1:2A:855:G:O2'	22:20:27:GLU:OE2	2.18	0.61
32:1a:171:A:H2'	32:1a:172:A:C8	2.35	0.61
1:2A:2116:G:N1	1:2A:2162:G:OP1	2.31	0.61
50:2s:28:LYS:HB3	50:2s:29:ARG:CA	2.30	0.61
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.82	0.61
32:2a:620:C:C2	35:2d:135:LEU:HG	2.36	0.61
32:2a:1086:U:H3	32:2a:1099:G:H22	1.49	0.61
41:2j:21:GLN:HE22	41:2j:25:GLU:HG2	1.65	0.61
21:1Z:132:ASN:HD22	21:1Z:160:GLY:HA3	1.65	0.61
34:1c:6:HIS:CD2	34:1c:8:ILE:H	2.16	0.61
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.81	0.61
1:2A:1938:A:OP2	61:2A:3921:HOH:O	2.16	0.61
32:2a:662:G:H2'	32:2a:663:A:C8	2.36	0.61
32:2a:1099:G:OP2	33:2b:144:ARG:NH2	2.34	0.61
1:1A:1058:G:H1	1:1A:1080:C:H42	1.48	0.61
16:1U:81:HIS:CE1	16:1U:85:LYS:HD2	2.36	0.61
27:15:40:LYS:NZ	27:15:44:THR:O	2.34	0.61
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	1.82	0.61
1:1A:2102:U:H3	1:1A:2187:G:H1	1.49	0.61
54:1w:18:G:O2'	54:1w:57:G:N2	2.25	0.61
32:2a:1002:G:C2	32:2a:1003:G:H1'	2.36	0.61
42:2k:54:ARG:NH2	54:2y:39:PSU:O2'	2.28	0.61
32:1a:70:G:H1	32:1a:99:U:H3	1.49	0.60
32:1a:1416:G:N7	61:1a:1819:HOH:O	2.30	0.60
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.83	0.60
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.81	0.60
32:2a:406:G:H21	35:2d:119:GLN:NE2	1.96	0.60
1:1A:2844:G:O6	61:1A:4121:HOH:O	2.15	0.60
37:1f:68:PRO:HG2	37:1f:71:ARG:HD2	1.84	0.60
1:2A:1508:A:H4'	1:2A:1509(A):A:C4	2.35	0.60
1:2A:2807:G:H22	1:2A:2892:A:N6	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.83	0.60
54:2y:55:PSU:HN1	54:2y:57:G:H5'	1.65	0.60
21:1Z:52:SER:O	21:1Z:54:HIS:N	2.34	0.60
50:1s:63:THR:OG1	50:1s:65:ASN:OD1	2.19	0.60
1:2A:793:A:O2'	61:2A:3919:HOH:O	2.15	0.60
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.34	0.60
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.15	0.60
12:2Q:17:LEU:HB3	12:2Q:39:PRO:HB2	1.83	0.60
26:24:55:ARG:O	26:24:60:GLN:NE2	2.33	0.60
32:2a:539:A:OP2	43:2l:115:LYS:NZ	2.33	0.60
40:2i:85:LEU:HB3	40:2i:92:TYR:HD2	1.66	0.60
1:1A:1948:G:O6	61:1A:4122:HOH:O	2.16	0.60
42:1k:87:THR:O	42:1k:87:THR:OG1	2.18	0.60
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.34	0.60
32:1a:933:G:O6	38:1g:3:ARG:NH2	2.34	0.60
1:2A:1639:U:H2'	1:2A:1640:C:H5''	1.83	0.60
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.84	0.60
1:2A:2100:G:H1	1:2A:2189:U:H3	1.47	0.60
21:2Z:154:ASP:N	21:2Z:154:ASP:OD1	2.34	0.60
32:2a:1255:G:N7	41:2j:43:ARG:NH2	2.49	0.60
32:2a:1302:U:OP2	44:2m:21:TYR:OH	2.11	0.60
36:2e:60:TYR:OH	36:2e:64:ARG:NH1	2.34	0.60
1:1A:1041:C:H42	1:1A:1114:G:H1	1.48	0.60
9:1N:62:VAL:HG22	9:1N:66:LYS:HD2	1.84	0.60
40:1i:21:PRO:HA	40:1i:59:PHE:HA	1.84	0.60
1:1A:2100:G:H1	1:1A:2189:U:H3	1.48	0.60
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.34	0.60
33:2b:103:THR:HA	33:2b:180:LEU:HD11	1.84	0.60
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.37	0.60
32:1a:78:G:O6	32:1a:92:C:N4	2.34	0.60
40:1i:110:GLU:OE2	40:1i:113:LYS:NZ	2.35	0.60
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.36	0.60
1:1A:880:G:H2'	1:1A:881:G:H8	1.66	0.60
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.36	0.60
51:1t:86:ARG:O	51:1t:90:GLN:NE2	2.35	0.60
32:2a:1271:G:N2	32:2a:1272:G:N7	2.49	0.60
32:2a:1347:G:H5''	40:2i:107:ARG:HB3	1.83	0.60
1:2A:332:A:O2'	1:2A:334:C:OP2	2.19	0.59
12:2Q:43:THR:HG22	12:2Q:94:VAL:HG12	1.84	0.59
40:2i:9:ARG:H	40:2i:79:LEU:HD23	1.67	0.59
1:1A:1026:U:OP1	61:1A:4117:HOH:O	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.02	0.59
1:2A:253:C:O2'	61:2A:3922:HOH:O	2.16	0.59
1:2A:602:G:O2'	1:2A:655:A:N6	2.35	0.59
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.84	0.59
1:2A:2150:U:H2'	1:2A:2151:G:H8	1.66	0.59
32:2a:79:G:H1	32:2a:90:U:H3	1.49	0.59
36:2e:74:GLY:HA3	36:2e:116:THR:HG22	1.84	0.59
1:1A:1039:G:H1	1:1A:1116:C:H42	1.50	0.59
29:17:33:ARG:NH2	61:17:201:HOH:O	2.34	0.59
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.17	0.59
41:1j:5:ARG:HG3	41:1j:71:LEU:HD11	1.84	0.59
32:2a:148:G:H2'	32:2a:149:A:C8	2.36	0.59
54:2y:8:4SU:H1'	54:2y:48:C:H1'	1.84	0.59
1:1A:998:C:OP1	61:1A:4124:HOH:O	2.17	0.59
1:1A:2319:G:H1	14:1S:3:ARG:HD3	1.67	0.59
1:1A:2350:C:OP2	61:1A:4123:HOH:O	2.17	0.59
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.38	0.59
32:1a:96:U:H2'	32:1a:97:G:C8	2.38	0.59
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.18	0.59
18:2W:1:MET:HE2	18:2W:62:HIS:HB3	1.85	0.59
35:2d:61:LYS:NZ	35:2d:72:GLU:OE1	2.33	0.59
50:2s:64:GLU:OE2	50:2s:65:ASN:ND2	2.34	0.59
32:1a:1006:C:N4	32:1a:1023:G:H1	2.01	0.59
33:1b:195:ASP:O	39:1h:68:ARG:NH2	2.30	0.59
1:2A:509:C:OP1	61:2A:3923:HOH:O	2.17	0.59
32:1a:1027:C:C2	32:1a:1034:G:N2	2.67	0.59
1:2A:893:C:H2'	1:2A:894:C:C4	2.38	0.59
9:2N:28:THR:HG22	9:2N:29:LYS:HG2	1.85	0.59
32:2a:673:G:H2'	32:2a:674:G:C8	2.38	0.59
32:2a:1312:G:H5'	50:2s:5:LEU:HD11	1.85	0.59
7:2H:86:GLU:OE2	7:2H:130:ARG:NH1	2.35	0.59
14:2S:78:LEU:HD11	14:2S:109:GLY:HA3	1.85	0.59
33:2b:43:ASP:OD2	33:2b:46:LYS:N	2.36	0.59
32:1a:567:G:N3	61:1a:1821:HOH:O	2.32	0.59
40:1i:48:GLU:HA	40:1i:51:ARG:HD3	1.85	0.59
32:2a:1010:G:N2	32:2a:1020:U:O2'	2.36	0.59
1:1A:2133:G:O2'	1:1A:2157:G:N2	2.35	0.59
1:2A:2138:C:N4	1:2A:2153:G:H1	2.00	0.59
19:2X:46:ALA:HB1	24:22:33:MET:HE1	1.83	0.59
35:2d:20:TYR:HD1	35:2d:26:CYS:HB3	1.67	0.59
37:2f:95:GLU:O	49:2r:32:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:8:U:O3'	14:1S:25:ARG:NH2	2.35	0.59
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.35	0.59
54:1w:1:G:C2	54:1w:72:C:O2	2.55	0.59
1:2A:1771:C:OP1	61:2A:3924:HOH:O	2.17	0.59
21:2Z:73:GLN:O	21:2Z:87:ASP:N	2.36	0.59
23:21:32:LYS:O	61:21:201:HOH:O	2.17	0.59
32:2a:838:G:H1	32:2a:848:C:H42	1.50	0.59
33:2b:217:ARG:HA	33:2b:220:ASP:HB2	1.85	0.59
38:2g:27:ILE:HD12	38:2g:40:ALA:HA	1.85	0.59
51:2t:50:GLU:O	51:2t:100:ILE:HD11	2.03	0.59
1:1A:2276:G:N7	61:1A:4164:HOH:O	2.32	0.58
15:1T:84:GLN:HG2	15:1T:85:LYS:HG2	1.84	0.58
1:2A:2206:G:H5''	1:2A:2207:G:C8	2.38	0.58
21:2Z:28:MET:HE2	21:2Z:37:VAL:HG11	1.85	0.58
32:2a:1029:C:N4	32:2a:1032:G:N1	2.51	0.58
38:2g:111:ARG:NH2	38:2g:126:ASP:OD2	2.36	0.58
39:2h:64:LYS:HG2	39:2h:79:VAL:HG21	1.85	0.58
1:1A:1062:G:H1	1:1A:1077:A:N6	1.97	0.58
1:1A:1595:G:O6	61:1A:4125:HOH:O	2.17	0.58
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.84	0.58
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.03	0.58
32:2a:1202:G:O4'	45:2n:29:ARG:NH1	2.36	0.58
44:2m:58:GLU:O	44:2m:62:ASN:ND2	2.23	0.58
48:2q:45:HIS:HB3	48:2q:72:ARG:HG2	1.84	0.58
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.68	0.58
1:2A:568:U:H5'	1:2A:945:A:N1	2.18	0.58
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.02	0.58
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.36	0.58
35:2d:79:PHE:HE1	35:2d:204:ILE:HD13	1.67	0.58
35:2d:104:VAL:HG21	35:2d:140:VAL:HG21	1.86	0.58
1:1A:1300:U:H4'	1:1A:1301:A:H5''	1.85	0.58
1:1A:2554:U:H3	54:1w:74:C:N4	1.97	0.58
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.35	0.58
34:1c:89:GLU:OE1	34:1c:90:GLU:N	2.35	0.58
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.38	0.58
1:2A:2319:G:N2	14:2S:3:ARG:HD2	2.19	0.58
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.37	0.58
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.84	0.58
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.85	0.58
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.36	0.58
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:1y:53:G:H3'	54:1y:54:5MU:H73	1.84	0.58
32:2a:67:C:H2'	32:2a:68:G:C8	2.38	0.58
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.84	0.58
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.22	0.58
1:2A:1721:G:H8	1:2A:1741:A:H62	1.49	0.58
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.85	0.58
32:2a:297:G:N2	32:2a:300:A:OP2	2.36	0.58
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.03	0.58
32:1a:1414:U:H3	32:1a:1486:G:H1	1.50	0.58
50:1s:27:GLU:HB2	50:1s:28:LYS:HA	1.84	0.58
1:2A:2805:G:H2'	1:2A:2807:G:H8	1.67	0.58
33:2b:74:LYS:O	33:2b:78:GLN:HG2	2.03	0.58
54:2y:14:A:H3'	54:2y:15:G:C8	2.39	0.58
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.68	0.58
1:1A:2614:A:N7	61:1A:4168:HOH:O	2.32	0.58
21:1Z:136:PHE:O	21:1Z:137:ILE:HG13	2.04	0.58
46:1o:3:ILE:HG21	46:1o:34:LEU:HD21	1.85	0.58
32:2a:1191:A:OP2	34:2c:3:ASN:ND2	2.37	0.58
35:2d:187:ARG:NH1	35:2d:190:ASP:OD1	2.37	0.58
40:2i:9:ARG:HG2	40:2i:14:VAL:HG22	1.84	0.58
32:1a:45:U:H2'	32:1a:46:G:C8	2.39	0.58
32:1a:1530:G:H2'	32:1a:1531:A:C8	2.39	0.58
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.39	0.58
6:2G:113:ARG:HH11	26:24:33:VAL:HG23	1.69	0.58
32:2a:56:U:H2'	32:2a:57:G:C8	2.39	0.58
32:2a:1271:G:C2	32:2a:1272:G:N7	2.72	0.58
34:2c:8:ILE:HG12	34:2c:184:TYR:HB3	1.86	0.58
40:2i:15:ALA:HB2	40:2i:65:VAL:HG23	1.84	0.58
1:1A:84:A:H5''	20:1Y:8:LYS:HE3	1.86	0.58
32:2a:1002:G:N3	32:2a:1003:G:H1'	2.19	0.58
32:2a:1218:C:OP2	45:2n:9:LYS:NZ	2.35	0.58
36:2e:57:LYS:HG2	36:2e:61:TYR:CE2	2.38	0.58
40:2i:33:PHE:HE2	40:2i:43:ALA:HB1	1.68	0.58
1:2A:1038:C:H42	1:2A:1117:G:H1	1.53	0.57
1:2A:1604:C:OP1	61:2A:3925:HOH:O	2.17	0.57
6:2G:11:TYR:HB2	6:2G:176:LEU:HD21	1.85	0.57
31:29:15:LYS:HD3	31:29:26:ILE:HD11	1.85	0.57
39:2h:113:SER:HB2	39:2h:134:ILE:HD11	1.86	0.57
21:1Z:125:LEU:HG	21:1Z:164:ALA:HB3	1.87	0.57
47:1p:27:LYS:HG3	47:1p:30:GLY:HA3	1.86	0.57
32:2a:1279:A:H4'	32:2a:1280:A:OP1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:16:HIS:HB3	33:2b:210:SER:CB	2.33	0.57
39:2h:10:LEU:HD22	39:2h:83:ILE:HD11	1.86	0.57
36:1e:78:HIS:CD2	39:1h:104:ARG:HD2	2.39	0.57
44:1m:3:ARG:HG3	44:1m:4:ILE:H	1.69	0.57
1:2A:668:G:H5'	1:2A:669:G:OP2	2.04	0.57
1:2A:2590:A:O3'	3:2D:239:ARG:NH2	2.37	0.57
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.68	0.57
47:2p:53:VAL:HG13	47:2p:79:VAL:HG22	1.85	0.57
1:1A:1359:A:H2'	1:1A:1360:A:H5'	1.85	0.57
8:1I:95:LYS:HE3	8:1I:99:GLU:HG3	1.85	0.57
15:1T:108:ARG:HA	15:1T:111:ARG:HH11	1.70	0.57
12:2Q:122:GLY:HA2	12:2Q:125:LEU:HD12	1.86	0.57
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.40	0.57
54:2y:62:C:H2'	54:2y:63:G:C8	2.39	0.57
6:1G:126:ASP:HB2	6:1G:130:ASN:H	1.69	0.57
32:1a:1030(D):A:H2'	32:1a:1031:G:H4'	1.87	0.57
33:2b:78:GLN:O	33:2b:94:ASN:ND2	2.38	0.57
1:1A:1187:G:H5''	17:1V:81:TYR:CE1	2.40	0.57
54:1w:1:G:C5	54:1w:72:C:N3	2.72	0.57
1:2A:880:G:N2	1:2A:898:C:O2	2.38	0.57
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.85	0.57
44:2m:22:ILE:HG21	44:2m:66:LEU:HD13	1.86	0.57
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.20	0.57
32:1a:17:U:H2'	32:1a:18:C:C6	2.39	0.57
1:2A:2166:G:H3'	1:2A:2167:U:H5''	1.86	0.57
5:2F:116:ASP:OD2	11:2P:1:MET:N	2.35	0.57
16:2U:90:VAL:HG12	16:2U:95:LEU:HG	1.87	0.57
32:2a:1286:A:H2	52:2u:18:TYR:HH	1.51	0.57
40:2i:42:ARG:NH2	40:2i:71:SER:OG	2.37	0.57
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.87	0.57
48:1q:45:HIS:NE2	48:1q:47:PRO:HG3	2.19	0.57
22:20:49:LYS:HE3	22:20:82:ARG:HG3	1.87	0.57
33:2b:8:LYS:HD3	33:2b:217:ARG:HG3	1.87	0.57
45:2n:23:ARG:NH1	45:2n:28:GLY:O	2.33	0.57
1:1A:2611:U:C4	27:15:3:LYS:HG2	2.40	0.57
33:1b:165:VAL:HG23	33:1b:166:ASP:H	1.69	0.57
36:1e:12:LEU:HB3	36:1e:31:LEU:HB2	1.86	0.57
1:2A:2316:C:O2'	6:2G:128:ARG:NH2	2.38	0.57
9:2N:73:THR:HG22	9:2N:84:LYS:HG2	1.87	0.57
14:2S:67:ARG:HG2	14:2S:71:ARG:HD2	1.87	0.57
32:2a:1272:G:N2	32:2a:1273:G:C5	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:2s:17:GLU:O	50:2s:21:GLU:N	2.30	0.57
32:1a:757:U:H2'	32:1a:758:G:O4'	2.05	0.57
48:1q:9:VAL:HG23	48:1q:56:VAL:HG22	1.87	0.57
14:2S:3:ARG:NH2	14:2S:4:LEU:O	2.38	0.57
21:2Z:51:ALA:O	21:2Z:52:SER:HB3	2.05	0.56
32:2a:376:G:H5''	47:2p:5:ARG:HB2	1.86	0.56
32:2a:405:U:O4	35:2d:2:GLY:N	2.38	0.56
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.20	0.56
32:2a:1352:C:OP1	52:2u:3:LYS:NZ	2.37	0.56
44:2m:13:LYS:HA	44:2m:44:ARG:HE	1.69	0.56
1:1A:881:G:N2	1:1A:897:C:O2	2.39	0.56
1:2A:922:U:H2'	1:2A:923:C:C6	2.40	0.56
1:2A:2171:A:N3	1:2A:2172:U:N3	2.52	0.56
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.87	0.56
20:2Y:55:TYR:H	20:2Y:56:PRO:HD3	1.69	0.56
34:2c:20:SER:HB3	34:2c:22:TRP:HE1	1.70	0.56
1:1A:278:A:O2'	1:1A:279:C:OP1	2.20	0.56
1:1A:530:G:N1	1:1A:2023:G:OP1	2.31	0.56
1:1A:952:G:OP1	12:1Q:16:ARG:NH2	2.38	0.56
11:1P:89:ALA:HA	11:1P:121:LYS:HD3	1.86	0.56
32:1a:1060:C:H5''	41:1j:51:ARG:HG2	1.88	0.56
32:1a:1183:A:O2'	32:1a:1184:G:OP1	2.23	0.56
32:1a:1239:A:H62	32:1a:1299:A:N6	2.04	0.56
51:1t:57:ARG:HH12	51:1t:100:ILE:HD12	1.70	0.56
1:2A:2317:C:N4	1:2A:2318:G:O6	2.38	0.56
6:2G:44:GLY:HA2	6:2G:88:ILE:HG22	1.86	0.56
9:2N:67:LEU:HB3	9:2N:88:GLU:HG3	1.87	0.56
14:2S:48:LEU:HD23	14:2S:82:ILE:HD11	1.87	0.56
32:2a:651:C:N4	32:2a:753:A:OP2	2.38	0.56
32:2a:737:A:H1'	37:2f:73:ASN:HD21	1.70	0.56
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.20	0.56
50:2s:19:VAL:O	50:2s:23:ASN:ND2	2.38	0.56
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.69	0.56
35:1d:187:ARG:NH2	35:1d:193:ASP:OD2	2.32	0.56
37:1f:27:GLN:HA	37:1f:30:LEU:HD12	1.87	0.56
32:2a:1032:G:H2'	32:2a:1033:G:C8	2.40	0.56
26:14:55:ARG:N	26:14:56:VAL:HA	2.19	0.56
32:1a:73:G:H1	32:1a:96:U:H3	1.53	0.56
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.39	0.56
34:1c:79:ARG:O	34:1c:82:GLU:HG2	2.06	0.56
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:32:LEU:O	34:2c:36:ASP:HB2	2.03	0.56
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.04	0.56
35:1d:119:GLN:HG2	35:1d:123:HIS:CD2	2.40	0.56
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.20	0.56
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.05	0.56
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.35	0.56
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.05	0.56
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.87	0.56
33:1b:188:ALA:HB3	33:1b:200:ILE:HD11	1.87	0.56
1:2A:2110:G:OP1	1:2A:2118:U:N3	2.31	0.56
17:2V:72:VAL:HB	17:2V:85:LYS:HB3	1.86	0.56
32:2a:134:A:H61	47:2p:25:ARG:NH1	2.04	0.56
35:2d:173:TRP:CD2	35:2d:189:PRO:HB3	2.41	0.56
36:2e:100:VAL:O	36:2e:107:ARG:NH2	2.39	0.56
55:2x:23:C:H2'	55:2x:24:U:C6	2.41	0.56
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.39	0.56
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.86	0.56
35:1d:60:GLU:HG3	35:1d:202:LEU:HD12	1.88	0.56
36:1e:89:ILE:HG12	36:1e:135:THR:HG22	1.87	0.56
49:1r:47:THR:O	49:1r:83:GLU:N	2.38	0.56
1:2A:2319:G:H22	14:2S:3:ARG:HD2	1.71	0.56
2:2B:103:G:H21	21:2Z:73:GLN:HE22	1.52	0.56
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.39	0.56
44:2m:80:ARG:HH22	50:2s:69:HIS:HE1	1.53	0.56
1:1A:153:C:OP2	23:11:92:LYS:NZ	2.39	0.56
33:1b:92:TYR:HH	33:1b:150:SER:HG	1.50	0.56
54:1w:18:G:HO2'	54:1w:57:G:H22	1.53	0.56
1:2A:884:C:H3'	1:2A:885:C:C6	2.41	0.56
25:23:40:THR:HG22	25:23:42:ALA:H	1.71	0.56
32:2a:1163:C:H42	32:2a:1173:G:H1	1.54	0.56
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.40	0.56
1:2A:621:A:OP2	11:2P:108:LYS:NZ	2.35	0.56
44:2m:10:PRO:HB2	44:2m:13:LYS:HD2	1.88	0.56
1:1A:668:G:H5'	1:1A:669:G:OP2	2.06	0.55
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.20	0.55
9:1N:46:VAL:HG23	9:1N:48:MET:HG2	1.88	0.55
1:2A:468:G:N7	29:27:39:ARG:NH2	2.50	0.55
12:2Q:78:PRO:HG2	12:2Q:81:VAL:HG11	1.86	0.55
32:2a:1026:G:H5'	32:2a:1027:C:O5'	2.06	0.55
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.39	0.55
1:1A:444:C:H5''	61:1A:4496:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.35	0.55
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.19	0.55
32:1a:560:U:O2'	32:1a:561:U:OP2	2.23	0.55
34:1c:22:TRP:CZ2	45:1n:54:PRO:HG2	2.41	0.55
41:1j:8:LEU:HD22	41:1j:96:ILE:HG22	1.88	0.55
50:1s:22:LEU:HD12	50:1s:31:ILE:HD11	1.89	0.55
6:2G:48:GLU:O	6:2G:51:ARG:NH1	2.39	0.55
34:2c:111:LEU:HD21	34:2c:146:ALA:HB2	1.88	0.55
35:2d:196:LEU:O	35:2d:198:VAL:N	2.39	0.55
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.39	0.55
33:1b:33:TYR:HB2	33:1b:43:ASP:HB2	1.89	0.55
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.39	0.55
32:2a:64:G:H4'	32:2a:65:U:H3'	1.89	0.55
32:2a:986:A:H2'	32:2a:987:G:O4'	2.06	0.55
32:2a:1310:G:H5'	44:2m:77:ASN:ND2	2.21	0.55
1:1A:2316:C:O2'	6:1G:128:ARG:NH2	2.39	0.55
61:1A:5448:HOH:O	11:1P:44:GLY:HA2	2.05	0.55
2:1B:33:G:H5'	6:1G:2:PRO:HD3	1.88	0.55
32:1a:67:C:H2'	32:1a:68:G:C8	2.42	0.55
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.04	0.55
40:1i:23:ASN:OD1	40:1i:23:ASN:N	2.38	0.55
54:1w:5:G:H1	54:1w:68:C:H42	1.54	0.55
1:2A:2134:A:H62	1:2A:2157:G:H4'	1.72	0.55
1:1A:602:G:O2'	1:1A:655:A:N6	2.39	0.55
1:1A:2096:U:H3	1:1A:2193:G:H1	1.55	0.55
12:2Q:77:LYS:NZ	12:2Q:86:GLY:O	2.39	0.55
21:2Z:53:ILE:HA	21:2Z:71:VAL:HG23	1.89	0.55
32:2a:17:U:H2'	32:2a:18:C:C6	2.42	0.55
40:2i:21:PRO:HA	40:2i:59:PHE:HA	1.89	0.55
46:2o:87:ILE:O	46:2o:88:ARG:HB2	2.05	0.55
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.07	0.55
16:2U:49:HIS:HA	16:2U:52:ARG:HB2	1.87	0.55
32:2a:903:G:OP1	61:2a:1908:HOH:O	2.18	0.55
32:2a:1316:G:N2	32:2a:1319:A:H5''	2.18	0.55
54:2w:4:C:H42	54:2w:69:G:H1	1.52	0.55
1:1A:528:A:O2'	1:1A:529:A:H5'	2.06	0.55
8:1I:109:ILE:HG23	8:1I:130:TYR:CZ	2.42	0.55
34:1c:150:LYS:HG3	34:1c:169:ALA:HB2	1.89	0.55
48:1q:22:LEU:HD11	48:1q:39:SER:HB2	1.87	0.55
1:2A:667:U:O2	30:28:2:PRO:HD2	2.07	0.55
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1645:G:H5'	1:2A:1646:C:H5'	1.88	0.55
32:2a:187:C:O2'	51:2t:89:ARG:NH2	2.39	0.55
34:2c:7:PRO:HG2	34:2c:184:TYR:HB2	1.89	0.55
36:2e:12:LEU:HB3	36:2e:31:LEU:HB2	1.89	0.55
1:1A:1055:G:H3'	1:1A:1056:G:H8	1.71	0.55
1:1A:2319:G:H1	14:1S:3:ARG:HA	1.71	0.55
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.06	0.55
32:1a:1023:G:H3'	32:1a:1024:G:H8	1.72	0.55
32:1a:1456:G:O3'	51:1t:39:LYS:NZ	2.40	0.55
6:2G:63:ILE:HD11	6:2G:144:ILE:HG13	1.88	0.55
7:2H:125:VAL:HG22	7:2H:131:VAL:HG22	1.88	0.55
37:2f:35:ALA:HA	37:2f:67:MET:HB3	1.89	0.55
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.89	0.55
32:1a:96:U:H2'	32:1a:97:G:H8	1.70	0.55
32:1a:236:G:OP1	48:1q:40:LYS:NZ	2.40	0.55
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.22	0.55
32:2a:1263:C:H1'	32:2a:1273:G:N2	2.21	0.55
54:2y:59:U:OP1	54:2y:60:U:N3	2.38	0.55
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.39	0.55
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.71	0.55
12:2Q:137:TYR:CE1	21:2Z:83:PRO:HG3	2.43	0.55
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.07	0.54
43:1l:53:ARG:HB3	43:1l:69:TYR:HE1	1.72	0.54
14:2S:58:LEU:HD13	14:2S:65:VAL:HB	1.89	0.54
32:2a:748:C:H4'	32:2a:749:C:O5'	2.08	0.54
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.88	0.54
32:1a:1039:C:H2'	32:1a:1040:U:C6	2.42	0.54
1:2A:890:A:H2'	1:2A:892:G:H8	1.71	0.54
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.43	0.54
6:2G:121:ASN:HD21	6:2G:123:ASN:HB2	1.73	0.54
32:2a:1278:U:H5'	32:2a:1279:A:C5'	2.37	0.54
46:2o:6:GLU:OE1	46:2o:6:GLU:N	2.39	0.54
1:1A:1762:A:H2'	61:1A:5810:HOH:O	2.07	0.54
1:1A:2182:G:H2'	1:1A:2183:C:C6	2.42	0.54
32:1a:972:C:O2'	41:1j:55:LYS:O	2.25	0.54
1:2A:1012:U:C5	9:2N:28:THR:HG21	2.42	0.54
32:2a:1095:U:H2'	32:2a:1096:C:C6	2.41	0.54
33:2b:8:LYS:NZ	33:2b:217:ARG:HB2	2.22	0.54
44:2m:81:LEU:HA	44:2m:84:ILE:HG12	1.89	0.54
1:1A:882:G:H1	1:1A:894:C:H42	1.55	0.54
1:1A:1038:C:H42	1:1A:1117:G:H1	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.42	0.54
1:1A:2206:G:H3'	1:1A:2207:G:N7	2.22	0.54
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.43	0.54
32:1a:877:C:OP1	39:1h:88:LYS:NZ	2.29	0.54
36:2e:33:VAL:HG13	36:2e:112:LEU:HD22	1.88	0.54
39:2h:21:LYS:O	39:2h:65:TYR:OH	2.25	0.54
54:2y:26:A:N1	54:2y:44:G:C6	2.75	0.54
1:1A:120:U:OP2	61:1A:4127:HOH:O	2.18	0.54
20:1Y:34:LYS:NZ	61:1Y:301:HOH:O	2.40	0.54
1:2A:271(M):G:OP1	8:2I:50:ARG:NH2	2.40	0.54
1:2A:1300:U:H4'	1:2A:1301:A:H5''	1.89	0.54
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.26	0.54
21:2Z:156:LYS:HE3	21:2Z:158:PRO:HD3	1.89	0.54
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.75	0.54
33:2b:109:SER:O	33:2b:112:VAL:HG12	2.07	0.54
33:2b:218:ALA:O	33:2b:222:ILE:HG23	2.08	0.54
45:2n:24:CYS:HB2	45:2n:40:CYS:HB3	1.90	0.54
6:1G:66:GLN:HG3	26:14:1:MET:HE1	1.88	0.54
38:1g:74:GLU:HG2	38:1g:91:VAL:HG22	1.90	0.54
1:2A:271(M):G:N2	8:2I:50:ARG:HD3	2.21	0.54
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.23	0.54
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.72	0.54
1:2A:2334:G:H5'	14:2S:9:ARG:HG2	1.89	0.54
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.23	0.54
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.42	0.54
32:2a:1102:A:O3'	33:2b:96:ARG:NH2	2.40	0.54
1:1A:1055:G:H1	1:1A:1104:C:N4	2.04	0.54
32:1a:473:G:OP2	47:1p:75:ARG:NH1	2.41	0.54
40:1i:40:LEU:HD11	40:1i:70:LYS:HD3	1.90	0.54
42:1k:15:ALA:HB1	42:1k:78:GLN:HE21	1.71	0.54
54:1y:4:C:H2'	54:1y:5:G:O4'	2.08	0.54
41:2j:46:ARG:NH2	41:2j:64:GLU:OE1	2.39	0.54
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.08	0.54
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.43	0.54
44:1m:23:TYR:HB3	44:1m:67:GLU:HA	1.90	0.54
1:2A:247:G:H4'	1:2A:386:G:C5	2.43	0.54
6:2G:113:ARG:NH2	6:2G:139:LEU:O	2.40	0.54
21:2Z:28:MET:HE1	21:2Z:61:LEU:HD21	1.89	0.54
34:2c:125:GLU:HB2	34:2c:190:ARG:HH21	1.73	0.54
1:1A:897:C:N3	1:1A:898:C:N4	2.55	0.54
32:1a:974:A:H8	32:1a:974:A:OP1	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:792:G:O6	61:2A:3911:HOH:O	2.12	0.54
32:2a:1299:A:H2'	32:2a:1299:A:N3	2.23	0.54
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.43	0.54
50:2s:41:VAL:HG12	50:2s:44:MET:HG3	1.90	0.54
51:2t:43:LEU:HD13	51:2t:51:GLU:HB3	1.90	0.54
1:1A:7:G:H2'	1:1A:8:A:O4'	2.07	0.54
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.08	0.54
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.07	0.54
13:1R:2:ARG:HA	13:1R:5:LYS:HD2	1.90	0.54
39:1h:34:GLU:OE1	39:1h:37:ARG:NH1	2.41	0.54
39:1h:81:HIS:N	39:1h:138:TRP:O	2.41	0.54
1:2A:531:C:OP1	1:2A:561:G:N1	2.39	0.54
1:2A:2807:G:H22	1:2A:2892:A:H62	1.56	0.54
32:2a:137:C:H2'	32:2a:138:G:H8	1.73	0.54
32:2a:1346:A:N1	32:2a:1374:A:H5''	2.22	0.54
36:2e:71:LEU:C	36:2e:72:GLN:HE21	2.16	0.54
47:2p:58:TYR:O	47:2p:61:SER:OG	2.19	0.54
1:1A:1013:C:OP2	61:1A:4107:HOH:O	2.18	0.53
1:2A:2127:G:H1	1:2A:2161:C:N4	2.06	0.53
27:25:40:LYS:NZ	27:25:44:THR:O	2.41	0.53
32:2a:429:U:O3'	35:2d:22:LYS:NZ	2.41	0.53
32:2a:1076:C:OP1	33:2b:179:LYS:NZ	2.41	0.53
1:1A:800:A:H8	1:1A:800:A:OP1	1.91	0.53
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.07	0.53
32:1a:184:G:H2'	32:1a:185:A:H8	1.73	0.53
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.89	0.53
1:2A:801:G:O6	5:2F:53:THR:OG1	2.26	0.53
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.90	0.53
1:2A:2156:G:H2'	1:2A:2157:G:C2	2.43	0.53
32:2a:1030(A):G:N2	32:2a:1030(C):G:H3'	2.23	0.53
38:2g:89:MET:SD	38:2g:155:ARG:HB2	2.49	0.53
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.90	0.53
26:14:59:PHE:CD2	50:1s:64:GLU:HB3	2.43	0.53
54:1y:48:C:C2	54:1y:59:U:H1'	2.44	0.53
6:2G:51:ARG:NE	6:2G:51:ARG:H	2.06	0.53
7:2H:143:GLN:NE2	7:2H:147:ASN:OD1	2.41	0.53
32:2a:1251:A:H2'	32:2a:1252:A:C8	2.43	0.53
54:2y:53:G:H3'	54:2y:54:5MU:H73	1.89	0.53
1:1A:2690:C:OP1	13:1R:17:ARG:NH2	2.40	0.53
5:1F:9:ILE:HD13	5:1F:22:ALA:HB3	1.89	0.53
11:1P:38:GLN:O	11:1P:39:LYS:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:110:THR:HG23	12:1Q:113:GLN:HB2	1.91	0.53
35:1d:173:TRP:CD2	35:1d:189:PRO:HG3	2.43	0.53
40:1i:43:ALA:HA	40:1i:74:ILE:HD13	1.90	0.53
47:1p:43:LYS:HA	47:1p:48:TRP:CD1	2.44	0.53
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.26	0.53
1:2A:1830:C:OP2	61:2A:3928:HOH:O	2.19	0.53
9:2N:15:LEU:HB2	9:2N:135:PRO:HB2	1.90	0.53
21:2Z:138:GLU:N	21:2Z:156:LYS:HE2	2.20	0.53
9:1N:96:GLU:H	9:1N:96:GLU:CD	2.15	0.53
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.09	0.53
32:1a:711:G:OP1	37:1f:54:LYS:NZ	2.41	0.53
32:1a:1499:A:OP2	61:1a:1801:HOH:O	2.18	0.53
1:1A:1420:U:O2'	1:1A:1421:G:OP1	2.25	0.53
1:1A:2153:G:H2'	1:1A:2154:G:C8	2.43	0.53
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.91	0.53
21:1Z:92:SER:OG	21:1Z:93:ASP:N	2.41	0.53
32:1a:1218:C:OP2	45:1n:9:LYS:NZ	2.37	0.53
41:1j:38:ILE:HG13	41:1j:71:LEU:HB3	1.90	0.53
1:2A:973:A:OP2	61:2A:3927:HOH:O	2.18	0.53
1:2A:1568:G:N7	61:2A:3988:HOH:O	2.34	0.53
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	1.90	0.53
32:2a:973:G:H3'	32:2a:974:A:H5''	1.90	0.53
36:2e:105:VAL:HB	36:2e:106:PRO:HD3	1.90	0.53
1:1A:1062:G:H1'	1:1A:1088:A:C8	2.44	0.53
1:1A:2107:C:H42	1:1A:2182:G:H1	1.55	0.53
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.74	0.53
8:1I:109:ILE:HD12	8:1I:130:TYR:CE2	2.43	0.53
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.43	0.53
12:1Q:16:ARG:HG2	12:1Q:18:LYS:HG3	1.91	0.53
32:1a:542:G:H5'	35:1d:41:GLY:HA3	1.91	0.53
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.09	0.53
15:2T:64:ARG:HB2	15:2T:73:GLU:HG2	1.89	0.53
38:2g:46:ALA:O	38:2g:50:ILE:HG13	2.09	0.53
1:1A:1054:A:H3'	1:1A:1055:G:H8	1.74	0.53
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.44	0.53
1:1A:2149:G:C2	1:1A:2150:U:H1'	2.44	0.53
1:1A:2168:G:O6	1:1A:2171:A:H5''	2.09	0.53
1:2A:646:A:H2'	1:2A:647:G:O4'	2.09	0.53
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.44	0.53
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.09	0.53
1:2A:2507:C:H5''	1:2A:2573:C:N4	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:56:PRO:HA	4:2E:59:VAL:HG23	1.90	0.53
6:2G:120:LEU:N	6:2G:179:PRO:O	2.34	0.53
32:2a:1263:C:C4	32:2a:1272:G:O6	2.61	0.53
1:1A:1843:C:H5'	3:1D:253:GLN:OE1	2.09	0.53
6:1G:122:PRO:HG3	6:1G:182:LYS:H	1.73	0.53
14:1S:20:ARG:NH2	22:10:51:VAL:O	2.41	0.53
32:1a:625:G:H4'	47:1p:16:HIS:CD2	2.44	0.53
1:2A:796:C:H2'	1:2A:797:C:C6	2.43	0.53
1:2A:1193:G:OP1	11:2P:14:LYS:NZ	2.34	0.53
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.27	0.53
6:2G:124:SER:O	6:2G:124:SER:OG	2.17	0.53
46:2o:39:LEU:HD13	46:2o:56:LEU:HB2	1.90	0.53
1:1A:2503:2MA:H8	57:1A:4098:WC9:O	2.09	0.53
47:1p:53:VAL:HG22	47:1p:79:VAL:HG22	1.91	0.53
1:2A:191:A:H2'	1:2A:192:C:C6	2.44	0.53
1:2A:2127:G:H1	1:2A:2161:C:H42	1.57	0.53
9:2N:58:ASP:OD1	9:2N:58:ASP:N	2.42	0.53
11:2P:3:LEU:HD23	11:2P:6:LEU:HD12	1.90	0.53
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.90	0.53
32:2a:8:A:H5'	36:2e:101:ILE:HG22	1.91	0.53
32:2a:1069:C:O2'	32:2a:1192:C:H1'	2.09	0.53
34:1c:36:ASP:O	34:1c:40:ARG:HG3	2.09	0.52
36:1e:78:HIS:CE1	36:1e:143:ARG:H	2.26	0.52
1:2A:1171:G:H1	1:2A:1178:C:H42	1.56	0.52
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.07	0.52
1:2A:2238:G:H5''	61:2A:4255:HOH:O	2.08	0.52
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.92	0.52
14:2S:11:LYS:HG3	14:2S:91:PRO:HB3	1.91	0.52
8:1I:38:LEU:HD23	8:1I:38:LEU:H	1.75	0.52
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.92	0.52
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.45	0.52
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	1.91	0.52
40:1i:49:PRO:HD3	40:1i:78:LYS:HG3	1.90	0.52
43:1l:88:GLY:O	43:1l:99:HIS:HD2	1.92	0.52
54:1w:26:A:N6	54:1w:44:G:H1	2.05	0.52
1:2A:249:C:O2	30:28:12:LYS:NZ	2.37	0.52
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.25	0.52
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.44	0.52
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	1.91	0.52
17:1V:1:MET:HE3	17:1V:43:GLU:HB2	1.91	0.52
32:1a:545:C:OP1	35:1d:61:LYS:NZ	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:922:G:H4'	36:1e:20:GLN:HA	1.92	0.52
32:2a:1265:G:C2	32:2a:1271:G:C2	2.98	0.52
32:2a:1320:C:H42	50:2s:36:ARG:HE	1.56	0.52
37:2f:2:ARG:NE	37:2f:69:GLU:HG2	2.25	0.52
37:2f:9:VAL:HB	37:2f:87:ARG:HB2	1.91	0.52
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.09	0.52
32:1a:1095:U:OP2	61:1a:1809:HOH:O	2.19	0.52
1:2A:184:C:H2'	1:2A:185:U:C6	2.45	0.52
1:2A:1482:G:H1	1:2A:1506:C:H42	1.57	0.52
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.10	0.52
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.42	0.52
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.92	0.52
32:2a:53:A:OP2	61:2a:1910:HOH:O	2.19	0.52
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.45	0.52
48:2q:45:HIS:CD2	48:2q:47:PRO:HG3	2.45	0.52
26:14:53:GLU:CD	26:14:54:GLY:H	2.18	0.52
32:1a:945:G:OP1	61:1a:1810:HOH:O	2.19	0.52
32:1a:1152:A:OP1	41:1j:68:HIS:ND1	2.41	0.52
1:2A:848:G:H2'	1:2A:849:A:C8	2.44	0.52
40:2i:99:LEU:HB3	40:2i:101:PHE:CD2	2.44	0.52
15:1T:65:LYS:HE2	15:1T:67:SER:HB2	1.90	0.52
40:1i:28:VAL:HG22	40:1i:63:ILE:HB	1.92	0.52
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.45	0.52
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.09	0.52
1:2A:1713:U:H2'	1:2A:1714:G:H8	1.75	0.52
26:24:58:ARG:HH21	50:2s:69:HIS:CE1	2.28	0.52
32:2a:337:C:H2'	32:2a:338:A:C8	2.45	0.52
33:2b:71:VAL:HB	33:2b:164:VAL:HG13	1.91	0.52
1:1A:882:G:H4'	54:1w:19:G:O6	2.10	0.52
18:1W:4:LYS:HD3	18:1W:6:ILE:HD11	1.90	0.52
1:2A:6:A:H2	9:2N:133:GLN:HE22	1.56	0.52
23:21:8:SER:HB3	23:21:66:HIS:CD2	2.45	0.52
34:2c:164:ARG:HG2	34:2c:165:THR:H	1.75	0.52
37:2f:2:ARG:CZ	37:2f:69:GLU:HG2	2.40	0.52
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	1.92	0.52
32:1a:159:G:N2	32:1a:162:A:OP2	2.42	0.52
32:1a:232:G:H1'	32:1a:262:A:N1	2.25	0.52
32:1a:881:G:P	43:1l:12:ARG:HH22	2.32	0.52
54:1y:19:G:O4'	54:1y:57:G:N2	2.42	0.52
1:2A:1604:C:OP2	61:2A:3929:HOH:O	2.19	0.52
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:21:83:GLU:OE1	23:21:83:GLU:N	2.43	0.52
24:22:9:GLN:HE22	24:22:56:GLN:HB3	1.75	0.52
35:2d:72:GLU:OE2	35:2d:207:TYR:OH	2.25	0.52
44:2m:37:THR:O	44:2m:55:ARG:NH1	2.32	0.52
54:2y:49:C:H42	54:2y:65:G:H1	1.57	0.52
11:1P:126:VAL:HG12	11:1P:148:LEU:HD13	1.92	0.52
47:1p:15:PRO:O	47:1p:16:HIS:ND1	2.43	0.52
8:2I:110:ASP:H	8:2I:130:TYR:HH	1.54	0.52
32:2a:73:G:H1	32:2a:96:U:H3	1.57	0.52
1:1A:2124:G:H1	1:1A:2174:C:H42	1.58	0.52
32:1a:501:C:H2'	32:1a:502:G:C8	2.45	0.52
32:1a:673:G:H2'	32:1a:674:G:C8	2.45	0.52
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.92	0.52
32:1a:1148:U:O4'	40:1i:16:ARG:HD2	2.10	0.52
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.45	0.52
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.91	0.52
2:2B:44:G:OP1	6:2G:98:ARG:NH2	2.43	0.52
24:22:25:VAL:HG13	24:22:57:ILE:HG23	1.90	0.52
26:24:50:VAL:HG21	44:2m:65:LYS:HA	1.91	0.52
28:26:38:LYS:HB2	28:26:49:HIS:CE1	2.44	0.52
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.92	0.52
37:2f:99:ALA:HB1	49:2r:23:LYS:HZ2	1.75	0.52
41:2j:46:ARG:HB2	41:2j:46:ARG:HH11	1.75	0.52
44:2m:45:VAL:HA	44:2m:48:LEU:HG	1.91	0.52
1:1A:2128:C:H42	1:1A:2160:G:H1	1.57	0.51
1:1A:2611:U:H5'	1:1A:2611:U:H6	1.75	0.51
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.90	0.51
18:1W:1:MET:HE3	18:1W:2:GLU:H	1.75	0.51
32:1a:1529:G:H4'	32:1a:1530:G:OP2	2.10	0.51
33:1b:15:VAL:HG21	33:1b:213:LEU:HD22	1.91	0.51
35:1d:194:LEU:HD12	35:1d:195:ALA:H	1.74	0.51
6:2G:70:VAL:HA	6:2G:90:LEU:HD23	1.91	0.51
8:2I:82:ARG:NH1	8:2I:90:GLY:H	2.08	0.51
21:2Z:121:HIS:N	21:2Z:171:ILE:O	2.43	0.51
32:2a:1111:A:H2'	32:2a:1112:C:H6	1.74	0.51
54:2w:51:U:H3	54:2w:63:G:H1	1.58	0.51
1:1A:9:U:H3	1:1A:2629:A:H2	1.55	0.51
1:1A:1315:C:OP2	61:1A:4104:HOH:O	2.19	0.51
15:1T:125:ARG:HD3	15:1T:129:ARG:HH21	1.75	0.51
32:1a:1030:C:H42	32:1a:1031:G:H1	1.58	0.51
44:1m:4:ILE:HD12	44:1m:57:ARG:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:1o:39:LEU:HD13	46:1o:56:LEU:HB2	1.92	0.51
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.92	0.51
1:2A:370:G:OP2	61:2A:3926:HOH:O	2.18	0.51
1:2A:810:U:C4	11:2P:29:LYS:O	2.64	0.51
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.10	0.51
21:2Z:74:VAL:HB	21:2Z:86:VAL:HG23	1.93	0.51
26:24:60:GLN:O	26:24:62:ARG:NH1	2.43	0.51
33:2b:223:ILE:HA	33:2b:226:ARG:HG2	1.92	0.51
1:1A:1062:G:C8	1:1A:1088:A:H2'	2.45	0.51
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.46	0.51
32:1a:376:G:H5''	47:1p:5:ARG:HB2	1.92	0.51
47:1p:60:LEU:HD11	47:1p:66:PRO:HD3	1.91	0.51
1:2A:1778:U:OP1	61:2A:3930:HOH:O	2.19	0.51
1:2A:2096:U:H2'	1:2A:2097:C:C6	2.45	0.51
4:2E:50:GLY:HA3	4:2E:75:VAL:HG21	1.93	0.51
32:2a:1264:C:N4	32:2a:1265:G:O6	2.44	0.51
43:2l:71:PRO:O	43:2l:102:ARG:NH1	2.41	0.51
1:1A:2789:C:O2	1:1A:2894:G:N1	2.37	0.51
40:1i:20:ARG:O	40:1i:60:ASP:N	2.25	0.51
1:2A:706:A:OP1	3:2D:7:LYS:NZ	2.39	0.51
1:2A:1183:G:H5''	25:23:30:ARG:NH2	2.26	0.51
2:2B:7:G:N2	14:2S:38:GLN:HE22	1.98	0.51
19:2X:35:THR:HG22	19:2X:38:GLU:H	1.75	0.51
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.28	0.51
32:2a:1216:G:H5''	45:2n:5:ALA:HB2	1.92	0.51
50:2s:31:ILE:O	50:2s:50:ALA:N	2.36	0.51
50:2s:49:ILE:HG22	50:2s:62:ILE:HD11	1.93	0.51
16:1U:85:LYS:HE2	16:1U:117:GLN:O	2.10	0.51
32:1a:405:U:OP2	35:1d:3:ARG:NH1	2.43	0.51
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.46	0.51
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.44	0.51
1:2A:2016:U:OP1	61:2A:3910:HOH:O	2.19	0.51
7:2H:11:VAL:HG13	7:2H:15:VAL:HG22	1.91	0.51
32:2a:1381:U:H1'	38:2g:79:ARG:HG2	1.93	0.51
34:2c:6:HIS:HD2	34:2c:8:ILE:H	1.58	0.51
38:2g:54:THR:O	38:2g:56:GLN:N	2.42	0.51
41:2j:42:THR:HG23	41:2j:68:HIS:HA	1.92	0.51
1:1A:897:C:H5'	54:1w:56:C:OP1	2.11	0.51
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.93	0.51
1:1A:2099:U:H3	1:1A:2190:G:H1	1.56	0.51
19:1X:11:PRO:HB3	19:1X:92:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:138:GLU:H	21:1Z:156:LYS:HE3	1.76	0.51
32:1a:1033:G:H2'	32:1a:1034:G:H8	1.75	0.51
32:1a:1149:C:H2'	32:1a:1150:U:C6	2.46	0.51
11:2P:99:LEU:HD12	11:2P:102:ARG:NH2	2.26	0.51
20:2Y:87:LYS:HB3	20:2Y:95:LYS:HD2	1.92	0.51
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.93	0.51
32:2a:815:A:N7	32:2a:1509:C:O2'	2.40	0.51
34:2c:100:ALA:O	34:2c:102:ASN:ND2	2.44	0.51
6:1G:72:ARG:HH12	6:1G:87:PRO:HG3	1.75	0.51
32:1a:1032:G:H2'	32:1a:1033:G:O4'	2.11	0.51
34:1c:21:ARG:HD2	34:1c:58:GLU:HG2	1.92	0.51
34:1c:89:GLU:O	34:1c:93:LYS:N	2.39	0.51
51:1t:36:LEU:HD12	51:1t:62:LEU:HD12	1.92	0.51
1:2A:2125:G:H1'	1:2A:2173:A:H61	1.75	0.51
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.44	0.51
12:2Q:65:PHE:HB2	12:2Q:105:GLU:HB2	1.93	0.51
32:2a:826:C:O2	39:2h:15:ASN:ND2	2.44	0.51
32:2a:1178:G:N2	32:2a:1180:A:H3'	2.26	0.51
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.46	0.51
32:1a:1112:C:C4	34:1c:178:LEU:HD12	2.46	0.51
32:1a:1334:G:OP2	61:1a:1811:HOH:O	2.20	0.51
46:1o:29:VAL:HG13	46:1o:63:ARG:HG3	1.93	0.51
1:2A:2183:C:H2'	1:2A:2184:G:C8	2.45	0.51
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.28	0.51
21:2Z:54:HIS:CD2	21:2Z:101:PRO:HG3	2.46	0.51
1:1A:1047:G:H2'	1:1A:1110:G:N2	2.26	0.51
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.46	0.51
1:1A:2417:C:OP1	11:1P:65:ARG:NH2	2.44	0.51
15:1T:127:ALA:C	15:1T:129:ARG:H	2.18	0.51
28:16:28:ARG:NH1	28:16:29:ASN:OD1	2.44	0.51
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.76	0.51
35:1d:178:VAL:HG12	35:1d:179:GLU:H	1.76	0.51
37:1f:69:GLU:H	37:1f:69:GLU:CD	2.19	0.51
1:2A:566:U:H5''	11:2P:29:LYS:HE3	1.92	0.51
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.45	0.51
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.46	0.51
1:2A:2340:G:H2'	1:2A:2341:G:H8	1.76	0.51
1:2A:2889:C:H2'	1:2A:2891:G:O4'	2.11	0.51
2:2B:51:G:OP2	14:2S:61:ASN:HA	2.10	0.51
44:2m:37:THR:HB	44:2m:55:ARG:HD2	1.92	0.51
1:1A:2154:G:C2	1:1A:2155:G:H1'	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:90:ARG:HG2	11:1P:90:ARG:HH11	1.76	0.51
32:1a:179:A:H2'	32:1a:180:U:C6	2.46	0.51
11:2P:42:SER:O	61:2P:301:HOH:O	2.19	0.51
14:2S:10:ARG:NE	14:2S:91:PRO:O	2.44	0.51
21:2Z:146:ILE:HG12	21:2Z:174:VAL:HG12	1.92	0.51
32:2a:1002:G:H1	32:2a:1038:C:H42	1.59	0.51
33:2b:80:ILE:HD11	33:2b:212:GLN:HB2	1.93	0.51
34:2c:71:ALA:HA	34:2c:106:VAL:HB	1.93	0.51
6:1G:167:GLU:OE1	6:1G:167:GLU:N	2.44	0.50
32:1a:353:A:H5'	32:1a:353:A:H8	1.76	0.50
50:1s:80:TYR:CZ	50:1s:82:GLY:HA2	2.47	0.50
1:2A:639:U:H2'	1:2A:640:C:C6	2.47	0.50
1:2A:987:G:O2'	1:2A:1000:A:N3	2.40	0.50
2:2B:7:G:H21	14:2S:38:GLN:NE2	1.99	0.50
29:27:24:THR:HG22	29:27:27:GLY:H	1.75	0.50
32:2a:137:C:H2'	32:2a:138:G:C8	2.46	0.50
40:2i:48:GLU:HB3	40:2i:101:PHE:HE1	1.75	0.50
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.46	0.50
9:1N:13:TRP:CE2	9:1N:133:GLN:HG2	2.46	0.50
11:1P:39:LYS:HG3	11:1P:45:LEU:HD22	1.92	0.50
26:14:53:GLU:HB2	26:14:55:ARG:C	2.35	0.50
32:1a:1216:G:H5''	45:1n:5:ALA:HB2	1.93	0.50
42:1k:91:ARG:NH1	42:1k:110:ASP:OD1	2.43	0.50
47:1p:48:TRP:CE3	47:1p:49:LEU:HB2	2.46	0.50
32:2a:460:G:N2	32:2a:471:G:N7	2.59	0.50
32:2a:1030(A):G:N2	32:2a:1030(D):A:OP2	2.40	0.50
33:2b:192:SER:O	33:2b:194:PRO:HD3	2.10	0.50
1:1A:639:U:H2'	1:1A:640:C:C6	2.47	0.50
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.46	0.50
1:2A:2822:G:O2'	1:2A:2825:C:N4	2.43	0.50
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.76	0.50
21:2Z:70:LEU:HD12	21:2Z:71:VAL:H	1.76	0.50
32:2a:7:G:O2'	36:2e:120:THR:O	2.28	0.50
38:2g:65:ALA:O	38:2g:69:VAL:HG23	2.11	0.50
44:2m:15:VAL:HG13	44:2m:45:VAL:HG12	1.93	0.50
1:1A:1970:A:OP1	61:1A:4129:HOH:O	2.20	0.50
7:1H:88:LEU:HD23	7:1H:130:ARG:HG2	1.93	0.50
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.47	0.50
32:1a:250:A:H4'	32:1a:251:G:O5'	2.11	0.50
32:1a:1130:A:OP1	40:1i:16:ARG:NH2	2.41	0.50
33:1b:20:GLU:HG2	33:1b:23:ARG:NH1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:163:PHE:HA	33:1b:185:ILE:HG12	1.93	0.50
1:2A:644:A:H4'	1:2A:645:C:C4	2.46	0.50
1:2A:2125:G:H1'	1:2A:2173:A:N6	2.25	0.50
32:2a:4:U:O4	39:2h:105:ARG:HD3	2.11	0.50
32:2a:757:U:H2'	32:2a:758:G:O4'	2.10	0.50
34:2c:191:THR:OG1	34:2c:194:GLY:O	2.28	0.50
44:2m:13:LYS:O	44:2m:45:VAL:HG13	2.12	0.50
5:1F:143:ALA:HB1	5:1F:148:LEU:HB2	1.93	0.50
26:14:63:TYR:N	26:14:63:TYR:CD1	2.79	0.50
34:1c:131:ARG:NH1	34:1c:166:GLU:HG3	2.27	0.50
51:1t:22:ARG:O	51:1t:26:ASN:ND2	2.44	0.50
1:2A:829:A:N7	1:2A:2248:C:H5'	2.26	0.50
32:2a:1148:U:H2'	32:2a:1149:C:O4'	2.11	0.50
32:2a:1328:C:OP1	52:2u:21:TYR:OH	2.26	0.50
37:2f:91:VAL:HG11	49:2r:72:ARG:NH1	2.26	0.50
40:2i:31:GLN:HB3	40:2i:35:GLU:HB3	1.94	0.50
40:2i:99:LEU:HB3	40:2i:101:PHE:HD2	1.76	0.50
54:2w:39:PSU:H2'	54:2w:40:C:H6	1.77	0.50
1:1A:2206:G:H5''	1:1A:2207:G:C5	2.47	0.50
8:1I:101:LEU:HD12	8:1I:107:VAL:HB	1.93	0.50
13:1R:2:ARG:HG2	13:1R:5:LYS:HB2	1.94	0.50
31:19:17:ILE:HD13	31:19:26:ILE:HD13	1.94	0.50
32:1a:738:C:OP2	37:1f:92:LYS:NZ	2.40	0.50
32:1a:1316:G:N1	32:1a:1319:A:OP2	2.41	0.50
32:1a:1469:G:N7	61:1a:1827:HOH:O	2.35	0.50
39:1h:25:ASP:OD2	39:1h:60:ARG:HG3	2.12	0.50
45:1n:48:ALA:HB2	45:1n:53:LEU:HD12	1.93	0.50
1:2A:748:G:C8	18:2W:89:ALA:HB1	2.47	0.50
1:2A:2135:A:C5	1:2A:2136:C:H5	2.29	0.50
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	1.94	0.50
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.12	0.50
32:2a:1517:G:H3'	32:2a:1518:MA6:H8	1.93	0.50
41:2j:78:ASN:O	41:2j:80:LYS:N	2.45	0.50
42:2k:45:GLY:O	42:2k:50:TYR:HB2	2.11	0.50
1:1A:1783:A:H5'	1:1A:2608:G:H4'	1.93	0.50
4:1E:50:GLY:HA3	4:1E:75:VAL:HG21	1.92	0.50
8:1I:126:TYR:HB2	8:1I:142:VAL:HG23	1.93	0.50
12:1Q:10:ARG:HH12	12:1Q:90:VAL:H	1.58	0.50
21:1Z:103:ARG:O	21:1Z:138:GLU:HA	2.12	0.50
31:19:15:LYS:HD3	31:19:26:ILE:HD11	1.93	0.50
38:1g:113:GLU:HG2	38:1g:119:ARG:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:153:C:OP1	23:21:92:LYS:HD3	2.10	0.50
1:2A:304:G:O6	61:2A:3931:HOH:O	2.19	0.50
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.46	0.50
21:2Z:47:VAL:O	21:2Z:50:GLN:NE2	2.44	0.50
35:2d:191:ARG:NH1	35:2d:191:ARG:O	2.45	0.50
1:1A:1053:C:H42	1:1A:1106:G:H1	1.60	0.50
10:1O:97:ARG:NH1	32:1a:339:C:OP2	2.43	0.50
32:1a:437:U:H5''	35:1d:155:LEU:HD21	1.94	0.50
32:1a:1445:C:H2'	32:1a:1446:U:O4'	2.12	0.50
50:1s:22:LEU:HD22	50:1s:27:GLU:HA	1.94	0.50
51:1t:33:ILE:O	51:1t:37:SER:OG	2.23	0.50
1:2A:455:C:N3	1:2A:472:A:H2'	2.27	0.50
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.12	0.50
1:2A:2058:MA6:H91	57:2A:3809:WC9:CAE	2.41	0.50
2:2B:83:G:H5''	25:23:52:HIS:CD2	2.47	0.50
1:1A:247:G:H4'	1:1A:386:G:C5	2.47	0.50
1:1A:987:G:O2'	1:1A:1000:A:N3	2.40	0.50
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.47	0.50
26:14:68:ARG:HD3	26:14:69:LYS:N	2.27	0.50
32:1a:222:U:H2'	32:1a:223:U:C6	2.46	0.50
32:1a:276:G:O3'	48:1q:68:ARG:NH1	2.45	0.50
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.47	0.50
32:1a:1531:A:H8	32:1a:1531:A:O5'	1.95	0.50
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.12	0.50
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.45	0.50
2:2B:31:C:H4'	6:2G:29:TRP:CZ2	2.47	0.50
2:2B:66:A:N6	2:2B:108:U:H3'	2.27	0.50
6:2G:41:GLN:O	6:2G:43:LEU:N	2.44	0.50
8:2I:81:VAL:O	8:2I:146:ALA:HA	2.12	0.50
32:2a:179:A:H2'	32:2a:180:U:C6	2.47	0.50
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.47	0.50
32:2a:1151:A:O2'	32:2a:1152:A:H8	1.95	0.50
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.77	0.50
32:2a:1456:G:O6	51:2t:54:LYS:NZ	2.35	0.50
44:2m:13:LYS:HA	44:2m:44:ARG:HH21	1.77	0.50
1:1A:588:U:H2'	1:1A:589:C:C6	2.47	0.49
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.27	0.49
21:1Z:155:LEU:HD12	21:1Z:156:LYS:H	1.76	0.49
32:1a:749:C:H2'	32:1a:750:G:H8	1.77	0.49
32:1a:1145:C:H4'	32:1a:1146:A:H5'	1.94	0.49
36:1e:91:LEU:HB3	36:1e:118:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1503:U:H2'	1:2A:1504:C:C6	2.47	0.49
32:2a:1004:A:C8	32:2a:1005:A:H4'	2.47	0.49
32:2a:1092:A:H5''	38:2g:4:ARG:NH1	2.27	0.49
39:2h:51:VAL:HG21	39:2h:60:ARG:HB2	1.93	0.49
44:2m:40:ASN:HD22	44:2m:41:PRO:HD2	1.77	0.49
47:2p:28:ARG:HG2	47:2p:28:ARG:HH11	1.77	0.49
1:1A:248:G:OP1	61:1A:4128:HOH:O	2.19	0.49
1:1A:484:C:H2'	1:1A:485:C:C6	2.47	0.49
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.12	0.49
1:1A:752:A:H3'	29:17:1:MET:HE1	1.94	0.49
1:1A:2134:A:N3	1:1A:2159:G:O2'	2.43	0.49
5:1F:132:VAL:HA	5:1F:138:GLU:HB3	1.93	0.49
26:14:58:ARG:HE	50:1s:68:GLY:H	1.60	0.49
32:1a:1525:G:OP1	42:1k:120:ARG:NH2	2.45	0.49
1:2A:884:C:H3'	1:2A:885:C:H6	1.76	0.49
1:2A:892:G:H3'	1:2A:893:C:C5'	2.42	0.49
1:2A:2839:G:H5'	13:2R:46:GLY:CA	2.41	0.49
1:1A:288:C:H2'	1:1A:289:A:H8	1.77	0.49
1:1A:2790:A:H3'	1:1A:2790:A:N3	2.27	0.49
32:1a:56:U:H2'	32:1a:57:G:C8	2.47	0.49
32:1a:200:G:H1	32:1a:217:C:N4	2.10	0.49
32:1a:1285:A:H4'	32:1a:1286:A:O5'	2.12	0.49
36:1e:151:LEU:HD11	39:1h:77:GLU:OE1	2.12	0.49
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.94	0.49
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.44	0.49
1:2A:2269:A:OP1	61:2A:3933:HOH:O	2.20	0.49
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.40	0.49
33:2b:224:GLN:HE21	33:2b:225:ALA:HB2	1.77	0.49
34:2c:110:ASN:HD21	34:2c:140:ARG:HH21	1.59	0.49
34:2c:184:TYR:HD1	34:2c:201:TYR:CE1	2.30	0.49
36:2e:41:VAL:HG23	36:2e:69:VAL:HG21	1.94	0.49
39:2h:9:MET:HB2	39:2h:32:LYS:HE3	1.92	0.49
1:1A:1448:G:H4'	1:1A:1542:A:OP1	2.12	0.49
6:1G:64:THR:HB	6:1G:94:LEU:HD21	1.94	0.49
32:1a:1060:C:C5	34:1c:2:GLY:HA3	2.48	0.49
38:1g:79:ARG:HD2	38:1g:80:VAL:HA	1.93	0.49
40:1i:9:ARG:HG2	40:1i:14:VAL:HG13	1.93	0.49
1:2A:2318:G:H21	14:2S:3:ARG:CD	2.25	0.49
25:23:18:ASP:OD1	25:23:18:ASP:N	2.40	0.49
26:24:41:PRO:HG3	26:24:49:PHE:CE1	2.47	0.49
32:2a:642:A:N3	39:2h:113:SER:OG	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:60:GLU:HG3	35:2d:202:LEU:HD12	1.95	0.49
41:2j:47:PHE:N	41:2j:63:PHE:O	2.45	0.49
1:1A:910:A:N1	1:1A:2277:G:H1'	2.27	0.49
1:1A:1744:C:H2'	1:1A:1745:C:C6	2.47	0.49
3:1D:147:LEU:HD22	3:1D:155:LEU:HD21	1.93	0.49
19:1X:44:GLU:HG2	19:1X:49:VAL:O	2.11	0.49
32:1a:973:G:H3'	32:1a:974:A:H5''	1.94	0.49
54:1w:1:G:O6	54:1w:72:C:C4	2.64	0.49
55:1x:23:C:H2'	55:1x:24:U:C6	2.48	0.49
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.11	0.49
1:2A:1847:A:H3'	1:2A:1848:A:H5'	1.93	0.49
18:2W:65:LEU:HD12	18:2W:68:ARG:HE	1.77	0.49
1:1A:1173:G:O2'	1:1A:1174:A:O4'	2.27	0.49
32:1a:486:U:H2'	32:1a:487:A:C8	2.48	0.49
32:1a:1239:A:H62	32:1a:1299:A:H62	1.58	0.49
1:2A:1779:U:H2'	61:2A:4214:HOH:O	2.11	0.49
1:2A:2291:U:OP1	1:2A:2380:C:O2'	2.30	0.49
21:2Z:138:GLU:HB2	21:2Z:156:LYS:HD3	1.93	0.49
9:1N:67:LEU:HB3	9:1N:88:GLU:HG3	1.94	0.49
45:1n:23:ARG:NH1	45:1n:30:ALA:HB2	2.28	0.49
1:2A:1653:G:H3'	13:2R:2:ARG:HD3	1.93	0.49
6:2G:109:VAL:HG11	26:24:14:ILE:HG21	1.94	0.49
6:2G:115:ARG:NH1	6:2G:137:GLU:OE2	2.45	0.49
32:2a:1005:A:H3'	32:2a:1006:C:C6	2.47	0.49
32:2a:1029:C:H1'	32:2a:1033:G:N2	2.27	0.49
32:2a:1053:G:H4'	32:2a:1054:C:H3'	1.95	0.49
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.13	0.49
49:2r:53:ARG:HH21	49:2r:59:SER:HA	1.78	0.49
1:1A:1074:G:C2	1:1A:1075:C:H1'	2.47	0.49
1:1A:1079:C:H2'	1:1A:1080:C:O4'	2.12	0.49
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.48	0.49
1:1A:1740:G:H2'	1:1A:1741:A:C8	2.48	0.49
1:1A:2576:G:H1'	61:1A:4441:HOH:O	2.13	0.49
14:1S:71:ARG:NH1	14:1S:107:GLU:OE1	2.41	0.49
15:1T:24:PRO:HA	15:1T:49:VAL:HG22	1.95	0.49
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	1.94	0.49
32:1a:1368:G:OP1	40:1i:111:ARG:NH2	2.46	0.49
35:1d:83:SER:HA	35:1d:89:THR:HG21	1.94	0.49
1:2A:2816:C:O3'	13:2R:99:LYS:NZ	2.44	0.49
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.48	0.49
21:2Z:9:TYR:CE1	21:2Z:35:ARG:HD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:560:U:H5'	32:2a:566:G:N2	2.28	0.49
32:2a:646:U:H2'	32:2a:647:C:C6	2.48	0.49
32:2a:1133:G:H1	32:2a:1141:C:N4	2.08	0.49
35:2d:176:LEU:HD12	35:2d:182:LYS:O	2.13	0.49
51:2t:98:PRO:O	51:2t:99:LEU:HB2	2.13	0.49
54:2w:19:G:N2	54:2w:57:G:H1'	2.27	0.49
1:1A:796:C:H2'	1:1A:797:C:C6	2.48	0.49
3:1D:206:LEU:HD22	3:1D:211:ARG:HG2	1.95	0.49
8:1I:77:LEU:HB3	8:1I:142:VAL:HG12	1.94	0.49
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.43	0.49
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.47	0.49
36:1e:105:VAL:HG21	36:1e:128:PRO:HB3	1.95	0.49
50:1s:27:GLU:HG3	50:1s:28:LYS:HE3	1.95	0.49
54:1w:1:G:C6	54:1w:72:C:C2	3.01	0.49
1:2A:422:A:OP2	61:2A:3926:HOH:O	2.20	0.49
5:2F:20:LEU:HD22	5:2F:125:LEU:HD13	1.94	0.49
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.13	0.49
30:28:62:LEU:HB3	30:28:65:GLU:HG2	1.95	0.49
32:2a:728:A:H2'	32:2a:729:A:C8	2.48	0.49
32:2a:1111:A:N1	34:2c:177:THR:OG1	2.41	0.49
32:2a:1226:C:O2'	44:2m:111:LYS:NZ	2.45	0.49
42:2k:84:VAL:HG21	42:2k:95:ILE:HD11	1.93	0.49
46:2o:55:GLY:HA2	46:2o:58:MET:HE3	1.93	0.49
54:2y:9:A:H4'	54:2y:46:G7M:H5'	1.95	0.49
1:1A:1588:C:H2'	1:1A:1589:C:C6	2.48	0.49
1:1A:1671:U:O4	61:1A:4102:HOH:O	2.20	0.49
1:1A:2080:G:OP1	23:11:35:THR:HG21	2.13	0.49
1:1A:2134:A:H2'	1:1A:2159:G:O2'	2.12	0.49
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.27	0.49
11:1P:59:LEU:HD21	30:18:10:ALA:HB2	1.94	0.49
48:1q:26:GLN:HG2	48:1q:37:LYS:HG2	1.95	0.49
1:2A:2529:G:O6	31:29:31:LYS:NZ	2.46	0.49
2:2B:20:C:H42	2:2B:63:G:H1	1.61	0.49
32:2a:134:A:H61	47:2p:25:ARG:HH12	1.61	0.49
32:2a:718:G:H5'	42:2k:117:ASN:CG	2.38	0.49
32:2a:922:G:N3	32:2a:1398:A:H2	2.11	0.49
32:2a:1325:C:OP1	52:2u:15:ARG:NH1	2.46	0.49
55:2x:50:U:H2'	55:2x:51:C:C6	2.48	0.49
1:1A:1173:G:H22	1:1A:1177:A:P	2.36	0.48
1:1A:1406:U:H2'	1:1A:1407:C:H6	1.78	0.48
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:105:PHE:C	33:1b:107:THR:H	2.21	0.48
1:2A:881:G:H3'	1:2A:882:G:H8	1.78	0.48
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.44	0.48
9:2N:73:THR:HB	9:2N:82:LEU:HD11	1.95	0.48
32:2a:1111:A:H2'	32:2a:1112:C:C6	2.48	0.48
54:2w:51:U:H2'	54:2w:52:G:C8	2.48	0.48
32:1a:1260:C:O5'	32:1a:1284:C:H4'	2.13	0.48
33:1b:71:VAL:HB	33:1b:164:VAL:HG12	1.95	0.48
37:1f:10:LEU:HB2	37:1f:59:TYR:HB3	1.95	0.48
1:2A:212:G:H2'	1:2A:213:A:O4'	2.13	0.48
1:2A:900:A:HO2'	1:2A:901:A:P	2.35	0.48
1:2A:2143:C:N4	1:2A:2148:G:H1	2.08	0.48
6:2G:129:GLY:O	6:2G:161:THR:HB	2.13	0.48
36:2e:110:LEU:HD13	36:2e:118:ILE:HD13	1.95	0.48
1:1A:1009:A:OP2	9:1N:37:LYS:NZ	2.35	0.48
1:1A:1062:G:O5'	1:1A:1070:A:O2'	2.28	0.48
8:1I:31:LEU:HD21	8:1I:38:LEU:HD22	1.95	0.48
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.46	0.48
55:1x:8:4SU:O2	55:1x:21:A:H2	1.96	0.48
1:2A:645:C:H5''	1:2A:646:A:OP2	2.12	0.48
1:2A:910:A:N1	1:2A:2277:G:H1'	2.28	0.48
5:2F:11:VAL:HG21	5:2F:20:LEU:HD13	1.95	0.48
6:2G:41:GLN:NE2	6:2G:153:ARG:HB3	2.28	0.48
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.79	0.48
1:1A:1075:C:C2'	1:1A:1076:C:H5'	2.42	0.48
1:1A:2136:C:N4	1:1A:2155:G:N1	2.41	0.48
1:1A:2747:G:O6	1:1A:2755:C:H5''	2.13	0.48
26:14:56:VAL:HB	26:14:60:GLN:HG3	1.95	0.48
32:1a:343:U:O2'	32:1a:346:G:O6	2.25	0.48
32:1a:1442:G:O6	32:1a:1461:G:N2	2.45	0.48
34:1c:152:ILE:HG23	34:1c:167:TRP:HB3	1.95	0.48
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.12	0.48
12:2Q:11:LYS:NZ	12:2Q:88:GLY:O	2.36	0.48
17:2V:40:LEU:HB2	17:2V:46:VAL:HB	1.96	0.48
21:2Z:27:VAL:HG12	21:2Z:85:HIS:HE1	1.78	0.48
54:2y:26:A:N1	54:2y:44:G:O6	2.46	0.48
1:1A:106:C:H1'	20:1Y:1:MET:HE2	1.95	0.48
1:1A:907:U:HO2'	12:1Q:101:ARG:HH22	1.61	0.48
1:1A:2448:A:OP1	61:1A:4113:HOH:O	2.20	0.48
2:1B:75:G:H22	21:1Z:73:GLN:NE2	2.11	0.48
14:1S:61:ASN:HB3	14:1S:64:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:130:PRO:HA	21:1Z:133:ILE:HG13	1.96	0.48
32:1a:584:G:H5'	48:1q:91:ARG:HH21	1.78	0.48
41:1j:11:PHE:HE1	41:1j:67:THR:HG22	1.77	0.48
43:1l:39:VAL:HG11	43:1l:41:ARG:HH11	1.77	0.48
48:1q:67:LYS:O	48:1q:68:ARG:HB2	2.13	0.48
1:2A:1181:C:H2'	1:2A:1182:A:H8	1.77	0.48
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.48	0.48
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.48	0.48
32:2a:381:C:H2'	32:2a:382:A:O4'	2.13	0.48
32:2a:1221:G:O3'	50:2s:77:THR:OG1	2.24	0.48
33:2b:118:LEU:O	33:2b:122:PHE:HB3	2.13	0.48
34:2c:69:HIS:CD2	34:2c:104:GLN:HG2	2.48	0.48
36:2e:42:GLY:HA2	36:2e:65:ASN:O	2.13	0.48
41:2j:16:LEU:HD12	41:2j:68:HIS:HB2	1.94	0.48
51:2t:9:ASN:OD1	51:2t:9:ASN:N	2.46	0.48
1:1A:1268:A:C2	1:1A:2013:A:C4	3.02	0.48
3:1D:37:LEU:HD13	3:1D:87:ASN:ND2	2.28	0.48
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.96	0.48
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.49	0.48
32:1a:836:G:OP1	49:1r:61:LYS:NZ	2.32	0.48
33:1b:134:GLU:O	33:1b:138:LEU:HG	2.13	0.48
44:1m:19:LEU:HD21	44:1m:56:LEU:HD21	1.94	0.48
45:1n:4:LYS:O	45:1n:7:ILE:HG22	2.14	0.48
1:2A:2386:C:H2'	1:2A:2387:U:C6	2.49	0.48
3:2D:132:PRO:HD3	3:2D:190:TYR:CZ	2.48	0.48
9:2N:21:LYS:NZ	9:2N:140:VAL:OXT	2.40	0.48
10:2O:111:PHE:HB3	10:2O:114:ILE:HD12	1.96	0.48
14:2S:87:PHE:CE1	14:2S:102:ALA:HB2	2.48	0.48
32:2a:1503:A:O2'	53:2v:13:A:N1	2.45	0.48
35:2d:15:GLU:OE2	35:2d:66:ARG:NH1	2.46	0.48
42:2k:110:ASP:HB3	49:2r:85:LEU:HB3	1.96	0.48
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.96	0.48
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.12	0.48
32:1a:1044:A:C5	32:1a:1045:C:H1'	2.49	0.48
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.49	0.48
51:1t:99:LEU:HA	51:1t:100:ILE:O	2.14	0.48
1:2A:2121:G:H1	1:2A:2177:C:H42	1.62	0.48
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.49	0.48
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.95	0.48
8:2I:40:THR:O	8:2I:44:LEU:HB2	2.14	0.48
32:2a:946:A:H2'	32:2a:947:G:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1026:G:H3'	32:2a:1026:G:N3	2.28	0.48
32:2a:1321:C:O2'	50:2s:77:THR:HG21	2.14	0.48
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.78	0.48
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.48	0.48
5:1F:53:THR:HG22	5:1F:55:GLY:H	1.78	0.48
1:2A:579:G:H2'	1:2A:580:C:C6	2.48	0.48
1:2A:1032:A:H2	1:2A:1122:G:H22	1.60	0.48
15:2T:24:PRO:HA	15:2T:49:VAL:HG12	1.94	0.48
20:2Y:5:MET:HB2	20:2Y:5:MET:HE2	1.70	0.48
32:2a:779:C:H2'	32:2a:780:A:O4'	2.14	0.48
33:2b:77:ALA:HA	33:2b:80:ILE:HG22	1.95	0.48
33:2b:222:ILE:HG13	33:2b:223:ILE:N	2.27	0.48
1:1A:264:C:O2'	1:1A:265:A:H2'	2.14	0.48
1:1A:2155:G:H2'	1:1A:2155:G:N3	2.29	0.48
32:1a:103:C:OP2	51:1t:14:LYS:NZ	2.31	0.48
44:1m:14:ARG:HB2	44:1m:17:VAL:HG12	1.95	0.48
50:1s:32:LYS:HA	50:1s:50:ALA:HB3	1.95	0.48
1:2A:1364:G:P	23:21:3:LYS:HG3	2.53	0.48
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.14	0.48
8:2I:59:ALA:HA	8:2I:62:LYS:HB2	1.96	0.48
32:2a:1051:C:H2'	32:2a:1052:U:C6	2.49	0.48
43:2l:117:ARG:HB3	43:2l:122:THR:HB	1.95	0.48
49:2r:26:LEU:HD11	49:2r:42:ARG:HD3	1.95	0.48
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.48	0.48
32:1a:148:G:H2'	32:1a:149:A:C8	2.45	0.48
32:1a:731:G:OP1	32:1a:766:A:H1'	2.13	0.48
43:1l:70:ILE:HD13	43:1l:77:LEU:HD12	1.96	0.48
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.43	0.48
12:2Q:103:MET:HE1	12:2Q:125:LEU:HD13	1.96	0.48
13:2R:12:ARG:O	13:2R:17:ARG:NH1	2.46	0.48
17:2V:1:MET:HE2	17:2V:43:GLU:H	1.79	0.48
50:2s:53:ASN:OD1	50:2s:54:GLY:N	2.46	0.48
1:1A:97:C:OP1	24:12:2:LYS:NZ	2.39	0.47
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.14	0.47
1:1A:2128:C:N4	1:1A:2160:G:H1	2.12	0.47
1:1A:2171:A:O2'	1:1A:2172:U:H5''	2.13	0.47
32:1a:309:G:O2'	32:1a:607:A:N1	2.46	0.47
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.96	0.47
32:1a:1002:G:H3'	32:1a:1003:G:C4'	2.44	0.47
36:1e:31:LEU:HD23	36:1e:31:LEU:HA	1.79	0.47
54:1w:4:C:H2'	54:1w:5:G:H8	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:479:A:N3	1:2A:481:G:H5''	2.28	0.47
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.49	0.47
21:2Z:52:SER:OG	21:2Z:54:HIS:ND1	2.37	0.47
21:2Z:153:SER:HB2	21:2Z:167:PRO:HB3	1.95	0.47
32:2a:165:C:H2'	32:2a:166:G:C8	2.49	0.47
32:2a:1016:A:H2'	32:2a:1017:G:O4'	2.14	0.47
32:2a:1279:A:OP2	41:2j:9:ARG:NH2	2.42	0.47
36:2e:53:LEU:HD12	36:2e:53:LEU:H	1.78	0.47
39:2h:86:ILE:HG21	39:2h:133:LEU:HD23	1.96	0.47
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.50	0.47
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.49	0.47
32:1a:863:U:OP1	61:1a:1812:HOH:O	2.20	0.47
37:1f:33:TYR:CD2	37:1f:75:LEU:HD23	2.49	0.47
1:2A:2110:G:H3'	1:2A:2111:C:C5'	2.43	0.47
5:2F:137:LYS:HE2	5:2F:137:LYS:HB3	1.69	0.47
5:2F:197:ASP:O	5:2F:200:GLU:HB3	2.14	0.47
9:2N:96:GLU:CD	9:2N:96:GLU:H	2.22	0.47
13:2R:38:VAL:HG22	13:2R:112:ALA:HB2	1.96	0.47
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.96	0.47
32:2a:1326:C:H2'	32:2a:1327:C:C6	2.48	0.47
38:2g:153:HIS:ND1	42:2k:58:PRO:HD2	2.29	0.47
48:2q:9:VAL:HG21	48:2q:84:LEU:HD12	1.96	0.47
1:1A:2612:C:OP2	27:15:2:ALA:N	2.47	0.47
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.50	0.47
9:1N:1:MET:O	9:1N:2:LYS:HB2	2.14	0.47
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.29	0.47
35:1d:107:ARG:NH2	35:1d:194:LEU:HD11	2.29	0.47
1:2A:574:C:N3	4:2E:145:LYS:NZ	2.57	0.47
1:2A:2319:G:H22	14:2S:3:ARG:NH1	2.03	0.47
2:2B:104:U:O2'	21:2Z:72:ARG:HG2	2.13	0.47
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.31	0.47
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.50	0.47
32:2a:446:G:O6	61:2a:1907:HOH:O	2.15	0.47
40:2i:23:ASN:OD1	40:2i:25:LYS:HG2	2.14	0.47
46:2o:87:ILE:HG22	46:2o:88:ARG:N	2.29	0.47
49:2r:53:ARG:HA	49:2r:56:THR:OG1	2.15	0.47
50:2s:36:ARG:HD2	50:2s:52:TYR:O	2.14	0.47
1:1A:271(M):G:H21	8:1I:50:ARG:CZ	2.27	0.47
1:1A:566:U:H5''	11:1P:29:LYS:HE3	1.97	0.47
1:1A:1094:U:H1'	1:1A:1097:U:C4	2.49	0.47
1:1A:1924:C:H4'	55:1x:13:C:O2'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2153:G:H2'	1:1A:2154:G:H8	1.79	0.47
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.97	0.47
4:1E:4:ILE:HD11	4:1E:29:GLY:HA2	1.96	0.47
32:1a:256:U:OP1	48:1q:17:LYS:NZ	2.46	0.47
32:1a:1080:A:H5'	36:1e:14:ARG:HH21	1.79	0.47
33:1b:59:GLU:HB2	33:1b:221:LEU:HD11	1.96	0.47
43:1l:70:ILE:HG12	43:1l:100:ILE:HD12	1.96	0.47
1:2A:287:C:H2'	1:2A:288:C:H6	1.79	0.47
1:2A:2150:U:H2'	1:2A:2151:G:C8	2.47	0.47
32:2a:396:G:O2'	32:2a:398:C:OP1	2.25	0.47
9:1N:61:ARG:HD3	9:1N:61:ARG:HA	1.69	0.47
32:1a:946:A:H2'	32:1a:947:G:C8	2.48	0.47
1:2A:881:G:C2	1:2A:882:G:H1'	2.49	0.47
1:2A:1434:A:H61	1:2A:1558:A:H62	1.61	0.47
1:2A:1639:U:C2'	1:2A:1640:C:H5''	2.45	0.47
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.30	0.47
6:2G:43:LEU:C	6:2G:45:GLU:H	2.23	0.47
21:2Z:92:SER:O	21:2Z:130:PRO:HG3	2.14	0.47
32:2a:838:G:H1	32:2a:848:C:N4	2.12	0.47
32:2a:1055:A:N7	32:2a:1200:C:N4	2.60	0.47
32:2a:1133:G:H2'	32:2a:1134:G:H8	1.80	0.47
32:2a:1517:G:N7	32:2a:1518:MA6:H103	2.29	0.47
34:2c:112:SER:HB3	34:2c:115:LEU:HD12	1.95	0.47
38:2g:38:LEU:O	38:2g:42:ILE:HG13	2.14	0.47
39:2h:41:ARG:NH2	39:2h:123:GLU:OE2	2.48	0.47
46:2o:87:ILE:HG22	46:2o:88:ARG:H	1.80	0.47
1:1A:1039:G:H1	1:1A:1116:C:N4	2.12	0.47
1:1A:1946:U:H2'	1:1A:1947:C:C6	2.49	0.47
3:1D:2:ALA:O	3:1D:20:ASP:HB3	2.15	0.47
14:1S:3:ARG:HD3	14:1S:3:ARG:HA	1.59	0.47
18:1W:92:ARG:NH2	61:1W:302:HOH:O	2.40	0.47
32:1a:1148:U:H2'	32:1a:1149:C:O4'	2.14	0.47
32:1a:1318:A:H5''	50:1s:3:ARG:HH12	1.80	0.47
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.50	0.47
54:1w:46:G7M:H3'	54:1w:47:U:H5''	1.97	0.47
54:1y:19:G:C4'	54:1y:57:G:H22	2.28	0.47
1:2A:657:U:H2'	1:2A:658:C:C6	2.50	0.47
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.15	0.47
32:2a:1005:A:H5''	32:2a:1006:C:C5	2.50	0.47
32:2a:1118:C:H1'	32:2a:1179:A:C5	2.50	0.47
37:2f:8:ILE:HD13	37:2f:26:ILE:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:2q:45:HIS:NE2	48:2q:47:PRO:HG3	2.30	0.47
54:2y:18:G:N2	54:2y:55:PSU:C4	2.83	0.47
1:1A:899:A:H2'	1:1A:899:A:N3	2.28	0.47
1:1A:1607:C:H4'	1:1A:1608:A:O5'	2.14	0.47
8:1I:38:LEU:H	8:1I:38:LEU:CD2	2.27	0.47
33:1b:97:TRP:CZ2	33:1b:102:LEU:HD13	2.50	0.47
41:1j:11:PHE:CE1	41:1j:67:THR:HG22	2.49	0.47
54:1w:4:C:H2'	54:1w:5:G:C8	2.50	0.47
54:1w:23:A:H2'	54:1w:24:G:C8	2.48	0.47
1:2A:223:A:O2'	1:2A:420:C:O2	2.27	0.47
1:2A:839:U:H2'	1:2A:840:C:C6	2.50	0.47
1:2A:1359:A:H2	1:2A:1372:U:O4	1.97	0.47
1:2A:1651:G:OP1	13:2R:40:LYS:NZ	2.48	0.47
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.32	0.47
1:2A:2103:C:H2'	1:2A:2104:G:C8	2.50	0.47
1:2A:2784:C:H1'	4:2E:37:ARG:NH1	2.30	0.47
1:2A:2888:C:H2'	1:2A:2889:C:H6	1.80	0.47
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.08	0.47
7:2H:23:ARG:HE	7:2H:23:ARG:HB2	1.48	0.47
27:25:49:CYS:SG	27:25:51:TYR:HB2	2.55	0.47
32:2a:222:U:H2'	32:2a:223:U:C6	2.49	0.47
32:2a:266:G:H2'	32:2a:266:G:N3	2.29	0.47
32:2a:890:G:O2'	32:2a:906:G:O6	2.31	0.47
33:2b:63:MET:HG2	33:2b:225:ALA:HB1	1.97	0.47
34:2c:139:GLN:O	34:2c:143:GLU:HG2	2.15	0.47
36:2e:31:LEU:HD22	36:2e:43:LEU:HD11	1.96	0.47
38:2g:59:LEU:HD23	38:2g:63:LYS:HE2	1.96	0.47
43:2l:56:ALA:HB2	43:2l:70:ILE:HD11	1.95	0.47
45:2n:48:ALA:HB2	45:2n:53:LEU:HD12	1.97	0.47
47:2p:17:TYR:HE2	47:2p:41:PRO:HG3	1.79	0.47
48:2q:37:LYS:O	48:2q:38:ARG:NH2	2.48	0.47
52:2u:5:ASP:O	52:2u:11:GLY:HA3	2.15	0.47
55:2x:15:G:H2'	55:2x:59:A:N1	2.29	0.47
54:2y:65:G:H2'	54:2y:66:U:C6	2.49	0.47
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.50	0.47
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.50	0.47
1:1A:2121:G:H1	1:1A:2177:C:H42	1.61	0.47
23:11:72:GLU:OE2	23:11:76:ARG:NH2	2.48	0.47
32:1a:1315:U:H2'	32:1a:1316:G:O4'	2.15	0.47
1:2A:271(O):C:H2'	1:2A:271(P):C:C6	2.49	0.47
1:2A:492:A:H2'	1:2A:493:G:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2823:A:OP1	4:2E:159:HIS:NE2	2.46	0.47
2:2B:105:A:H5'	2:2B:106:G:OP2	2.15	0.47
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.96	0.47
15:2T:127:ALA:C	15:2T:129:ARG:H	2.22	0.47
32:2a:407:G:H5''	35:2d:115:ARG:HB3	1.97	0.47
32:2a:841:U:C5	32:2a:848:C:H1'	2.50	0.47
32:2a:1029:C:N4	32:2a:1032:G:C6	2.82	0.47
33:2b:53:ARG:HB3	33:2b:53:ARG:HH11	1.79	0.47
36:2e:7:GLU:CD	36:2e:37:ARG:HH21	2.22	0.47
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.15	0.47
20:1Y:38:ILE:HD11	20:1Y:66:PRO:HG3	1.97	0.47
32:1a:262:A:H2'	32:1a:263:A:C8	2.50	0.47
32:1a:269:C:H2'	32:1a:270:A:C8	2.50	0.47
32:1a:1039:C:H2'	32:1a:1040:U:H6	1.80	0.47
36:1e:105:VAL:HB	36:1e:106:PRO:HD3	1.96	0.47
1:2A:330:A:H2	1:2A:1210:A:O2'	1.96	0.47
1:2A:774:A:H2'	1:2A:774:A:N3	2.30	0.47
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.49	0.47
4:2E:56:PRO:C	4:2E:58:ARG:H	2.23	0.47
8:2I:87:LYS:HE3	8:2I:87:LYS:HB2	1.70	0.47
32:2a:15:G:H21	36:2e:18:ARG:HA	1.79	0.47
32:2a:523:A:N1	43:2l:92:0TD:H6	2.30	0.47
32:2a:1190:G:O2'	34:2c:3:ASN:HB2	2.15	0.47
32:2a:1226:C:OP2	44:2m:91:ARG:NH1	2.41	0.47
33:2b:17:PHE:HA	33:2b:44:LEU:HD21	1.97	0.47
50:2s:44:MET:O	50:2s:47:HIS:HB2	2.14	0.47
54:2w:23:A:H2'	54:2w:24:G:C8	2.49	0.47
54:2y:14:A:H61	54:2y:21:A:H2	1.63	0.47
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.97	0.47
26:14:62:ARG:HB2	26:14:63:TYR:CD1	2.49	0.47
32:1a:110:C:H2'	32:1a:111:G:O4'	2.14	0.47
32:1a:193:C:H2'	32:1a:194:C:C6	2.49	0.47
36:1e:6:PHE:HB3	36:1e:34:VAL:HG22	1.96	0.47
1:2A:1359:A:C2	1:2A:1372:U:O4	2.68	0.47
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.50	0.47
2:2B:103:G:H21	21:2Z:73:GLN:NE2	2.12	0.47
10:2O:68:GLU:HB3	10:2O:78:ARG:HD3	1.97	0.47
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.96	0.47
32:2a:853:G:H2'	32:2a:854:G:H8	1.80	0.47
34:2c:11:ARG:NH2	34:2c:177:THR:O	2.40	0.47
44:2m:30:ALA:O	44:2m:34:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:2n:22:THR:HB	45:2n:33:VAL:HG11	1.97	0.47
54:2w:12:U:H2'	54:2w:13:C:H5''	1.97	0.47
1:1A:1155:A:OP1	16:1U:55:ARG:HD2	2.15	0.46
1:1A:2277:G:OP2	22:10:10:THR:HG21	2.15	0.46
32:1a:175:C:H2'	32:1a:176:C:C6	2.51	0.46
33:1b:84:GLU:HB3	33:1b:219:VAL:HG21	1.96	0.46
38:1g:16:LEU:HD23	40:1i:42:ARG:HA	1.97	0.46
38:1g:78:ARG:HD3	38:1g:79:ARG:HG3	1.97	0.46
1:2A:885:C:H2'	1:2A:886:C:O4'	2.15	0.46
1:2A:900:A:O2'	1:2A:901:A:OP1	2.26	0.46
1:2A:1356:G:OP2	61:2A:3934:HOH:O	2.20	0.46
6:2G:59:GLU:O	6:2G:63:ILE:HG12	2.15	0.46
9:2N:12:ARG:HH21	9:2N:38:HIS:HE2	1.62	0.46
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.48	0.46
35:2d:112:VAL:H	35:2d:116:GLN:NE2	2.12	0.46
54:2w:5:G:H2'	54:2w:6:G:H8	1.79	0.46
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.14	0.46
1:1A:2629:A:HO2'	1:1A:2630:G:P	2.36	0.46
6:1G:109:VAL:C	6:1G:112:PRO:HD2	2.39	0.46
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.97	0.46
32:1a:672:U:O2'	32:1a:673:G:O5'	2.31	0.46
32:1a:731:G:H5'	32:1a:766:A:H4'	1.97	0.46
33:1b:82:ARG:HD2	33:1b:92:TYR:OH	2.14	0.46
54:1w:51:U:H2'	54:1w:52:G:C8	2.50	0.46
1:2A:459:U:H5''	29:27:40:TRP:CD2	2.51	0.46
1:2A:652(A):A:H3'	1:2A:652(B):A:C5'	2.44	0.46
14:2S:5:THR:OG1	14:2S:8:GLU:HG3	2.15	0.46
21:2Z:29:TYR:HB3	21:2Z:34:ASN:HD22	1.79	0.46
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.97	0.46
22:20:49:LYS:HE2	22:20:80:HIS:HB3	1.97	0.46
32:2a:45:U:H2'	32:2a:46:G:C8	2.50	0.46
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.97	0.46
32:2a:1292:U:H2'	32:2a:1293:G:C8	2.49	0.46
32:2a:1305:G:H22	32:2a:1331:G:H1'	1.79	0.46
33:2b:8:LYS:NZ	33:2b:214:ILE:HA	2.31	0.46
35:2d:20:TYR:CD1	35:2d:26:CYS:HB3	2.48	0.46
36:2e:72:GLN:C	36:2e:73:ASN:HD22	2.24	0.46
41:2j:11:PHE:HE1	41:2j:67:THR:HG22	1.80	0.46
1:1A:721:C:H2'	1:1A:722:A:C8	2.50	0.46
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.20	0.46
26:14:58:ARG:HD3	50:1s:67:VAL:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:59:PHE:HD2	50:1s:64:GLU:HB3	1.80	0.46
32:1a:736:C:H2'	32:1a:737:A:C8	2.50	0.46
32:1a:741:G:H2'	32:1a:742:G:O4'	2.15	0.46
32:1a:1194:U:H4'	36:1e:22:GLY:HA2	1.96	0.46
51:1t:36:LEU:HD13	51:1t:58:LYS:HG3	1.98	0.46
1:2A:534:U:H5'	16:2U:42:ALA:HB1	1.96	0.46
1:2A:2769:C:H2'	1:2A:2770:G:O4'	2.15	0.46
7:2H:70:THR:HG22	7:2H:74:ASN:HD21	1.80	0.46
16:2U:50:ARG:NH2	17:2V:72:VAL:HG22	2.29	0.46
18:2W:2:GLU:OE2	18:2W:72:LYS:NZ	2.27	0.46
21:2Z:93:ASP:HA	21:2Z:131:ARG:HH22	1.81	0.46
32:2a:818:G:O2'	32:2a:819:A:H5'	2.14	0.46
32:2a:1051:C:H2'	32:2a:1052:U:H6	1.81	0.46
32:2a:1260:C:O5'	32:2a:1284:C:H4'	2.16	0.46
32:2a:1347:G:H22	32:2a:1373:G:H2'	1.81	0.46
33:2b:167:PRO:HD3	33:2b:187:LEU:O	2.16	0.46
34:2c:179:ARG:HH12	34:2c:206:GLU:CD	2.24	0.46
40:2i:50:LEU:HA	40:2i:53:VAL:HG22	1.96	0.46
1:1A:284:U:H2'	1:1A:285:C:C6	2.50	0.46
1:1A:288:C:H2'	1:1A:289:A:C8	2.50	0.46
1:1A:1973:G:OP1	61:1A:4131:HOH:O	2.21	0.46
1:1A:2106:G:H2'	1:1A:2107:C:C6	2.51	0.46
2:1B:23:G:O6	61:1B:302:HOH:O	2.20	0.46
11:1P:101:VAL:HA	11:1P:106:LEU:O	2.15	0.46
12:1Q:10:ARG:NH1	12:1Q:90:VAL:H	2.13	0.46
32:1a:963:G:H5'	61:1a:1934:HOH:O	2.16	0.46
46:1o:9:GLN:HA	46:1o:9:GLN:HE21	1.80	0.46
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.40	0.46
1:2A:1038:C:N4	1:2A:1117:G:H1	2.12	0.46
1:2A:1996:C:OP1	10:2O:31:LYS:HE3	2.16	0.46
6:2G:126:ASP:HB2	6:2G:130:ASN:O	2.15	0.46
32:2a:1031:G:H2'	32:2a:1032:G:C8	2.50	0.46
32:2a:1452:C:H5'	32:2a:1457:G:H1'	1.98	0.46
32:1a:186:C:H2'	32:1a:187:C:C6	2.50	0.46
32:1a:266:G:H5''	32:1a:268:C:H41	1.79	0.46
32:1a:271:C:H2'	32:1a:272:C:C6	2.50	0.46
32:1a:767:A:H2'	32:1a:768:A:O4'	2.16	0.46
33:1b:48:MET:HA	33:1b:51:LEU:HB2	1.98	0.46
1:2A:336:C:HO2'	20:2Y:35:TYR:HH	1.63	0.46
1:2A:1198:U:H2'	1:2A:1199:U:C6	2.51	0.46
3:2D:5:LYS:HG2	3:2D:17:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:20:ASP:OD1	3:2D:20:ASP:N	2.43	0.46
4:2E:178:GLU:H	4:2E:178:GLU:CD	2.20	0.46
9:2N:59:LYS:O	9:2N:61:ARG:NH2	2.48	0.46
20:2Y:43:ASN:O	20:2Y:65:ALA:N	2.36	0.46
32:2a:23:C:H5	32:2a:561:U:O4	1.98	0.46
32:2a:1029:C:C2	32:2a:1032:G:N2	2.76	0.46
32:2a:1375:A:H4'	38:2g:29:LYS:HE3	1.98	0.46
33:2b:211:ILE:O	33:2b:215:LEU:HB2	2.16	0.46
37:2f:96:PRO:HB3	49:2r:30:ASP:CG	2.40	0.46
38:2g:65:ALA:HB1	38:2g:127:ALA:HB3	1.97	0.46
40:2i:79:LEU:HG	40:2i:83:ARG:HD2	1.96	0.46
44:2m:4:ILE:HG23	44:2m:5:ALA:H	1.79	0.46
51:2t:90:GLN:O	51:2t:93:GLU:HG3	2.15	0.46
1:1A:893:C:H2'	1:1A:894:C:C6	2.51	0.46
1:1A:1055:G:H3'	1:1A:1056:G:C8	2.49	0.46
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.46	0.46
14:1S:93:LYS:HG2	14:1S:95:HIS:HB2	1.97	0.46
21:1Z:102:LEU:HD23	21:1Z:123:ASP:HA	1.97	0.46
32:1a:271:C:H2'	32:1a:272:C:H6	1.80	0.46
32:1a:618:C:H5''	32:1a:619:U:H5''	1.97	0.46
36:1e:122:GLU:O	36:1e:126:ARG:NH1	2.47	0.46
54:1w:5:G:H2'	54:1w:6:G:C8	2.50	0.46
54:1y:23:A:H2'	54:1y:24:G:C8	2.50	0.46
1:2A:184:C:H2'	1:2A:185:U:H6	1.79	0.46
1:2A:392:C:H5''	1:2A:409:C:H5''	1.98	0.46
1:2A:709:U:H2'	1:2A:710:G:C8	2.51	0.46
12:2Q:10:ARG:HH11	12:2Q:11:LYS:HE2	1.80	0.46
36:2e:95:ALA:O	36:2e:97:GLY:N	2.44	0.46
41:2j:46:ARG:HB2	41:2j:46:ARG:NH1	2.31	0.46
1:1A:2820:A:P	13:1R:2:ARG:HH22	2.38	0.46
8:1I:46:ALA:O	8:1I:50:ARG:HG2	2.16	0.46
32:1a:487:A:H2'	32:1a:488:C:O4'	2.15	0.46
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.45	0.46
34:1c:61:ALA:C	34:1c:63:ASN:H	2.23	0.46
36:1e:95:ALA:HB1	36:1e:96:PRO:HD2	1.98	0.46
6:2G:41:GLN:HB3	6:2G:43:LEU:HD22	1.96	0.46
9:2N:20:GLY:H	9:2N:61:ARG:HH21	1.63	0.46
32:2a:201:C:H5'	32:2a:202:U:OP2	2.16	0.46
32:2a:1241:G:H2'	32:2a:1242:C:C6	2.51	0.46
34:2c:101:LEU:HD22	34:2c:102:ASN:N	2.31	0.46
42:2k:44:SER:OG	42:2k:47:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:2q:32:TYR:O	48:2q:34:LYS:N	2.48	0.46
1:1A:870:A:OP1	12:1Q:6:ARG:NH1	2.48	0.46
1:1A:880:G:H1	1:1A:898:C:N4	2.14	0.46
1:1A:2693:A:H2'	1:1A:2694:G:C8	2.51	0.46
2:1B:73:A:C4	2:1B:105:A:C2	3.04	0.46
36:1e:131:ILE:O	36:1e:135:THR:HG23	2.16	0.46
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	1.98	0.46
1:2A:2096:U:H3	1:2A:2193:G:H1	1.64	0.46
2:2B:24:G:N7	2:2B:56:G:H2'	2.30	0.46
6:2G:20:ILE:HA	6:2G:25:TYR:HD2	1.81	0.46
26:24:49:PHE:HD2	26:24:50:VAL:HG22	1.80	0.46
32:2a:136:C:H42	32:2a:227:G:H1	1.64	0.46
33:2b:33:TYR:HB2	33:2b:43:ASP:HA	1.97	0.46
32:1a:161:A:H2'	32:1a:162:A:C8	2.51	0.46
1:2A:38:A:H2'	1:2A:39:C:C6	2.51	0.46
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.51	0.46
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.80	0.46
1:2A:2611:U:H6	1:2A:2611:U:H5'	1.81	0.46
1:2A:2785:C:OP1	4:2E:41:LYS:NZ	2.49	0.46
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.30	0.46
8:2I:77:LEU:HD21	8:2I:100:ALA:HB3	1.98	0.46
16:2U:106:PHE:O	16:2U:110:VAL:HG23	2.16	0.46
32:2a:189(K):U:H2'	32:2a:189(L):G:C8	2.51	0.46
32:2a:1174:G:N7	61:2a:1927:HOH:O	2.36	0.46
32:2a:1381:U:O2'	38:2g:79:ARG:HD3	2.16	0.46
1:1A:185:U:H4'	1:1A:218:A:H4'	1.98	0.46
1:1A:271(K):U:H4'	1:1A:271(L):U:OP2	2.13	0.46
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.50	0.46
11:1P:94:GLU:CD	11:1P:124:LYS:HE3	2.41	0.46
32:1a:72:C:H2'	32:1a:73:G:C8	2.51	0.46
32:1a:109:A:C6	32:1a:326:G:C6	3.04	0.46
32:1a:433:C:H2'	32:1a:434:U:C6	2.51	0.46
32:1a:841:U:C4	32:1a:848:C:H1'	2.50	0.46
1:2A:271(L):U:H4'	8:2I:50:ARG:NH2	2.31	0.46
1:2A:1697:G:OP2	1:2A:1698:A:O2'	2.30	0.46
1:2A:2134:A:H2'	1:2A:2134:A:N3	2.31	0.46
5:2F:28:ILE:HA	5:2F:112:MET:HG2	1.98	0.46
26:24:24:THR:OG1	26:24:25:TYR:N	2.30	0.46
26:24:45:GLY:C	26:24:47:GLN:H	2.23	0.46
32:2a:372:C:O2	61:2a:1909:HOH:O	2.18	0.46
32:2a:737:A:H2'	32:2a:738:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:920:U:H2'	32:2a:921:U:C6	2.50	0.46
39:2h:121:ASP:N	39:2h:121:ASP:OD1	2.49	0.46
1:1A:958:U:OP1	12:1Q:74:TYR:OH	2.21	0.45
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.16	0.45
6:1G:45:GLU:H	6:1G:45:GLU:CD	2.24	0.45
12:1Q:111:GLU:O	12:1Q:115:MET:HG2	2.16	0.45
32:1a:1073:U:O2'	33:1b:104:ASN:OD1	2.32	0.45
36:1e:43:LEU:HB2	36:1e:136:MET:HG3	1.97	0.45
1:2A:217:G:OP2	61:2A:3936:HOH:O	2.21	0.45
1:2A:1012:U:H5	9:2N:28:THR:HG21	1.82	0.45
1:2A:1721:G:H2'	1:2A:1740:G:O6	2.16	0.45
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.81	0.45
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.51	0.45
9:2N:35:ARG:O	9:2N:42:TRP:NE1	2.49	0.45
23:21:67:ILE:N	23:21:68:PRO:HD2	2.31	0.45
32:2a:524:G:H2'	32:2a:525:C:C6	2.51	0.45
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.51	0.45
55:2x:61:C:H2'	55:2x:62:C:H6	1.80	0.45
1:1A:2375:G:O2'	1:1A:2377:A:N7	2.41	0.45
1:1A:2693:A:H2'	1:1A:2694:G:H8	1.80	0.45
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.99	0.45
32:1a:78:G:O2'	32:1a:79:G:O5'	2.34	0.45
32:1a:501:C:H2'	32:1a:502:G:H8	1.81	0.45
32:1a:925:G:H1'	32:1a:1502:A:C4	2.51	0.45
32:1a:955:U:O2'	50:1s:83:HIS:HD2	2.00	0.45
34:1c:56:ASP:HB2	34:1c:67:THR:HB	1.99	0.45
42:1k:99:GLN:HG3	42:1k:105:VAL:HG21	1.97	0.45
51:1t:33:ILE:HG12	51:1t:62:LEU:HB3	1.97	0.45
1:2A:1417:C:H2'	1:2A:1418:G:O4'	2.16	0.45
1:2A:2505:G:OP1	57:2A:3809:WC9:OAI	2.34	0.45
19:2X:60:ARG:HH22	29:27:47:ARG:HH12	1.65	0.45
32:2a:1003:G:H2'	32:2a:1004:A:O4'	2.16	0.45
33:2b:58:ILE:O	33:2b:62:ALA:N	2.44	0.45
41:2j:40:LEU:HB2	41:2j:69:ASN:HB3	1.98	0.45
47:2p:18:ARG:HD3	47:2p:35:LYS:HD2	1.98	0.45
1:1A:184:C:H2'	1:1A:185:U:C6	2.51	0.45
1:1A:536:A:H2'	1:1A:537:C:C6	2.51	0.45
1:1A:576:U:H2'	1:1A:577:G:C8	2.51	0.45
1:1A:586:A:N1	1:1A:809:G:O2'	2.48	0.45
1:1A:2245:U:O2'	1:1A:2436:G:OP2	2.30	0.45
4:1E:77:ILE:HD12	4:1E:195:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:78:G:H8	32:1a:78:G:OP2	2.00	0.45
35:1d:98:GLU:OE1	35:1d:103:ASN:ND2	2.50	0.45
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.16	0.45
27:25:41:PRO:O	27:25:44:THR:OG1	2.30	0.45
32:2a:130:A:O2'	32:2a:131:C:O5'	2.29	0.45
32:2a:345:C:H4'	32:2a:346:G:O5'	2.16	0.45
32:2a:653:A:OP1	39:2h:56:LYS:NZ	2.34	0.45
32:2a:975:A:N1	41:2j:48:THR:OG1	2.49	0.45
32:2a:1327:C:H2'	32:2a:1328:C:H6	1.81	0.45
44:2m:122:LYS:HG3	44:2m:123:ALA:H	1.81	0.45
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.32	0.45
1:1A:1851:U:H2'	1:1A:1852:C:O4'	2.16	0.45
2:1B:42:C:O2'	6:1G:66:GLN:HG2	2.16	0.45
32:1a:486:U:H2'	32:1a:487:A:H8	1.81	0.45
54:1w:1:G:H2'	54:1w:2:C:C6	2.51	0.45
1:2A:2741:A:H2'	1:2A:2742:C:O4'	2.16	0.45
5:2F:31:HIS:NE2	5:2F:35:GLU:OE2	2.46	0.45
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.97	0.45
32:2a:7:G:H5'	32:2a:298:A:O4'	2.16	0.45
32:2a:738:C:H5''	37:2f:69:GLU:HB3	1.98	0.45
33:2b:55:PHE:HE1	33:2b:218:ALA:HA	1.82	0.45
41:2j:16:LEU:HD23	41:2j:16:LEU:HA	1.72	0.45
1:1A:829:A:N7	1:1A:2248:C:H5'	2.31	0.45
1:1A:1803:A:H4'	3:1D:259:THR:HG23	1.97	0.45
1:1A:1899:G:O2'	1:1A:1900:A:OP2	2.30	0.45
1:1A:2064:C:H2'	1:1A:2065:C:C6	2.51	0.45
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.51	0.45
1:1A:2864:G:OP1	15:1T:119:LYS:HD2	2.17	0.45
2:1B:66:A:H61	2:1B:108:U:H2'	1.81	0.45
3:1D:71:ASP:CB	3:1D:103:ARG:HH12	2.29	0.45
3:1D:145:VAL:HG12	3:1D:146:GLU:O	2.16	0.45
4:1E:9:VAL:HG13	15:1T:3:ARG:HG2	1.99	0.45
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.17	0.45
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.49	0.45
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.17	0.45
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.51	0.45
32:1a:438:G:H4'	35:1d:123:HIS:ND1	2.32	0.45
32:1a:743:U:H2'	32:1a:744:C:C6	2.51	0.45
32:1a:942:G:H21	40:1i:124:GLN:NE2	2.14	0.45
32:1a:1349:A:H5''	40:1i:121:ARG:HB2	1.99	0.45
34:1c:116:VAL:HG21	34:1c:202:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:173:TRP:CE3	35:1d:189:PRO:HG3	2.52	0.45
36:1e:90:VAL:O	36:1e:120:THR:HA	2.16	0.45
40:1i:53:VAL:O	40:1i:55:ALA:N	2.50	0.45
41:1j:78:ASN:O	41:1j:80:LYS:N	2.49	0.45
54:1y:26:A:H61	54:1y:44:G:H1	1.59	0.45
54:1y:66:U:C4	54:1y:67:C:C4	3.05	0.45
1:2A:1537:G:H2'	1:2A:1538:G:H8	1.82	0.45
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.32	0.45
32:2a:21:G:H2'	32:2a:22:G:C8	2.50	0.45
32:2a:448:A:P	32:2a:485:G:H22	2.37	0.45
32:2a:1288:A:N1	32:2a:1371:G:H1'	2.32	0.45
35:2d:150:GLU:OE1	35:2d:151:LYS:N	2.43	0.45
35:2d:153:ARG:HG2	35:2d:181:MET:HE2	1.97	0.45
1:1A:1094:U:N3	1:1A:1097:U:OP2	2.45	0.45
1:1A:2685:G:H5'	10:1O:68:GLU:OE2	2.16	0.45
1:1A:2794:C:H42	1:1A:2802:G:H22	1.65	0.45
3:1D:71:ASP:HB3	3:1D:103:ARG:HH12	1.82	0.45
5:1F:12:LEU:HD12	5:1F:17:ARG:HE	1.82	0.45
5:1F:150:GLY:HA2	5:1F:172:TRP:CD2	2.51	0.45
6:1G:98:ARG:CZ	26:14:1:MET:HE3	2.46	0.45
21:1Z:1:MET:HG3	21:1Z:56:VAL:H	1.81	0.45
32:1a:1320:C:OP1	50:1s:70:LYS:NZ	2.46	0.45
34:1c:15:THR:HG21	34:1c:181:ASN:HA	1.97	0.45
1:2A:811:U:H2'	11:2P:21:ARG:HA	1.99	0.45
1:2A:2124:G:O6	1:2A:2125:G:N2	2.49	0.45
1:2A:2303:G:O2'	6:2G:132:ASN:HB2	2.16	0.45
1:2A:2640:G:P	9:2N:97:ARG:HH22	2.39	0.45
4:2E:47:VAL:HG12	4:2E:84:PHE:HB3	1.99	0.45
12:2Q:66:ILE:HG23	12:2Q:104:PHE:CE1	2.51	0.45
13:2R:72:ASP:O	13:2R:76:VAL:HG23	2.17	0.45
21:2Z:105:VAL:N	21:2Z:139:VAL:O	2.49	0.45
32:2a:1264:C:C4	32:2a:1272:G:O6	2.69	0.45
44:2m:108:ARG:HD3	44:2m:108:ARG:HA	1.77	0.45
1:1A:271(I):G:N7	1:1A:271(J):C:N4	2.65	0.45
1:1A:671:C:N4	61:1A:4291:HOH:O	2.49	0.45
1:1A:2160:G:C6	1:1A:2161:C:N4	2.85	0.45
1:1A:2378:A:H2'	14:1S:21:THR:HG21	1.99	0.45
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	1.99	0.45
6:1G:133:LEU:HD11	6:1G:157:ILE:HD12	1.99	0.45
32:1a:375:U:OP1	47:1p:69:THR:OG1	2.17	0.45
32:1a:977:A:H1'	32:1a:982:U:O4	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:95:GLN:NE2	33:1b:147:LYS:O	2.50	0.45
54:1y:36:A:H2'	54:1y:37:MIA:O4'	2.17	0.45
1:2A:55:G:O2'	1:2A:127:A:N1	2.49	0.45
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.32	0.45
1:2A:1824:G:N3	3:2D:254:THR:OG1	2.50	0.45
1:2A:2471:C:N4	1:2A:2476:A:O2'	2.48	0.45
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.52	0.45
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.98	0.45
9:2N:73:THR:HA	9:2N:83:LYS:O	2.17	0.45
21:2Z:31:ARG:NH1	21:2Z:94:GLU:HG2	2.32	0.45
26:24:19:GLY:O	26:24:21:VAL:HG23	2.17	0.45
32:2a:20:U:H2'	32:2a:21:G:O4'	2.16	0.45
33:2b:82:ARG:HB2	33:2b:92:TYR:CZ	2.51	0.45
34:2c:164:ARG:NH1	34:2c:166:GLU:OE1	2.50	0.45
37:2f:99:ALA:HB1	49:2r:23:LYS:NZ	2.32	0.45
38:2g:78:ARG:HE	38:2g:79:ARG:HG3	1.81	0.45
54:2w:18:G:H4'	54:2w:60:U:C5	2.52	0.45
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.64	0.45
32:1a:890:G:O2'	32:1a:906:G:O6	2.24	0.45
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.52	0.45
36:1e:85:GLY:C	36:1e:87:SER:H	2.25	0.45
38:1g:26:PHE:CE2	38:1g:30:ILE:HD11	2.52	0.45
40:1i:70:LYS:O	40:1i:74:ILE:HG13	2.16	0.45
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.99	0.45
1:2A:2304:G:OP1	6:2G:124:SER:HB2	2.17	0.45
10:2O:15:GLY:O	10:2O:47:ILE:HG12	2.17	0.45
21:2Z:55:HIS:CE1	21:2Z:135:GLU:HB2	2.51	0.45
32:2a:165:C:H2'	32:2a:166:G:H8	1.81	0.45
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.15	0.45
32:2a:966:M2G:HM22	55:2x:34:C:H5'	1.98	0.45
32:2a:1109:C:H2'	32:2a:1110:A:O4'	2.17	0.45
32:2a:1226:C:H4'	50:2s:80:TYR:CZ	2.52	0.45
34:2c:122:GLU:HA	34:2c:125:GLU:HG2	1.98	0.45
38:2g:113:GLU:OE1	38:2g:122:HIS:ND1	2.44	0.45
40:2i:26:VAL:HG22	40:2i:61:ALA:HB3	1.97	0.45
1:1A:139(A):G:O2'	1:1A:140:G:H5'	2.17	0.45
1:1A:2131:G:H5'	1:1A:2133:G:C8	2.51	0.45
1:1A:2649:U:H2'	1:1A:2650:U:C6	2.52	0.45
32:1a:28:G:O2'	32:1a:296:U:OP1	2.27	0.45
32:1a:109:A:H2'	32:1a:326:G:N2	2.32	0.45
32:1a:266:G:H2'	32:1a:266:G:N3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:418:C:H1'	32:1a:540:G:O2'	2.17	0.45
54:1w:2:C:N3	54:1w:71:G:N2	2.53	0.45
1:2A:71:A:H5''	1:2A:73:A:C8	2.52	0.45
1:2A:1709:U:H2'	1:2A:1710:C:C6	2.52	0.45
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.17	0.45
26:24:61:ARG:NH1	26:24:62:ARG:O	2.49	0.45
32:2a:520:A:N1	32:2a:536:C:H1'	2.31	0.45
32:2a:620:C:H2'	32:2a:621:A:O4'	2.17	0.45
32:2a:685:G:C2	32:2a:686:U:C4	3.05	0.45
33:2b:98:LEU:H	33:2b:101:MET:HE3	1.81	0.45
43:2l:33:ARG:HD2	43:2l:33:ARG:HA	1.89	0.45
54:2y:51:U:H3	54:2y:63:G:H1	1.64	0.45
8:1I:76:THR:HG22	8:1I:141:LYS:HE2	1.99	0.45
12:1Q:16:ARG:HG3	12:1Q:17:LEU:H	1.82	0.45
21:1Z:1:MET:HA	21:1Z:2:GLU:HA	1.69	0.45
32:1a:278:G:OP2	48:1q:92:ARG:NH2	2.49	0.45
32:1a:961:U:OP2	32:1a:1223:C:O2'	2.25	0.45
32:1a:1370:G:C2	32:1a:1371:G:C8	3.05	0.45
38:1g:151:TYR:OH	42:1k:54:ARG:NH1	2.50	0.45
1:2A:699:A:H2'	1:2A:700:G:O4'	2.17	0.45
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.51	0.45
1:2A:1843:C:H5'	3:2D:253:GLN:OE1	2.17	0.45
2:2B:48:A:OP1	14:2S:30:ARG:NH2	2.50	0.45
6:2G:16:ARG:NE	6:2G:31:VAL:HG11	2.31	0.45
7:2H:3:ARG:HD2	7:2H:3:ARG:HA	1.70	0.45
18:2W:12:ILE:HD13	18:2W:17:VAL:HG13	1.98	0.45
21:2Z:9:TYR:OH	21:2Z:61:LEU:HD23	2.17	0.45
32:2a:232:G:H1'	32:2a:262:A:N1	2.32	0.45
40:2i:43:ALA:HA	40:2i:74:ILE:HD13	1.99	0.45
47:2p:28:ARG:NH1	47:2p:29:ASP:OD2	2.50	0.45
48:2q:27:PHE:CE1	48:2q:36:ILE:HD11	2.52	0.45
1:1A:118:A:C8	1:1A:119:A:C8	3.05	0.44
1:1A:637:A:H4'	1:1A:638:G:O5'	2.17	0.44
1:1A:1012:U:C5	9:1N:28:THR:HG21	2.52	0.44
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.52	0.44
1:1A:1183:G:O2'	25:13:29:ARG:NH1	2.50	0.44
3:1D:26:LYS:HE2	3:1D:28:GLU:O	2.17	0.44
21:1Z:45:ASP:O	21:1Z:49:ARG:HB2	2.18	0.44
22:10:10:THR:HG22	22:10:12:ASN:N	2.24	0.44
32:1a:390:C:H2'	32:1a:391:G:C8	2.51	0.44
32:1a:1196:U:N3	53:1v:24:A:O2'	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:105:VAL:HG13	35:1d:110:PHE:HB2	1.99	0.44
35:1d:172:PRO:C	35:1d:174:LEU:H	2.25	0.44
47:1p:15:PRO:HD2	47:1p:42:ARG:HD3	1.99	0.44
51:1t:90:GLN:O	51:1t:93:GLU:HB2	2.16	0.44
1:2A:287:C:H2'	1:2A:288:C:C6	2.51	0.44
1:2A:307:G:N1	1:2A:310:A:OP2	2.46	0.44
1:2A:856:C:H2'	1:2A:857:C:C6	2.52	0.44
1:2A:1019:U:H2'	1:2A:1020:A:H8	1.82	0.44
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.32	0.44
1:2A:2299:G:N1	1:2A:2318:G:N7	2.66	0.44
1:2A:2439:A:H5'	1:2A:2439:A:C8	2.52	0.44
1:2A:2783:G:H2'	1:2A:2784:C:C6	2.52	0.44
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.50	0.44
6:2G:110:ALA:HB1	6:2G:140:ILE:HG23	1.99	0.44
7:2H:27:LYS:HE3	7:2H:27:LYS:HB2	1.84	0.44
32:2a:865:A:H5'	32:2a:1078:U:C5	2.52	0.44
32:2a:1142:G:H2'	32:2a:1143:G:O4'	2.17	0.44
32:2a:1212:U:H5'	32:2a:1213:A:C8	2.51	0.44
32:2a:1530:G:OP1	32:2a:1530:G:H4'	2.17	0.44
34:2c:113:ALA:HB2	34:2c:202:ILE:HG13	1.98	0.44
38:2g:69:VAL:HG11	38:2g:134:ALA:HB1	1.98	0.44
38:2g:108:ALA:HA	38:2g:111:ARG:HD2	2.00	0.44
44:2m:15:VAL:O	44:2m:19:LEU:HG	2.17	0.44
54:2y:42:C:H2'	54:2y:43:C:C6	2.52	0.44
1:1A:593:G:H4'	30:18:4:MET:HE2	2.00	0.44
1:1A:2280:G:O2'	1:1A:2388:A:N1	2.48	0.44
1:1A:2615:U:H2'	1:1A:2616:C:H6	1.82	0.44
10:1O:104:ARG:NH2	15:1T:36:GLU:OE2	2.38	0.44
25:13:7:LYS:HE3	25:13:32:GLN:HE21	1.81	0.44
32:1a:382:A:H2'	32:1a:383:A:C8	2.52	0.44
32:1a:580:U:H2'	32:1a:581:G:O4'	2.17	0.44
32:1a:840:C:H4'	32:1a:841:U:OP1	2.17	0.44
37:1f:8:ILE:HD11	37:1f:79:LEU:HD13	2.00	0.44
51:1t:50:GLU:HG3	51:1t:100:ILE:HD13	1.99	0.44
1:2A:2105:C:H2'	1:2A:2106:G:H8	1.82	0.44
1:2A:2376:A:H2'	1:2A:2377:A:O4'	2.17	0.44
2:2B:2:C:H2'	2:2B:3:C:H6	1.82	0.44
7:2H:137:ASP:HB3	7:2H:140:LYS:HB3	1.98	0.44
12:2Q:12:GLN:NE2	12:2Q:72:LYS:HG3	2.32	0.44
18:2W:18:ARG:HG2	18:2W:76:VAL:HB	1.99	0.44
20:2Y:55:TYR:N	20:2Y:56:PRO:HD3	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.52	0.44
32:2a:1280:A:O2'	32:2a:1281:U:H5'	2.17	0.44
33:2b:178:ARG:NH2	39:2h:74:PRO:HB3	2.32	0.44
40:2i:4:TYR:CE2	40:2i:88:TYR:HD1	2.34	0.44
44:2m:92:HIS:HD2	44:2m:110:ARG:NH2	2.15	0.44
45:2n:4:LYS:HA	45:2n:7:ILE:HG22	1.99	0.44
50:2s:63:THR:OG1	50:2s:64:GLU:N	2.50	0.44
54:2w:3:C:O2	54:2w:3:C:H2'	2.17	0.44
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.51	0.44
1:1A:1176:G:N2	1:1A:1178:C:OP2	2.50	0.44
1:1A:2031:A:C6	1:1A:2498:C:H1'	2.52	0.44
3:1D:70:TRP:HB3	3:1D:190:TYR:CE2	2.52	0.44
5:1F:14:PRO:HD2	5:1F:127:GLU:OE1	2.17	0.44
11:1P:121:LYS:HB3	11:1P:121:LYS:HE2	1.69	0.44
32:1a:7:G:H5'	32:1a:298:A:O4'	2.16	0.44
32:1a:848:C:H2'	32:1a:849:C:H6	1.82	0.44
32:1a:1298:C:H2'	38:1g:114:ARG:HH21	1.81	0.44
33:1b:155:LEU:HD11	33:1b:159:PRO:HG3	1.99	0.44
40:1i:17:VAL:HB	40:1i:63:ILE:HG23	2.00	0.44
54:1w:66:U:H2'	54:1w:67:C:C6	2.52	0.44
1:2A:880:G:C2	1:2A:881:G:C8	3.05	0.44
1:2A:1448:G:H2'	1:2A:1449:A:C8	2.52	0.44
1:2A:1478:G:O2'	1:2A:1558:A:N1	2.45	0.44
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.30	0.44
1:2A:2065:C:H4'	1:2A:2251:OMG:HM22	1.99	0.44
4:2E:181:LEU:HD12	4:2E:181:LEU:HA	1.73	0.44
5:2F:112:MET:HE3	5:2F:112:MET:HB2	1.72	0.44
10:2O:49:ARG:NH1	32:2a:1422:G:O3'	2.48	0.44
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.52	0.44
32:2a:428:G:OP2	35:2d:10:ARG:NH1	2.51	0.44
32:2a:1277:C:O2'	32:2a:1279:A:H8	2.00	0.44
37:2f:69:GLU:CD	37:2f:69:GLU:H	2.23	0.44
54:2y:52:G:H5'	54:2y:53:G:OP2	2.17	0.44
1:1A:55:G:O2'	1:1A:127:A:N1	2.46	0.44
1:1A:226:G:N2	1:1A:228:A:H62	2.15	0.44
1:1A:1080:C:H5'	1:1A:1081:U:OP2	2.17	0.44
1:1A:1359:A:C2	1:1A:1372:U:O4	2.70	0.44
30:18:26:LYS:HD2	30:18:48:PHE:CD2	2.52	0.44
32:1a:532:A:N6	32:1a:1206:G:O2'	2.51	0.44
32:1a:920:U:H2'	32:1a:921:U:C6	2.52	0.44
32:1a:1060:C:OP1	45:1n:45:ARG:NH2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1241:G:H2'	32:1a:1242:C:C6	2.53	0.44
40:1i:56:LEU:H	40:1i:56:LEU:HD12	1.83	0.44
1:2A:483:A:O2'	20:2Y:49:VAL:O	2.33	0.44
1:2A:630:G:OP1	30:28:47:LYS:NZ	2.44	0.44
1:2A:1022:G:N7	9:2N:66:LYS:HE2	2.32	0.44
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.18	0.44
1:2A:2484:G:C2	1:2A:2485:G:C8	3.06	0.44
2:2B:118:G:H2'	2:2B:119:G:O4'	2.17	0.44
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.53	0.44
16:2U:104:GLN:NE2	16:2U:105:VAL:HG23	2.33	0.44
32:2a:583:A:H2'	32:2a:584:G:O4'	2.17	0.44
32:2a:1277:C:O2'	32:2a:1279:A:C8	2.69	0.44
33:2b:185:ILE:HG22	33:2b:199:TYR:CD2	2.53	0.44
47:2p:15:PRO:HD2	47:2p:42:ARG:HD3	1.98	0.44
47:2p:28:ARG:HG2	47:2p:29:ASP:OD1	2.17	0.44
1:1A:479:A:N3	1:1A:481:G:H5''	2.32	0.44
1:1A:647:G:H2'	1:1A:648:G:O4'	2.18	0.44
1:1A:1058:G:H1	1:1A:1080:C:N4	2.12	0.44
1:1A:1506:C:H2'	1:1A:1507:A:H8	1.82	0.44
1:1A:2312:U:H5'	6:1G:88:ILE:HD11	2.00	0.44
7:1H:11:VAL:HG13	7:1H:15:VAL:HG22	1.99	0.44
10:1O:7:TYR:HE2	10:1O:20:MET:HE3	1.82	0.44
20:1Y:21:LYS:HE2	20:1Y:21:LYS:HB3	1.78	0.44
32:1a:262:A:C6	32:1a:263:A:C6	3.05	0.44
34:1c:143:GLU:C	34:1c:145:GLY:H	2.24	0.44
42:1k:51:LYS:HA	42:1k:51:LYS:HD2	1.72	0.44
54:1y:9:A:O3'	54:1y:45:U:O2'	2.35	0.44
1:2A:27:G:N2	1:2A:512:G:H1'	2.33	0.44
1:2A:311:A:C6	1:2A:328:U:C4	3.06	0.44
1:2A:744:G:OP1	4:2E:132:HIS:ND1	2.42	0.44
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.53	0.44
1:2A:2639:A:O3'	9:2N:97:ARG:NH2	2.51	0.44
6:2G:122:PRO:HG3	6:2G:182:LYS:C	2.42	0.44
21:2Z:44:PHE:HA	21:2Z:47:VAL:HG12	1.99	0.44
32:2a:565:U:OP2	32:2a:566:G:O2'	2.31	0.44
32:2a:1134:G:C2	32:2a:1135:U:H1'	2.52	0.44
34:2c:41:GLY:O	34:2c:45:LYS:HE3	2.18	0.44
34:2c:52:LEU:HA	34:2c:70:VAL:HG12	2.00	0.44
37:2f:100:ASN:HB2	49:2r:28:GLU:HA	1.99	0.44
44:2m:20:THR:HG22	44:2m:26:GLY:C	2.43	0.44
44:2m:80:ARG:HH22	50:2s:69:HIS:CE1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:236:C:H2'	1:1A:237:C:C6	2.52	0.44
1:1A:747:U:H1'	18:1W:92:ARG:NH2	2.32	0.44
1:1A:1059:G:H2'	1:1A:1060:U:C5	2.53	0.44
1:1A:1680:U:H2'	1:1A:1681:G:O4'	2.17	0.44
1:1A:1864:U:OP1	1:1A:2410:G:O2'	2.29	0.44
5:1F:172:TRP:CD1	5:1F:172:TRP:H	2.35	0.44
7:1H:3:ARG:HD2	7:1H:3:ARG:HA	1.41	0.44
32:1a:748:C:H4'	32:1a:749:C:O5'	2.18	0.44
33:1b:122:PHE:HE2	33:1b:139:LYS:HB2	1.82	0.44
33:1b:167:PRO:HG3	33:1b:188:ALA:HB2	1.99	0.44
37:1f:97:PHE:CD2	49:1r:31:LEU:HD11	2.48	0.44
42:1k:20:TYR:CE1	42:1k:83:ILE:HD12	2.52	0.44
46:1o:10:LYS:HB2	46:1o:10:LYS:HE2	1.69	0.44
1:2A:897:C:O4'	54:2w:56:C:H5	2.01	0.44
1:2A:1243:G:H2'	1:2A:1244:G:O4'	2.18	0.44
1:2A:1686:C:H2'	1:2A:1687:G:O4'	2.17	0.44
1:2A:1815:A:P	3:2D:54:ARG:HH22	2.41	0.44
1:2A:2867:G:OP2	15:2T:119:LYS:NZ	2.30	0.44
2:2B:58:A:H2'	2:2B:59:A:O4'	2.17	0.44
6:2G:33:ARG:NH2	6:2G:162:THR:HG21	2.32	0.44
6:2G:36:LYS:HD3	6:2G:95:ARG:HH12	1.81	0.44
6:2G:106:LEU:O	6:2G:110:ALA:HB3	2.17	0.44
8:2I:122:GLU:O	8:2I:126:TYR:OH	2.32	0.44
14:2S:105:ALA:HB1	14:2S:110:LEU:HD12	1.99	0.44
15:2T:16:ARG:NH2	15:2T:18:ASP:OD2	2.51	0.44
21:2Z:31:ARG:HD2	21:2Z:94:GLU:CD	2.42	0.44
21:2Z:55:HIS:HE1	21:2Z:135:GLU:HB2	1.83	0.44
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.32	0.44
33:2b:8:LYS:O	33:2b:9:GLU:HB2	2.17	0.44
33:2b:27:LYS:O	33:2b:194:PRO:HG2	2.18	0.44
34:2c:101:LEU:HD22	34:2c:102:ASN:H	1.82	0.44
1:1A:1075:C:O2	1:1A:1076:C:H2'	2.17	0.44
1:1A:2238:G:N3	1:1A:2238:G:H2'	2.32	0.44
1:1A:2336:A:H61	22:10:43:THR:HG22	1.82	0.44
4:1E:7:VAL:HG23	4:1E:51:PHE:HE2	1.82	0.44
5:1F:7:TYR:CD2	5:1F:24:LEU:HB2	2.53	0.44
6:1G:109:VAL:HG11	26:14:14:ILE:HG21	1.98	0.44
26:14:61:ARG:O	26:14:62:ARG:C	2.61	0.44
28:16:12:GLU:OE1	28:16:52:VAL:HG11	2.18	0.44
32:1a:165:C:H2'	32:1a:166:G:C8	2.41	0.44
32:1a:1343:G:H1'	40:1i:121:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1g:16:LEU:HD21	40:1i:45:ALA:HB2	1.99	0.44
50:1s:3:ARG:NE	50:1s:8:GLY:O	2.50	0.44
51:1t:26:ASN:OD1	51:1t:71:THR:OG1	2.21	0.44
1:2A:1342:A:OP1	19:2X:36:LYS:NZ	2.47	0.44
1:2A:2127:G:H22	1:2A:2160:G:H1	1.65	0.44
1:2A:2176:A:H2'	1:2A:2177:C:H6	1.83	0.44
18:2W:14:PRO:O	18:2W:18:ARG:HG3	2.18	0.44
32:2a:1128:C:HO2'	32:2a:1129:C:P	2.39	0.44
32:2a:1330:U:H4'	44:2m:23:TYR:CE1	2.52	0.44
33:2b:8:LYS:HB2	33:2b:8:LYS:HE2	1.65	0.44
40:2i:4:TYR:CE1	40:2i:88:TYR:HA	2.53	0.44
1:1A:2121:G:H2'	1:1A:2122:U:C6	2.53	0.44
1:1A:2376:A:H2'	1:1A:2377:A:O4'	2.18	0.44
3:1D:232:PRO:HB3	3:1D:244:ARG:CZ	2.48	0.44
8:1I:37:VAL:HG13	8:1I:38:LEU:HD23	2.00	0.44
25:13:50:VAL:HB	25:13:53:LEU:HD12	2.00	0.44
32:1a:881:G:OP2	43:1l:12:ARG:NH2	2.51	0.44
32:1a:1513:A:H2'	32:1a:1514:C:C6	2.53	0.44
42:1k:62:GLN:OE1	42:1k:93:GLN:NE2	2.50	0.44
1:2A:1508:A:H5'	1:2A:1509(A):A:C8	2.52	0.44
10:2O:70:LYS:HB3	10:2O:70:LYS:HE2	1.85	0.44
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.17	0.44
32:2a:719:C:H42	49:2r:71:LYS:HE2	1.83	0.44
32:2a:989:C:H2'	32:2a:990:C:C6	2.52	0.44
32:2a:1149:C:OP1	40:2i:9:ARG:HD3	2.17	0.44
34:2c:190:ARG:NE	34:2c:190:ARG:O	2.51	0.44
40:2i:42:ARG:HH21	40:2i:71:SER:HG	1.64	0.44
54:2y:14:A:O2'	54:2y:15:G:OP1	2.32	0.44
1:1A:1278:A:OP1	13:1R:36:THR:HG23	2.17	0.44
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.18	0.44
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.52	0.44
10:1O:36:GLY:HA2	10:1O:106:LEU:HD23	2.00	0.44
32:1a:591:U:H2'	32:1a:592:G:H8	1.82	0.44
32:1a:1016:A:H2'	32:1a:1017:G:O4'	2.18	0.44
32:1a:1054:C:C5	54:1w:34:G:H1'	2.53	0.44
33:1b:97:TRP:HZ2	33:1b:102:LEU:HD13	1.83	0.44
1:2A:2689:U:P	1:2A:2719:G:H22	2.41	0.44
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.32	0.44
8:2I:93:THR:H	8:2I:96:ASP:HB2	1.83	0.44
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	2.00	0.44
29:27:24:THR:HG22	29:27:26:GLY:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:29:27:CYS:SG	31:29:28:GLU:N	2.90	0.44
32:2a:109:A:C6	32:2a:326:G:C6	3.06	0.44
32:2a:811:C:O2'	32:2a:901:A:N1	2.47	0.44
32:2a:1518:MA6:H93	32:2a:1519:MA6:C9	2.46	0.44
33:2b:101:MET:HA	33:2b:108:ILE:HD12	1.99	0.44
33:2b:170:GLU:HB3	33:2b:173:ALA:HB3	2.00	0.44
34:2c:45:LYS:H	34:2c:45:LYS:HG3	1.62	0.44
36:2e:143:ARG:NE	39:2h:77:GLU:OE2	2.49	0.44
47:2p:74:LEU:O	47:2p:79:VAL:HG23	2.18	0.44
50:2s:80:TYR:O	50:2s:81:ARG:HG2	2.18	0.44
1:1A:881:G:C2	1:1A:882:G:H1'	2.53	0.43
2:1B:24:G:N7	2:1B:56:G:H2'	2.33	0.43
5:1F:29:ASN:H	5:1F:112:MET:HE3	1.83	0.43
12:1Q:19:GLY:O	12:1Q:98:LYS:HE3	2.18	0.43
33:1b:20:GLU:HG2	33:1b:23:ARG:HH11	1.82	0.43
36:1e:144:THR:H	36:1e:147:ASP:HB2	1.83	0.43
44:1m:20:THR:HA	44:1m:25:ILE:O	2.18	0.43
1:2A:1006:C:C2	1:2A:1138:G:N2	2.86	0.43
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.53	0.43
2:2B:103:G:N2	21:2Z:73:GLN:HE22	2.15	0.43
17:2V:28:GLU:HG3	17:2V:29:PRO:HD2	2.00	0.43
32:2a:542:G:H5'	35:2d:41:GLY:HA3	1.99	0.43
32:2a:1256:A:N1	32:2a:1278:U:H1'	2.33	0.43
32:2a:1272:G:N2	32:2a:1273:G:C8	2.86	0.43
32:2a:1442:G:O2'	32:2a:1442(A):G:H5'	2.18	0.43
33:2b:31:TYR:HE2	33:2b:200:ILE:HD13	1.81	0.43
33:2b:47:THR:HA	33:2b:202:PRO:HG2	1.99	0.43
36:2e:36:ASP:C	36:2e:38:GLN:H	2.25	0.43
36:2e:68:GLU:OE2	36:2e:70:PRO:HG3	2.17	0.43
38:2g:46:ALA:HA	38:2g:49:ILE:HD12	1.99	0.43
39:2h:6:ILE:O	39:2h:10:LEU:HG	2.18	0.43
40:2i:3:GLN:HG3	40:2i:20:ARG:HE	1.83	0.43
1:1A:27:G:C2	1:1A:512:G:N3	2.86	0.43
1:1A:1022:G:N7	9:1N:66:LYS:HE2	2.32	0.43
1:1A:1071:G:H1	1:1A:1100:C:H42	1.66	0.43
1:1A:1814:G:C4'	3:1D:51:VAL:HG21	2.48	0.43
32:1a:78:G:C6	32:1a:91:C:N4	2.86	0.43
37:1f:38:GLU:OE1	37:1f:64:GLN:NE2	2.42	0.43
41:1j:30:SER:HB3	41:1j:81:THR:HG23	2.00	0.43
1:2A:42:G:H2'	1:2A:43:A:O4'	2.18	0.43
1:2A:71:A:N7	19:2X:31:HIS:HE1	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:484:C:H2'	1:2A:485:C:H6	1.83	0.43
1:2A:878:A:H61	1:2A:899:A:H1'	1.83	0.43
1:2A:1665:A:H2'	1:2A:1666:G:O4'	2.18	0.43
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.18	0.43
2:2B:3:C:H2'	2:2B:4:C:C6	2.53	0.43
11:2P:37:GLY:O	11:2P:40:SER:OG	2.25	0.43
26:24:20:ASN:C	26:24:20:ASN:HD22	2.26	0.43
32:2a:302:G:N3	32:2a:556:C:H4'	2.33	0.43
32:2a:1360:A:H8	32:2a:1360:A:OP1	2.01	0.43
1:1A:922:U:H2'	1:1A:923:C:C6	2.53	0.43
1:1A:1038:C:N4	1:1A:1117:G:H1	2.16	0.43
1:1A:1698:A:C8	1:1A:1700:A:O4'	2.71	0.43
24:12:51:ARG:HD3	24:12:55:ARG:NH1	2.33	0.43
26:14:58:ARG:NE	50:1s:68:GLY:H	2.15	0.43
32:1a:1292:U:H5'	40:1i:38:GLN:OE1	2.18	0.43
35:1d:119:GLN:HE21	35:1d:123:HIS:HD2	1.66	0.43
1:2A:643:A:C8	28:26:44:ARG:NH1	2.86	0.43
1:2A:700:G:O2'	1:2A:1632:A:N3	2.43	0.43
1:2A:1991:U:H2'	1:2A:1992:G:H5''	2.00	0.43
1:2A:2037:G:H2'	1:2A:2038:G:C8	2.54	0.43
7:2H:27:LYS:HG2	7:2H:32:GLU:HB3	2.01	0.43
15:2T:106:SER:N	15:2T:109:GLU:OE1	2.42	0.43
18:2W:19:LEU:HB3	27:25:25:LEU:HG	2.00	0.43
21:2Z:74:VAL:HA	21:2Z:86:VAL:HA	1.99	0.43
44:2m:14:ARG:HA	44:2m:44:ARG:HA	2.00	0.43
47:2p:1:MET:HE2	47:2p:1:MET:HB3	1.82	0.43
54:2y:18:G:N1	54:2y:55:PSU:C4	2.86	0.43
1:1A:1059:G:H1	1:1A:1079:C:N4	2.12	0.43
1:1A:2336:A:H61	22:10:43:THR:CG2	2.31	0.43
6:1G:110:ALA:HB1	6:1G:140:ILE:HD12	2.00	0.43
17:1V:71:LEU:HD23	17:1V:71:LEU:HA	1.87	0.43
20:1Y:6:HIS:H	20:1Y:6:HIS:CD2	2.36	0.43
31:19:25:VAL:O	31:19:33:LYS:HA	2.19	0.43
32:1a:447:G:H2'	32:1a:485:G:N2	2.34	0.43
33:1b:17:PHE:HA	33:1b:44:LEU:HD21	2.00	0.43
33:1b:21:ARG:O	33:1b:23:ARG:HG2	2.17	0.43
34:1c:105:GLU:HG2	34:1c:106:VAL:N	2.33	0.43
1:2A:361:G:O2'	1:2A:362:U:H5'	2.18	0.43
1:2A:373:U:H2'	1:2A:374:A:H8	1.83	0.43
1:2A:375:C:H2'	1:2A:376:C:C6	2.54	0.43
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2118:U:OP1	1:2A:2148:G:H4'	2.18	0.43
1:2A:2138:C:H2'	1:2A:2139:C:O4'	2.19	0.43
1:2A:2340:G:H2'	1:2A:2341:G:C8	2.54	0.43
2:2B:75:G:N2	21:2Z:87:ASP:OD1	2.51	0.43
3:2D:24:ILE:HD13	3:2D:84:TYR:HB2	2.00	0.43
32:2a:157:G:N2	32:2a:164:U:O2	2.37	0.43
32:2a:826:C:H4'	39:2h:12:ARG:HG2	1.99	0.43
33:2b:82:ARG:HB3	33:2b:94:ASN:OD1	2.18	0.43
49:2r:33:ASP:OD2	49:2r:36:ASN:HB2	2.19	0.43
50:2s:63:THR:HG22	50:2s:66:MET:HE2	1.99	0.43
54:2y:34:G:H2'	54:2y:35:A:C8	2.54	0.43
1:1A:2019:A:O4'	16:1U:34:LYS:HE2	2.19	0.43
25:13:16:PRO:HB2	25:13:18:ASP:OD1	2.18	0.43
32:1a:975:A:H5'	32:1a:975:A:H8	1.84	0.43
35:1d:178:VAL:C	35:1d:180:GLY:H	2.27	0.43
47:1p:59:TRP:HA	47:1p:62:VAL:HG12	2.00	0.43
54:1w:48:C:C2	54:1w:59:U:H1'	2.54	0.43
1:2A:484:C:H2'	1:2A:485:C:C6	2.53	0.43
1:2A:2104:G:C2	1:2A:2186:G:C2	3.06	0.43
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.53	0.43
2:2B:14:U:H1'	2:2B:108:U:O2'	2.18	0.43
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	2.00	0.43
32:2a:397:A:H5'	32:2a:398:C:OP1	2.18	0.43
32:2a:542:G:P	35:2d:10:ARG:HH22	2.41	0.43
32:2a:1049:U:O4	45:2n:3:ARG:NH1	2.51	0.43
40:2i:16:ARG:HE	40:2i:64:THR:HG21	1.83	0.43
1:1A:2319:G:H22	14:1S:3:ARG:CD	2.32	0.43
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.19	0.43
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.62	0.43
32:1a:8:A:N6	35:1d:205:GLU:O	2.52	0.43
32:1a:167:G:H2'	32:1a:168:G:C8	2.54	0.43
32:1a:572:A:OP1	61:1a:1813:HOH:O	2.21	0.43
32:1a:815:A:N7	32:1a:1509:C:O2'	2.45	0.43
1:2A:275:G:H2'	1:2A:276:A:O4'	2.19	0.43
1:2A:1260:G:C6	1:2A:1261:C:C4	3.07	0.43
1:2A:2108:C:H42	1:2A:2181:G:H1	1.66	0.43
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.82	0.43
26:24:62:ARG:HB2	26:24:63:TYR:CE2	2.54	0.43
32:2a:141:A:H1'	32:2a:182:U:O2	2.19	0.43
32:2a:1327:C:H2'	32:2a:1328:C:C6	2.53	0.43
33:2b:118:LEU:HD23	33:2b:142:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:2n:53:LEU:HD23	45:2n:53:LEU:HA	1.80	0.43
1:1A:1176:G:H1'	1:1A:1177:A:H5''	2.01	0.43
1:1A:2320:A:H2'	1:1A:2320:A:N3	2.34	0.43
1:1A:2794:C:N4	1:1A:2802:G:H22	2.16	0.43
32:1a:100:C:H2'	32:1a:101:A:C8	2.54	0.43
32:1a:748:C:O5'	32:1a:748:C:H6	2.01	0.43
41:1j:43:ARG:HB3	41:1j:67:THR:OG1	2.18	0.43
1:2A:2128:C:H6	1:2A:2128:C:O5'	2.02	0.43
32:2a:1271:G:N2	32:2a:1272:G:C8	2.87	0.43
54:2y:14:A:H3'	54:2y:15:G:H8	1.80	0.43
1:1A:2001:A:H2'	1:1A:2002:G:C8	2.53	0.43
1:1A:2103:C:H42	1:1A:2186:G:H1	1.66	0.43
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.62	0.43
32:1a:1106:G:C6	32:1a:1107:C:C4	3.06	0.43
32:1a:1202:G:H1'	45:1n:29:ARG:HD2	2.00	0.43
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	2.01	0.43
33:1b:63:MET:HE2	33:1b:63:MET:HB3	1.90	0.43
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.54	0.43
1:2A:1029:A:N1	1:2A:2465:C:O2'	2.40	0.43
1:2A:2166:G:O6	1:2A:2171:A:N6	2.48	0.43
1:2A:2811:G:N2	1:2A:2891:G:H1'	2.34	0.43
3:2D:70:TRP:CE2	3:2D:150:LYS:HD3	2.53	0.43
14:2S:62:LYS:HB3	14:2S:97:ARG:NE	2.33	0.43
32:2a:157:G:H2'	32:2a:158:G:C8	2.53	0.43
32:2a:174:C:H2'	32:2a:175:C:H6	1.84	0.43
33:2b:124:SER:HB3	33:2b:125:PRO:HD3	1.99	0.43
38:2g:16:LEU:HD12	40:2i:41:VAL:O	2.19	0.43
46:2o:26:GLU:HG3	46:2o:81:LEU:HD13	2.00	0.43
1:1A:721:C:H2'	1:1A:722:A:H8	1.84	0.43
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.19	0.43
1:1A:2461:C:H2'	1:1A:2462:U:C6	2.54	0.43
12:1Q:65:PHE:HB2	12:1Q:105:GLU:HB2	2.00	0.43
25:13:23:LEU:HD13	25:13:50:VAL:HG11	2.01	0.43
32:1a:857:C:H2'	32:1a:858:G:O4'	2.18	0.43
34:1c:44:GLU:HA	34:1c:52:LEU:HD23	2.01	0.43
40:1i:26:VAL:HG22	40:1i:61:ALA:HB3	2.00	0.43
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.54	0.43
1:2A:2336:A:H61	22:20:43:THR:CG2	2.32	0.43
21:2Z:53:ILE:HG22	21:2Z:71:VAL:HG23	2.00	0.43
32:2a:1187:G:OP1	40:2i:113:LYS:NZ	2.51	0.43
32:2a:1239:A:H62	32:2a:1299:A:N6	2.13	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1274:G:N2	32:2a:1275:A:N7	2.66	0.43
33:2b:188:ALA:HB1	33:2b:192:SER:OG	2.18	0.43
46:2o:10:LYS:HB3	46:2o:10:LYS:HE2	1.93	0.43
49:2r:73:ALA:HB3	49:2r:79:LEU:HD12	2.00	0.43
1:1A:484:C:OP1	20:1Y:51:VAL:HG22	2.18	0.43
1:1A:615:G:OP1	5:1F:40:GLN:NE2	2.41	0.43
1:1A:657:U:H2'	1:1A:658:C:C6	2.54	0.43
1:1A:969:U:H2'	1:1A:970:C:C6	2.54	0.43
1:1A:2347:C:H2'	1:1A:2348:U:C6	2.54	0.43
1:1A:2518:A:OP1	61:1A:4133:HOH:O	2.22	0.43
2:1B:66:A:H61	2:1B:109:C:H5'	1.83	0.43
32:1a:130:A:N3	32:1a:263:A:O2'	2.50	0.43
32:1a:434:U:H2'	32:1a:435:C:O4'	2.19	0.43
32:1a:828:A:H2'	32:1a:829:G:O4'	2.18	0.43
32:1a:1025:U:C2	32:1a:1036:G:O6	2.71	0.43
44:1m:3:ARG:HG3	44:1m:4:ILE:N	2.32	0.43
54:1w:67:C:H2'	54:1w:68:C:O4'	2.19	0.43
1:2A:271(X):G:C2	1:2A:271(Y):U:O4	2.72	0.43
1:2A:1301:A:O2'	1:2A:1302:A:H3'	2.19	0.43
1:2A:1805:U:O2	3:2D:50:THR:HB	2.19	0.43
1:2A:2497:A:H5''	61:2A:4326:HOH:O	2.19	0.43
57:2A:3809:WC9:NAL	57:2A:3809:WC9:OAW	2.51	0.43
8:2I:38:LEU:HB2	8:2I:40:THR:HG23	2.01	0.43
16:2U:102:GLU:HG3	17:2V:2:PHE:CZ	2.54	0.43
17:2V:24:LYS:HB3	17:2V:24:LYS:HE2	1.75	0.43
32:2a:404:U:H2'	32:2a:405:U:C6	2.53	0.43
33:2b:114:ARG:O	33:2b:118:LEU:N	2.50	0.43
51:2t:10:LEU:HG	51:2t:12:ALA:H	1.84	0.43
54:2y:8:4SU:O4'	54:2y:48:C:O2'	2.32	0.43
1:1A:271(K):U:O2	8:1I:50:ARG:HG3	2.19	0.42
1:1A:615:G:OP2	5:1F:43:LYS:NZ	2.47	0.42
1:1A:2167:U:O2	1:1A:2167:U:H2'	2.19	0.42
1:1A:2273:A:H2'	1:1A:2274:A:C8	2.53	0.42
1:1A:2615:U:H2'	1:1A:2616:C:C6	2.54	0.42
11:1P:46:LYS:HB3	11:1P:46:LYS:HE3	1.83	0.42
25:13:18:ASP:OD1	25:13:18:ASP:N	2.51	0.42
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.33	0.42
38:1g:65:ALA:HB1	38:1g:127:ALA:HB3	2.01	0.42
39:1h:49:GLU:HG2	39:1h:62:TYR:HE2	1.84	0.42
1:2A:30:G:H2'	1:2A:31:C:C6	2.53	0.42
1:2A:271(S):G:C6	1:2A:271(T):C:C4	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:715:G:C2	46:2o:56:LEU:HD21	2.53	0.42
1:2A:2331:G:O2'	22:20:43:THR:HG22	2.18	0.42
5:2F:102:PRO:HB2	5:2F:105:VAL:HG23	2.01	0.42
8:2I:78:THR:HA	8:2I:143:SER:HB3	2.01	0.42
9:2N:38:HIS:NE2	9:2N:50:ASP:OD2	2.48	0.42
11:2P:81:GLN:NE2	11:2P:105:LEU:O	2.43	0.42
18:2W:45:TYR:CZ	18:2W:49:LYS:HE3	2.54	0.42
24:22:51:ARG:O	24:22:55:ARG:HG3	2.19	0.42
32:2a:130:A:H1'	32:2a:263:A:O2'	2.19	0.42
32:2a:271:C:H2'	32:2a:272:C:C6	2.54	0.42
32:2a:458:C:H2'	32:2a:460:G:O4'	2.19	0.42
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.18	0.42
32:2a:1194:U:H2'	32:2a:1195:C:C6	2.54	0.42
41:2j:32:ALA:HB1	41:2j:33:GLN:HG3	2.01	0.42
47:2p:69:THR:HG23	47:2p:72:ARG:HH12	1.84	0.42
1:1A:242:G:C8	30:18:5:LYS:HG2	2.54	0.42
1:1A:1021:A:H3'	1:1A:1021:A:N3	2.34	0.42
24:12:53:LEU:HD12	24:12:53:LEU:HA	1.79	0.42
25:13:26:LEU:O	25:13:35:ARG:NE	2.49	0.42
32:1a:184:G:H2'	32:1a:185:A:C8	2.53	0.42
32:1a:664:G:N2	32:1a:741:G:H1	2.07	0.42
32:1a:1504:G:OP1	32:1a:1507:A:H4'	2.20	0.42
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.87	0.42
38:1g:70:LYS:HG2	38:1g:96:GLN:HB3	2.01	0.42
39:1h:81:HIS:ND1	39:1h:138:TRP:OXT	2.45	0.42
45:1n:4:LYS:HA	45:1n:7:ILE:HG22	2.00	0.42
50:1s:22:LEU:HB3	50:1s:27:GLU:HB3	2.00	0.42
54:1w:37:MIA:H162	54:1w:37:MIA:H121	1.86	0.42
1:2A:141:A:C8	1:2A:1408:C:O2'	2.70	0.42
1:2A:675:A:OP1	5:2F:63:LYS:NZ	2.50	0.42
1:2A:702:G:C2	1:2A:731:C:C2	3.07	0.42
1:2A:881:G:H3'	1:2A:882:G:C8	2.54	0.42
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.20	0.42
6:2G:46:ALA:HB2	6:2G:53:LEU:HG	2.01	0.42
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.54	0.42
9:2N:1:MET:HE1	16:2U:94:ASN:ND2	2.33	0.42
13:2R:36:THR:HG22	13:2R:37:THR:H	1.84	0.42
21:2Z:100:VAL:HG21	21:2Z:134:PRO:HG2	2.01	0.42
28:26:23:THR:OG1	28:26:24:GLU:N	2.51	0.42
32:2a:353:A:H5'	32:2a:353:A:H8	1.84	0.42
32:2a:1292:U:H2'	32:2a:1293:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	2.01	0.42
33:2b:16:HIS:CE1	33:2b:44:LEU:HD11	2.54	0.42
38:2g:99:LEU:HD23	38:2g:102:ARG:NH1	2.34	0.42
40:2i:23:ASN:ND2	40:2i:25:LYS:HE2	2.33	0.42
54:2w:4:C:N4	54:2w:69:G:H1	2.16	0.42
1:1A:746:A:H2'	1:1A:2612:C:H5''	2.01	0.42
1:1A:1096:A:N6	1:1A:1097:U:O2	2.51	0.42
1:1A:1359:A:N1	1:1A:1372:U:C4	2.87	0.42
1:1A:1858:G:N2	1:1A:1883:G:H2'	2.34	0.42
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.84	0.42
15:1T:112:ARG:HG3	15:1T:115:ARG:NH2	2.34	0.42
32:1a:591:U:H2'	32:1a:592:G:C8	2.55	0.42
32:1a:865:A:H2	32:1a:918:A:H4'	1.84	0.42
32:1a:1189:C:OP1	41:1j:51:ARG:NH2	2.37	0.42
32:1a:1503:A:O2'	53:1v:13:A:N1	2.52	0.42
33:1b:118:LEU:HD23	33:1b:142:LEU:HB2	2.01	0.42
40:1i:42:ARG:NH1	40:1i:71:SER:OG	2.49	0.42
1:2A:602:G:N1	1:2A:655:A:OP2	2.47	0.42
1:2A:1820:U:C2	3:2D:202:LYS:HD2	2.54	0.42
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.54	0.42
1:2A:2577:A:H5''	1:2A:2578:G:H5'	2.01	0.42
2:2B:54:G:OP2	61:2B:301:HOH:O	2.22	0.42
32:2a:328:C:H4'	32:2a:329:A:H5'	2.01	0.42
32:2a:741:G:H2'	32:2a:742:G:O4'	2.19	0.42
32:2a:1133:G:H2'	32:2a:1134:G:C8	2.54	0.42
32:2a:1186:G:H21	45:2n:61:TRP:C	2.26	0.42
33:2b:74:LYS:HG2	33:2b:75:LYS:H	1.84	0.42
35:2d:77:ASN:HD22	35:2d:77:ASN:HA	1.68	0.42
38:2g:47:CYS:HA	38:2g:50:ILE:HD12	2.00	0.42
40:2i:28:VAL:HA	40:2i:63:ILE:O	2.19	0.42
48:2q:67:LYS:O	48:2q:68:ARG:HB2	2.20	0.42
50:2s:53:ASN:HD21	50:2s:56:GLN:HB3	1.83	0.42
1:1A:1364:G:OP2	23:11:3:LYS:HG3	2.18	0.42
61:1A:5744:HOH:O	9:1N:28:THR:HG23	2.19	0.42
20:1Y:106:LEU:O	20:1Y:107:ASP:HB2	2.17	0.42
32:1a:421:U:O4	34:1c:127:ARG:NH2	2.53	0.42
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.54	0.42
34:1c:35:GLU:CD	34:1c:59:ARG:HH22	2.27	0.42
35:1d:194:LEU:HD13	35:1d:194:LEU:HA	1.74	0.42
42:1k:45:GLY:O	42:1k:50:TYR:HB2	2.18	0.42
1:2A:125:G:O2'	29:27:48:LYS:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1023:U:OP2	61:2A:3935:HOH:O	2.21	0.42
1:2A:1557:C:H5''	1:2A:1558:A:OP2	2.20	0.42
11:2P:39:LYS:HB2	11:2P:45:LEU:HD13	2.01	0.42
11:2P:79:ARG:HE	11:2P:79:ARG:HB2	1.66	0.42
21:2Z:150:LEU:O	21:2Z:171:ILE:HG12	2.19	0.42
26:24:69:LYS:HE2	26:24:69:LYS:HB2	1.85	0.42
32:2a:445:G:H1	32:2a:489:C:H42	1.67	0.42
32:2a:512:U:H2'	32:2a:513:C:C6	2.54	0.42
32:2a:977:A:O2'	32:2a:981:U:N3	2.52	0.42
33:2b:162:ILE:HD11	33:2b:184:VAL:HG22	2.02	0.42
38:2g:78:ARG:O	38:2g:84:ASN:HA	2.19	0.42
55:2x:31:G:C8	55:2x:32:5MC:HM53	2.55	0.42
1:1A:1065:U:H1'	1:1A:1074:G:C2	2.54	0.42
1:1A:2156:G:OP2	1:1A:2156:G:H8	2.01	0.42
2:1B:78:A:C2	2:1B:100:A:C4	3.06	0.42
5:1F:136:THR:HA	5:1F:166:ALA:O	2.19	0.42
12:1Q:18:LYS:O	12:1Q:98:LYS:NZ	2.31	0.42
21:1Z:139:VAL:HG12	21:1Z:140:ASP:H	1.84	0.42
32:1a:1402:4OC:O5'	32:1a:1402:4OC:H6	2.19	0.42
40:1i:32:ASP:OD1	40:1i:33:PHE:N	2.52	0.42
40:1i:85:LEU:O	40:1i:88:TYR:HB3	2.20	0.42
1:2A:11:G:C2'	1:2A:12:U:H5'	2.50	0.42
1:2A:907:U:O2'	12:2Q:101:ARG:NH2	2.37	0.42
1:2A:2872:G:O2'	1:2A:2873:A:H5'	2.19	0.42
6:2G:43:LEU:O	6:2G:45:GLU:HG2	2.20	0.42
32:2a:921:U:O2	36:2e:19:MET:HB2	2.19	0.42
37:2f:91:VAL:HG11	49:2r:72:ARG:HH12	1.85	0.42
41:2j:5:ARG:N	41:2j:99:LYS:O	2.52	0.42
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.44	0.42
1:1A:125:G:H5'	29:17:14:LYS:HD3	2.00	0.42
1:1A:996:A:H4'	16:1U:91:ASP:OD2	2.20	0.42
1:1A:1069:A:H2'	1:1A:1073:A:N7	2.35	0.42
1:1A:1213:A:N3	1:1A:1238:G:O2'	2.50	0.42
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.54	0.42
1:1A:2029:G:H2'	1:1A:2031:A:OP1	2.19	0.42
8:1I:125:GLU:OE2	8:1I:143:SER:HB2	2.19	0.42
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.35	0.42
32:1a:341:C:H2'	32:1a:342:C:C6	2.55	0.42
32:1a:431:A:H2'	32:1a:432:A:O4'	2.18	0.42
32:1a:1002:G:C5	32:1a:1003:G:H1'	2.54	0.42
32:1a:1030(C):G:H2'	32:1a:1030(D):A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:528:A:O2'	1:2A:529:A:H5'	2.19	0.42
1:2A:747:U:O2	1:2A:2014:A:H1'	2.19	0.42
1:2A:1813:G:H1'	3:2D:50:THR:OG1	2.19	0.42
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.20	0.42
4:2E:96:PHE:O	4:2E:175:VAL:HG21	2.19	0.42
6:2G:161:THR:HG22	6:2G:163:ALA:N	2.28	0.42
8:2I:134:PRO:C	8:2I:136:VAL:H	2.26	0.42
32:2a:189(C):C:H2'	32:2a:189(D):C:O4'	2.19	0.42
32:2a:203:U:H2'	32:2a:203:U:OP2	2.20	0.42
32:2a:529:G:O6	43:2l:49:ASN:HA	2.19	0.42
32:2a:1029:C:H1'	32:2a:1033:G:H22	1.85	0.42
32:2a:1042:G:H2'	32:2a:1043:C:O4'	2.19	0.42
32:2a:1261:A:H3'	32:2a:1262:C:C6	2.55	0.42
32:2a:1279:A:O2'	32:2a:1281:U:OP2	2.21	0.42
33:2b:111:ARG:HD3	33:2b:111:ARG:HA	1.87	0.42
34:2c:6:HIS:CG	45:2n:49:HIS:HB3	2.54	0.42
34:2c:143:GLU:C	34:2c:145:GLY:H	2.27	0.42
1:1A:747:U:O2	1:1A:2014:A:H1'	2.19	0.42
1:1A:1815:A:P	3:1D:54:ARG:HH22	2.41	0.42
1:1A:2313:C:H4'	6:1G:91:ARG:HG3	2.00	0.42
1:1A:2789:C:O2'	1:1A:2790:A:H4'	2.19	0.42
2:1B:13:A:N1	2:1B:69:G:O2'	2.47	0.42
21:1Z:52:SER:C	21:1Z:54:HIS:N	2.75	0.42
32:1a:1057:G:H2'	32:1a:1058:G:O4'	2.20	0.42
47:1p:1:MET:N	47:1p:1:MET:HE2	2.35	0.42
1:2A:315:G:H2'	1:2A:316:C:C6	2.55	0.42
1:2A:590:A:H2'	1:2A:591:C:O4'	2.20	0.42
1:2A:1268:A:C2	1:2A:2013:A:C4	3.08	0.42
9:2N:69:GLN:O	9:2N:71:ILE:HG13	2.20	0.42
32:2a:828:A:H5''	32:2a:859:A:C2	2.55	0.42
32:2a:1004:A:N6	32:2a:1037:C:O2	2.35	0.42
32:2a:1103:C:P	33:2b:96:ARG:HH22	2.42	0.42
41:2j:13:HIS:HB3	41:2j:68:HIS:CE1	2.55	0.42
44:2m:91:ARG:HH11	44:2m:96:LEU:HD13	1.85	0.42
1:1A:878:A:N6	1:1A:899:A:O2'	2.52	0.42
1:1A:1074:G:N1	1:1A:1075:C:H1'	2.35	0.42
4:1E:54:GLN:HE22	4:1E:76:ARG:HE	1.68	0.42
6:1G:59:GLU:OE2	6:1G:138:GLN:NE2	2.40	0.42
32:1a:196:A:N3	32:1a:222:U:H1'	2.35	0.42
32:1a:685:G:O2'	32:1a:686:U:H5'	2.20	0.42
32:1a:1037:C:H2'	32:1a:1038:C:H6	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1140:C:H2'	32:1a:1141:C:C6	2.54	0.42
32:1a:1323:G:H2'	32:1a:1324:A:C8	2.55	0.42
39:1h:51:VAL:HG12	39:1h:52:ASP:N	2.31	0.42
54:1w:5:G:H1	54:1w:68:C:N4	2.16	0.42
54:1y:26:A:N6	54:1y:44:G:H1	2.18	0.42
1:2A:643:A:N1	1:2A:2369:A:O2'	2.50	0.42
1:2A:2759:G:OP2	61:2A:3938:HOH:O	2.22	0.42
2:2B:50:G:OP1	14:2S:63:THR:OG1	2.35	0.42
6:2G:101:ILE:HG22	6:2G:105:LYS:HE2	2.02	0.42
21:2Z:145:GLU:HB3	21:2Z:148:ASP:HB2	2.01	0.42
32:2a:909:A:H2'	32:2a:910:C:O4'	2.20	0.42
41:2j:32:ALA:HA	41:2j:33:GLN:HA	1.86	0.42
50:2s:51:VAL:O	50:2s:58:VAL:N	2.52	0.42
51:2t:92:LEU:HD12	51:2t:92:LEU:HA	1.84	0.42
1:1A:251:A:C5	1:1A:252:G:H1'	2.54	0.42
1:1A:878:A:H61	1:1A:899:A:C2'	2.32	0.42
1:1A:1506:C:H2'	1:1A:1507:A:C8	2.55	0.42
1:1A:1865:G:N2	1:1A:1877:A:OP2	2.48	0.42
1:1A:2149:G:N1	1:1A:2150:U:O2	2.52	0.42
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	2.01	0.42
21:1Z:126:VAL:HG11	21:1Z:161:VAL:HB	2.02	0.42
32:1a:584:G:H5'	48:1q:91:ARG:NH2	2.34	0.42
32:1a:662:G:H2'	32:1a:663:A:C8	2.55	0.42
41:1j:38:ILE:HD11	41:1j:71:LEU:HD23	2.00	0.42
1:2A:208:C:H2'	1:2A:209:C:C6	2.55	0.42
1:2A:570:G:H2'	1:2A:2030:A:C5	2.54	0.42
1:2A:900:A:H2'	1:2A:901:A:H8	1.85	0.42
1:2A:1270:C:H5''	1:2A:1271:G:O5'	2.20	0.42
3:2D:77:ALA:HB2	3:2D:97:TYR:CD1	2.54	0.42
5:2F:32:LEU:O	5:2F:36:VAL:HG23	2.19	0.42
7:2H:90:LYS:HE3	7:2H:90:LYS:HB2	1.83	0.42
10:2O:63:VAL:HG23	10:2O:64:ARG:HG3	2.01	0.42
32:2a:300:A:H1'	32:2a:565:U:O2	2.20	0.42
32:2a:1265:G:C4	32:2a:1271:G:N2	2.87	0.42
40:2i:65:VAL:HG21	40:2i:73:GLN:HB3	2.01	0.42
54:2y:61:C:H2'	54:2y:62:C:C6	2.55	0.42
1:1A:692:C:O2'	3:1D:38:LYS:NZ	2.46	0.42
1:1A:774:A:N3	1:1A:774:A:H2'	2.34	0.42
1:1A:2441:C:OP2	1:1A:2586:C:O2'	2.34	0.42
6:1G:22:ARG:HH12	6:1G:175:LEU:HD21	1.85	0.42
28:16:11:LEU:HD23	28:16:11:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:219:C:H2'	32:1a:220:G:O4'	2.20	0.42
32:1a:783:C:OP1	32:1a:1515:C:O2'	2.33	0.42
32:1a:1025:U:O2	32:1a:1036:G:C6	2.72	0.42
32:1a:1027:C:H5	32:1a:1028:C:C4	2.38	0.42
32:1a:1134:G:H2'	32:1a:1134:G:N3	2.35	0.42
32:1a:1263:C:H2'	32:1a:1264:C:C6	2.55	0.42
32:1a:1298:C:H4'	32:1a:1299:A:C4	2.55	0.42
32:1a:1367:C:H5'	41:1j:60:ARG:NH1	2.34	0.42
50:1s:66:MET:HB2	50:1s:74:PHE:CZ	2.55	0.42
54:1w:18:G:H4'	54:1w:60:U:C5	2.55	0.42
1:2A:320:A:H4'	1:2A:322:A:N7	2.35	0.42
6:2G:7:LEU:HD13	6:2G:104:GLU:HA	2.01	0.42
9:2N:138:LEU:HD23	9:2N:138:LEU:HA	1.81	0.42
32:2a:730:G:C5	32:2a:731:G:H1'	2.55	0.42
32:2a:735:C:H2'	32:2a:736:C:H6	1.83	0.42
32:2a:955:U:O2'	50:2s:83:HIS:HD2	2.03	0.42
33:2b:187:LEU:HD12	33:2b:214:ILE:HG21	2.02	0.42
39:2h:51:VAL:CG2	39:2h:60:ARG:HB2	2.49	0.42
39:2h:51:VAL:HG11	39:2h:60:ARG:NH1	2.35	0.42
50:2s:37:ARG:O	50:2s:70:LYS:HE3	2.20	0.42
1:1A:884:C:C4	1:1A:885:C:H1'	2.55	0.41
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.31	0.41
1:1A:1622:G:OP2	61:1A:4132:HOH:O	2.21	0.41
1:1A:2233:U:H2'	1:1A:2234:G:C8	2.55	0.41
2:1B:88:C:H2'	2:1B:89:G:O4'	2.19	0.41
11:1P:132:LYS:O	11:1P:136:GLU:HG3	2.20	0.41
13:1R:59:ASP:OD1	13:1R:59:ASP:N	2.45	0.41
19:1X:94:GLY:H	19:1X:95:LEU:C	2.28	0.41
20:1Y:5:MET:HE2	20:1Y:5:MET:HB2	1.77	0.41
21:1Z:158:PRO:O	21:1Z:161:VAL:HG22	2.20	0.41
27:15:8:LYS:O	27:15:9:LYS:HD2	2.20	0.41
32:1a:685:G:C2	32:1a:686:U:C4	3.07	0.41
32:1a:695:A:OP2	42:1k:53:SER:N	2.51	0.41
34:1c:172:ARG:HG3	34:1c:174:PRO:HD3	2.02	0.41
37:1f:100:ASN:HB2	49:1r:28:GLU:HA	2.01	0.41
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.19	0.41
1:2A:363:G:H2'	1:2A:363(A):A:H8	1.84	0.41
1:2A:859:G:N2	1:2A:917:A:OP2	2.43	0.41
1:2A:1181:C:H2'	1:2A:1182:A:C8	2.55	0.41
1:2A:1227:G:OP1	16:2U:13:LYS:HG2	2.20	0.41
1:2A:1287:A:H8	13:2R:104:ARG:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2892:A:H2'	1:2A:2893:G:H5'	2.01	0.41
5:2F:119:ARG:CZ	5:2F:119:ARG:HB3	2.48	0.41
5:2F:126:VAL:HG21	5:2F:129:PHE:CZ	2.55	0.41
6:2G:111:LEU:HD21	6:2G:120:LEU:HD21	2.02	0.41
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.45	0.41
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.20	0.41
26:24:58:ARG:HB2	50:2s:64:GLU:O	2.19	0.41
28:26:10:LEU:HG	28:26:54:ILE:HG13	2.02	0.41
31:29:13:LYS:HD3	31:29:13:LYS:HA	1.87	0.41
32:2a:1126:U:H3	41:2j:40:LEU:HD11	1.84	0.41
39:2h:26:VAL:HG23	39:2h:59:LEU:O	2.19	0.41
40:2i:3:GLN:HG3	40:2i:20:ARG:NE	2.35	0.41
41:2j:11:PHE:CE1	41:2j:67:THR:HG22	2.55	0.41
1:1A:185:U:H2'	1:1A:186:G:C8	2.55	0.41
1:1A:1048:A:N1	1:1A:1112:G:O2'	2.42	0.41
1:1A:1965:C:OP1	1:1A:1966:A:O2'	2.35	0.41
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	2.01	0.41
32:1a:332:G:OP2	51:1t:10:LEU:HD12	2.20	0.41
32:1a:1486:G:H2'	32:1a:1487:G:O4'	2.20	0.41
41:1j:19:SER:OG	41:1j:91:PRO:HD2	2.20	0.41
46:1o:82:ILE:O	46:1o:86:GLY:N	2.53	0.41
1:2A:784:A:N6	3:2D:229:VAL:HG11	2.35	0.41
1:2A:969:U:H2'	1:2A:970:C:C6	2.55	0.41
1:2A:1163:G:OP1	17:2V:24:LYS:NZ	2.34	0.41
1:2A:1671:U:OP2	61:2A:3904:HOH:O	2.21	0.41
1:2A:1837:C:OP1	32:2a:784:C:H4'	2.20	0.41
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.20	0.41
1:2A:2612:C:OP2	27:25:2:ALA:N	2.53	0.41
1:2A:2626:C:H2'	1:2A:2627:G:O4'	2.20	0.41
21:2Z:30:ASN:HA	21:2Z:89:PHE:HE1	1.84	0.41
32:2a:130:A:N3	32:2a:263:A:O2'	2.48	0.41
32:2a:542:G:OP1	35:2d:10:ARG:NH2	2.40	0.41
32:2a:1002:G:H1	32:2a:1038:C:N4	2.17	0.41
36:2e:47:LYS:HB2	36:2e:47:LYS:HE2	1.86	0.41
36:2e:99:GLY:O	36:2e:117:ASP:HA	2.20	0.41
54:2y:36:A:H2'	54:2y:37:MIA:O4'	2.21	0.41
1:1A:271(M):G:O2'	1:1A:271(N):U:H5''	2.21	0.41
1:1A:388:G:O2'	1:1A:389:G:N7	2.49	0.41
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.20	0.41
32:1a:254:G:OP1	48:1q:67:LYS:O	2.39	0.41
32:1a:679:C:H2'	32:1a:680:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1f:33:TYR:OH	37:1f:78:GLU:HG3	2.20	0.41
43:1l:56:ALA:HB2	43:1l:70:ILE:HD11	2.02	0.41
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	2.02	0.41
46:1o:56:LEU:O	46:1o:60:VAL:HG23	2.20	0.41
1:2A:586:A:N1	1:2A:809:G:O2'	2.49	0.41
1:2A:910:A:C5	12:2Q:13:GLN:HG3	2.55	0.41
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.20	0.41
1:2A:1371:G:H2'	1:2A:1372:U:H5	1.84	0.41
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.35	0.41
1:2A:2647:U:H2'	1:2A:2648:C:C6	2.55	0.41
5:2F:10:PRO:HB3	5:2F:17:ARG:CZ	2.51	0.41
6:2G:16:ARG:HB2	6:2G:17:PRO:HD3	2.01	0.41
14:2S:80:LEU:HD12	14:2S:80:LEU:HA	1.89	0.41
21:2Z:23:LYS:HB3	21:2Z:38:TYR:CD1	2.55	0.41
23:21:73:LEU:HD23	23:21:73:LEU:HA	1.80	0.41
32:2a:1316:G:N2	32:2a:1318:A:H3'	2.35	0.41
32:2a:1359:C:H1'	32:2a:1362:C:H41	1.84	0.41
36:2e:76:ILE:O	36:2e:93:PRO:HB3	2.20	0.41
50:2s:62:ILE:HA	50:2s:66:MET:CE	2.50	0.41
54:2y:55:PSU:N1	54:2y:57:G:H5'	2.34	0.41
1:1A:221:A:N1	1:1A:265:A:O2'	2.51	0.41
1:1A:857:C:N4	1:1A:858:U:O4	2.53	0.41
1:1A:1354:A:H2'	1:1A:1355:G:O4'	2.21	0.41
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.86	0.41
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.55	0.41
6:1G:9:ARG:NH1	6:1G:13:GLU:OE2	2.53	0.41
8:1I:77:LEU:HD23	8:1I:77:LEU:HA	1.84	0.41
13:1R:56:LYS:NZ	13:1R:90:ARG:O	2.54	0.41
14:1S:9:ARG:O	14:1S:13:ARG:HB2	2.21	0.41
19:1X:35:THR:HG22	19:1X:38:GLU:H	1.86	0.41
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.84	0.41
21:1Z:151:HIS:HB3	21:1Z:169:GLU:O	2.19	0.41
32:1a:160:A:H2'	32:1a:161:A:O4'	2.20	0.41
32:1a:1053:G:N7	32:1a:1200:C:H5''	2.36	0.41
34:1c:122:GLU:O	34:1c:126:ARG:HD2	2.20	0.41
51:1t:100:ILE:H	51:1t:100:ILE:HG12	1.67	0.41
54:1y:58:A:H4'	54:1y:59:U:OP1	2.21	0.41
1:2A:909:A:C6	1:2A:912:C:C2	3.08	0.41
1:2A:1027:A:C6	1:2A:1126:A:C4	3.09	0.41
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.35	0.41
1:2A:2169:A:H1'	54:2y:56:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2533:A:OP1	1:2A:2665:A:O2'	2.36	0.41
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.56	0.41
2:2B:40:U:C5	26:24:2:LYS:HG3	2.56	0.41
3:2D:29:PRO:HA	3:2D:83:GLU:OE1	2.21	0.41
3:2D:121:PRO:HB3	3:2D:135:PHE:CE2	2.53	0.41
4:2E:112:GLY:O	4:2E:159:HIS:HA	2.20	0.41
8:2I:77:LEU:HD23	8:2I:97:ILE:HG23	2.03	0.41
11:2P:59:LEU:HD11	30:28:10:ALA:HA	2.03	0.41
12:2Q:63:LYS:HD3	12:2Q:65:PHE:CZ	2.56	0.41
15:2T:91:ARG:HB2	15:2T:121:ILE:HG13	2.03	0.41
32:2a:189(D):C:H2'	32:2a:189(E):U:O4'	2.20	0.41
32:2a:473:G:H2'	32:2a:474:G:H8	1.85	0.41
32:2a:1047:G:H5''	45:2n:4:LYS:HD3	2.02	0.41
32:2a:1049:U:OP1	45:2n:3:ARG:HB3	2.21	0.41
34:2c:136:GLN:O	34:2c:140:ARG:HG3	2.20	0.41
35:2d:19:LEU:O	35:2d:21:LEU:N	2.53	0.41
36:2e:146:ALA:O	36:2e:150:ARG:HG2	2.21	0.41
55:2x:61:C:H2'	55:2x:62:C:C6	2.56	0.41
1:1A:207:A:H2'	1:1A:208:C:O4'	2.19	0.41
1:1A:876:C:H2'	1:1A:877:U:O4'	2.20	0.41
1:1A:1512:U:H2'	1:1A:1513:C:C6	2.55	0.41
3:1D:35:LYS:HB2	3:1D:36:PRO:HD2	2.02	0.41
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	2.01	0.41
32:1a:160:A:H1'	32:1a:344:A:C5	2.56	0.41
32:1a:620:C:H2'	32:1a:621:A:O4'	2.20	0.41
32:1a:922:G:C6	32:1a:923:A:C6	3.09	0.41
32:1a:1401:G:C2	32:1a:1402:4OC:H1'	2.55	0.41
35:1d:122:ARG:HA	35:1d:122:ARG:HD2	1.74	0.41
40:1i:55:ALA:HB1	40:1i:58:HIS:HB2	2.03	0.41
1:2A:242:G:C8	30:28:5:LYS:HG2	2.55	0.41
1:2A:263:C:H2'	1:2A:264:C:O4'	2.20	0.41
1:2A:514:A:N3	1:2A:581:C:O2'	2.52	0.41
1:2A:686:G:N2	1:2A:788:A:H61	2.19	0.41
1:2A:784:A:C8	1:2A:792:G:C5	3.09	0.41
1:2A:1263:U:C4	1:2A:1264:G:C6	3.08	0.41
1:2A:1647:G:H3'	1:2A:1647:G:OP2	2.19	0.41
1:2A:2151:G:H2'	1:2A:2152:G:H8	1.85	0.41
2:2B:2:C:H2'	2:2B:3:C:C6	2.56	0.41
3:2D:16:MET:HE3	3:2D:16:MET:HB2	1.85	0.41
6:2G:45:GLU:H	6:2G:45:GLU:HG2	1.43	0.41
21:2Z:130:PRO:O	21:2Z:133:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:397:A:H3'	32:2a:397:A:N3	2.35	0.41
32:2a:435:C:H2'	32:2a:436:C:H6	1.85	0.41
32:2a:1427:U:H2'	32:2a:1428:A:C8	2.55	0.41
38:2g:151:TYR:OH	42:2k:54:ARG:NH1	2.51	0.41
39:2h:51:VAL:HG12	39:2h:52:ASP:N	2.35	0.41
47:2p:48:TRP:HH2	47:2p:76:GLN:HE22	1.67	0.41
49:2r:35:ARG:O	49:2r:37:VAL:N	2.54	0.41
50:2s:41:VAL:HG22	50:2s:42:PRO:HD2	2.03	0.41
51:2t:79:ARG:O	51:2t:83:ARG:HG3	2.21	0.41
1:1A:883:G:N2	1:1A:893:C:H42	2.18	0.41
1:1A:1371:G:O6	61:1A:4134:HOH:O	2.22	0.41
1:1A:1453:U:O2'	1:1A:1455:G:N7	2.48	0.41
1:1A:2038:G:H2'	1:1A:2039:C:O4'	2.21	0.41
1:1A:2107:C:N4	1:1A:2182:G:H1	2.18	0.41
6:1G:18:GLU:OE2	6:1G:21:ARG:NH1	2.53	0.41
6:1G:110:ALA:HA	6:1G:140:ILE:O	2.21	0.41
11:1P:95:VAL:HG22	11:1P:125:VAL:HG12	2.03	0.41
21:1Z:131:ARG:H	21:1Z:131:ARG:HG2	1.55	0.41
23:11:64:ALA:HA	23:11:67:ILE:HG13	2.02	0.41
32:1a:277:C:P	48:1q:68:ARG:HH12	2.44	0.41
32:1a:297:G:H4'	32:1a:557:G:H4'	2.03	0.41
32:1a:1318:A:H5''	50:1s:3:ARG:NH1	2.35	0.41
39:1h:73:ASP:OD1	39:1h:75:ARG:NE	2.53	0.41
42:1k:48:ILE:O	42:1k:50:TYR:N	2.44	0.41
43:1l:32:PHE:HB3	43:1l:84:LEU:HD11	2.02	0.41
1:2A:64:A:O3'	19:2X:71:GLY:HA3	2.21	0.41
1:2A:141:A:H8	1:2A:1408:C:O2'	2.04	0.41
1:2A:1752:C:H2'	1:2A:1753:G:C8	2.55	0.41
1:2A:1913:A:H4'	1:2A:1914:C:O5'	2.20	0.41
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.56	0.41
1:2A:2846:G:H2'	1:2A:2847:U:O4'	2.20	0.41
7:2H:7:LEU:HD23	7:2H:69:ARG:NH2	2.36	0.41
16:2U:16:LYS:HB3	16:2U:16:LYS:HE2	1.84	0.41
25:23:4:LEU:HD23	25:23:4:LEU:HA	1.91	0.41
32:2a:19:C:H5''	36:2e:86:ALA:HB3	2.03	0.41
32:2a:157:G:H2'	32:2a:158:G:H8	1.86	0.41
32:2a:993:G:N3	32:2a:993:G:H2'	2.35	0.41
32:2a:1320:C:N3	50:2s:36:ARG:NH2	2.68	0.41
35:2d:191:ARG:HA	35:2d:191:ARG:HD2	1.95	0.41
36:2e:7:GLU:O	36:2e:34:VAL:HA	2.21	0.41
42:2k:77:MET:HE2	42:2k:77:MET:HB2	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:14:A:H61	54:2w:21:A:H2	1.67	0.41
1:1A:218:A:C2	1:1A:235:U:H4'	2.55	0.41
1:1A:1108:U:H2'	1:1A:1109:C:O4'	2.21	0.41
1:1A:1364:G:P	23:11:3:LYS:HG3	2.59	0.41
1:1A:1508:A:H4'	1:1A:1509(A):A:C5	2.56	0.41
1:1A:1557:C:H5''	1:1A:1558:A:OP2	2.20	0.41
1:1A:2389:G:H5''	1:1A:2390:U:O4'	2.21	0.41
1:1A:2801(A):A:N3	1:1A:2895:U:H1'	2.36	0.41
7:1H:11:VAL:HG21	7:1H:50:VAL:HG23	2.03	0.41
32:1a:35:G:O2'	43:1l:118:SER:O	2.26	0.41
32:1a:130:A:O2'	32:1a:131:C:O5'	2.35	0.41
32:1a:433:C:H2'	32:1a:434:U:H6	1.85	0.41
32:1a:562:C:O2	43:1l:16:GLU:N	2.50	0.41
32:1a:567:G:H2'	32:1a:568:G:O4'	2.20	0.41
32:1a:1348:U:H4'	40:1i:120:ARG:HD2	2.03	0.41
33:1b:95:GLN:HE22	33:1b:147:LYS:HG3	1.85	0.41
41:1j:85:LEU:HD23	41:1j:85:LEU:HA	1.86	0.41
44:1m:22:ILE:HB	44:1m:25:ILE:HD12	2.02	0.41
51:1t:62:LEU:HD23	51:1t:62:LEU:HA	1.93	0.41
1:2A:271(L):U:H5'	8:2I:50:ARG:NH1	2.35	0.41
1:2A:608:A:H2'	1:2A:609:A:C8	2.56	0.41
1:2A:760:G:H2'	1:2A:761:A:O4'	2.20	0.41
1:2A:813:U:H2'	1:2A:814:C:C6	2.56	0.41
1:2A:1810:A:H2'	1:2A:1811:G:O4'	2.20	0.41
1:2A:2299:G:H2'	1:2A:2300:G:H8	1.86	0.41
1:2A:2364:C:H4'	22:20:56:ASP:OD1	2.20	0.41
1:2A:2563:U:O2'	10:2O:28:SER:HB2	2.19	0.41
1:2A:2684:U:H1'	10:2O:70:LYS:HD2	2.02	0.41
1:2A:2751:G:H5'	7:2H:2:SER:HA	2.02	0.41
1:2A:2788:C:O2'	1:2A:2809:A:N3	2.52	0.41
2:2B:17:C:H2'	2:2B:18:G:O4'	2.21	0.41
2:2B:48:A:P	14:2S:30:ARG:HH22	2.44	0.41
11:2P:101:VAL:HA	11:2P:106:LEU:O	2.21	0.41
14:2S:15:ARG:HB3	14:2S:19:LYS:NZ	2.35	0.41
23:21:23:LYS:HB3	23:21:29:GLY:HA3	2.02	0.41
25:23:59:VAL:HG12	25:23:60:GLU:H	1.85	0.41
32:2a:532:A:N6	32:2a:1206:G:O2'	2.54	0.41
32:2a:582:U:C2	32:2a:760:G:C6	3.09	0.41
32:2a:1150:U:H4'	41:2j:41:PRO:HG3	2.03	0.41
35:2d:134:ASP:OD1	35:2d:134:ASP:N	2.51	0.41
39:2h:51:VAL:HG21	39:2h:60:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2k:17:GLY:O	42:2k:80:VAL:HA	2.20	0.41
1:1A:863:A:OP1	12:1Q:22:LYS:HG3	2.21	0.41
1:1A:1010:A:N3	1:1A:1153:C:H1'	2.36	0.41
1:1A:2654:A:N1	1:1A:2665:A:H5''	2.36	0.41
1:1A:2695:C:H2'	1:1A:2696:U:C6	2.56	0.41
6:1G:135:LEU:HD13	6:1G:140:ILE:HD11	2.02	0.41
7:1H:101:ARG:HH22	7:1H:122:THR:HA	1.86	0.41
13:1R:10:LEU:HD23	13:1R:10:LEU:HA	1.86	0.41
28:16:38:LYS:HB3	28:16:38:LYS:HE3	1.83	0.41
32:1a:216:G:H2'	32:1a:217:C:C6	2.56	0.41
32:1a:935:A:C2	32:1a:936:C:C2	3.09	0.41
32:1a:1262:C:H2'	32:1a:1263:C:C6	2.56	0.41
32:1a:1456:G:O6	51:1t:54:LYS:NZ	2.42	0.41
35:1d:53:ASP:O	35:1d:57:ARG:HG3	2.21	0.41
35:1d:86:LYS:HE2	35:1d:86:LYS:HB3	1.96	0.41
39:1h:64:LYS:HG2	39:1h:79:VAL:HG21	2.02	0.41
49:1r:35:ARG:O	49:1r:37:VAL:N	2.54	0.41
1:2A:580:C:H2'	1:2A:581:C:C6	2.56	0.41
1:2A:581:C:H2'	1:2A:582:G:C8	2.55	0.41
1:2A:652(B):A:N6	1:2A:655:A:O2'	2.43	0.41
1:2A:937:U:H2'	1:2A:938:G:O4'	2.20	0.41
1:2A:1321:A:H2'	1:2A:1322:A:O4'	2.21	0.41
1:2A:1857:G:C6	1:2A:1858:G:C6	3.09	0.41
1:2A:2126:A:N3	1:2A:2127:G:H1'	2.36	0.41
1:2A:2130:U:H4'	1:2A:2133:G:H4'	2.01	0.41
1:2A:2788:C:N4	1:2A:2789:C:H41	2.19	0.41
5:2F:53:THR:HG22	5:2F:56:GLU:HG3	2.03	0.41
32:2a:164:U:H2'	32:2a:165:C:H6	1.86	0.41
32:2a:1049:U:C6	32:2a:1201:A:H5'	2.56	0.41
33:2b:93:VAL:HG11	33:2b:97:TRP:HE3	1.86	0.41
35:2d:61:LYS:HD2	35:2d:207:TYR:OH	2.21	0.41
39:2h:51:VAL:HG11	39:2h:60:ARG:HH12	1.86	0.41
1:1A:271(I):G:H2'	1:1A:271(J):C:C6	2.56	0.41
1:1A:1065:U:H5''	1:1A:1066:U:OP2	2.21	0.41
1:1A:1164:G:H2'	1:1A:1165:U:C6	2.56	0.41
1:1A:1750:G:O2'	1:1A:2860:A:N1	2.42	0.41
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.36	0.41
1:1A:2116:G:H2'	1:1A:2117:A:C5	2.56	0.41
1:1A:2224:G:H4'	1:1A:2226:C:C2	2.56	0.41
1:1A:2572:A:C8	4:1E:144:ARG:HD3	2.55	0.41
5:1F:165:ARG:HA	5:1F:168:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:47:LEU:O	8:1I:51:ILE:HG13	2.21	0.41
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	2.03	0.41
19:1X:12:VAL:HG21	19:1X:27:THR:HG22	2.03	0.41
24:12:1:MET:HE3	24:12:5:GLU:HB3	2.03	0.41
32:1a:688:G:H2'	32:1a:689:C:H6	1.86	0.41
32:1a:694:A:OP1	42:1k:53:SER:OG	2.32	0.41
32:1a:1146:A:H2'	32:1a:1147:C:O4'	2.20	0.41
33:1b:188:ALA:HB1	33:1b:192:SER:OG	2.21	0.41
34:1c:16:ARG:NH1	34:1c:183:ASP:OD1	2.53	0.41
39:1h:40:ALA:HA	39:1h:45:ILE:HG13	2.03	0.41
54:1w:8:4SU:O5'	54:1w:8:4SU:H6	2.21	0.41
1:2A:236:C:H2'	1:2A:237:C:C6	2.56	0.41
1:2A:445:C:OP1	16:2U:2:PRO:HA	2.21	0.41
1:2A:945:A:C4	1:2A:2448:A:C2	3.09	0.41
1:2A:1037:G:H2'	1:2A:1038:C:O4'	2.21	0.41
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.56	0.41
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.56	0.41
1:2A:1668:A:H4'	1:2A:1669:A:O5'	2.20	0.41
1:2A:2006:C:O2'	1:2A:2823:A:N3	2.50	0.41
1:2A:2112:G:H2'	1:2A:2113:U:O4'	2.21	0.41
1:2A:2151:G:H2'	1:2A:2152:G:C8	2.55	0.41
1:2A:2540:C:O2'	1:2A:2740:A:N3	2.51	0.41
2:2B:8:U:O2'	14:2S:40:ILE:HD13	2.20	0.41
3:2D:34:VAL:HA	3:2D:62:TYR:O	2.21	0.41
6:2G:114:ILE:HB	6:2G:117:PHE:HD1	1.86	0.41
8:2I:82:ARG:HH12	8:2I:90:GLY:H	1.68	0.41
8:2I:102:SER:OG	8:2I:103:ARG:N	2.54	0.41
10:2O:26:LYS:O	10:2O:30:ALA:HB2	2.20	0.41
19:2X:5:TYR:HD1	24:22:33:MET:HE2	1.86	0.41
19:2X:40:LYS:HG3	19:2X:51:VAL:HB	2.02	0.41
24:22:17:SER:N	24:22:20:GLU:OE1	2.37	0.41
25:23:46:ASN:O	25:23:50:VAL:HG22	2.20	0.41
32:2a:298:A:H2'	32:2a:299:G:O4'	2.21	0.41
32:2a:1057:G:C4	32:2a:1204:A:C2	3.09	0.41
32:2a:1273:G:H3'	32:2a:1274:G:H8	1.85	0.41
32:2a:1355:G:H2'	32:2a:1356:G:C8	2.56	0.41
32:2a:1431:C:H2'	32:2a:1432:G:O4'	2.20	0.41
34:2c:6:HIS:HB3	45:2n:49:HIS:CD2	2.56	0.41
41:2j:29:ARG:H	41:2j:29:ARG:HG2	1.71	0.41
41:2j:50:ILE:HB	45:2n:41:ARG:NH1	2.36	0.41
41:2j:81:THR:C	41:2j:83:GLU:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2k:59:TYR:O	42:2k:62:GLN:HB3	2.21	0.41
43:2l:39:VAL:HG11	43:2l:41:ARG:HH11	1.85	0.41
45:2n:42:ILE:O	45:2n:46:GLU:HG3	2.21	0.41
1:1A:534:U:H2'	1:1A:535:C:C6	2.56	0.41
1:1A:548:A:H1'	1:1A:549:G:OP1	2.20	0.41
1:1A:784:A:C8	1:1A:792:G:C5	3.09	0.41
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.36	0.41
1:1A:2143:C:H2'	1:1A:2144:U:O4'	2.20	0.41
22:10:43:THR:OG1	22:10:46:LYS:HG2	2.20	0.41
32:1a:737:A:H2'	32:1a:738:C:C6	2.56	0.41
32:1a:1003:G:C4	32:1a:1004:A:H2	2.39	0.41
32:1a:1326:C:H5''	52:1u:12:LYS:HE3	2.03	0.41
37:1f:10:LEU:HD21	37:1f:61:LEU:HD22	2.03	0.41
38:1g:69:VAL:HG21	38:1g:104:LEU:HD22	2.02	0.41
49:1r:58:LEU:HB3	49:1r:62:GLU:HB2	2.04	0.41
54:1y:9:A:H4'	54:1y:46:G7M:OP2	2.19	0.41
1:2A:300:A:P	20:2Y:86:ARG:HH12	2.43	0.41
1:2A:478:A:N1	1:2A:500:G:H4'	2.36	0.41
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.86	0.41
9:2N:71:ILE:CG2	9:2N:84:LYS:HB3	2.51	0.41
32:2a:1035:A:HO2'	32:2a:1036:G:H8	1.69	0.41
32:2a:1360:A:OP2	45:2n:35:ARG:NH2	2.54	0.41
32:2a:1368:G:OP1	40:2i:111:ARG:NH2	2.54	0.41
34:2c:109:PRO:C	34:2c:111:LEU:H	2.29	0.41
41:2j:33:GLN:O	41:2j:75:ILE:N	2.40	0.41
43:2l:77:LEU:HD21	43:2l:107:ALA:HA	2.03	0.41
50:2s:80:TYR:C	50:2s:82:GLY:H	2.28	0.41
1:1A:1054:A:C6	1:1A:1055:G:C6	3.10	0.40
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.21	0.40
1:1A:2591:C:H2'	1:1A:2592:G:H8	1.86	0.40
5:1F:28:ILE:O	5:1F:30:PRO:HD3	2.21	0.40
10:1O:66:LYS:HA	10:1O:79:PHE:O	2.22	0.40
16:1U:104:GLN:HE21	16:1U:105:VAL:HG23	1.86	0.40
53:1v:14:A:H3'	53:1v:15:A:H8	1.87	0.40
1:2A:893:C:H5'	1:2A:894:C:C5	2.56	0.40
1:2A:1297:C:OP1	1:2A:2710:C:H4'	2.21	0.40
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.56	0.40
1:2A:1607:C:H4'	1:2A:1608:A:O5'	2.20	0.40
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	2.03	0.40
2:2B:20:C:N4	2:2B:63:G:H1	2.19	0.40
6:2G:170:ARG:NH2	6:2G:182:LYS:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:15:ARG:O	14:2S:19:LYS:HG3	2.21	0.40
27:25:20:ARG:HG2	27:25:23:HIS:ND1	2.36	0.40
32:2a:255:G:C6	32:2a:256:U:C4	3.09	0.40
32:2a:1151:A:O4'	41:2j:39:PRO:HB2	2.20	0.40
32:2a:1446:U:H2'	32:2a:1452:C:C5	2.56	0.40
36:2e:24:ARG:H	36:2e:24:ARG:HG2	1.63	0.40
38:2g:28:ASN:HD21	38:2g:36:LYS:NZ	2.19	0.40
38:2g:113:GLU:O	38:2g:119:ARG:HD3	2.20	0.40
43:2l:53:ARG:HG3	43:2l:93:LEU:HD21	2.04	0.40
54:2w:34:G:H2'	54:2w:35:A:C8	2.56	0.40
54:2y:14:A:N3	54:2y:14:A:H2'	2.35	0.40
1:1A:286:C:H2'	1:1A:287:C:H6	1.86	0.40
1:1A:414:C:H2'	1:1A:415:A:C8	2.56	0.40
1:1A:760:G:H2'	1:1A:761:A:O4'	2.22	0.40
1:1A:768:G:O2'	1:1A:1379:A:N1	2.51	0.40
1:1A:819:A:C4	1:1A:1189:A:C2	3.09	0.40
1:1A:1041:C:N4	1:1A:1114:G:H1	2.16	0.40
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.57	0.40
13:1R:87:TYR:OH	13:1R:116:LEU:HB3	2.21	0.40
32:1a:328:C:H4'	32:1a:329:A:H5'	2.03	0.40
32:1a:942:G:C2	32:1a:1342:C:C2	3.09	0.40
32:1a:1369:C:H2'	32:1a:1370:G:C8	2.56	0.40
1:2A:309:G:N3	1:2A:329:G:O2'	2.50	0.40
1:2A:829:A:N7	1:2A:2247:A:O2'	2.51	0.40
1:2A:1001:A:H2'	1:2A:1002:G:O4'	2.22	0.40
1:2A:1408:C:H2'	1:2A:1409:C:C6	2.56	0.40
1:2A:1866:C:H2'	1:2A:1876:A:O4'	2.20	0.40
1:2A:2064:C:H2'	1:2A:2065:C:C6	2.56	0.40
1:2A:2135:A:N7	1:2A:2136:C:H5	2.18	0.40
1:2A:2305:A:H2'	1:2A:2306:C:O4'	2.21	0.40
5:2F:116:ASP:O	5:2F:120:GLU:HG2	2.21	0.40
5:2F:137:LYS:H	5:2F:137:LYS:HG2	1.74	0.40
11:2P:95:VAL:HA	11:2P:99:LEU:HD22	2.02	0.40
21:2Z:19:ARG:HD3	21:2Z:84:GLU:HA	2.03	0.40
32:2a:923:A:OP1	36:2e:21:ALA:HB2	2.21	0.40
32:2a:1291:G:C6	32:2a:1292:U:C4	3.09	0.40
39:2h:93:VAL:O	39:2h:132:GLU:HA	2.21	0.40
54:2y:9:A:O2'	54:2y:11:C:N4	2.40	0.40
54:2y:40:C:H2'	54:2y:41:C:C6	2.56	0.40
1:1A:274:G:H2'	1:1A:275:G:C8	2.55	0.40
1:1A:2283:C:H2'	1:1A:2284:C:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:54:GLN:HB2	4:1E:76:ARG:HG2	2.03	0.40
8:1I:6:LEU:O	8:1I:7:GLU:HG3	2.22	0.40
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.57	0.40
29:17:41:ARG:HG2	61:17:202:HOH:O	2.21	0.40
32:1a:358:U:H2'	32:1a:359:U:C6	2.56	0.40
34:1c:16:ARG:HE	34:1c:16:ARG:HB3	1.75	0.40
43:1l:57:LYS:NZ	43:1l:65:GLU:OE2	2.53	0.40
1:2A:41:C:H2'	1:2A:42:G:H8	1.87	0.40
1:2A:1220:A:OP2	16:2U:19:LYS:NZ	2.39	0.40
1:2A:1325:G:OP1	1:2A:1647:G:O2'	2.17	0.40
1:2A:2394:C:N3	54:2y:76:A:O2'	2.49	0.40
1:2A:2406:U:C2	11:2P:72:PRO:HG2	2.56	0.40
2:2B:94:C:H2'	2:2B:95:C:C6	2.57	0.40
5:2F:118:ALA:HB2	5:2F:123:LEU:HD23	2.02	0.40
7:2H:90:LYS:HD2	7:2H:159:GLU:HG2	2.03	0.40
8:2I:82:ARG:NH1	8:2I:82:ARG:O	2.42	0.40
32:2a:1049:U:C5	32:2a:1201:A:H5'	2.56	0.40
32:2a:1273:G:C6	32:2a:1274:G:C4	3.09	0.40
36:2e:41:VAL:CG2	36:2e:69:VAL:HG21	2.51	0.40
38:2g:79:ARG:HH21	38:2g:80:VAL:HA	1.87	0.40
48:2q:89:LEU:HA	48:2q:89:LEU:HD23	1.85	0.40
1:1A:213:A:H2'	1:1A:214:G:O4'	2.21	0.40
2:1B:28:C:OP1	14:1S:36:TYR:OH	2.35	0.40
13:1R:1:MET:HE3	13:1R:1:MET:HB2	1.93	0.40
32:1a:129(A):G:C6	32:1a:189(E):U:H4'	2.57	0.40
32:1a:381:C:H2'	32:1a:382:A:O4'	2.21	0.40
32:1a:435:C:H2'	32:1a:436:C:H6	1.87	0.40
32:1a:666:G:H5'	32:1a:726:C:H1'	2.03	0.40
32:1a:964:A:N3	32:1a:969:A:O2'	2.43	0.40
32:1a:1036:G:H5''	32:1a:1037:C:H5	1.83	0.40
36:1e:8:GLU:HG3	36:1e:34:VAL:HG23	2.03	0.40
39:1h:49:GLU:O	39:1h:51:VAL:HG23	2.21	0.40
41:1j:38:ILE:CG1	41:1j:71:LEU:HB3	2.52	0.40
47:1p:47:ASP:OD1	47:1p:47:ASP:N	2.48	0.40
47:1p:74:LEU:HG	47:1p:79:VAL:HG21	2.03	0.40
54:1w:52:G:H2'	54:1w:53:G:O4'	2.21	0.40
54:1y:32:PSU:N3	54:1y:33:U:H5	2.20	0.40
1:2A:500:G:N1	1:2A:503:A:OP2	2.54	0.40
1:2A:844:C:C5	1:2A:845:G:C6	3.09	0.40
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.57	0.40
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:29:15:LYS:HB3	31:29:26:ILE:HG13	2.02	0.40
32:2a:451:A:N6	32:2a:480:U:H2'	2.36	0.40
32:2a:573:A:N3	32:2a:883:C:O2'	2.47	0.40
32:2a:1095:U:H5''	32:2a:1109:C:O2	2.21	0.40
32:2a:1106:G:H4'	34:2c:171:GLY:O	2.22	0.40
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.56	0.40
34:2c:151:VAL:HG23	34:2c:199:LYS:O	2.22	0.40
34:2c:195:VAL:C	34:2c:196:LEU:HD23	2.47	0.40
44:2m:56:LEU:O	44:2m:60:VAL:HG12	2.20	0.40
1:1A:817:C:H4'	1:1A:932:G:C5	2.56	0.40
1:1A:1087:G:H1	1:1A:1102:C:N4	2.19	0.40
1:1A:1902:C:H5'	3:1D:246:PRO:HD3	2.04	0.40
1:1A:2305:A:H5''	6:1G:134:GLY:HA3	2.03	0.40
4:1E:181:LEU:HD12	4:1E:181:LEU:HA	1.82	0.40
21:1Z:46:LYS:HE2	21:1Z:46:LYS:HB3	1.89	0.40
32:1a:524:G:H2'	32:1a:525:C:C6	2.57	0.40
32:1a:1346:A:N1	32:1a:1374:A:H5''	2.36	0.40
35:1d:101:LEU:HB2	35:1d:138:TYR:HB3	2.02	0.40
47:1p:4:ILE:HA	47:1p:20:VAL:O	2.22	0.40
48:1q:45:HIS:O	48:1q:73:VAL:HG23	2.21	0.40
1:2A:569:U:C4	1:2A:570:G:C6	3.10	0.40
1:2A:1759:A:H1'	1:2A:2711:A:C2	2.56	0.40
9:2N:102:ALA:O	9:2N:106:MET:HG3	2.22	0.40
12:2Q:110:THR:HG23	12:2Q:113:GLN:HB2	2.03	0.40
32:2a:628:G:H2'	32:2a:629:G:C8	2.57	0.40
32:2a:736:C:H2'	32:2a:737:A:C8	2.57	0.40
32:2a:1060:C:H5''	41:2j:51:ARG:HB3	2.03	0.40
33:2b:168:THR:HG21	33:2b:191:ASP:O	2.21	0.40
40:2i:3:GLN:HE21	40:2i:20:ARG:NH2	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

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%)	199 (93%)	16 (7%)	13	17
3	2D	215/218 (99%)	205 (95%)	10 (5%)	23	36
4	1E	164/166 (99%)	159 (97%)	5 (3%)	36	53
4	2E	164/166 (99%)	159 (97%)	5 (3%)	36	53
5	1F	160/166 (96%)	146 (91%)	14 (9%)	9	12
5	2F	159/166 (96%)	151 (95%)	8 (5%)	22	33
6	1G	143/156 (92%)	128 (90%)	15 (10%)	6	8
6	2G	143/156 (92%)	126 (88%)	17 (12%)	5	5
7	1H	144/148 (97%)	133 (92%)	11 (8%)	12	17
7	2H	144/148 (97%)	128 (89%)	16 (11%)	6	6
8	1I	113/124 (91%)	99 (88%)	14 (12%)	4	4
8	2I	105/124 (85%)	93 (89%)	12 (11%)	5	6
9	1N	118/119 (99%)	107 (91%)	11 (9%)	8	10
9	2N	118/119 (99%)	111 (94%)	7 (6%)	18	27
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28	42
10	2O	100/100 (100%)	93 (93%)	7 (7%)	14	19
11	1P	115/116 (99%)	106 (92%)	9 (8%)	11	16
11	2P	115/116 (99%)	108 (94%)	7 (6%)	17	25
12	1Q	111/111 (100%)	106 (96%)	5 (4%)	24	38
12	2Q	111/111 (100%)	108 (97%)	3 (3%)	39	58
13	1R	101/101 (100%)	98 (97%)	3 (3%)	36	53
13	2R	101/101 (100%)	99 (98%)	2 (2%)	48	67
14	1S	86/88 (98%)	77 (90%)	9 (10%)	6	8
14	2S	85/88 (97%)	77 (91%)	8 (9%)	8	10
15	1T	115/127 (91%)	108 (94%)	7 (6%)	17	25
15	2T	113/127 (89%)	107 (95%)	6 (5%)	20	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	91 (98%)	2 (2%)	45	64
16	2U	93/94 (99%)	88 (95%)	5 (5%)	20	30
17	1V	80/82 (98%)	78 (98%)	2 (2%)	42	60
17	2V	80/82 (98%)	75 (94%)	5 (6%)	16	23
18	1W	90/92 (98%)	88 (98%)	2 (2%)	45	64
18	2W	90/92 (98%)	86 (96%)	4 (4%)	25	38
19	1X	77/78 (99%)	76 (99%)	1 (1%)	61	76
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28	43
20	1Y	85/91 (93%)	79 (93%)	6 (7%)	13	19
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	13	19
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11	15
21	2Z	137/179 (76%)	123 (90%)	14 (10%)	7	8
22	10	61/67 (91%)	60 (98%)	1 (2%)	55	73
22	20	65/67 (97%)	64 (98%)	1 (2%)	57	74
23	11	80/83 (96%)	78 (98%)	2 (2%)	42	60
23	21	80/83 (96%)	78 (98%)	2 (2%)	42	60
24	12	65/67 (97%)	63 (97%)	2 (3%)	35	53
24	22	65/67 (97%)	63 (97%)	2 (3%)	35	53
25	13	51/52 (98%)	47 (92%)	4 (8%)	11	16
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	15
26	14	59/63 (94%)	50 (85%)	9 (15%)	3	2
26	24	53/63 (84%)	46 (87%)	7 (13%)	4	4
27	15	50/52 (96%)	48 (96%)	2 (4%)	28	42
27	25	50/52 (96%)	45 (90%)	5 (10%)	7	9
28	16	51/52 (98%)	49 (96%)	2 (4%)	28	43
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	9
29	17	41/42 (98%)	37 (90%)	4 (10%)	7	9
29	27	41/42 (98%)	38 (93%)	3 (7%)	13	18
30	18	54/55 (98%)	52 (96%)	2 (4%)	30	45
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	45
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	164 (85%)	28 (15%)	3	2
33	2b	187/220 (85%)	153 (82%)	34 (18%)	2	1
34	1c	142/188 (76%)	132 (93%)	10 (7%)	14	19
34	2c	140/188 (74%)	124 (89%)	16 (11%)	5	6
35	1d	169/181 (93%)	157 (93%)	12 (7%)	13	19
35	2d	173/181 (96%)	161 (93%)	12 (7%)	14	20
36	1e	113/123 (92%)	106 (94%)	7 (6%)	16	24
36	2e	114/123 (93%)	106 (93%)	8 (7%)	14	19
37	1f	84/90 (93%)	75 (89%)	9 (11%)	6	7
37	2f	85/90 (94%)	80 (94%)	5 (6%)	18	27
38	1g	119/127 (94%)	107 (90%)	12 (10%)	7	8
38	2g	120/127 (94%)	114 (95%)	6 (5%)	22	33
39	1h	114/119 (96%)	111 (97%)	3 (3%)	40	59
39	2h	114/119 (96%)	107 (94%)	7 (6%)	17	25
40	1i	90/99 (91%)	83 (92%)	7 (8%)	11	16
40	2i	89/99 (90%)	77 (86%)	12 (14%)	4	3
41	1j	66/92 (72%)	60 (91%)	6 (9%)	9	11
41	2j	69/92 (75%)	60 (87%)	9 (13%)	4	4
42	1k	82/99 (83%)	78 (95%)	4 (5%)	22	34
42	2k	83/99 (84%)	78 (94%)	5 (6%)	17	26
43	1l	96/108 (89%)	91 (95%)	5 (5%)	21	32
43	2l	96/108 (89%)	90 (94%)	6 (6%)	16	23
44	1m	93/101 (92%)	83 (89%)	10 (11%)	6	7
44	2m	92/101 (91%)	81 (88%)	11 (12%)	5	5
45	1n	49/50 (98%)	45 (92%)	4 (8%)	10	14
45	2n	49/50 (98%)	45 (92%)	4 (8%)	10	14
46	1o	78/80 (98%)	73 (94%)	5 (6%)	16	23
46	2o	78/80 (98%)	75 (96%)	3 (4%)	29	44
47	1p	69/74 (93%)	60 (87%)	9 (13%)	4	4
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	85 (90%)	9 (10%)	8	9
48	2q	94/97 (97%)	90 (96%)	4 (4%)	26	39
49	1r	59/77 (77%)	55 (93%)	4 (7%)	14	20
49	2r	59/77 (77%)	52 (88%)	7 (12%)	5	5
50	1s	69/80 (86%)	63 (91%)	6 (9%)	9	13
50	2s	67/80 (84%)	61 (91%)	6 (9%)	9	11
51	1t	70/82 (85%)	64 (91%)	6 (9%)	10	13
51	2t	70/82 (85%)	65 (93%)	5 (7%)	13	19
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9299/10064 (92%)	8624 (93%)	675 (7%)	13	18

All (675) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	14	ARG
3	1D	32	SER
3	1D	37	LEU
3	1D	38	LYS
3	1D	71	ASP
3	1D	89	SER
3	1D	106	ILE
3	1D	142	VAL
3	1D	173	VAL
3	1D	204	ILE
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	270	ILE
3	1D	273	ARG
4	1E	59	VAL
4	1E	73	GLU
4	1E	116	VAL
4	1E	181	LEU
4	1E	184	VAL
5	1F	9	ILE
5	1F	24	LEU

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Mol	Chain	Res	Type
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	106	ARG
5	1F	108	LYS
5	1F	132	VAL
5	1F	140	LEU
5	1F	162	LEU
5	1F	168	ARG
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	3	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	22	ARG
6	1G	28	VAL
6	1G	31	VAL
6	1G	43	LEU
6	1G	47	LYS
6	1G	60	LEU
6	1G	82	LEU
6	1G	126	ASP
6	1G	140	ILE
6	1G	148	MET
6	1G	150	ASP
6	1G	159	VAL
7	1H	3	ARG
7	1H	13	LYS
7	1H	15	VAL
7	1H	24	VAL
7	1H	49	VAL
7	1H	56	SER
7	1H	84	SER
7	1H	92	ILE
7	1H	95	ARG
7	1H	124	GLU
7	1H	127	GLU
8	1I	9	LEU
8	1I	12	LEU
8	1I	20	ASP
8	1I	38	LEU

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Mol	Chain	Res	Type
8	1I	47	LEU
8	1I	61	ARG
8	1I	77	LEU
8	1I	92	VAL
8	1I	101	LEU
8	1I	108	THR
8	1I	129	THR
8	1I	133	HIS
8	1I	140	LEU
8	1I	144	VAL
9	1N	1	MET
9	1N	8	GLN
9	1N	10	GLU
9	1N	14	VAL
9	1N	28	THR
9	1N	61	ARG
9	1N	62	VAL
9	1N	65	LYS
9	1N	96	GLU
9	1N	134	ARG
9	1N	137	LYS
10	1O	52	VAL
10	1O	66	LYS
10	1O	113	LYS
10	1O	116	SER
11	1P	1	MET
11	1P	45	LEU
11	1P	75	ILE
11	1P	95	VAL
11	1P	98	GLU
11	1P	126	VAL
11	1P	147	LEU
11	1P	148	LEU
11	1P	149	GLU
12	1Q	8	LYS
12	1Q	56	ARG
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	110	THR
13	1R	36	THR
13	1R	99	LYS
13	1R	114	VAL

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Mol	Chain	Res	Type
14	1S	3	ARG
14	1S	13	ARG
14	1S	14	VAL
14	1S	36	TYR
14	1S	46	VAL
14	1S	69	VAL
14	1S	73	LEU
14	1S	85	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	30	VAL
15	1T	34	VAL
15	1T	49	VAL
15	1T	65	LYS
15	1T	96	ARG
15	1T	128	GLU
16	1U	8	VAL
16	1U	74	LEU
17	1V	61	VAL
17	1V	79	VAL
18	1W	11	ARG
18	1W	17	VAL
19	1X	35	THR
20	1Y	1	MET
20	1Y	7	VAL
20	1Y	21	LYS
20	1Y	31	LEU
20	1Y	88	LYS
20	1Y	99	CYS
21	1Z	31	ARG
21	1Z	42	VAL
21	1Z	49	ARG
21	1Z	61	LEU
21	1Z	92	SER
21	1Z	138	GLU
21	1Z	139	VAL
21	1Z	140	ASP
21	1Z	154	ASP
21	1Z	170	THR
21	1Z	171	ILE
22	10	49	LYS
23	11	3	LYS

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Mol	Chain	Res	Type
23	11	40	ARG
24	12	8	LYS
24	12	65	ASN
25	13	23	LEU
25	13	31	LEU
25	13	54	VAL
25	13	60	GLU
26	14	1	MET
26	14	49	PHE
26	14	50	VAL
26	14	52	THR
26	14	53	GLU
26	14	61	ARG
26	14	63	TYR
26	14	67	TYR
26	14	69	LYS
27	15	6	VAL
27	15	35	GLU
28	16	44	ARG
28	16	47	THR
29	17	24	THR
29	17	43	THR
29	17	46	VAL
29	17	48	LYS
30	18	14	VAL
30	18	29	LYS
31	19	4	ARG
33	1b	8	LYS
33	1b	10	LEU
33	1b	12	GLU
33	1b	24	TRP
33	1b	35	GLU
33	1b	39	ILE
33	1b	45	GLN
33	1b	80	ILE
33	1b	93	VAL
33	1b	107	THR
33	1b	108	ILE
33	1b	112	VAL
33	1b	122	PHE
33	1b	127	ILE
33	1b	128	GLU

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Mol	Chain	Res	Type
33	1b	137	ARG
33	1b	160	ASP
33	1b	165	VAL
33	1b	170	GLU
33	1b	185	ILE
33	1b	196	LEU
33	1b	208	ILE
33	1b	212	GLN
33	1b	221	LEU
33	1b	222	ILE
33	1b	229	VAL
33	1b	231	GLU
33	1b	236	TYR
34	1c	3	ASN
34	1c	15	THR
34	1c	21	ARG
34	1c	40	ARG
34	1c	49	SER
34	1c	64	VAL
34	1c	70	VAL
34	1c	89	GLU
34	1c	101	LEU
34	1c	195	VAL
35	1d	3	ARG
35	1d	5	ILE
35	1d	19	LEU
35	1d	83	SER
35	1d	127	THR
35	1d	135	LEU
35	1d	170	VAL
35	1d	175	SER
35	1d	177	ASP
35	1d	178	VAL
35	1d	188	LEU
35	1d	194	LEU
36	1e	9	LYS
36	1e	12	LEU
36	1e	31	LEU
36	1e	41	VAL
36	1e	51	VAL
36	1e	64	ARG
36	1e	67	VAL

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Mol	Chain	Res	Type
37	1f	19	LEU
37	1f	25	ILE
37	1f	37	VAL
37	1f	45	LEU
37	1f	55	ASP
37	1f	72	VAL
37	1f	75	LEU
37	1f	81	ILE
37	1f	92	LYS
38	1g	12	LEU
38	1g	16	LEU
38	1g	27	ILE
38	1g	32	ARG
38	1g	50	ILE
38	1g	57	GLU
38	1g	78	ARG
38	1g	104	LEU
38	1g	110	GLN
38	1g	113	GLU
38	1g	115	ARG
38	1g	138	LYS
39	1h	39	LEU
39	1h	52	ASP
39	1h	120	THR
40	1i	14	VAL
40	1i	17	VAL
40	1i	23	ASN
40	1i	41	VAL
40	1i	50	LEU
40	1i	53	VAL
40	1i	128	ARG
41	1j	38	ILE
41	1j	44	VAL
41	1j	46	ARG
41	1j	49	VAL
41	1j	81	THR
41	1j	92	THR
42	1k	48	ILE
42	1k	87	THR
42	1k	109	VAL
42	1k	117	ASN
43	1l	18	VAL

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Mol	Chain	Res	Type
43	1l	55	VAL
43	1l	58	VAL
43	1l	83	VAL
43	1l	117	ARG
44	1m	4	ILE
44	1m	11	ARG
44	1m	14	ARG
44	1m	15	VAL
44	1m	19	LEU
44	1m	43	THR
44	1m	49	THR
44	1m	70	LEU
44	1m	106	ASN
44	1m	109	THR
45	1n	3	ARG
45	1n	13	THR
45	1n	18	VAL
45	1n	29	ARG
46	1o	9	GLN
46	1o	39	LEU
46	1o	47	LYS
46	1o	76	GLU
46	1o	87	ILE
47	1p	1	MET
47	1p	5	ARG
47	1p	11	SER
47	1p	20	VAL
47	1p	27	LYS
47	1p	43	LYS
47	1p	45	THR
47	1p	60	LEU
47	1p	67	THR
48	1q	9	VAL
48	1q	16	GLN
48	1q	34	LYS
48	1q	52	LYS
48	1q	70	ARG
48	1q	89	LEU
48	1q	90	ILE
48	1q	97	SER
48	1q	99	SER
49	1r	31	LEU

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Mol	Chain	Res	Type
49	1r	38	GLU
49	1r	66	LEU
49	1r	76	LEU
50	1s	5	LEU
50	1s	12	ASP
50	1s	37	ARG
50	1s	41	VAL
50	1s	56	GLN
50	1s	79	THR
51	1t	10	LEU
51	1t	13	LEU
51	1t	24	LEU
51	1t	71	THR
51	1t	74	LYS
51	1t	90	GLN
3	2D	3	VAL
3	2D	5	LYS
3	2D	14	ARG
3	2D	37	LEU
3	2D	38	LYS
3	2D	99	ASP
3	2D	106	ILE
3	2D	142	VAL
3	2D	242	ARG
3	2D	259	THR
4	2E	7	VAL
4	2E	59	VAL
4	2E	73	GLU
4	2E	116	VAL
4	2E	181	LEU
5	2F	33	LEU
5	2F	70	THR
5	2F	112	MET
5	2F	126	VAL
5	2F	135	LYS
5	2F	183	VAL
5	2F	192	LEU
5	2F	201	VAL
6	2G	5	VAL
6	2G	28	VAL
6	2G	31	VAL
6	2G	43	LEU

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Mol	Chain	Res	Type
6	2G	45	GLU
6	2G	53	LEU
6	2G	60	LEU
6	2G	70	VAL
6	2G	79	ASN
6	2G	92	VAL
6	2G	116	ASP
6	2G	124	SER
6	2G	139	LEU
6	2G	140	ILE
6	2G	152	LEU
6	2G	159	VAL
6	2G	165	THR
7	2H	2	SER
7	2H	15	VAL
7	2H	23	ARG
7	2H	53	GLU
7	2H	70	THR
7	2H	90	LYS
7	2H	92	ILE
7	2H	104	GLU
7	2H	119	GLU
7	2H	122	THR
7	2H	127	GLU
7	2H	130	ARG
7	2H	133	VAL
7	2H	136	ILE
7	2H	149	ARG
7	2H	163	TYR
8	2I	15	VAL
8	2I	38	LEU
8	2I	44	LEU
8	2I	58	LEU
8	2I	82	ARG
8	2I	87	LYS
8	2I	92	VAL
8	2I	102	SER
8	2I	117	GLU
8	2I	122	GLU
8	2I	127	VAL
8	2I	142	VAL
9	2N	1	MET

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Mol	Chain	Res	Type
9	2N	8	GLN
9	2N	28	THR
9	2N	62	VAL
9	2N	67	LEU
9	2N	83	LYS
9	2N	134	ARG
10	2O	28	SER
10	2O	52	VAL
10	2O	66	LYS
10	2O	85	VAL
10	2O	108	GLU
10	2O	113	LYS
10	2O	116	SER
11	2P	1	MET
11	2P	39	LYS
11	2P	45	LEU
11	2P	75	ILE
11	2P	95	VAL
11	2P	98	GLU
11	2P	135	LEU
12	2Q	75	THR
12	2Q	98	LYS
12	2Q	110	THR
13	2R	36	THR
13	2R	114	VAL
14	2S	3	ARG
14	2S	15	ARG
14	2S	46	VAL
14	2S	48	LEU
14	2S	52	SER
14	2S	58	LEU
14	2S	63	THR
14	2S	80	LEU
15	2T	28	VAL
15	2T	40	THR
15	2T	64	ARG
15	2T	85	LYS
15	2T	115	ARG
15	2T	124	ASP
16	2U	5	LYS
16	2U	8	VAL
16	2U	17	ILE

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Mol	Chain	Res	Type
16	2U	55	ARG
16	2U	74	LEU
17	2V	7	THR
17	2V	61	VAL
17	2V	73	SER
17	2V	79	VAL
17	2V	98	GLU
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	63	ASP
19	2X	35	THR
19	2X	38	GLU
19	2X	49	VAL
20	2Y	1	MET
20	2Y	7	VAL
20	2Y	9	LYS
20	2Y	11	ASP
20	2Y	14	LEU
20	2Y	99	CYS
21	2Z	33	LEU
21	2Z	40	ASP
21	2Z	42	VAL
21	2Z	53	ILE
21	2Z	71	VAL
21	2Z	74	VAL
21	2Z	100	VAL
21	2Z	129	SER
21	2Z	140	ASP
21	2Z	150	LEU
21	2Z	154	ASP
21	2Z	157	LEU
21	2Z	161	VAL
21	2Z	170	THR
22	20	3	HIS
23	21	35	THR
23	21	40	ARG
24	22	19	VAL
24	22	59	ARG
25	23	31	LEU
25	23	37	LEU
25	23	54	VAL

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Mol	Chain	Res	Type
25	23	59	VAL
26	24	20	ASN
26	24	26	SER
26	24	34	GLU
26	24	49	PHE
26	24	59	PHE
26	24	62	ARG
26	24	68	ARG
27	25	6	VAL
27	25	33	CYS
27	25	40	LYS
27	25	58	LEU
27	25	59	GLU
28	26	6	ARG
28	26	19	ARG
28	26	23	THR
28	26	32	ASN
28	26	48	VAL
29	27	41	ARG
29	27	43	THR
29	27	46	VAL
30	28	14	VAL
30	28	23	VAL
33	2b	7	VAL
33	2b	9	GLU
33	2b	23	ARG
33	2b	44	LEU
33	2b	48	MET
33	2b	49	GLU
33	2b	53	ARG
33	2b	67	THR
33	2b	71	VAL
33	2b	76	GLN
33	2b	90	MET
33	2b	94	ASN
33	2b	112	VAL
33	2b	115	LEU
33	2b	117	GLU
33	2b	127	ILE
33	2b	136	VAL
33	2b	138	LEU
33	2b	144	ARG

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Mol	Chain	Res	Type
33	2b	158	LEU
33	2b	164	VAL
33	2b	165	VAL
33	2b	185	ILE
33	2b	189	ASP
33	2b	195	ASP
33	2b	196	LEU
33	2b	201	ILE
33	2b	204	ASN
33	2b	208	ILE
33	2b	212	GLN
33	2b	224	GLN
33	2b	229	VAL
33	2b	230	VAL
33	2b	235	SER
34	2c	15	THR
34	2c	44	GLU
34	2c	55	VAL
34	2c	77	ILE
34	2c	82	GLU
34	2c	85	ARG
34	2c	87	LEU
34	2c	91	LEU
34	2c	103	VAL
34	2c	116	VAL
34	2c	152	ILE
34	2c	164	ARG
34	2c	190	ARG
34	2c	191	THR
34	2c	192	THR
34	2c	202	ILE
35	2d	5	ILE
35	2d	8	VAL
35	2d	19	LEU
35	2d	34	GLU
35	2d	58	LEU
35	2d	135	LEU
35	2d	150	GLU
35	2d	162	LEU
35	2d	168	ARG
35	2d	175	SER
35	2d	196	LEU

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Mol	Chain	Res	Type
35	2d	198	VAL
36	2e	13	ILE
36	2e	18	ARG
36	2e	20	GLN
36	2e	41	VAL
36	2e	55	VAL
36	2e	72	GLN
36	2e	75	THR
36	2e	151	LEU
37	2f	37	VAL
37	2f	63	TYR
37	2f	70	ASP
37	2f	75	LEU
37	2f	93	SER
38	2g	9	VAL
38	2g	51	GLN
38	2g	78	ARG
38	2g	94	ARG
38	2g	98	SER
38	2g	155	ARG
39	2h	24	THR
39	2h	26	VAL
39	2h	37	ARG
39	2h	112	LEU
39	2h	114	THR
39	2h	120	THR
39	2h	129	VAL
40	2i	32	ASP
40	2i	41	VAL
40	2i	54	ASP
40	2i	56	LEU
40	2i	64	THR
40	2i	65	VAL
40	2i	70	LYS
40	2i	77	ILE
40	2i	87	GLN
40	2i	99	LEU
40	2i	108	VAL
40	2i	128	ARG
41	2j	8	LEU
41	2j	9	ARG
41	2j	23	ILE

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Mol	Chain	Res	Type
41	2j	29	ARG
41	2j	33	GLN
41	2j	38	ILE
41	2j	72	VAL
41	2j	95	GLU
41	2j	98	ILE
42	2k	14	VAL
42	2k	48	ILE
42	2k	54	ARG
42	2k	78	GLN
42	2k	84	VAL
43	2l	18	VAL
43	2l	36	VAL
43	2l	55	VAL
43	2l	62	SER
43	2l	78	GLN
43	2l	83	VAL
44	2m	3	ARG
44	2m	4	ILE
44	2m	15	VAL
44	2m	32	GLU
44	2m	45	VAL
44	2m	50	GLU
44	2m	81	LEU
44	2m	88	ARG
44	2m	90	LEU
44	2m	106	ASN
44	2m	117	VAL
45	2n	3	ARG
45	2n	7	ILE
45	2n	18	VAL
45	2n	22	THR
46	2o	39	LEU
46	2o	76	GLU
46	2o	83	GLU
47	2p	1	MET
47	2p	2	VAL
47	2p	20	VAL
47	2p	21	VAL
47	2p	57	ARG
47	2p	73	LEU
47	2p	74	LEU

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Mol	Chain	Res	Type
48	2q	9	VAL
48	2q	60	ILE
48	2q	63	ARG
48	2q	70	ARG
49	2r	21	LYS
49	2r	31	LEU
49	2r	38	GLU
49	2r	41	LYS
49	2r	46	GLU
49	2r	54	ARG
49	2r	76	LEU
50	2s	12	ASP
50	2s	37	ARG
50	2s	41	VAL
50	2s	43	GLU
50	2s	47	HIS
50	2s	71	LEU
51	2t	9	ASN
51	2t	50	GLU
51	2t	92	LEU
51	2t	93	GLU
51	2t	100	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (148) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	126	GLN
4	1E	48	GLN
5	1F	8	GLN
5	1F	69	HIS
6	1G	26	GLN
8	1I	74	ASN
8	1I	133	HIS
9	1N	8	GLN
9	1N	56	ASN
9	1N	94	HIS
9	1N	131	GLN
12	1Q	12	GLN
12	1Q	57	HIS
12	1Q	123	HIS
13	1R	31	HIS

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Mol	Chain	Res	Type
13	1R	50	HIS
13	1R	71	GLN
14	1S	68	GLN
14	1S	95	HIS
15	1T	58	ASN
15	1T	84	GLN
16	1U	72	HIS
16	1U	81	HIS
16	1U	94	ASN
19	1X	31	HIS
19	1X	82	GLN
21	1Z	34	ASN
21	1Z	73	GLN
23	11	19	GLN
23	11	56	GLN
24	12	56	GLN
25	13	32	GLN
30	18	35	GLN
30	18	43	GLN
33	1b	16	HIS
33	1b	40	HIS
33	1b	94	ASN
33	1b	140	HIS
33	1b	212	GLN
34	1c	6	HIS
34	1c	98	ASN
34	1c	162	GLN
35	1d	116	GLN
35	1d	123	HIS
35	1d	160	GLN
36	1e	73	ASN
36	1e	78	HIS
37	1f	13	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	106	GLN
40	1i	3	GLN
40	1i	31	GLN
40	1i	124	GLN
41	1j	56	HIS
42	1k	78	GLN

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Mol	Chain	Res	Type
43	1l	99	HIS
44	1m	77	ASN
44	1m	92	HIS
46	1o	9	GLN
48	1q	26	GLN
50	1s	23	ASN
50	1s	47	HIS
50	1s	83	HIS
51	1t	16	HIS
51	1t	42	GLN
51	1t	73	HIS
3	2D	87	ASN
3	2D	126	GLN
4	2E	48	GLN
5	2F	69	HIS
5	2F	75	HIS
6	2G	132	ASN
7	2H	143	GLN
7	2H	147	ASN
8	2I	105	HIS
9	2N	8	GLN
10	2O	3	GLN
11	2P	35	HIS
12	2Q	12	GLN
12	2Q	123	HIS
13	2R	71	GLN
14	2S	38	GLN
14	2S	95	HIS
15	2T	58	ASN
16	2U	94	ASN
19	2X	31	HIS
19	2X	82	GLN
20	2Y	6	HIS
21	2Z	34	ASN
21	2Z	55	HIS
21	2Z	73	GLN
22	20	29	GLN
23	21	56	GLN
24	22	9	GLN
25	23	32	GLN
26	24	20	ASN
28	26	20	ASN

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Mol	Chain	Res	Type
30	28	35	GLN
33	2b	95	GLN
33	2b	135	GLN
33	2b	224	GLN
34	2c	69	HIS
34	2c	110	ASN
34	2c	162	GLN
35	2d	45	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
36	2e	65	ASN
36	2e	72	GLN
36	2e	73	ASN
36	2e	141	GLN
37	2f	73	ASN
37	2f	100	ASN
38	2g	13	GLN
38	2g	28	ASN
40	2i	3	GLN
40	2i	29	ASN
40	2i	58	HIS
40	2i	117	HIS
41	2j	21	GLN
41	2j	33	GLN
41	2j	69	ASN
42	2k	22	HIS
42	2k	38	ASN
42	2k	78	GLN
42	2k	104	GLN
42	2k	117	ASN
43	2l	99	HIS
44	2m	40	ASN
44	2m	77	ASN
44	2m	92	HIS
46	2o	62	GLN
47	2p	16	HIS
48	2q	26	GLN
50	2s	23	ASN
50	2s	56	GLN

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Mol	Chain	Res	Type
50	2s	65	ASN
50	2s	69	HIS
50	2s	83	HIS
51	2t	45	GLN
51	2t	75	ASN
51	2t	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2863/2915 (98%)	404 (14%)	22 (0%)
1	2A	2791/2915 (95%)	420 (15%)	27 (0%)
2	1B	119/121 (98%)	9 (7%)	0
2	2B	118/121 (97%)	23 (19%)	0
32	1a	1497/1521 (98%)	216 (14%)	0
32	2a	1501/1521 (98%)	244 (16%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	2 (16%)	0
54	1w	70/76 (92%)	17 (24%)	0
54	1y	72/76 (94%)	23 (31%)	0
54	2w	66/76 (86%)	18 (27%)	0
54	2y	70/76 (92%)	19 (27%)	0
55	1x	74/77 (96%)	9 (12%)	0
55	2x	74/77 (96%)	8 (10%)	0
All	All	9339/9620 (97%)	1413 (15%)	49 (0%)

All (1413) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	181	A

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Mol	Chain	Res	Type
1	1A	196	A
1	1A	197	A
1	1A	199	A
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	271(C)	C
1	1A	271(I)	G
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	272(B)	G
1	1A	272(H)	C
1	1A	272(I)	U
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	330	A
1	1A	352	G
1	1A	357	A
1	1A	363	G
1	1A	380	U
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	456	C
1	1A	457	A

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Mol	Chain	Res	Type
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	563	G
1	1A	573	G
1	1A	575	A
1	1A	586	A
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(F)	G
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	746	A
1	1A	747	U
1	1A	764	A
1	1A	765	G
1	1A	774	A
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G

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Mol	Chain	Res	Type
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	880	G
1	1A	882	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	900	A
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	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	1045	A

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Mol	Chain	Res	Type
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G
1	1A	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	1081	U
1	1A	1082	U
1	1A	1085	A
1	1A	1087	G
1	1A	1088	A
1	1A	1090	U
1	1A	1091	G
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	1109	C
1	1A	1112	G
1	1A	1116	C
1	1A	1128	A
1	1A	1135	C
1	1A	1136	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	1220	A

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Mol	Chain	Res	Type
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1281	G
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1308	A
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1370	C
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	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	1532	C
1	1A	1543	C
1	1A	1558	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G
1	1A	1582	C
1	1A	1584	C
1	1A	1608	A

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Mol	Chain	Res	Type
1	1A	1609	A
1	1A	1610	A
1	1A	1648	C
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1722	A
1	1A	1739	U
1	1A	1745	C
1	1A	1747	G
1	1A	1756	G
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1829	A
1	1A	1847	A
1	1A	1848	A
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	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

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Mol	Chain	Res	Type
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2102	U
1	1A	2108	C
1	1A	2110	G
1	1A	2113	U
1	1A	2116	G
1	1A	2121	G
1	1A	2122	U
1	1A	2126	A
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	2150	U
1	1A	2151	G
1	1A	2152	G
1	1A	2154	G
1	1A	2156	G

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Mol	Chain	Res	Type
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2160	G
1	1A	2161	C
1	1A	2166	G
1	1A	2167	U
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2174	C
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2283	C
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
1	1A	2379	G
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2407	G
1	1A	2414	G
1	1A	2422	A
1	1A	2424	C
1	1A	2425	A

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Mol	Chain	Res	Type
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2434	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2476	A
1	1A	2478	A
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
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	2727	G
1	1A	2733	A
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C

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Mol	Chain	Res	Type
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2803	C
1	1A	2805	G
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2839	G
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	13	A
2	1B	25	A
2	1B	35	U
2	1B	56	G
2	1B	73	A
2	1B	84	C
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	61	G
32	1a	76	C
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	115	G
32	1a	116	A
32	1a	121	C
32	1a	131	C

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Mol	Chain	Res	Type
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(A)	C
32	1a	189(H)	G
32	1a	195	A
32	1a	197	A
32	1a	203	U
32	1a	204	U
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	306	G
32	1a	316	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	342	C
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	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	457	C
32	1a	461	A

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Mol	Chain	Res	Type
32	1a	470	C
32	1a	471	G
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	527	G7M
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	666	G
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	703	G
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	755	G
32	1a	766	A
32	1a	774	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A

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Mol	Chain	Res	Type
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	870	U
32	1a	874	G
32	1a	902	G
32	1a	913	A
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	998	G
32	1a	1000	U
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C

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Mol	Chain	Res	Type
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1034	G
32	1a	1039	C
32	1a	1043	C
32	1a	1044	A
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1124	G
32	1a	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	1159	U
32	1a	1160	G
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
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	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U

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Mol	Chain	Res	Type
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	1320	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1380	U
32	1a	1419	G
32	1a	1442	G
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
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	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	24	A
54	1w	2	C
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	34	G
54	1w	45	U
54	1w	46	G7M
54	1w	47	U
54	1w	48	C
54	1w	68	C

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Mol	Chain	Res	Type
54	1w	69	G
54	1w	71	G
54	1w	72	C
54	1w	73	A
54	1w	74	C
55	1x	6	G
55	1x	9	G
55	1x	13	C
55	1x	19	G
55	1x	20	U
55	1x	21	A
55	1x	47	U
55	1x	61	C
55	1x	69	C
54	1y	5	G
54	1y	6	G
54	1y	7	A
54	1y	8	4SU
54	1y	14	A
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	23	A
54	1y	31	A
54	1y	34	G
54	1y	35	A
54	1y	44	G
54	1y	45	U
54	1y	46	G7M
54	1y	47	U
54	1y	48	C
54	1y	53	G
54	1y	54	5MU
54	1y	56	C
54	1y	58	A
54	1y	59	U
54	1y	70	G
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C

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Mol	Chain	Res	Type
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	92	A
1	2A	94	C
1	2A	95	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	141	A
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	197	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	232	G
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(O)	C
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	311	A

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Mol	Chain	Res	Type
1	2A	312	G
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	363(B)	G
1	2A	386	G
1	2A	396	G
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	443	A
1	2A	444	C
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	494	G
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A

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Mol	Chain	Res	Type
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	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	765	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	874	G
1	2A	875	G
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	892	G
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A

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Mol	Chain	Res	Type
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	983	A
1	2A	996	A
1	2A	1012	U
1	2A	1013	C
1	2A	1018	C
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1117	G
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1171	G
1	2A	1188	U
1	2A	1195	G
1	2A	1211	U
1	2A	1220	A
1	2A	1236	G
1	2A	1244	G
1	2A	1253	A

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Mol	Chain	Res	Type
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1321	A
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1384	A
1	2A	1385	G
1	2A	1395	A
1	2A	1396	U
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1533	G

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Mol	Chain	Res	Type
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1608	A
1	2A	1609	A
1	2A	1639	U
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1743	C
1	2A	1756	G
1	2A	1763	G
1	2A	1764	G
1	2A	1769	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A

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Mol	Chain	Res	Type
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	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2099	U
1	2A	2108	C
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2122	U
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G

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Mol	Chain	Res	Type
1	2A	2134	A
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C
1	2A	2141	G
1	2A	2142	C
1	2A	2146	C
1	2A	2150	U
1	2A	2151	G
1	2A	2154	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2174	C
1	2A	2176	A
1	2A	2178	C
1	2A	2182	G
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
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	2283	C
1	2A	2287	A
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A
1	2A	2319	G

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Mol	Chain	Res	Type
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2406	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2434	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2468	G
1	2A	2469	A
1	2A	2476	A
1	2A	2490	G
1	2A	2491	U
1	2A	2502	G
1	2A	2505	G
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2554	U
1	2A	2555	U
1	2A	2562	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U

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Mol	Chain	Res	Type
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2758	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	2803	C
1	2A	2808	U
1	2A	2810	A
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2836	U
1	2A	2839	G
1	2A	2872	G
1	2A	2873	A
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	9	G
2	2B	13	A
2	2B	17	C
2	2B	25	A

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Mol	Chain	Res	Type
2	2B	34	U
2	2B	41	U
2	2B	42	C
2	2B	51	G
2	2B	53	A
2	2B	56	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	88	C
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	111	G
2	2B	116	G
2	2B	119	G
2	2B	120	A
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	65	U
32	2a	66	G
32	2a	73	G
32	2a	88	A
32	2a	89	C
32	2a	98	G
32	2a	101	A
32	2a	105	G
32	2a	116	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	156	G
32	2a	161	A
32	2a	163	C
32	2a	182	U

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Mol	Chain	Res	Type
32	2a	189(G)	G
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	281	G
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	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	470	C
32	2a	471	G
32	2a	484	G

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Mol	Chain	Res	Type
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	527	G7M
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	536	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
32	2a	630	G
32	2a	650	G
32	2a	653	A
32	2a	661	G
32	2a	665	A
32	2a	673	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	723	U
32	2a	731	G
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	817	C
32	2a	821	G

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Mol	Chain	Res	Type
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	859	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	958	A
32	2a	960	U
32	2a	961	U
32	2a	963	G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	991	U
32	2a	992	U
32	2a	993	G
32	2a	996	A
32	2a	997	U
32	2a	998	G
32	2a	999	C
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1010	G
32	2a	1011	G
32	2a	1017	G
32	2a	1020	U
32	2a	1021	G

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Mol	Chain	Res	Type
32	2a	1023	G
32	2a	1025	U
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1035	A
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1044	A
32	2a	1046	A
32	2a	1051	C
32	2a	1053	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1086	U
32	2a	1092	A
32	2a	1094	G
32	2a	1095	U
32	2a	1097	C
32	2a	1101	A
32	2a	1108	G
32	2a	1122	U
32	2a	1128	C
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1135	U
32	2a	1136	U
32	2a	1137	C
32	2a	1139	G
32	2a	1140	C
32	2a	1146	A
32	2a	1150	U

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Mol	Chain	Res	Type
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1172	C
32	2a	1182	G
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	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	1272	G
32	2a	1273	G
32	2a	1276	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1286	A
32	2a	1287	A
32	2a	1300	G
32	2a	1305	G
32	2a	1320	C
32	2a	1338	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1358	U
32	2a	1363	C
32	2a	1370	G
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G

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Mol	Chain	Res	Type
32	2a	1492	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	14	A
53	2v	24	A
54	2w	3	C
54	2w	4	C
54	2w	5	G
54	2w	7	A
54	2w	9	A
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	28	G
54	2w	46	G7M
54	2w	47	U
54	2w	48	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
55	2x	9	G
55	2x	13	C
55	2x	20	U
55	2x	21	A
55	2x	47	U
55	2x	52	G
55	2x	69	C
55	2x	70	G
54	2y	15	G
54	2y	19	G
54	2y	27	G
54	2y	43	C

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Mol	Chain	Res	Type
54	2y	45	U
54	2y	48	C
54	2y	49	C
54	2y	52	G
54	2y	53	G
54	2y	54	5MU
54	2y	55	PSU
54	2y	56	C
54	2y	57	G
54	2y	58	A
54	2y	59	U
54	2y	62	C
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	195	A
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	1174	A
1	1A	1176	G
1	1A	1420	U
1	1A	1508	A
1	1A	1608	A
1	1A	1658	C
1	1A	1944	U
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2439	A
1	1A	2629	A
1	1A	2689	U
1	2A	196	A

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Mol	Chain	Res	Type
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	764	A
1	2A	774	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1395	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	2126	A
1	2A	2406	U
1	2A	2439	A
1	2A	2689	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	OMC	1A	1920	1	19,22,23	0.80	0	25,31,34	0.87	0
1	5MU	2A	1915	1	19,22,23	1.46	5 (26%)	27,32,35	2.20	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	5MU	2w	54	54	19,22,23	1.34	3 (15%)	27,32,35	1.87	7 (25%)
32	5MC	1a	967	32	19,22,23	1.73	2 (10%)	26,32,35	1.13	2 (7%)
32	G7M	1a	527	32	23,26,27	1.53	3 (13%)	34,39,42	1.63	4 (11%)
1	2MA	1A	2503	56,1	22,25,26	1.45	5 (22%)	32,37,40	2.32	9 (28%)
32	5MC	2a	1400	32	19,22,23	1.67	3 (15%)	26,32,35	1.21	3 (11%)
54	5MU	1y	54	54	19,22,23	1.46	5 (26%)	27,32,35	1.72	6 (22%)
32	2MG	2a	1207	32	23,26,27	1.24	4 (17%)	33,38,41	2.23	8 (24%)
32	MA6	1a	1518	32	23,26,27	0.42	0	33,38,41	1.99	9 (27%)
32	M2G	1a	966	32	24,27,28	1.32	4 (16%)	33,40,43	1.84	6 (18%)
1	OMG	1A	2251	55,56,1	23,26,27	1.24	3 (13%)	32,38,41	1.97	7 (21%)
32	M2G	2a	966	32	24,27,28	1.28	3 (12%)	33,40,43	1.86	6 (18%)
54	PSU	2w	55	54	18,21,22	1.37	2 (11%)	21,30,33	1.97	3 (14%)
54	5MU	1w	54	54	19,22,23	1.35	4 (21%)	27,32,35	2.07	6 (22%)
1	5MU	1A	1939	56,1	19,22,23	1.50	6 (31%)	27,32,35	2.01	5 (18%)
1	PSU	1A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	1.99	4 (19%)
1	MA6	1A	2058	56,1	23,26,27	0.53	0	33,38,41	2.45	13 (39%)
32	5MC	2a	967	32	19,22,23	1.66	3 (15%)	26,32,35	1.08	2 (7%)
32	5MC	2a	1404	32	19,22,23	1.81	3 (15%)	26,32,35	1.18	2 (7%)
32	MA6	2a	1518	32	23,26,27	0.45	0	33,38,41	2.03	9 (27%)
32	5MC	1a	1404	32	19,22,23	1.73	3 (15%)	26,32,35	1.20	2 (7%)
1	2MA	2A	2503	56,1	22,25,26	1.49	5 (22%)	32,37,40	2.34	8 (25%)
54	4SU	2y	8	54	18,21,22	1.74	4 (22%)	25,30,33	2.21	4 (16%)
1	MA6	2A	2058	1	23,26,27	0.49	0	33,38,41	2.20	12 (36%)
32	UR3	1a	1498	32	19,22,23	1.00	1 (5%)	26,32,35	1.79	4 (15%)
55	5MC	1x	32	55	19,22,23	1.65	3 (15%)	26,32,35	1.21	3 (11%)
54	G7M	2w	46	54	23,26,27	1.47	5 (21%)	34,39,42	1.62	4 (11%)
43	0TD	1l	92	43	8,9,10	4.35	1 (12%)	6,11,13	7.57	2 (33%)
54	PSU	1y	39	54	18,21,22	1.38	2 (11%)	21,30,33	1.82	3 (14%)
1	OMU	2A	2552	56,1	19,22,23	1.16	2 (10%)	25,31,34	1.78	5 (20%)
1	OMU	1A	2552	56,1	19,22,23	1.26	3 (15%)	25,31,34	1.83	5 (20%)
32	PSU	1a	516	56,32	18,21,22	1.39	2 (11%)	21,30,33	2.09	6 (28%)
32	5MC	1a	1407	32	19,22,23	1.60	2 (10%)	26,32,35	1.05	2 (7%)
54	MIA	1w	37	54	28,31,32	2.36	6 (21%)	38,44,47	2.85	13 (34%)
54	G7M	2y	46	54	23,26,27	1.52	3 (13%)	34,39,42	1.75	4 (11%)
54	G7M	1y	46	54	23,26,27	1.52	4 (17%)	34,39,42	1.70	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	31H	1x	76	55,56,60	31,34,35	1.25	4 (12%)	35,47,50	2.05	13 (37%)
32	MA6	2a	1519	32	23,26,27	0.41	0	33,38,41	2.12	9 (27%)
32	UR3	2a	1498	32	19,22,23	1.06	1 (5%)	26,32,35	1.74	3 (11%)
54	PSU	1y	32	54	18,21,22	1.32	2 (11%)	21,30,33	1.97	3 (14%)
1	OMC	2A	1920	1	19,22,23	0.80	0	25,31,34	0.90	1 (4%)
1	PSU	1A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	2.02	3 (14%)
54	PSU	2y	55	54	18,21,22	1.44	2 (11%)	21,30,33	1.94	5 (23%)
1	5MC	1A	1962	56,1	19,22,23	1.63	3 (15%)	26,32,35	1.19	2 (7%)
54	PSU	1w	32	56,54	18,21,22	1.35	2 (11%)	21,30,33	1.98	3 (14%)
55	PSU	2x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.06	4 (19%)
43	0TD	2l	92	43	8,9,10	4.46	1 (12%)	6,11,13	3.72	3 (50%)
1	5MU	2A	1939	56,1	19,22,23	1.45	6 (31%)	27,32,35	2.33	6 (22%)
55	PSU	1x	55	55	18,21,22	1.33	2 (11%)	21,30,33	1.98	4 (19%)
1	5MC	2A	1962	56,1	19,22,23	1.68	3 (15%)	26,32,35	1.16	3 (11%)
54	G7M	1w	46	54	23,26,27	1.53	4 (17%)	34,39,42	1.61	4 (11%)
54	PSU	1w	39	54	18,21,22	1.34	2 (11%)	21,30,33	1.94	3 (14%)
54	PSU	2y	32	54	18,21,22	1.34	2 (11%)	21,30,33	1.98	3 (14%)
32	5MC	2a	1407	56,32	19,22,23	1.57	2 (10%)	26,32,35	1.16	2 (7%)
55	5MU	2x	54	55	19,22,23	1.37	5 (26%)	27,32,35	2.17	6 (22%)
54	MIA	2y	37	54	21,24,32	1.63	3 (14%)	30,35,47	1.99	7 (23%)
1	5MC	1A	1942	1	19,22,23	1.63	3 (15%)	26,32,35	1.24	2 (7%)
54	PSU	2y	39	54	18,21,22	1.38	2 (11%)	21,30,33	1.85	4 (19%)
55	4SU	2x	8	55	18,21,22	2.06	6 (33%)	25,30,33	1.38	5 (20%)
1	PSU	1A	2605	56,1	18,21,22	1.43	3 (16%)	21,30,33	2.00	4 (19%)
1	5MU	1A	1915	1	19,22,23	1.42	4 (21%)	27,32,35	2.21	6 (22%)
32	MA6	1a	1519	32	23,26,27	0.45	0	33,38,41	2.10	9 (27%)
1	PSU	2A	1917	1	18,21,22	1.32	2 (11%)	21,30,33	1.91	4 (19%)
54	PSU	1y	55	54	18,21,22	1.39	2 (11%)	21,30,33	2.00	3 (14%)
54	5MU	2y	54	54	19,22,23	1.42	4 (21%)	27,32,35	2.09	7 (25%)
1	OMG	2A	2251	55,1	23,26,27	1.22	3 (13%)	32,38,41	2.03	6 (18%)
55	5MC	2x	32	55	19,22,23	1.59	3 (15%)	26,32,35	1.27	3 (11%)
32	4OC	1a	1402	32	20,23,24	0.73	0	25,32,35	1.05	1 (4%)
1	5MC	2A	1942	1	19,22,23	1.60	3 (15%)	26,32,35	1.07	2 (7%)
32	2MG	1a	1207	32	23,26,27	1.23	2 (8%)	33,38,41	2.20	8 (24%)
54	MIA	1y	37	54	21,24,32	1.67	4 (19%)	30,35,47	2.00	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	4SU	1y	8	54	18,21,22	1.81	6 (33%)	25,30,33	1.80	4 (16%)
54	PSU	2w	39	54	18,21,22	1.36	2 (11%)	21,30,33	1.94	3 (14%)
1	PSU	2A	2605	1	18,21,22	1.37	3 (16%)	21,30,33	2.07	4 (19%)
54	PSU	1w	55	54	18,21,22	1.38	2 (11%)	21,30,33	2.09	3 (14%)
32	5MC	1a	1400	32	19,22,23	1.66	3 (15%)	26,32,35	1.17	2 (7%)
54	4SU	1w	8	54	18,21,22	1.77	5 (27%)	25,30,33	1.80	5 (20%)
54	PSU	2w	32	54	18,21,22	1.38	2 (11%)	21,30,33	1.93	4 (19%)
1	PSU	2A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	2.00	4 (19%)
55	31H	2x	76	55,56,60	31,34,35	1.24	4 (12%)	35,47,50	1.97	11 (31%)
54	MIA	2w	37	54	24,27,32	2.11	6 (25%)	32,39,47	2.59	11 (34%)
55	5MU	1x	54	55,56	19,22,23	1.44	5 (26%)	27,32,35	2.01	6 (22%)
32	4OC	2a	1402	32	20,23,24	0.78	0	25,32,35	0.96	1 (4%)
32	PSU	2a	516	32	18,21,22	1.29	2 (11%)	21,30,33	2.10	4 (19%)
55	4SU	1x	8	55	18,21,22	2.35	6 (33%)	25,30,33	1.83	7 (28%)
54	4SU	2w	8	54	18,21,22	1.78	5 (27%)	25,30,33	2.02	5 (20%)
32	G7M	2a	527	56,32	23,26,27	1.47	4 (17%)	34,39,42	1.71	5 (14%)

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	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	5MU	2A	1915	1	-	1/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32	-	3/7/25/26	0/3/3/3
1	2MA	1A	2503	56,1	-	0/7/25/26	0/3/3/3
32	5MC	2a	1400	32	-	1/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	2/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	OMG	1A	2251	55,56,1	-	0/9/27/28	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	1A	1939	56,1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	MA6	1A	2058	56,1	-	0/11/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	56,1	-	2/7/25/26	0/3/3/3
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2
1	MA6	2A	2058	1	-	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
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
43	0TD	1l	92	43	-	2/7/12/14	-
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	56,1	-	0/9/27/28	0/2/2/2
1	OMU	1A	2552	56,1	-	0/9/27/28	0/2/2/2
32	PSU	1a	516	56,32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/15/33/34	0/3/3/3
54	G7M	2y	46	54	-	2/7/25/26	0/3/3/3
54	G7M	1y	46	54	-	1/7/25/26	0/3/3/3
55	31H	1x	76	55,56,60	-	5/22/40/41	0/3/3/3
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	3/7/25/26	0/2/2/2
1	5MC	1A	1962	56,1	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	56,54	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	4/7/12/14	-
1	5MU	2A	1939	56,1	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	56,1	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	56,32	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	MIA	2y	37	54	-	1/7/25/34	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	56,1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	1/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	3/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/9/27/28	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
54	MIA	1y	37	54	-	0/7/25/34	0/3/3/3
54	4SU	1y	8	54	-	3/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	31H	2x	76	55,56,60	-	4/22/40/41	0/3/3/3
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
55	5MU	1x	54	55,56	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	56,32	-	3/7/25/26	0/3/3/3

All (252) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.18	1.70	1.82
43	1l	92	0TD	CB-SB	-11.84	1.70	1.82
54	1w	37	MIA	C2-S10	-7.18	1.69	1.75
54	1w	37	MIA	C13-C14	6.81	1.52	1.32
54	2w	37	MIA	C2-S10	-6.57	1.70	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1404	5MC	C5-C4	6.57	1.49	1.44
32	1a	967	5MC	C5-C4	6.32	1.48	1.44
32	1a	1404	5MC	C5-C4	6.27	1.48	1.44
1	2A	1962	5MC	C5-C4	6.24	1.48	1.44
32	2a	967	5MC	C5-C4	6.12	1.48	1.44
32	2a	1400	5MC	C5-C4	6.06	1.48	1.44
32	1a	1400	5MC	C5-C4	6.01	1.48	1.44
1	1A	1962	5MC	C5-C4	5.97	1.48	1.44
55	1x	8	4SU	C4-N3	-5.93	1.31	1.37
55	1x	32	5MC	C5-C4	5.90	1.48	1.44
32	1a	1407	5MC	C5-C4	5.89	1.48	1.44
1	1A	1942	5MC	C5-C4	5.78	1.48	1.44
55	2x	32	5MC	C5-C4	5.62	1.48	1.44
1	2A	1942	5MC	C5-C4	5.61	1.48	1.44
32	2a	1407	5MC	C5-C4	5.54	1.48	1.44
54	1y	37	MIA	C5-C4	5.36	1.48	1.39
54	2w	37	MIA	C5-C4	5.22	1.48	1.39
54	2y	37	MIA	C5-C4	5.20	1.48	1.39
54	1w	37	MIA	C5-C4	4.99	1.48	1.39
32	1a	527	G7M	C5-N7	-4.84	1.33	1.39
55	2x	8	4SU	C4-N3	-4.80	1.32	1.37
54	2y	8	4SU	C4-S4	-4.79	1.60	1.68
54	2w	8	4SU	C4-S4	-4.78	1.60	1.68
55	1x	8	4SU	C4-S4	-4.68	1.60	1.68
54	1w	46	G7M	C5-N7	-4.64	1.33	1.39
54	1w	8	4SU	C4-S4	-4.64	1.60	1.68
54	1y	8	4SU	C4-S4	-4.59	1.60	1.68
54	1y	46	G7M	C5-N7	-4.49	1.34	1.39
54	2y	46	G7M	C5-N7	-4.40	1.34	1.39
55	2x	8	4SU	C4-S4	-4.34	1.61	1.68
1	2A	2503	2MA	C5-C4	4.31	1.46	1.39
55	1x	8	4SU	C2-N3	-4.22	1.30	1.38
1	1A	2503	2MA	C5-C4	4.19	1.46	1.39
32	2a	527	G7M	C5-N7	-4.14	1.34	1.39
54	2w	46	G7M	C5-N7	-4.13	1.34	1.39
54	1w	55	PSU	C6-C5	3.98	1.39	1.35
54	1y	55	PSU	C6-C5	3.98	1.39	1.35
55	2x	76	31H	C5-N7	-3.93	1.31	1.39
54	2w	55	PSU	C6-C5	3.88	1.39	1.35
55	1x	76	31H	C5-N7	-3.86	1.32	1.39
54	2y	32	PSU	C6-C5	3.85	1.39	1.35
54	2w	32	PSU	C6-C5	3.82	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	32	PSU	C6-C5	3.79	1.39	1.35
54	1y	39	PSU	C6-C5	3.79	1.39	1.35
54	1y	32	PSU	C6-C5	3.69	1.39	1.35
54	2w	39	PSU	C6-C5	3.69	1.39	1.35
1	1A	1911	PSU	C6-C5	3.67	1.39	1.35
54	2y	39	PSU	C6-C5	3.67	1.39	1.35
55	2x	55	PSU	C6-C5	3.64	1.39	1.35
32	1a	516	PSU	C6-C5	3.62	1.39	1.35
32	2a	516	PSU	C6-C5	3.55	1.39	1.35
54	1y	8	4SU	C4-N3	-3.54	1.34	1.37
54	1y	46	G7M	C5-C4	3.52	1.47	1.38
54	2y	46	G7M	C5-C4	3.49	1.47	1.38
1	2A	1911	PSU	C6-C5	3.48	1.39	1.35
1	1A	1917	PSU	C6-C5	3.46	1.39	1.35
54	2y	55	PSU	C6-C5	3.45	1.39	1.35
1	2A	2605	PSU	C6-C5	3.43	1.39	1.35
1	2A	1917	PSU	C6-C5	3.42	1.39	1.35
54	2w	46	G7M	C5-C4	3.35	1.46	1.38
32	2a	527	G7M	C5-C4	3.32	1.46	1.38
55	2x	8	4SU	C2-N3	-3.32	1.32	1.38
1	1A	2605	PSU	C6-C5	3.32	1.39	1.35
54	2w	8	4SU	C4-N3	-3.31	1.34	1.37
55	1x	55	PSU	C6-C5	3.28	1.38	1.35
55	1x	76	31H	C5-C4	-3.28	1.33	1.39
54	1w	46	G7M	C5-C4	3.26	1.46	1.38
55	1x	8	4SU	C5-C4	-3.25	1.38	1.42
32	1a	527	G7M	C5-C4	3.25	1.46	1.38
55	2x	76	31H	C5-C4	-3.25	1.33	1.39
54	1w	39	PSU	C6-C5	3.24	1.38	1.35
32	2a	1207	2MG	C5-C4	3.22	1.47	1.38
32	2a	1404	5MC	C6-C5	3.20	1.39	1.34
54	1w	8	4SU	C4-N3	-3.19	1.34	1.37
1	1A	1942	5MC	C6-C5	3.12	1.39	1.34
1	2A	2251	OMG	C5-C4	3.09	1.47	1.38
32	2a	966	M2G	C5-C4	3.08	1.47	1.38
32	1a	966	M2G	C5-C4	3.07	1.47	1.38
1	1A	1939	5MU	C4-N3	-3.07	1.33	1.38
32	1a	1207	2MG	C5-C4	3.07	1.47	1.38
32	1a	967	5MC	C6-C5	3.05	1.39	1.34
55	2x	8	4SU	C5-C4	-3.04	1.38	1.42
54	2w	37	MIA	C5-C6	3.03	1.49	1.41
54	2y	37	MIA	C5-C6	2.98	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1915	5MU	C6-C5	2.98	1.39	1.34
55	1x	54	5MU	C6-C5	2.96	1.39	1.34
1	2A	1939	5MU	C6-C5	2.96	1.39	1.34
1	1A	1939	5MU	C2-N3	-2.95	1.32	1.38
1	1A	1915	5MU	C2-N1	2.94	1.43	1.38
1	1A	2605	PSU	C4-N3	-2.93	1.33	1.38
54	2y	54	5MU	C2-N1	2.93	1.43	1.38
54	1y	37	MIA	C5-C6	2.92	1.49	1.41
1	1A	2251	OMG	C5-C4	2.92	1.46	1.38
32	2a	1407	5MC	C6-C5	2.91	1.39	1.34
32	1a	1404	5MC	C6-C5	2.90	1.39	1.34
54	1y	54	5MU	C6-C5	2.90	1.39	1.34
54	2y	8	4SU	C4-N3	-2.90	1.34	1.37
32	1a	966	M2G	C2-N2	2.89	1.40	1.35
1	2A	1942	5MC	C6-C5	2.87	1.39	1.34
55	1x	54	5MU	C4-N3	-2.84	1.33	1.38
1	1A	1939	5MU	C6-C5	2.81	1.39	1.34
54	2y	54	5MU	C6-C5	2.81	1.39	1.34
32	1a	1407	5MC	C6-C5	2.81	1.39	1.34
1	1A	2552	OMU	C4-N3	-2.80	1.33	1.38
55	2x	54	5MU	C6-C5	2.79	1.39	1.34
55	1x	32	5MC	C6-C5	2.79	1.39	1.34
1	2A	1939	5MU	C4-N3	-2.78	1.33	1.38
55	2x	32	5MC	C6-C5	2.78	1.39	1.34
1	1A	1915	5MU	C6-C5	2.77	1.39	1.34
1	1A	2251	OMG	C6-N1	-2.74	1.33	1.38
32	2a	966	M2G	C2-N2	2.71	1.40	1.35
54	1w	37	MIA	C5-C6	2.70	1.48	1.41
32	2a	1400	5MC	C6-C5	2.69	1.39	1.34
54	1y	54	5MU	C4-N3	-2.69	1.33	1.38
1	2A	1911	PSU	C4-N3	-2.65	1.33	1.38
54	2y	39	PSU	C4-N3	-2.65	1.33	1.38
54	1w	39	PSU	C4-N3	-2.64	1.33	1.38
32	1a	516	PSU	C4-N3	-2.63	1.33	1.38
1	1A	1911	PSU	C4-N3	-2.62	1.33	1.38
54	1w	54	5MU	C6-C5	2.62	1.38	1.34
54	2y	55	PSU	C4-N3	-2.62	1.33	1.38
1	2A	1915	5MU	C2-N1	2.62	1.42	1.38
32	1a	1400	5MC	C6-C5	2.61	1.38	1.34
54	2w	54	5MU	C6-C5	2.60	1.38	1.34
1	1A	2552	OMU	C2-N3	-2.59	1.33	1.38
54	1y	54	5MU	C2-N1	2.58	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2503	2MA	C5-N7	-2.57	1.34	1.39
1	2A	1915	5MU	C4-C5	2.57	1.49	1.44
54	1w	8	4SU	C5-C4	-2.56	1.39	1.42
55	1x	76	31H	C5-C6	-2.56	1.33	1.41
1	2A	1915	5MU	C4-N3	-2.56	1.34	1.38
1	2A	2552	OMU	C4-N3	-2.56	1.34	1.38
54	1y	39	PSU	C4-N3	-2.55	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.55	1.34	1.38
55	2x	76	31H	C5-C6	-2.55	1.33	1.41
32	2a	967	5MC	C6-C5	2.53	1.38	1.34
1	1A	1962	5MC	C6-C5	2.52	1.38	1.34
55	1x	55	PSU	C4-N3	-2.49	1.34	1.38
1	1A	1915	5MU	C4-C5	2.49	1.48	1.44
54	1w	37	MIA	C5-N7	-2.49	1.34	1.39
1	1A	2503	2MA	C5-C6	2.48	1.47	1.41
54	2w	39	PSU	C4-N3	-2.47	1.34	1.38
54	2y	37	MIA	C8-N7	2.47	1.36	1.31
32	1a	1207	2MG	C6-N1	-2.47	1.34	1.38
1	2A	2605	PSU	C4-N3	-2.46	1.34	1.38
55	2x	54	5MU	C4-N3	-2.45	1.34	1.38
54	2y	32	PSU	C4-N3	-2.45	1.34	1.38
1	1A	2503	2MA	C5-N7	-2.45	1.34	1.39
54	1w	32	PSU	C4-N3	-2.44	1.34	1.38
32	2a	1498	UR3	C2-N1	2.44	1.41	1.38
1	2A	1962	5MC	C6-N1	-2.44	1.33	1.38
54	2w	54	5MU	C4-N3	-2.44	1.34	1.38
54	2w	8	4SU	C5-C4	-2.44	1.39	1.42
54	2w	55	PSU	C4-N3	-2.44	1.34	1.38
54	2w	54	5MU	C4-C5	2.43	1.48	1.44
1	2A	1939	5MU	C2-N3	-2.43	1.33	1.38
55	2x	55	PSU	C4-N3	-2.43	1.34	1.38
1	2A	2251	OMG	C6-N1	-2.43	1.34	1.38
55	1x	32	5MC	C6-N1	-2.41	1.33	1.38
32	1a	966	M2G	C6-N1	-2.40	1.34	1.38
54	1y	37	MIA	C8-N7	2.39	1.36	1.31
54	1w	54	5MU	C4-C5	2.38	1.48	1.44
54	1y	55	PSU	C4-N3	-2.38	1.34	1.38
54	1y	8	4SU	C5-C4	-2.37	1.39	1.42
1	2A	2251	OMG	C5-N7	-2.37	1.34	1.39
54	1w	54	5MU	C4-N3	-2.37	1.34	1.38
54	2w	32	PSU	C4-N3	-2.37	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.36	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1939	5MU	C6-N1	-2.36	1.34	1.38
55	2x	54	5MU	C4-C5	2.36	1.48	1.44
54	2y	54	5MU	C4-C5	2.36	1.48	1.44
54	2y	46	G7M	C6-N1	-2.36	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.35	1.34	1.38
1	2A	1962	5MC	C6-C5	2.35	1.38	1.34
54	2y	8	4SU	C2-N1	2.35	1.42	1.38
32	1a	527	G7M	C6-N1	-2.35	1.34	1.38
1	2A	2503	2MA	C5-C6	2.34	1.47	1.41
54	2w	37	MIA	C5-N7	-2.34	1.34	1.39
1	1A	2251	OMG	C5-N7	-2.34	1.34	1.39
55	1x	54	5MU	C4-C5	2.34	1.48	1.44
1	1A	1939	5MU	C6-N1	-2.33	1.34	1.38
54	2y	54	5MU	C4-N3	-2.32	1.34	1.38
55	1x	8	4SU	O2-C2	2.31	1.27	1.23
54	1w	46	G7M	C6-N1	-2.31	1.34	1.38
1	1A	1915	5MU	C4-N3	-2.30	1.34	1.38
32	2a	527	G7M	C6-N1	-2.30	1.34	1.38
54	1y	32	PSU	C4-N3	-2.30	1.34	1.38
54	1y	54	5MU	C4-C5	2.29	1.48	1.44
32	2a	1404	5MC	C6-N1	-2.29	1.34	1.38
32	2a	966	M2G	C6-N1	-2.28	1.34	1.38
54	1w	55	PSU	C4-N3	-2.27	1.34	1.38
54	1y	8	4SU	C2-N3	-2.27	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.27	1.34	1.38
1	2A	1939	5MU	C4-C5	2.27	1.48	1.44
55	2x	32	5MC	C6-N1	-2.26	1.34	1.38
54	2y	8	4SU	C5-C4	-2.25	1.39	1.42
32	2a	1400	5MC	C6-N1	-2.24	1.34	1.38
1	1A	2503	2MA	C8-N7	2.24	1.36	1.31
54	2w	37	MIA	C2-N3	2.23	1.37	1.34
1	1A	1917	PSU	C4-N3	-2.22	1.34	1.38
55	1x	54	5MU	C2-N1	2.22	1.41	1.38
54	1y	8	4SU	C2-N1	2.22	1.41	1.38
54	2w	8	4SU	C2-N1	2.22	1.41	1.38
1	2A	1942	5MC	C6-N1	-2.21	1.34	1.38
55	2x	54	5MU	C2-N1	2.21	1.41	1.38
32	1a	1404	5MC	C6-N1	-2.20	1.34	1.38
54	1w	37	MIA	C8-N7	2.20	1.35	1.31
54	1y	46	G7M	C6-N1	-2.19	1.34	1.38
1	2A	2552	OMU	C2-N3	-2.19	1.34	1.38
32	2a	527	G7M	C5-C6	2.18	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	967	5MC	C6-N1	-2.18	1.34	1.38
54	1w	54	5MU	C2-N1	2.17	1.41	1.38
55	2x	8	4SU	O2-C2	2.15	1.26	1.23
54	1w	46	G7M	C4-N9	-2.15	1.32	1.38
54	1y	37	MIA	C5-N7	-2.15	1.35	1.39
32	1a	1498	UR3	C2-N1	2.15	1.41	1.38
32	2a	516	PSU	C4-N3	-2.14	1.34	1.38
54	1w	8	4SU	C2-N3	-2.14	1.34	1.38
1	1A	2552	OMU	C5-C4	-2.13	1.39	1.43
1	2A	1939	5MU	C2-N1	2.13	1.41	1.38
55	2x	8	4SU	C6-C5	2.12	1.40	1.35
1	1A	1942	5MC	C6-N1	-2.11	1.34	1.38
54	2w	46	G7M	C6-N1	-2.11	1.34	1.38
1	1A	2605	PSU	C2-N3	-2.11	1.34	1.37
55	2x	76	31H	C3'-N3'	2.10	1.49	1.45
55	1x	76	31H	C3'-N3'	2.10	1.49	1.45
54	1w	8	4SU	C2-N1	2.09	1.41	1.38
55	1x	54	5MU	C2-N3	-2.07	1.34	1.38
54	2w	37	MIA	C8-N7	2.07	1.35	1.31
54	2w	46	G7M	C5-C6	2.06	1.48	1.43
54	2w	46	G7M	C4-N9	-2.06	1.32	1.38
55	2x	54	5MU	C6-N1	-2.06	1.34	1.38
54	1y	8	4SU	C6-C5	2.06	1.39	1.35
1	1A	2503	2MA	C4-N9	-2.05	1.33	1.37
32	1a	966	M2G	C5-N7	-2.05	1.35	1.39
1	1A	1939	5MU	C2-N1	2.05	1.41	1.38
54	2w	8	4SU	C2-N3	-2.04	1.34	1.38
1	2A	2503	2MA	C8-N7	2.04	1.35	1.31
54	1y	54	5MU	C2-N3	-2.03	1.34	1.38
1	2A	2503	2MA	C4-N9	-2.03	1.33	1.37
54	1y	46	G7M	C5-C6	2.03	1.48	1.43
32	2a	1207	2MG	C5-N7	-2.03	1.35	1.39
1	2A	1915	5MU	C6-N1	-2.02	1.34	1.38
55	1x	8	4SU	C6-C5	2.02	1.39	1.35
1	1A	1939	5MU	C4-C5	2.02	1.48	1.44
1	2A	2605	PSU	C2-N3	-2.01	1.34	1.37
32	2a	1207	2MG	C2-N3	2.00	1.35	1.32

All (435) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-18.12	69.79	102.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	37	MIA	C12-C13-C14	-9.42	110.10	127.01
54	2w	37	MIA	C5-C4-N3	-9.08	117.61	127.18
54	1w	37	MIA	C5-C4-N3	-8.21	118.53	127.18
1	1A	2503	2MA	C5-C4-N3	-8.14	118.60	127.18
43	2l	92	0TD	CSB-SB-CB	8.10	116.92	102.36
1	2A	2503	2MA	C5-C4-N3	-8.06	118.69	127.18
54	2w	37	MIA	N3-C4-N9	7.49	136.49	126.99
32	2a	1207	2MG	C2-N3-C4	7.35	121.19	112.00
32	1a	1207	2MG	C2-N3-C4	7.03	120.79	112.00
32	1a	1498	UR3	C4-N3-C2	-6.94	119.00	124.58
32	2a	1498	UR3	C4-N3-C2	-6.77	119.13	124.58
1	2A	2503	2MA	N3-C4-N9	6.75	135.56	126.99
54	2y	8	4SU	C4-N3-C2	-6.64	120.95	127.31
32	1a	516	PSU	N1-C2-N3	6.52	122.05	115.17
54	1w	37	MIA	N3-C4-N9	6.49	135.22	126.99
54	1w	55	PSU	N1-C2-N3	6.42	121.94	115.17
55	2x	55	PSU	N1-C2-N3	6.42	121.94	115.17
1	2A	2605	PSU	N1-C2-N3	6.36	121.88	115.17
54	1y	55	PSU	N1-C2-N3	6.35	121.87	115.17
32	2a	516	PSU	N1-C2-N3	6.33	121.85	115.17
1	1A	2503	2MA	N3-C4-N9	6.33	135.03	126.99
1	2A	2251	OMG	C5-C4-N3	-6.33	118.32	128.39
54	1w	32	PSU	N1-C2-N3	6.21	121.72	115.17
32	2a	1207	2MG	C5-C4-N3	-6.19	118.53	128.39
1	1A	1911	PSU	N1-C2-N3	6.17	121.67	115.17
1	2A	1911	PSU	N1-C2-N3	6.16	121.66	115.17
54	2w	55	PSU	N1-C2-N3	6.10	121.61	115.17
54	2y	32	PSU	N1-C2-N3	6.09	121.59	115.17
54	2y	55	PSU	N1-C2-N3	6.07	121.57	115.17
54	1y	37	MIA	C5-C4-N3	-6.05	118.38	126.72
54	2w	32	PSU	N1-C2-N3	6.03	121.53	115.17
1	1A	1917	PSU	N1-C2-N3	6.02	121.52	115.17
54	2w	39	PSU	N1-C2-N3	6.01	121.51	115.17
1	1A	2251	OMG	C5-C4-N3	-5.98	118.87	128.39
32	2a	966	M2G	C5-C4-N3	-5.98	118.88	128.39
55	1x	55	PSU	N1-C2-N3	5.96	121.45	115.17
32	1a	966	M2G	C5-C4-N3	-5.95	118.92	128.39
54	1y	32	PSU	N1-C2-N3	5.94	121.44	115.17
54	1w	39	PSU	N1-C2-N3	5.94	121.43	115.17
1	1A	2605	PSU	N1-C2-N3	5.92	121.42	115.17
54	2w	8	4SU	C4-N3-C2	-5.88	121.68	127.31
54	2y	46	G7M	N9-C4-N3	5.87	137.69	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	39	PSU	N1-C2-N3	5.86	121.35	115.17
1	2A	1939	5MU	C4-N3-C2	-5.85	119.66	127.34
1	2A	1917	PSU	N1-C2-N3	5.77	121.26	115.17
54	2y	8	4SU	C5-C4-N3	5.76	120.11	114.75
55	2x	76	31H	N1-C2-N3	-5.76	119.86	128.58
55	1x	76	31H	N1-C2-N3	-5.74	119.89	128.58
54	2y	37	MIA	C5-C4-N3	-5.74	118.82	126.72
32	1a	1207	2MG	C5-C4-N3	-5.71	119.31	128.39
54	1y	39	PSU	N1-C2-N3	5.68	121.16	115.17
1	2A	1939	5MU	N3-C2-N1	5.65	122.24	114.89
1	2A	2058	MA6	N1-C2-N3	-5.62	120.07	128.58
54	1y	46	G7M	N9-C4-N3	5.53	137.01	125.95
32	2a	527	G7M	N9-C4-N3	5.47	136.89	125.95
1	2A	1915	5MU	C4-N3-C2	-5.38	120.29	127.34
1	1A	2058	MA6	N1-C2-N3	-5.36	120.47	128.58
32	2a	527	G7M	C5-C4-N3	-5.35	118.04	128.15
54	2w	8	4SU	C5-C4-N3	5.33	119.71	114.75
1	1A	1915	5MU	C4-N3-C2	-5.33	120.35	127.34
54	2y	46	G7M	C5-C4-N3	-5.31	118.11	128.15
55	2x	54	5MU	C4-N3-C2	-5.28	120.42	127.34
54	1y	46	G7M	C5-C4-N3	-5.25	118.22	128.15
1	1A	1915	5MU	N3-C2-N1	5.23	121.70	114.89
32	1a	527	G7M	N9-C4-N3	5.21	136.37	125.95
1	1A	2058	MA6	N3-C4-N9	5.15	135.92	127.17
1	1A	1939	5MU	C5-C4-N3	5.14	119.79	115.32
1	2A	1915	5MU	N3-C2-N1	5.11	121.55	114.89
54	1w	54	5MU	N3-C2-N1	5.11	121.54	114.89
54	1w	46	G7M	N9-C4-N3	5.07	136.09	125.95
54	1w	8	4SU	C5-C4-N3	5.05	119.45	114.75
55	2x	54	5MU	N3-C2-N1	5.04	121.45	114.89
54	1y	8	4SU	C4-N3-C2	-5.03	122.49	127.31
55	1x	76	31H	C5-C4-N3	-5.02	119.81	126.72
1	1A	2251	OMG	C2-N3-C4	5.01	120.93	112.30
1	2A	1939	5MU	C5-C4-N3	5.00	119.67	115.32
32	1a	527	G7M	C5-C4-N3	-4.99	118.72	128.15
1	2A	2251	OMG	C2-N3-C4	4.95	120.83	112.30
1	2A	2251	OMG	N9-C4-N3	4.95	135.85	125.95
32	2a	1519	MA6	N1-C2-N3	-4.95	121.09	128.58
54	1w	54	5MU	C4-N3-C2	-4.93	120.88	127.34
55	2x	76	31H	C5-C4-N3	-4.92	119.94	126.72
1	2A	1915	5MU	C5-C4-N3	4.92	119.60	115.32
1	1A	2552	OMU	C4-N3-C2	-4.88	120.55	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1518	MA6	N1-C2-N3	-4.87	121.21	128.58
55	1x	54	5MU	N3-C2-N1	4.87	121.22	114.89
54	1w	8	4SU	C4-N3-C2	-4.86	122.66	127.31
54	1y	37	MIA	N3-C4-N9	4.85	135.42	127.17
55	1x	54	5MU	C4-N3-C2	-4.81	121.04	127.34
54	2w	46	G7M	C5-C4-N3	-4.80	119.08	128.15
54	1y	8	4SU	C5-C4-N3	4.78	119.20	114.75
1	2A	2552	OMU	C4-N3-C2	-4.77	120.69	126.61
32	1a	1519	MA6	N1-C2-N3	-4.76	121.38	128.58
54	2w	46	G7M	N9-C4-N3	4.76	135.47	125.95
1	1A	1939	5MU	C4-N3-C2	-4.76	121.11	127.34
32	1a	1518	MA6	N1-C2-N3	-4.71	121.45	128.58
54	2y	54	5MU	C4-N3-C2	-4.70	121.17	127.34
32	2a	527	G7M	C2-N3-C4	4.70	120.39	112.30
54	1w	46	G7M	C5-C4-N3	-4.68	119.31	128.15
1	1A	1915	5MU	O4-C4-C5	-4.67	119.57	124.92
54	1y	46	G7M	C2-N3-C4	4.67	120.34	112.30
1	1A	1915	5MU	C5-C4-N3	4.64	119.35	115.32
1	2A	2058	MA6	C9-N6-C6	-4.64	108.73	120.52
32	1a	1519	MA6	C5-C4-N3	-4.63	120.34	126.72
54	2y	54	5MU	N3-C2-N1	4.62	120.90	114.89
54	2y	37	MIA	N3-C4-N9	4.61	135.01	127.17
54	2y	46	G7M	C2-N3-C4	4.60	120.22	112.30
55	2x	54	5MU	C5-C4-N3	4.59	119.31	115.32
32	2a	1518	MA6	C5-C4-N3	-4.59	120.40	126.72
1	1A	2251	OMG	N9-C4-N3	4.48	134.91	125.95
32	2a	966	M2G	C2-N3-C4	4.48	120.80	112.51
1	2A	2058	MA6	C2-N1-C6	4.47	122.75	111.83
54	2y	54	5MU	O4-C4-C5	-4.46	119.81	124.92
32	1a	516	PSU	C4-N3-C2	-4.46	120.23	126.37
32	2a	1519	MA6	C5-C4-N3	-4.42	120.63	126.72
32	1a	966	M2G	N9-C4-N3	4.37	134.69	125.95
1	1A	2058	MA6	C5-C4-N3	-4.37	120.70	126.72
1	2A	1939	5MU	C5-C6-N1	-4.36	118.58	123.31
32	2a	516	PSU	C4-N3-C2	-4.35	120.38	126.37
1	2A	1915	5MU	O4-C4-C5	-4.34	119.95	124.92
55	2x	54	5MU	O4-C4-C5	-4.34	119.95	124.92
32	2a	966	M2G	N9-C4-N3	4.34	134.62	125.95
1	1A	2552	OMU	N3-C2-N1	4.32	120.52	114.89
1	2A	2605	PSU	C4-N3-C2	-4.32	120.42	126.37
54	2w	54	5MU	N3-C2-N1	4.31	120.51	114.89
1	2A	1939	5MU	O4-C4-C5	-4.31	119.99	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	54	5MU	C5-C4-N3	4.31	119.07	115.32
55	2x	55	PSU	C4-N3-C2	-4.30	120.45	126.37
1	1A	1939	5MU	C5-C6-N1	-4.28	118.66	123.31
1	1A	1939	5MU	N3-C2-N1	4.28	120.46	114.89
55	1x	54	5MU	C5-C4-N3	4.28	119.04	115.32
54	2w	54	5MU	C4-N3-C2	-4.28	121.73	127.34
32	1a	527	G7M	C2-N3-C4	4.26	119.64	112.30
32	1a	966	M2G	C2-N3-C4	4.26	120.38	112.51
54	1w	46	G7M	C2-N3-C4	4.24	119.60	112.30
54	1w	54	5MU	O4-C4-C5	-4.23	120.08	124.92
54	2w	46	G7M	C2-N3-C4	4.20	119.54	112.30
54	1w	37	MIA	C15-C14-C13	-4.19	110.07	122.66
1	1A	2605	PSU	C4-N3-C2	-4.18	120.62	126.37
55	1x	55	PSU	C4-N3-C2	-4.17	120.62	126.37
32	1a	1518	MA6	C5-C4-N3	-4.17	120.98	126.72
1	1A	2058	MA6	C9-N6-C6	4.15	131.08	120.52
1	1A	2058	MA6	C5-C6-N6	-4.15	118.77	125.33
55	1x	8	4SU	O2-C2-N1	4.14	128.19	122.80
55	1x	8	4SU	C6-C5-C4	-4.12	116.39	119.95
54	1w	32	PSU	C4-N3-C2	-4.11	120.71	126.37
32	2a	516	PSU	O2-C2-N1	-4.10	118.56	122.79
32	2a	1519	MA6	C2-N1-C6	4.09	121.82	111.83
1	2A	1911	PSU	C4-N3-C2	-4.08	120.75	126.37
32	2a	1207	2MG	N9-C4-N3	4.06	134.07	125.95
54	1w	55	PSU	C4-N3-C2	-4.05	120.80	126.37
54	1y	54	5MU	N3-C2-N1	4.04	120.15	114.89
1	1A	1917	PSU	O2-C2-N1	-4.03	118.63	122.79
32	2a	1518	MA6	C2-N1-C6	4.03	121.68	111.83
1	1A	1911	PSU	C4-N3-C2	-4.03	120.82	126.37
1	1A	1917	PSU	C4-N3-C2	-4.03	120.82	126.37
1	2A	1917	PSU	C4-N3-C2	-4.02	120.83	126.37
1	2A	2552	OMU	C5-C4-N3	4.02	120.43	114.80
1	2A	2552	OMU	N3-C2-N1	4.01	120.11	114.89
54	2w	39	PSU	C4-N3-C2	-4.00	120.85	126.37
54	2y	8	4SU	N3-C2-N1	4.00	120.10	114.89
54	1w	54	5MU	C5-C4-N3	3.99	118.79	115.32
54	2y	32	PSU	C4-N3-C2	-3.98	120.88	126.37
32	2a	1519	MA6	C5-N7-C8	3.98	109.70	103.45
54	1y	32	PSU	C4-N3-C2	-3.97	120.90	126.37
32	1a	1519	MA6	C4-C5-N7	-3.95	106.06	110.58
32	2a	1519	MA6	C4-C5-N7	-3.95	106.07	110.58
32	1a	1519	MA6	C5-N7-C8	3.95	109.66	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1207	2MG	C6-C5-N7	3.94	137.46	130.29
54	1y	55	PSU	C4-N3-C2	-3.94	120.95	126.37
32	1a	1404	5MC	C5-C6-N1	-3.94	119.04	123.31
32	1a	1518	MA6	C2-N1-C6	3.92	121.40	111.83
54	2w	55	PSU	C4-N3-C2	-3.91	120.99	126.37
54	2w	54	5MU	C5-C4-N3	3.90	118.71	115.32
32	1a	967	5MC	C5-C6-N1	-3.88	119.09	123.31
54	2w	32	PSU	C4-N3-C2	-3.88	121.03	126.37
32	1a	1519	MA6	C2-N1-C6	3.87	121.29	111.83
1	1A	2058	MA6	C2-N3-C4	3.85	121.24	111.83
1	1A	1942	5MC	C5-C6-N1	-3.85	119.14	123.31
1	1A	2058	MA6	C4-N9-C8	3.84	109.77	105.74
54	1w	55	PSU	O2-C2-N1	-3.80	118.87	122.79
54	1w	37	MIA	C16-C14-C13	-3.79	111.28	122.66
55	1x	32	5MC	C5-C6-N1	-3.78	119.21	123.31
32	2a	1400	5MC	C5-C6-N1	-3.77	119.22	123.31
55	1x	54	5MU	C5-C6-N1	-3.77	119.22	123.31
54	1w	39	PSU	C4-N3-C2	-3.77	121.18	126.37
32	1a	1518	MA6	C5-N7-C8	3.76	109.36	103.45
32	1a	1207	2MG	N9-C4-N3	3.76	133.47	125.95
55	1x	8	4SU	S4-C4-N3	-3.75	116.28	120.20
54	2w	8	4SU	N3-C2-N1	3.73	119.75	114.89
32	1a	1400	5MC	C5-C6-N1	-3.72	119.28	123.31
54	2w	54	5MU	O4-C4-C5	-3.70	120.68	124.92
1	2A	2058	MA6	N9-C8-N7	-3.70	108.69	113.94
54	2y	8	4SU	C5-C4-S4	-3.69	120.09	124.31
54	1y	54	5MU	C4-N3-C2	-3.69	122.51	127.34
1	1A	2552	OMU	C5-C4-N3	3.68	119.95	114.80
54	2y	37	MIA	C2-N3-C4	3.67	120.81	111.83
1	2A	1915	5MU	C5-C6-N1	-3.67	119.33	123.31
55	1x	54	5MU	O4-C4-C5	-3.65	120.74	124.92
32	1a	1518	MA6	C4-C5-N7	-3.65	106.41	110.58
54	2y	55	PSU	C4-N3-C2	-3.63	121.36	126.37
1	2A	2503	2MA	N6-C6-N1	3.63	121.93	117.03
54	1w	39	PSU	O2-C2-N1	-3.62	119.05	122.79
32	2a	1518	MA6	C5-N7-C8	3.62	109.14	103.45
54	2y	39	PSU	C4-N3-C2	-3.62	121.38	126.37
54	1y	8	4SU	N3-C2-N1	3.62	119.60	114.89
54	1y	37	MIA	C2-N3-C4	3.60	120.62	111.83
54	1y	32	PSU	O2-C2-N1	-3.60	119.08	122.79
55	2x	32	5MC	C5-C6-N1	-3.59	119.41	123.31
32	2a	1518	MA6	C4-C5-N7	-3.58	106.48	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2503	2MA	C4-C5-N7	-3.58	106.49	110.58
55	2x	54	5MU	C5-C6-N1	-3.56	119.45	123.31
32	2a	1207	2MG	C6-C5-N7	3.56	136.76	130.29
54	1y	39	PSU	C4-N3-C2	-3.55	121.48	126.37
1	2A	1911	PSU	O2-C2-N1	-3.52	119.16	122.79
54	2y	32	PSU	O2-C2-N1	-3.52	119.16	122.79
32	2a	1519	MA6	N9-C8-N7	-3.52	108.94	113.94
54	1y	54	5MU	O4-C4-C5	-3.49	120.93	124.92
32	2a	1404	5MC	C5-C6-N1	-3.49	119.53	123.31
54	1y	54	5MU	C5-C4-N3	3.48	118.35	115.32
55	2x	76	31H	N9-C8-N7	-3.47	109.02	113.94
32	1a	1519	MA6	N9-C8-N7	-3.47	109.02	113.94
32	2a	1518	MA6	C2-N3-C4	3.46	120.27	111.83
32	1a	1519	MA6	C2-N3-C4	3.45	120.26	111.83
1	1A	2058	MA6	C2-N1-C6	3.45	120.25	111.83
55	1x	76	31H	N9-C8-N7	-3.44	109.05	113.94
32	2a	1519	MA6	C2-N3-C4	3.43	120.21	111.83
1	1A	1962	5MC	C5-C6-N1	-3.43	119.59	123.31
54	2w	37	MIA	C4-C5-N7	-3.42	106.67	110.58
32	2a	1407	5MC	C5-C4-N3	-3.41	118.25	121.75
1	2A	2058	MA6	C5-N7-C8	3.41	108.81	103.45
54	2y	37	MIA	C4-C5-N7	-3.41	106.69	110.58
54	1w	37	MIA	C4-C5-N7	-3.40	106.70	110.58
54	1y	37	MIA	C4-C5-N7	-3.39	106.70	110.58
54	2y	37	MIA	N3-C2-N1	-3.39	123.45	128.58
54	2y	55	PSU	O2-C2-N1	-3.39	119.29	122.79
55	1x	76	31H	C2-N3-C4	3.37	120.07	111.83
1	2A	1942	5MC	C5-C6-N1	-3.36	119.67	123.31
32	1a	1518	MA6	N9-C8-N7	-3.35	109.19	113.94
1	1A	1911	PSU	O2-C2-N1	-3.34	119.34	122.79
55	2x	76	31H	C2-N3-C4	3.33	119.97	111.83
54	1y	55	PSU	O2-C2-N1	-3.33	119.35	122.79
55	2x	55	PSU	O2-C2-N1	-3.33	119.36	122.79
54	2w	55	PSU	O2-C2-N1	-3.32	119.36	122.79
1	1A	2251	OMG	C6-C5-N7	3.31	136.31	130.29
32	2a	966	M2G	C6-C5-N7	3.29	136.28	130.29
1	1A	1942	5MC	C5-C4-N3	-3.29	118.38	121.75
54	1w	37	MIA	C6-C5-N7	3.29	136.01	132.43
32	1a	1518	MA6	C2-N3-C4	3.29	119.86	111.83
54	2w	37	MIA	C2-N3-C4	3.28	120.88	112.29
54	2w	8	4SU	C5-C4-S4	-3.27	120.57	124.31
1	2A	1962	5MC	C5-C6-N1	-3.24	119.79	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	37	MIA	C2-N3-C4	3.23	120.75	112.29
32	2a	1407	5MC	C5-C6-N1	-3.22	119.81	123.31
32	2a	1498	UR3	C5-C4-N3	3.21	119.27	115.04
54	1w	8	4SU	N3-C2-N1	3.19	119.05	114.89
32	1a	1498	UR3	C5-C4-N3	3.19	119.24	115.04
54	1y	37	MIA	N3-C2-N1	-3.16	123.80	128.58
1	2A	2605	PSU	O2-C2-N1	-3.16	119.53	122.79
32	1a	1207	2MG	C4-C5-N7	-3.16	105.67	110.67
1	2A	2503	2MA	C4-C5-N7	-3.14	106.99	110.58
1	2A	2058	MA6	C2-N3-C4	3.13	119.48	111.83
1	1A	1939	5MU	O4-C4-C5	-3.13	121.33	124.92
32	2a	1518	MA6	N9-C8-N7	-3.12	109.51	113.94
54	2w	32	PSU	O2-C2-N1	-3.12	119.58	122.79
1	2A	1917	PSU	O2-C2-N1	-3.10	119.59	122.79
1	2A	2503	2MA	C4-N9-C8	3.10	108.99	105.74
43	2l	92	0TD	OD2-CG-CB	3.09	119.82	113.15
32	1a	1407	5MC	C5-C6-N1	-3.08	119.97	123.31
1	1A	2552	OMU	O4-C4-C5	-3.07	119.86	125.16
43	1l	92	0TD	OD2-CG-CB	3.06	119.76	113.15
55	2x	76	31H	C5-N7-C8	3.04	108.23	103.45
55	1x	8	4SU	C5-C4-N3	3.04	117.58	114.75
32	1a	966	M2G	C6-C5-N7	3.02	135.78	130.29
55	2x	8	4SU	C6-C5-C4	-3.02	117.34	119.95
54	2w	39	PSU	O2-C2-N1	-3.02	119.67	122.79
55	1x	76	31H	O4'-C1'-N9	-3.01	102.31	108.09
32	1a	1404	5MC	C5-C4-N3	-3.01	118.67	121.75
1	1A	2058	MA6	N9-C8-N7	-3.00	109.68	113.94
55	1x	55	PSU	O2-C2-N1	-3.00	119.70	122.79
1	1A	2058	MA6	N1-C6-N6	2.99	120.50	116.86
1	2A	2251	OMG	C6-C5-N7	2.99	135.74	130.29
32	1a	1402	4OC	C6-C5-C4	2.97	120.58	117.00
54	1w	54	5MU	C5-C6-N1	-2.96	120.09	123.31
55	1x	76	31H	C5-N7-C8	2.96	108.10	103.45
55	1x	32	5MC	C5-C4-N3	-2.95	118.73	121.75
54	2y	54	5MU	C5-C6-N1	-2.95	120.11	123.31
54	1w	54	5MU	O2-C2-N1	-2.93	118.98	122.80
32	2a	967	5MC	C5-C6-N1	-2.93	120.14	123.31
1	2A	2058	MA6	C4-N9-C8	2.92	108.81	105.74
54	1w	8	4SU	C5-C4-S4	-2.92	120.97	124.31
32	2a	1404	5MC	C5-C4-N3	-2.92	118.77	121.75
1	1A	2503	2MA	C4-N9-C8	2.91	108.79	105.74
1	1A	2605	PSU	O2-C2-N1	-2.91	119.79	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	54	5MU	O2-C2-N1	-2.88	119.05	122.80
32	2a	1207	2MG	C4-C5-N7	-2.86	106.13	110.67
55	1x	76	31H	C4'-O4'-C1'	-2.85	103.18	109.47
32	2a	1518	MA6	N3-C4-N9	2.84	132.00	127.17
1	1A	2503	2MA	N6-C6-N1	2.84	120.85	117.03
1	2A	2552	OMU	O4-C4-C5	-2.84	120.27	125.16
1	2A	1939	5MU	O2-C2-N1	-2.83	119.11	122.80
54	2y	54	5MU	C1'-N1-C2	2.83	122.67	117.59
32	1a	1207	2MG	N1-C2-N2	2.82	119.44	116.56
1	2A	2058	MA6	C5-C4-N3	-2.82	122.84	126.72
1	1A	2058	MA6	C10-N6-C6	-2.81	113.38	120.52
1	2A	2058	MA6	C10-N6-C9	2.80	125.18	116.18
32	1a	1519	MA6	N3-C4-N9	2.78	131.89	127.17
55	2x	76	31H	C4'-O4'-C1'	-2.78	103.33	109.47
1	1A	1915	5MU	C5-C6-N1	-2.78	120.30	123.31
54	1w	32	PSU	O2-C2-N1	-2.77	119.93	122.79
55	2x	8	4SU	C1'-N1-C2	2.76	122.55	117.59
1	1A	1962	5MC	C5-C4-N3	-2.74	118.95	121.75
32	1a	516	PSU	O2-C2-N1	-2.73	119.97	122.79
54	1y	54	5MU	C5-C6-N1	-2.73	120.35	123.31
54	1w	37	MIA	C11-S10-C2	-2.73	100.20	102.25
55	2x	32	5MC	O2-C2-N3	-2.72	118.04	122.33
55	2x	76	31H	C5-C4-N9	2.72	108.78	105.81
54	2w	54	5MU	C5-C6-N1	-2.71	120.37	123.31
55	1x	76	31H	C5-C4-N9	2.70	108.75	105.81
32	2a	966	M2G	C4-C5-N7	-2.69	106.40	110.67
32	2a	1400	5MC	O2-C2-N3	-2.69	118.08	122.33
55	2x	32	5MC	C5-C4-N3	-2.69	119.00	121.75
32	2a	967	5MC	C5-C4-N3	-2.68	119.01	121.75
55	2x	8	4SU	O2-C2-N1	2.68	126.28	122.80
1	1A	2503	2MA	C5-N7-C8	2.67	107.65	103.45
32	1a	1407	5MC	C5-C4-N3	-2.67	119.02	121.75
55	2x	8	4SU	C5-C4-N3	2.66	117.22	114.75
1	2A	1962	5MC	C5-C4-N3	-2.66	119.03	121.75
32	2a	1519	MA6	N3-C4-N9	2.65	131.68	127.17
1	1A	2251	OMG	C4-C5-N7	-2.63	106.51	110.67
1	2A	1942	5MC	C5-C4-N3	-2.62	119.06	121.75
54	2w	37	MIA	C12-N6-C6	-2.61	120.42	122.85
54	2w	37	MIA	C5-N7-C8	2.61	107.56	103.45
1	1A	2058	MA6	C1'-N9-C8	-2.61	121.31	127.09
1	1A	2503	2MA	C2-N1-C6	2.61	122.11	118.10
54	2y	37	MIA	C4-N9-C8	2.60	108.47	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	966	M2G	C4-C5-N7	-2.60	106.56	110.67
54	2w	54	5MU	C5M-C5-C4	2.59	121.55	118.78
32	2a	1518	MA6	C4-C5-C6	2.57	118.57	115.91
55	1x	54	5MU	O2-C2-N1	-2.57	119.45	122.80
55	1x	8	4SU	O2-C2-N3	-2.56	116.77	121.49
54	1w	37	MIA	C2-N1-C6	2.55	122.38	117.54
32	1a	1518	MA6	N3-C4-N9	2.55	131.50	127.17
32	1a	1519	MA6	C4-C5-C6	2.54	118.54	115.91
54	1y	39	PSU	O2-C2-N1	-2.54	120.17	122.79
1	2A	2058	MA6	C4-C5-N7	-2.54	107.68	110.58
1	2A	2251	OMG	C4-C5-N7	-2.53	106.66	110.67
1	2A	2503	2MA	C2-N1-C6	2.53	121.99	118.10
32	2a	1207	2MG	N1-C2-N2	2.53	119.14	116.56
1	1A	2605	PSU	C5-C6-N1	-2.53	118.63	122.14
54	2y	54	5MU	C1'-N1-C6	-2.52	117.00	121.15
43	2l	92	0TD	OD1-CG-CB	-2.52	117.17	122.44
55	1x	8	4SU	C1'-N1-C2	2.51	122.11	117.59
55	1x	76	31H	N3-C4-N9	2.51	131.43	127.17
54	2y	39	PSU	O2-C2-N1	-2.50	120.21	122.79
32	1a	516	PSU	C5-C6-N1	-2.49	118.69	122.14
32	1a	967	5MC	C5-C4-N3	-2.48	119.21	121.75
54	1w	37	MIA	C5-N7-C8	2.47	107.33	103.45
1	2A	2503	2MA	C5-N7-C8	2.46	107.32	103.45
54	1w	46	G7M	O6-C6-C5	-2.46	122.52	128.01
54	2y	37	MIA	C5-N7-C8	2.46	107.31	103.45
32	2a	1402	4OC	C6-C5-C4	2.45	119.95	117.00
54	2w	54	5MU	O2-C2-N1	-2.45	119.61	122.80
54	1y	37	MIA	C5-N7-C8	2.44	107.29	103.45
32	1a	527	G7M	O6-C6-C5	-2.44	122.57	128.01
1	1A	2552	OMU	O2-C2-N1	-2.43	119.63	122.80
32	1a	1400	5MC	C5-C4-N3	-2.43	119.27	121.75
1	2A	2552	OMU	O2-C2-N1	-2.43	119.64	122.80
55	2x	76	31H	N3-C4-N9	2.42	131.28	127.17
32	1a	1498	UR3	C6-N1-C2	-2.41	119.83	121.80
54	2y	46	G7M	O6-C6-C5	-2.41	122.63	128.01
54	2w	46	G7M	O6-C6-C5	-2.39	122.67	128.01
32	2a	1519	MA6	C4-C5-C6	2.36	118.35	115.91
1	1A	1915	5MU	O2-C2-N1	-2.35	119.74	122.80
1	2A	2058	MA6	N3-C4-N9	2.35	131.16	127.17
54	2w	37	MIA	C1'-N9-C8	-2.34	121.89	127.09
1	2A	2251	OMG	O6-C6-C5	-2.34	120.35	126.53
54	2w	37	MIA	C4-C5-C6	2.33	118.72	116.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	76	31H	OCN-CN-N	-2.31	119.34	125.32
54	1y	46	G7M	O6-C6-C5	-2.31	122.86	128.01
32	2a	527	G7M	C5-C6-N1	2.30	116.60	111.84
55	1x	76	31H	C6-C5-C4	2.30	120.31	117.18
54	1w	37	MIA	C4-N9-C8	2.29	108.14	105.74
1	1A	2503	2MA	N9-C8-N7	-2.28	110.70	113.94
1	2A	1915	5MU	O2-C2-N1	-2.26	119.85	122.80
32	1a	966	M2G	O6-C6-C5	-2.24	120.61	126.53
1	1A	2058	MA6	C5-C4-N9	-2.24	103.38	105.81
54	1y	8	4SU	C5-C4-S4	-2.23	121.76	124.31
1	2A	1911	PSU	C5-C6-N1	-2.23	119.04	122.14
54	2y	39	PSU	C5-C6-N1	-2.22	119.05	122.14
32	1a	1207	2MG	N2-C2-N3	-2.22	117.68	120.51
55	1x	55	PSU	C5-C6-N1	-2.22	119.06	122.14
1	1A	2503	2MA	C6-C5-N7	2.22	136.36	132.09
32	2a	1400	5MC	C5-C4-N3	-2.21	119.49	121.75
54	2w	37	MIA	C4-N9-C8	2.21	108.06	105.74
54	2w	37	MIA	C2-N1-C6	2.21	121.73	117.54
55	2x	76	31H	C6-C5-C4	2.20	120.19	117.18
55	1x	76	31H	CA-N-CN	-2.20	119.44	122.82
32	2a	1207	2MG	N2-C2-N3	-2.20	117.71	120.51
32	2a	1498	UR3	C6-N1-C2	-2.19	120.01	121.80
54	1w	37	MIA	N3-C2-N1	-2.19	123.00	127.00
54	2w	8	4SU	C1'-N1-C2	2.19	121.53	117.59
1	2A	2058	MA6	C10-N6-C6	2.19	126.09	120.52
32	1a	516	PSU	O2-C2-N3	-2.18	117.98	121.86
1	2A	2605	PSU	C5-C6-N1	-2.18	119.11	122.14
55	2x	55	PSU	C5-C6-N1	-2.17	119.13	122.14
32	2a	516	PSU	O4'-C1'-C2'	2.16	108.14	105.15
32	1a	1207	2MG	C8-N7-C5	2.14	108.08	104.26
55	2x	76	31H	C4-C5-N7	-2.14	108.13	110.58
1	2A	1917	PSU	C5-C6-N1	-2.13	119.18	122.14
32	2a	527	G7M	O6-C6-C5	-2.13	123.26	128.01
55	1x	76	31H	C4-C5-N7	-2.12	108.15	110.58
32	1a	516	PSU	O4'-C1'-C2'	2.12	108.09	105.15
32	1a	1498	UR3	C1'-N1-C2	2.12	120.51	117.04
55	1x	32	5MC	O2-C2-N3	-2.12	118.98	122.33
1	2A	2503	2MA	N9-C8-N7	-2.11	110.94	113.94
54	1y	37	MIA	C4-N9-C8	2.11	107.95	105.74
1	1A	2251	OMG	O6-C6-C5	-2.09	121.00	126.53
32	2a	1207	2MG	C2-N1-C6	-2.09	122.02	124.55
55	2x	8	4SU	S4-C4-N3	-2.06	118.05	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	966	M2G	O6-C6-C5	-2.06	121.09	126.53
1	2A	1920	OMC	O2-C2-N3	-2.05	119.10	122.33
1	1A	1911	PSU	C5-C6-N1	-2.04	119.31	122.14
54	1y	54	5MU	C1'-N1-C2	2.03	121.24	117.59
1	1A	2251	OMG	C8-N7-C5	2.03	107.88	104.26
54	2y	55	PSU	C6-C5-C4	-2.02	116.81	118.17
55	1x	8	4SU	C4-N3-C2	2.02	129.25	127.31
54	2y	55	PSU	O4'-C1'-C2'	2.02	107.95	105.15
1	2A	1962	5MC	CM5-C5-C6	-2.02	120.12	122.85
54	1w	8	4SU	C1'-N1-C2	2.01	121.21	117.59
55	2x	76	31H	OCN-CN-N	-2.01	120.13	125.32
54	2w	37	MIA	C6-C5-N7	2.01	134.62	132.43
32	1a	1518	MA6	C4-C5-C6	2.00	117.98	115.91
54	2w	32	PSU	C5-C6-N1	-2.00	119.36	122.14

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	C12-C13-C14-C16
55	1x	76	31H	C-CA-CB-CG
54	1y	8	4SU	O4'-C4'-C5'-O5'
54	1y	46	G7M	C4'-C5'-O5'-P
43	2l	92	0TD	O-C-CA-CB
43	2l	92	0TD	SB-CB-CG-OD2
43	2l	92	0TD	SB-CB-CG-OD1
55	2x	76	31H	C-CA-CB-CG
54	2y	54	5MU	O4'-C4'-C5'-O5'
54	2y	55	PSU	C3'-C4'-C5'-O5'
55	1x	76	31H	C3'-C4'-C5'-O5'
55	2x	76	31H	C3'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
54	2y	54	5MU	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'
32	1a	527	G7M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
55	2x	76	31H	C4'-C5'-O5'-P
55	1x	76	31H	C4'-C5'-O5'-P
54	2w	46	G7M	C4'-C5'-O5'-P
54	2y	46	G7M	O4'-C1'-N9-C4
43	2l	92	0TD	CG-CB-SB-CSB
32	1a	1402	4OC	O4'-C4'-C5'-O5'
54	1y	54	5MU	C3'-C4'-C5'-O5'
1	2A	2503	2MA	O4'-C4'-C5'-O5'
54	2y	37	MIA	C3'-C4'-C5'-O5'
54	1w	46	G7M	C4'-C5'-O5'-P
54	1y	55	PSU	O4'-C1'-C5-C4
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
1	2A	1917	PSU	O4'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	527	G7M	C4'-C5'-O5'-P
32	2a	1519	MA6	C3'-C4'-C5'-O5'
54	2y	55	PSU	O4'-C1'-C5-C6
54	2w	37	MIA	N1-C2-S10-C11
32	2a	1402	4OC	O4'-C4'-C5'-O5'
54	2y	46	G7M	O4'-C1'-N9-C8
55	1x	76	31H	CB-CA-N-CN
54	2w	37	MIA	N3-C2-S10-C11
32	1a	1519	MA6	C4'-C5'-O5'-P
54	2y	54	5MU	C2'-C1'-N1-C2
1	2A	1915	5MU	O4'-C4'-C5'-O5'
1	2A	2503	2MA	C3'-C4'-C5'-O5'
32	2a	527	G7M	C4'-C5'-O5'-P
54	1y	8	4SU	C4'-C5'-O5'-P
1	1A	1920	OMC	C2'-C1'-N1-C2

There are no ring outliers.

31 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1915	5MU	1	0
1	1A	2503	2MA	1	0
54	1y	54	5MU	1	0
32	1a	1518	MA6	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	966	M2G	1	0
1	1A	2058	MA6	1	0
32	2a	1518	MA6	4	0
54	2y	8	4SU	2	0
1	2A	2058	MA6	3	0
1	1A	2552	OMU	1	0
54	1w	37	MIA	1	0
54	2y	46	G7M	1	0
54	1y	46	G7M	1	0
32	2a	1519	MA6	2	0
54	1y	32	PSU	1	0
54	2y	55	PSU	7	0
43	2l	92	0TD	1	0
1	2A	1939	5MU	1	0
54	1w	46	G7M	1	0
54	2y	37	MIA	1	0
54	2y	39	PSU	1	0
32	1a	1519	MA6	1	0
54	2y	54	5MU	1	0
1	2A	2251	OMG	1	0
55	2x	32	5MC	1	0
32	1a	1402	4OC	2	0
54	1y	37	MIA	1	0
54	1y	8	4SU	1	0
54	2w	39	PSU	1	0
54	1w	8	4SU	1	0
55	1x	8	4SU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2682 ligands modelled in this entry, 2678 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	$\# Z > 2$
59	SF4	2d	303	35	0,12,12	-	-	-		
57	WC9	2A	3809	-	34,37,37	1.36	5 (14%)	31,53,53	1.18	3 (9%)
59	SF4	1d	302	35	0,12,12	-	-	-		
57	WC9	1A	4098	-	34,37,37	1.45	5 (14%)	31,53,53	1.36	6 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	2d	303	35	-	-	0/6/5/5
57	WC9	2A	3809	-	-	2/28/71/71	0/3/4/4
59	SF4	1d	302	35	-	-	0/6/5/5
57	WC9	1A	4098	-	-	3/28/71/71	0/3/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2A	3809	WC9	CAM-CBF	-4.74	1.40	1.51
57	1A	4098	WC9	CAM-CBF	-4.54	1.40	1.51
57	1A	4098	WC9	CD2-CAZ	-2.90	1.50	1.53
57	1A	4098	WC9	CAF-CAE	-2.85	1.48	1.53
57	2A	3809	WC9	OAW-CB	2.81	1.45	1.42
57	1A	4098	WC9	CAB-CAK	-2.59	1.49	1.53
57	2A	3809	WC9	CD2-CAZ	-2.45	1.51	1.53
57	2A	3809	WC9	CG-CB	-2.36	1.49	1.53
57	1A	4098	WC9	CBF-CBH	2.20	1.40	1.31
57	2A	3809	WC9	CBF-CBH	2.17	1.40	1.31

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2A	3809	WC9	CBC-CBB-CAZ	-3.14	110.58	116.68
57	1A	4098	WC9	CBC-CBB-CAZ	-3.05	110.77	116.68
57	1A	4098	WC9	CAF-OAA-CAB	-2.99	110.25	114.17
57	1A	4098	WC9	OAA-CAF-CAE	-2.79	106.47	110.32
57	2A	3809	WC9	CAF-OAA-CAB	-2.61	110.75	114.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1A	4098	WC9	CD2-CAZ-CAY	-2.54	110.00	113.78
57	1A	4098	WC9	OAA-CAF-SAG	2.34	116.38	109.94
57	1A	4098	WC9	CAF-CAE-CAD	2.07	114.60	110.55
57	2A	3809	WC9	CD2-CAZ-CAY	-2.06	110.70	113.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

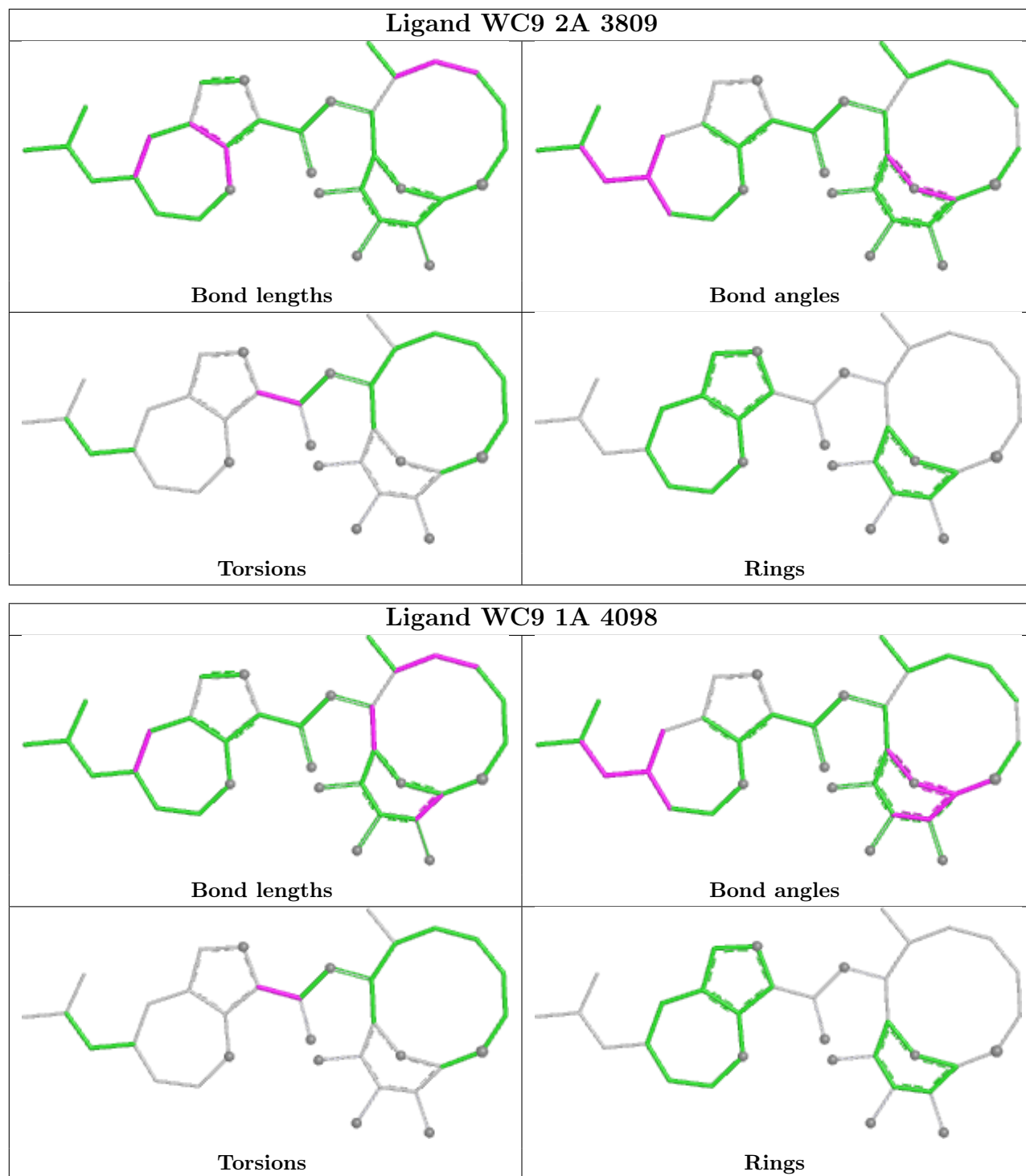
Mol	Chain	Res	Type	Atoms
57	1A	4098	WC9	O-C-CA-CB
57	2A	3809	WC9	O-C-CA-CB
57	1A	4098	WC9	NAL-C-CA-CB
57	2A	3809	WC9	NAL-C-CA-CB
57	1A	4098	WC9	O-C-CA-N

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	2A	3809	WC9	4	0
57	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	2859/2915 (98%)	-0.46	162 (5%)	29	29	24, 40, 98, 110	0
1	2A	2788/2915 (95%)	0.01	139 (4%)	34	33	35, 58, 96, 108	0
2	1B	120/121 (99%)	-0.28	0	100	100	35, 53, 67, 93	0
2	2B	120/121 (99%)	0.53	0	100	100	62, 75, 85, 97	0
3	1D	275/276 (99%)	-0.09	4 (1%)	72	73	24, 40, 53, 82	0
3	2D	275/276 (99%)	0.25	7 (2%)	58	59	33, 50, 62, 82	0
4	1E	204/206 (99%)	-0.13	2 (0%)	79	80	23, 42, 61, 74	0
4	2E	204/206 (99%)	0.58	7 (3%)	48	49	39, 60, 73, 83	0
5	1F	203/210 (96%)	0.14	7 (3%)	48	49	22, 46, 70, 89	0
5	2F	203/210 (96%)	0.63	10 (4%)	35	34	36, 68, 81, 87	0
6	1G	181/182 (99%)	0.67	11 (6%)	27	26	42, 62, 75, 89	0
6	2G	181/182 (99%)	1.35	29 (16%)	5	4	67, 77, 85, 92	0
7	1H	174/180 (96%)	0.30	3 (1%)	69	69	40, 55, 67, 77	0
7	2H	174/180 (96%)	1.91	70 (40%)	0	0	71, 85, 94, 96	0
8	1I	146/148 (98%)	0.99	7 (4%)	35	35	48, 75, 83, 86	0
8	2I	146/148 (98%)	1.07	13 (8%)	15	14	52, 74, 83, 88	0
9	1N	140/140 (100%)	-0.04	2 (1%)	73	74	30, 41, 61, 76	0
9	2N	140/140 (100%)	0.87	5 (3%)	46	47	52, 67, 80, 88	0
10	1O	122/122 (100%)	-0.04	1 (0%)	82	84	31, 43, 60, 66	0
10	2O	122/122 (100%)	0.63	3 (2%)	58	59	48, 61, 72, 76	0
11	1P	149/150 (99%)	0.21	2 (1%)	75	75	25, 50, 71, 78	0
11	2P	149/150 (99%)	0.83	11 (7%)	20	19	40, 68, 85, 91	0
12	1Q	141/141 (100%)	0.12	5 (3%)	47	48	30, 44, 62, 74	0
12	2Q	141/141 (100%)	1.11	20 (14%)	6	5	54, 68, 79, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.22	1 (0%) 82 84	28, 38, 51, 61	0
13	2R	118/118 (100%)	0.36	2 (1%) 69 69	44, 54, 64, 74	0
14	1S	110/112 (98%)	0.34	1 (0%) 81 83	42, 53, 66, 69	0
14	2S	110/112 (98%)	1.13	12 (10%) 10 10	63, 73, 79, 85	0
15	1T	131/146 (89%)	0.29	6 (4%) 37 38	36, 49, 74, 83	0
15	2T	131/146 (89%)	0.79	8 (6%) 27 26	52, 65, 79, 85	0
16	1U	116/118 (98%)	-0.33	1 (0%) 81 83	25, 33, 46, 68	0
16	2U	116/118 (98%)	0.67	3 (2%) 57 58	47, 63, 77, 83	0
17	1V	101/101 (100%)	-0.27	1 (0%) 79 80	25, 41, 58, 68	0
17	2V	101/101 (100%)	0.83	4 (3%) 42 43	44, 73, 81, 93	0
18	1W	112/113 (99%)	-0.24	1 (0%) 81 83	27, 34, 54, 82	0
18	2W	112/113 (99%)	0.28	2 (1%) 67 68	43, 51, 67, 95	0
19	1X	95/96 (98%)	0.11	3 (3%) 50 51	31, 44, 69, 84	0
19	2X	95/96 (98%)	0.67	5 (5%) 32 31	46, 61, 75, 86	0
20	1Y	107/110 (97%)	0.45	3 (2%) 55 56	37, 52, 69, 78	0
20	2Y	107/110 (97%)	1.18	17 (15%) 5 4	57, 71, 83, 90	0
21	1Z	154/206 (74%)	1.05	23 (14%) 5 5	40, 67, 89, 93	0
21	2Z	160/206 (77%)	2.00	71 (44%) 0 0	70, 84, 93, 96	0
22	10	77/85 (90%)	0.02	1 (1%) 75 75	30, 41, 55, 72	0
22	20	83/85 (97%)	1.33	13 (15%) 5 4	46, 65, 78, 87	0
23	11	97/98 (98%)	0.33	1 (1%) 79 80	31, 47, 75, 80	0
23	21	97/98 (98%)	0.53	1 (1%) 79 80	39, 55, 75, 80	0
24	12	70/72 (97%)	0.50	2 (2%) 53 55	41, 53, 65, 76	0
24	22	70/72 (97%)	0.85	2 (2%) 53 55	58, 72, 80, 85	0
25	13	59/60 (98%)	-0.02	3 (5%) 33 33	28, 38, 62, 81	0
25	23	59/60 (98%)	0.90	4 (6%) 23 22	60, 68, 81, 89	0
26	14	69/71 (97%)	1.34	15 (21%) 2 2	57, 77, 90, 95	0
26	24	69/71 (97%)	1.82	24 (34%) 1 0	76, 87, 95, 98	0
27	15	59/60 (98%)	-0.28	1 (1%) 69 69	24, 35, 53, 60	0
27	25	59/60 (98%)	0.32	2 (3%) 48 49	41, 53, 68, 82	0
28	16	53/54 (98%)	-0.11	0 100 100	37, 45, 58, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.59	1 (1%) 66 66	48, 61, 70, 75	0
29	17	48/49 (97%)	0.02	4 (8%) 17 17	24, 31, 64, 70	0
29	27	48/49 (97%)	0.36	4 (8%) 17 17	36, 42, 70, 76	0
30	18	64/65 (98%)	-0.21	0 100 100	29, 37, 44, 58	0
30	28	64/65 (98%)	0.62	0 100 100	48, 56, 64, 70	0
31	19	37/37 (100%)	-0.11	0 100 100	34, 42, 59, 62	0
31	29	37/37 (100%)	1.21	4 (10%) 11 10	66, 72, 79, 83	0
32	1a	1488/1521 (97%)	0.30	60 (4%) 42 43	38, 69, 96, 108	0
32	2a	1491/1521 (98%)	0.58	96 (6%) 25 24	48, 75, 96, 109	0
33	1b	231/256 (90%)	1.63	70 (30%) 1 0	67, 81, 90, 94	0
33	2b	231/256 (90%)	1.89	95 (41%) 0 0	73, 85, 91, 95	0
34	1c	206/239 (86%)	1.21	30 (14%) 6 5	64, 76, 86, 95	0
34	2c	206/239 (86%)	1.97	98 (47%) 0 0	75, 83, 90, 92	0
35	1d	208/209 (99%)	1.18	36 (17%) 4 3	55, 72, 81, 90	0
35	2d	208/209 (99%)	0.91	5 (2%) 59 61	60, 68, 76, 82	0
36	1e	148/162 (91%)	0.86	8 (5%) 31 31	53, 67, 77, 84	0
36	2e	148/162 (91%)	1.30	18 (12%) 8 7	60, 74, 82, 86	0
37	1f	100/101 (99%)	0.92	8 (8%) 18 18	59, 70, 78, 83	0
37	2f	100/101 (99%)	0.67	1 (1%) 79 80	60, 69, 77, 84	0
38	1g	155/156 (99%)	1.05	22 (14%) 6 5	64, 73, 85, 89	0
38	2g	155/156 (99%)	1.25	28 (18%) 3 3	68, 78, 88, 93	0
39	1h	137/138 (99%)	0.79	3 (2%) 62 63	55, 68, 74, 80	0
39	2h	137/138 (99%)	1.25	17 (12%) 8 7	67, 76, 81, 87	0
40	1i	127/128 (99%)	1.54	29 (22%) 2 2	59, 80, 87, 89	0
40	2i	127/128 (99%)	2.00	63 (49%) 0 0	72, 84, 90, 91	0
41	1j	97/105 (92%)	1.82	30 (30%) 1 0	59, 80, 89, 93	0
41	2j	96/105 (91%)	2.36	60 (62%) 0 0	75, 86, 92, 95	0
42	1k	114/129 (88%)	0.80	12 (10%) 11 11	45, 67, 78, 84	0
42	2k	114/129 (88%)	1.09	14 (12%) 8 7	55, 72, 82, 86	0
43	1l	121/132 (91%)	0.40	4 (3%) 49 50	46, 56, 70, 75	0
43	2l	121/132 (91%)	0.99	10 (8%) 17 17	54, 67, 78, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	1.08	11 (8%) 15 14	58, 73, 82, 90	0
44	2m	122/126 (96%)	1.78	37 (30%) 1 0	72, 83, 87, 93	0
45	1n	60/61 (98%)	1.39	12 (20%) 3 2	63, 72, 78, 80	0
45	2n	60/61 (98%)	2.62	45 (75%) 0 0	76, 83, 89, 93	0
46	1o	88/89 (98%)	0.83	6 (6%) 23 22	49, 67, 75, 82	0
46	2o	88/89 (98%)	0.90	4 (4%) 38 38	60, 72, 82, 85	0
47	1p	82/88 (93%)	1.46	13 (15%) 5 4	59, 72, 81, 86	0
47	2p	82/88 (93%)	1.09	7 (8%) 16 16	59, 69, 77, 82	0
48	1q	99/105 (94%)	0.91	4 (4%) 42 43	55, 68, 77, 80	0
48	2q	99/105 (94%)	0.88	5 (5%) 33 33	61, 72, 82, 84	0
49	1r	68/88 (77%)	0.79	4 (5%) 28 27	59, 67, 79, 82	0
49	2r	68/88 (77%)	0.82	2 (2%) 53 55	61, 70, 79, 83	0
50	1s	83/93 (89%)	1.13	8 (9%) 13 13	66, 76, 83, 89	0
50	2s	83/93 (89%)	2.19	45 (54%) 0 0	78, 86, 91, 96	0
51	1t	96/106 (90%)	1.34	21 (21%) 2 2	62, 73, 83, 85	0
51	2t	96/106 (90%)	1.12	11 (11%) 9 8	59, 71, 84, 85	0
52	1u	23/27 (85%)	1.32	5 (21%) 2 2	66, 70, 74, 79	0
52	2u	23/27 (85%)	2.50	17 (73%) 0 0	73, 79, 83, 85	0
53	1v	13/24 (54%)	0.37	0 100 100	50, 59, 81, 94	0
53	2v	13/24 (54%)	1.13	3 (23%) 2 1	64, 74, 92, 100	0
54	1w	65/76 (85%)	0.81	8 (12%) 8 7	58, 87, 98, 104	0
54	1y	67/76 (88%)	1.04	8 (11%) 9 8	39, 94, 101, 104	0
54	2w	62/76 (81%)	1.24	11 (17%) 4 3	74, 93, 102, 106	0
54	2y	66/76 (86%)	1.30	11 (16%) 4 3	52, 98, 103, 106	0
55	1x	71/77 (92%)	0.16	2 (2%) 55 56	32, 63, 81, 90	0
55	2x	71/77 (92%)	0.43	3 (4%) 40 41	49, 76, 88, 101	0
All	All	20860/21748 (95%)	0.49	1886 (9%) 15 14	22, 65, 90, 110	0

All (1886) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	10.0
1	1A	653	A	8.5

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Mol	Chain	Res	Type	RSRZ
45	2n	2	ALA	8.0
1	2A	652(U)	G	7.7
1	2A	652(V)	C	7.6
44	1m	123	ALA	7.6
1	1A	652(V)	C	7.3
44	2m	124	PRO	7.2
1	1A	654	A	7.0
1	2A	653	A	6.9
1	1A	652(U)	G	6.9
44	1m	124	PRO	6.9
1	2A	652(T)	C	6.6
21	2Z	172	ALA	6.3
45	1n	2	ALA	6.3
51	1t	103	GLY	6.1
38	1g	80	VAL	6.1
21	1Z	146	ILE	6.0
21	1Z	141	VAL	6.0
41	2j	65	LEU	5.8
21	2Z	146	ILE	5.8
44	2m	122	LYS	5.8
50	2s	2	PRO	5.8
41	2j	32	ALA	5.8
33	2b	237	ALA	5.7
1	2A	652(C)	G	5.7
42	2k	49	GLY	5.6
23	2l	2	SER	5.6
22	20	2	ALA	5.6
32	1a	1532	U	5.5
38	2g	84	ASN	5.5
1	2A	2802	G	5.5
1	2A	2146	C	5.4
7	2H	128	PRO	5.4
1	1A	652(C)	G	5.4
44	1m	2	ALA	5.4
1	2A	654	A	5.3
1	1A	652(S)	C	5.3
40	1i	2	GLU	5.3
20	2Y	1	MET	5.3
33	1b	237	ALA	5.2
3	1D	276	LYS	5.2
1	1A	1057	A	5.2
45	2n	38	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
32	2a	1030(B)	C	5.2
38	2g	83	ALA	5.1
26	24	56	VAL	5.1
23	11	2	SER	5.1
1	2A	2147	G	5.1
22	20	3	HIS	5.0
33	2b	165	VAL	5.0
51	2t	103	GLY	5.0
1	1A	1078	U	5.0
1	2A	652(B)	A	5.0
34	2c	8	ILE	4.9
32	1a	1531	A	4.9
38	2g	82	GLY	4.9
38	2g	154	TYR	4.9
41	2j	59	SER	4.8
45	2n	34	TYR	4.8
41	2j	47	PHE	4.8
7	1H	2	SER	4.8
50	1s	9	VAL	4.8
1	2A	883	G	4.8
15	1T	131	ALA	4.8
21	1Z	1	MET	4.8
1	1A	2804	C	4.8
45	2n	39	LEU	4.8
7	1H	174	GLY	4.7
1	1A	1058	G	4.7
40	2i	102	LEU	4.7
1	1A	652(T)	C	4.7
1	1A	885	C	4.6
1	2A	2145	C	4.6
54	1w	74	C	4.6
44	1m	122	LYS	4.6
33	2b	11	LEU	4.6
34	1c	2	GLY	4.6
1	2A	885	C	4.6
5	1F	208	GLY	4.6
1	2A	2893	G	4.6
32	2a	1033	G	4.6
29	27	48	LYS	4.6
22	20	84	LEU	4.5
33	2b	236	TYR	4.5
1	2A	2113	U	4.5

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Mol	Chain	Res	Type	RSRZ
1	1A	2793	G	4.5
22	20	5	LYS	4.5
1	2A	2803	C	4.5
32	1a	1257	U	4.5
41	2j	63	PHE	4.4
1	2A	1536	C	4.4
32	1a	1503	A	4.4
38	1g	154	TYR	4.4
42	1k	25	TYR	4.4
34	2c	207	VAL	4.4
7	2H	2	SER	4.4
1	1A	888	C	4.4
1	2A	2111	C	4.4
1	2A	2125	G	4.4
50	1s	13	ASP	4.4
1	2A	1509	C	4.4
34	2c	149	ALA	4.4
26	24	51	ASP	4.4
29	17	48	LYS	4.3
38	2g	80	VAL	4.3
35	1d	194	LEU	4.3
33	2b	7	VAL	4.3
22	20	4	LYS	4.3
33	1b	9	GLU	4.3
41	1j	32	ALA	4.3
32	2a	1001(A)	G	4.3
46	2o	89	GLY	4.3
1	1A	1094	U	4.2
50	2s	80	TYR	4.2
32	2a	1030	C	4.2
33	2b	70	PHE	4.2
44	2m	102	ARG	4.2
21	2Z	173	ALA	4.2
1	2A	884	C	4.2
26	14	45	GLY	4.2
32	2a	1030(A)	G	4.2
32	2a	1032	G	4.2
21	2Z	95	PRO	4.1
1	2A	2117	A	4.1
40	2i	11	LYS	4.1
1	2A	2155	G	4.1
33	1b	229	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
50	2s	9	VAL	4.1
21	2Z	150	LEU	4.1
33	1b	11	LEU	4.1
26	14	49	PHE	4.1
34	2c	190	ARG	4.1
43	2l	63	GLY	4.1
34	1c	39	ILE	4.1
43	2l	64	TYR	4.1
1	2A	882	G	4.1
1	2A	2112	G	4.1
1	2A	2805	G	4.1
26	14	50	VAL	4.1
44	2m	6	GLY	4.0
7	2H	175	LYS	4.0
33	1b	127	ILE	4.0
41	1j	4	ILE	4.0
45	2n	25	VAL	4.0
33	1b	230	VAL	4.0
42	2k	14	VAL	4.0
32	1a	1001(A)	G	4.0
52	2u	6	ARG	4.0
1	1A	1096	A	4.0
50	2s	13	ASP	4.0
50	2s	15	LEU	4.0
44	1m	121	LYS	4.0
32	2a	1002	G	4.0
1	2A	2119	A	4.0
54	2w	4	C	4.0
41	2j	91	PRO	4.0
34	2c	2	GLY	3.9
26	24	63	TYR	3.9
33	1b	236	TYR	3.9
1	1A	2119	A	3.9
1	2A	2793	G	3.9
19	2X	68	ARG	3.9
1	1A	2803	C	3.9
7	2H	43	VAL	3.9
47	2p	82	GLN	3.9
33	2b	121	LEU	3.9
38	1g	79	ARG	3.9
45	2n	3	ARG	3.9
1	2A	2896	C	3.9

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Mol	Chain	Res	Type	RSRZ
54	1w	72	C	3.9
54	2w	3	C	3.9
38	2g	85	TYR	3.9
40	2i	105	ASP	3.9
51	2t	98	PRO	3.9
52	2u	23	PRO	3.9
32	2a	1018	C	3.8
42	2k	25	TYR	3.8
38	2g	5	ARG	3.8
43	2l	18	VAL	3.8
15	2T	130	ALA	3.8
32	1a	1003	G	3.8
5	1F	14	PRO	3.8
21	2Z	149	SER	3.8
21	2Z	174	VAL	3.8
20	1Y	1	MET	3.8
12	2Q	10	ARG	3.8
33	2b	17	PHE	3.8
44	2m	121	LYS	3.8
52	2u	24	ARG	3.8
34	2c	201	TYR	3.8
6	2G	132	ASN	3.8
1	1A	889	C	3.8
32	1a	1027	C	3.8
40	1i	19	LEU	3.8
45	2n	18	VAL	3.8
25	23	2	PRO	3.8
1	2A	2148	G	3.8
33	1b	7	VAL	3.7
33	2b	136	VAL	3.7
7	2H	156	ALA	3.7
29	17	45	ALA	3.7
32	1a	1025	U	3.7
34	2c	52	LEU	3.7
38	2g	156	TRP	3.7
54	2w	73	A	3.7
26	24	65	ASP	3.7
1	2A	888	C	3.7
33	2b	132	LYS	3.7
9	1N	9	VAL	3.7
32	1a	630	G	3.7
41	2j	90	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
26	14	56	VAL	3.7
1	1A	1068	G	3.7
32	1a	346	G	3.7
15	1T	130	ALA	3.7
29	27	45	ALA	3.7
40	1i	106	ALA	3.7
26	14	59	PHE	3.7
34	2c	188	LEU	3.7
45	2n	6	LEU	3.7
48	1q	98	LEU	3.7
1	1A	1095	A	3.7
22	20	6	GLY	3.7
35	1d	167	GLY	3.7
38	2g	81	GLY	3.7
1	2A	2154	G	3.7
32	1a	1036	G	3.7
7	2H	136	ILE	3.7
41	2j	74	ILE	3.7
50	2s	22	LEU	3.7
1	2A	2897	U	3.7
33	1b	232	PRO	3.7
33	1b	97	TRP	3.6
21	1Z	170	THR	3.6
1	2A	2804	C	3.6
7	2H	96	ALA	3.6
44	2m	100	GLY	3.6
52	2u	16	GLY	3.6
1	2A	2115	G	3.6
32	1a	1030(A)	G	3.6
9	2N	9	VAL	3.6
21	2Z	96	VAL	3.6
20	1Y	91	GLU	3.6
34	2c	19	GLU	3.6
1	2A	2138	C	3.6
33	1b	10	LEU	3.6
33	1b	17	PHE	3.6
34	2c	194	GLY	3.6
41	2j	78	ASN	3.6
1	1A	2152	G	3.6
33	2b	77	ALA	3.6
50	2s	30	LEU	3.6
1	2A	652(D)	C	3.6

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Mol	Chain	Res	Type	RSRZ
1	2A	2137	C	3.6
21	1Z	2	GLU	3.6
21	1Z	139	VAL	3.6
32	1a	1034	G	3.6
32	2a	1034	G	3.6
34	2c	68	VAL	3.6
40	1i	126	SER	3.6
1	2A	2126	A	3.6
20	2Y	5	MET	3.6
32	1a	344	A	3.6
33	1b	188	ALA	3.6
33	2b	48	MET	3.6
54	1w	73	A	3.6
34	1c	47	LEU	3.6
33	1b	33	TYR	3.5
13	2R	14	SER	3.5
21	2Z	121	HIS	3.5
26	14	52	THR	3.5
33	2b	93	VAL	3.5
33	2b	112	VAL	3.5
41	2j	42	THR	3.5
38	1g	85	TYR	3.5
21	2Z	144	LEU	3.5
40	1i	13	ALA	3.5
1	2A	2801(A)	A	3.5
26	24	59	PHE	3.5
32	1a	1035	A	3.5
1	1A	884	C	3.5
1	1A	886	C	3.5
1	1A	898	C	3.5
29	17	47	ARG	3.5
32	2a	1038	C	3.5
34	2c	195	VAL	3.5
33	1b	125	PRO	3.5
35	1d	179	GLU	3.5
1	1A	1064	C	3.5
32	1a	1028	C	3.5
40	2i	19	LEU	3.5
33	1b	186	ALA	3.5
33	2b	161	ALA	3.5
41	1j	10	GLY	3.5
6	1G	182	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
26	14	51	ASP	3.4
8	2I	82	ARG	3.4
41	1j	33	GLN	3.4
47	1p	82	GLN	3.4
41	1j	100	THR	3.4
41	2j	48	THR	3.4
26	14	54	GLY	3.4
45	2n	51	GLY	3.4
45	2n	55	GLY	3.4
1	1A	2805	G	3.4
1	2A	2116	G	3.4
32	2a	1117	G	3.4
21	1Z	150	LEU	3.4
7	2H	39	PRO	3.4
8	2I	146	ALA	3.4
1	1A	1081	U	3.4
1	2A	1026	U	3.4
43	1l	64	TYR	3.4
33	2b	122	PHE	3.4
38	1g	156	TRP	3.4
52	2u	14	TRP	3.4
3	2D	38	LYS	3.4
38	1g	81	GLY	3.4
46	1o	89	GLY	3.4
51	1t	102	GLY	3.4
1	1A	652(E)	G	3.4
1	1A	1087	G	3.4
1	1A	2802	G	3.4
1	2A	2149	G	3.4
33	2b	123	ALA	3.4
34	2c	60	ALA	3.4
34	2c	6	HIS	3.4
33	2b	12	GLU	3.4
34	2c	48	TYR	3.4
50	2s	10	PHE	3.4
1	1A	897	C	3.4
1	2A	2139	C	3.4
33	2b	133	LYS	3.4
1	1A	896	A	3.4
19	1X	95	LEU	3.4
34	2c	5	ILE	3.4
42	2k	89	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
44	1m	5	ALA	3.4
50	2s	81	ARG	3.4
54	1w	20	U	3.3
3	2D	275	LYS	3.3
50	2s	16	LEU	3.3
1	1A	887	A	3.3
26	14	55	ARG	3.3
32	1a	1001	A	3.3
52	2u	15	ARG	3.3
21	2Z	171	ILE	3.3
45	2n	5	ALA	3.3
45	2n	7	ILE	3.3
26	24	49	PHE	3.3
1	1A	2145	C	3.3
1	2A	2136	C	3.3
41	1j	77	PRO	3.3
41	2j	37	PRO	3.3
7	2H	35	VAL	3.3
21	2Z	170	THR	3.3
40	2i	109	VAL	3.3
26	24	54	GLY	3.3
38	1g	82	GLY	3.3
32	2a	1286	A	3.3
26	24	32	TYR	3.3
33	2b	148	TYR	3.3
34	2c	23	TYR	3.3
1	1A	1056	G	3.3
32	1a	1002	G	3.3
32	1a	1026	G	3.3
33	2b	187	LEU	3.3
33	1b	19	HIS	3.3
18	2W	112	GLY	3.3
40	2i	2	GLU	3.3
33	2b	34	ALA	3.3
51	1t	97	ALA	3.3
1	1A	899	A	3.3
1	2A	2169	A	3.3
3	2D	276	LYS	3.3
32	2a	1004	A	3.3
54	2y	36	A	3.3
47	1p	80	PHE	3.3
24	12	70	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
42	2k	117	ASN	3.3
34	2c	87	LEU	3.3
1	1A	1093	G	3.3
32	1a	1033	G	3.3
34	1c	207	VAL	3.3
40	1i	17	VAL	3.3
32	1a	1030	C	3.3
41	2j	93	GLY	3.3
1	2A	2173	A	3.2
19	2X	69	TYR	3.2
1	2A	2150	U	3.2
7	2H	36	PRO	3.2
6	1G	48	GLU	3.2
20	2Y	54	LYS	3.2
41	2j	14	LYS	3.2
1	1A	1059	G	3.2
1	2A	2166	G	3.2
32	2a	1006	C	3.2
55	2x	70	G	3.2
40	2i	126	SER	3.2
1	2A	896	A	3.2
32	1a	1030(D)	A	3.2
32	2a	1005	A	3.2
38	2g	79	ARG	3.2
33	2b	10	LEU	3.2
45	2n	14	PRO	3.2
1	1A	2150	U	3.2
54	2y	33	U	3.2
50	1s	84	GLY	3.2
8	1I	146	ALA	3.2
45	2n	61	TRP	3.2
1	1A	2151	G	3.2
1	2A	2792	G	3.2
32	1a	1032	G	3.2
40	2i	91	ASP	3.2
1	1A	1098	A	3.2
1	1A	2790	A	3.2
50	2s	14	HIS	3.2
40	2i	114	TYR	3.2
32	1a	204	U	3.2
32	2a	1257	U	3.2
4	2E	115	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
7	2H	48	GLY	3.2
33	2b	214	ILE	3.2
34	2c	53	ALA	3.2
1	1A	2138	C	3.2
21	2Z	136	PHE	3.2
34	2c	128	PHE	3.2
7	2H	7	LEU	3.2
21	2Z	70	LEU	3.2
33	1b	61	LEU	3.2
41	2j	41	PRO	3.2
50	1s	71	LEU	3.2
21	2Z	141	VAL	3.2
21	2Z	147	GLY	3.2
33	1b	15	VAL	3.2
34	2c	9	GLY	3.2
44	2m	105	THR	3.2
6	1G	51	ARG	3.1
29	27	47	ARG	3.1
21	2Z	166	SER	3.1
45	2n	36	PHE	3.1
1	1A	652(D)	C	3.1
1	1A	2140	C	3.1
21	2Z	159	PRO	3.1
25	13	2	PRO	3.1
51	1t	10	LEU	3.1
1	1A	271(I)	G	3.1
1	2A	2156	G	3.1
1	2A	2114	A	3.1
32	2a	1001	A	3.1
40	2i	14	VAL	3.1
41	2j	10	GLY	3.1
42	2k	75	TYR	3.1
34	2c	124	ILE	3.1
35	2d	5	ILE	3.1
37	1f	46	ARG	3.1
41	2j	46	ARG	3.1
6	2G	182	LYS	3.1
41	2j	58	ASP	3.1
1	1A	1509	C	3.1
1	2A	11	G	3.1
1	2A	2157	G	3.1
1	2A	2165	G	3.1

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Mol	Chain	Res	Type	RSRZ
14	2S	35	ILE	3.1
32	2a	993	G	3.1
33	1b	136	VAL	3.1
41	2j	96	ILE	3.1
46	1o	3	ILE	3.1
50	2s	31	ILE	3.1
1	2A	2144	U	3.1
33	2b	207	ALA	3.1
34	2c	189	ALA	3.1
54	1y	20	U	3.1
11	2P	39	LYS	3.1
21	2Z	156	LYS	3.1
45	2n	4	LYS	3.1
33	2b	232	PRO	3.1
41	1j	86	MET	3.1
33	2b	189	ASP	3.1
34	2c	62	ASP	3.1
34	2c	196	LEU	3.1
40	1i	91	ASP	3.1
35	1d	173	TRP	3.1
19	1X	94	GLY	3.1
36	2e	114	GLY	3.1
29	27	46	VAL	3.1
39	1h	93	VAL	3.1
40	2i	10	ARG	3.1
48	1q	9	VAL	3.1
35	1d	5	ILE	3.1
41	1j	74	ILE	3.1
33	2b	31	TYR	3.1
42	1k	75	TYR	3.1
1	1A	1073	A	3.1
1	1A	1176	G	3.1
1	2A	2894	G	3.1
32	2a	1503	A	3.1
54	2w	71	G	3.1
1	1A	2897	U	3.1
21	1Z	104	PHE	3.1
51	1t	13	LEU	3.1
52	1u	24	ARG	3.1
41	2j	34	VAL	3.1
1	2A	894	C	3.1
32	2a	1027	C	3.1

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Mol	Chain	Res	Type	RSRZ
32	2a	1037	C	3.1
33	1b	120	ALA	3.0
40	1i	4	TYR	3.0
49	1r	24	ALA	3.0
1	1A	1054	A	3.0
33	1b	12	GLU	3.0
54	1y	35	A	3.0
1	1A	271(K)	U	3.0
1	1A	880	G	3.0
1	1A	2792	G	3.0
41	2j	77	PRO	3.0
7	2H	64	LEU	3.0
14	1S	3	ARG	3.0
40	2i	20	ARG	3.0
41	2j	31	GLY	3.0
21	2Z	53	ILE	3.0
6	1G	50	ALA	3.0
21	2Z	164	ALA	3.0
32	2a	1029	C	3.0
42	2k	23	ALA	3.0
22	20	68	GLU	3.0
36	2e	133	TYR	3.0
40	2i	125	TYR	3.0
1	1A	1082	U	3.0
32	1a	1447	A	3.0
34	2c	43	LEU	3.0
26	24	58	ARG	3.0
41	1j	66	ARG	3.0
41	2j	35	SER	3.0
3	1D	38	LYS	3.0
6	2G	52	ILE	3.0
34	2c	157	ILE	3.0
35	1d	70	ILE	3.0
40	2i	65	VAL	3.0
43	1l	18	VAL	3.0
33	1b	34	ALA	3.0
33	2b	134	GLU	3.0
44	2m	28	ALA	3.0
45	2n	10	ALA	3.0
26	14	63	TYR	3.0
32	1a	345	C	3.0
40	2i	36	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
21	2Z	158	PRO	3.0
1	1A	652(A)	A	3.0
1	1A	1065	U	3.0
1	2A	2118	U	3.0
32	1a	1286	A	3.0
32	2a	1531	A	3.0
41	1j	46	ARG	3.0
1	1A	1063	G	3.0
36	1e	85	GLY	3.0
7	2H	52	VAL	3.0
33	2b	71	VAL	3.0
41	2j	49	VAL	3.0
41	2j	72	VAL	3.0
43	2l	55	VAL	3.0
33	1b	123	ALA	3.0
50	2s	76	PRO	3.0
1	2A	889	C	3.0
7	2H	33	LEU	3.0
32	1a	1029	C	3.0
34	2c	32	LEU	3.0
45	2n	37	PHE	3.0
1	2A	1509(A)	A	3.0
32	2a	1030(D)	A	3.0
53	2v	12	A	3.0
11	2P	109	GLY	3.0
34	2c	158	GLY	3.0
52	2u	11	GLY	3.0
7	2H	19	VAL	2.9
7	2H	50	VAL	2.9
34	1c	57	ILE	2.9
40	2i	17	VAL	2.9
1	1A	2141	G	2.9
1	2A	1171	G	2.9
32	1a	1023	G	2.9
32	1a	1024	G	2.9
32	2a	1021	G	2.9
32	2a	1036	G	2.9
40	2i	82	ALA	2.9
9	2N	61	ARG	2.9
45	2n	12	ARG	2.9
41	2j	85	LEU	2.9
52	2u	18	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
40	1i	59	PHE	2.9
1	1A	1067	A	2.9
1	1A	1077	A	2.9
1	1A	2117	A	2.9
32	2a	1035	A	2.9
50	2s	4	SER	2.9
6	2G	127	GLY	2.9
9	1N	131	GLN	2.9
21	2Z	106	GLY	2.9
41	1j	76	ASN	2.9
7	2H	72	ILE	2.9
7	2H	89	ILE	2.9
41	2j	50	ILE	2.9
7	2H	133	VAL	2.9
50	2s	29	ARG	2.9
51	1t	95	ALA	2.9
1	1A	883	G	2.9
1	2A	2159	G	2.9
21	2Z	167	PRO	2.9
45	2n	17	LYS	2.9
47	1p	48	TRP	2.9
34	1c	87	LEU	2.9
4	2E	151	TYR	2.9
1	1A	1060	U	2.9
1	1A	2794	C	2.9
21	1Z	149	SER	2.9
32	2a	1039	C	2.9
33	1b	227	GLY	2.9
43	1l	63	GLY	2.9
1	1A	655	A	2.9
1	2A	2170	A	2.9
33	2b	127	ILE	2.9
5	2F	6	VAL	2.9
7	2H	113	VAL	2.9
40	2i	49	PRO	2.9
22	20	7	LEU	2.9
33	1b	187	LEU	2.9
1	1A	1089	G	2.9
54	2y	57	G	2.9
12	1Q	32	TYR	2.9
21	2Z	93	ASP	2.9
34	2c	193	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
7	2H	123	PHE	2.9
41	2j	61	GLU	2.9
1	2A	271(K)	U	2.9
1	1A	271(J)	C	2.9
33	1b	214	ILE	2.9
1	1A	548	A	2.9
1	2A	2134	A	2.9
7	2H	45	VAL	2.9
7	2H	79	VAL	2.9
32	2a	1016	A	2.9
44	2m	53	VAL	2.9
52	1u	15	ARG	2.9
54	2y	21	A	2.9
7	2H	10	PRO	2.9
21	2Z	51	ALA	2.9
21	2Z	152	ALA	2.9
49	1r	20	ALA	2.9
51	1t	94	ALA	2.9
40	2i	96	LEU	2.9
41	2j	40	LEU	2.9
50	2s	20	LEU	2.9
1	1A	652(F)	G	2.9
1	1A	879	G	2.9
1	1A	2207	G	2.9
1	2A	2110	G	2.9
1	2A	2127	G	2.9
1	2A	2751	G	2.9
36	2e	45	PHE	2.9
42	2k	13	GLN	2.9
54	1y	15	G	2.9
6	1G	35	GLU	2.9
6	2G	48	GLU	2.9
17	2V	101	GLY	2.9
33	1b	18	GLY	2.9
41	1j	36	GLY	2.9
26	24	55	ARG	2.8
33	1b	200	ILE	2.8
41	2j	76	ASN	2.8
47	1p	81	ARG	2.8
51	1t	100	ILE	2.8
21	1Z	105	VAL	2.8
31	29	16	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
34	2c	198	VAL	2.8
1	1A	2136	C	2.8
32	1a	163	C	2.8
32	2a	1043	C	2.8
32	2a	1115	C	2.8
3	2D	2	ALA	2.8
6	2G	139	LEU	2.8
21	2Z	2	GLU	2.8
26	24	57	GLU	2.8
33	2b	163	PHE	2.8
12	2Q	32	TYR	2.8
20	2Y	55	TYR	2.8
1	1A	2110	G	2.8
1	1A	2159	G	2.8
26	24	66	SER	2.8
32	2a	1003	G	2.8
34	2c	57	ILE	2.8
39	2h	26	VAL	2.8
44	2m	7	VAL	2.8
6	2G	17	PRO	2.8
34	2c	7	PRO	2.8
46	1o	19	PRO	2.8
41	2j	92	THR	2.8
1	2A	886	C	2.8
1	2A	2140	C	2.8
8	2I	55	ALA	2.8
32	2a	1019	C	2.8
32	2a	1045	C	2.8
1	1A	1088	A	2.8
1	1A	1103	A	2.8
1	1A	2114	A	2.8
6	2G	53	LEU	2.8
11	2P	86	LYS	2.8
21	1Z	99	TYR	2.8
34	1c	193	TYR	2.8
34	2c	181	ASN	2.8
42	2k	48	ILE	2.8
45	1n	7	ILE	2.8
1	2A	892	G	2.8
7	2H	173	PRO	2.8
44	2m	98	VAL	2.8
32	1a	1031	G	2.8

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Mol	Chain	Res	Type	RSRZ
50	2s	42	PRO	2.8
32	2a	1219	U	2.8
1	1A	34	C	2.8
1	1A	2896	C	2.8
1	1A	1086	A	2.8
21	1Z	148	ASP	2.8
12	2Q	104	PHE	2.8
31	29	20	HIS	2.8
50	2s	34	TRP	2.8
34	2c	182	ILE	2.8
50	2s	61	TYR	2.8
38	1g	84	ASN	2.8
7	2H	15	VAL	2.8
12	2Q	27	VAL	2.8
45	2n	33	VAL	2.8
1	1A	2113	U	2.8
21	2Z	125	LEU	2.8
34	2c	191	THR	2.8
1	2A	271(M)	G	2.8
1	2A	652(E)	G	2.8
1	1A	1076	C	2.8
7	2H	6	ARG	2.8
1	1A	1084	A	2.8
1	2A	887	A	2.8
32	1a	1030(B)	C	2.8
33	1b	50	GLU	2.8
51	2t	8	ARG	2.8
6	2G	4	ASP	2.8
12	1Q	15	GLY	2.7
34	2c	186	PHE	2.8
52	2u	2	GLY	2.7
26	14	67	TYR	2.7
33	1b	93	VAL	2.7
34	2c	55	VAL	2.7
21	2Z	157	LEU	2.7
38	2g	16	LEU	2.7
41	1j	8	LEU	2.7
44	2m	42	ALA	2.7
51	2t	97	ALA	2.7
1	1A	12	U	2.7
3	1D	275	LYS	2.7
32	2a	1020	U	2.7

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Mol	Chain	Res	Type	RSRZ
33	2b	90	MET	2.7
34	2c	4	LYS	2.7
7	2H	60	ARG	2.7
1	1A	11	G	2.7
32	2a	1031	G	2.7
54	2w	70	G	2.7
1	1A	890	A	2.7
1	1A	1053	C	2.7
1	2A	271(J)	C	2.7
1	2A	2794	C	2.7
32	1a	1038	C	2.7
10	2O	69	ILE	2.7
33	2b	222	ILE	2.7
34	1c	84	ILE	2.7
7	2H	11	VAL	2.7
33	2b	33	TYR	2.7
36	1e	69	VAL	2.7
40	2i	92	TYR	2.7
33	2b	221	LEU	2.7
9	2N	83	LYS	2.7
25	23	51	ALA	2.7
44	2m	72	ALA	2.7
11	2P	15	ARG	2.7
15	2T	111	ARG	2.7
24	12	69	ARG	2.7
38	2g	76	ARG	2.7
45	2n	31	ARG	2.7
32	2a	1532	U	2.7
1	1A	1071	G	2.7
1	1A	2894	G	2.7
1	2A	1112	G	2.7
1	2A	1170	G	2.7
1	2A	2133	G	2.7
17	1V	101	GLY	2.7
32	2a	1030(C)	G	2.7
33	1b	228	GLY	2.7
33	2b	72	GLY	2.7
54	2y	19	G	2.7
1	1A	2158	A	2.7
1	2A	2164	C	2.7
35	1d	154	ASN	2.7
6	1G	5	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
7	2H	17	VAL	2.7
7	2H	44	VAL	2.7
7	2H	125	VAL	2.7
7	2H	88	LEU	2.7
10	2O	113	LYS	2.7
21	2Z	90	VAL	2.7
33	2b	139	LYS	2.7
34	2c	184	TYR	2.7
47	2p	59	TRP	2.7
33	2b	21	ARG	2.7
33	2b	218	ALA	2.7
34	2c	129	ALA	2.7
40	1i	52	ALA	2.7
40	2i	106	ALA	2.7
51	2t	86	ARG	2.7
36	2e	8	GLU	2.7
54	1y	47	U	2.7
6	2G	20	ILE	2.7
36	1e	6	PHE	2.7
21	2Z	130	PRO	2.7
33	2b	234	PRO	2.7
40	2i	21	PRO	2.7
1	1A	271(M)	G	2.7
1	1A	2168	G	2.7
1	1A	2892	A	2.7
1	2A	880	G	2.7
22	20	12	ASN	2.7
40	2i	97	LYS	2.7
41	1j	80	LYS	2.7
19	2X	95	LEU	2.7
33	2b	145	LEU	2.7
36	1e	10	MET	2.7
21	2Z	129	SER	2.7
52	1u	9	ARG	2.7
52	2u	10	ARG	2.7
4	2E	163	GLU	2.7
21	2Z	168	GLU	2.7
26	14	32	TYR	2.7
33	2b	97	TRP	2.7
34	2c	15	THR	2.7
34	2c	95	THR	2.7
41	2j	87	THR	2.7

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Mol	Chain	Res	Type	RSRZ
18	1W	112	GLY	2.6
45	1n	51	GLY	2.6
51	2t	96	GLY	2.6
7	1H	175	LYS	2.6
34	2c	14	ILE	2.6
40	1i	21	PRO	2.6
41	1j	38	ILE	2.6
41	2j	80	LYS	2.6
33	2b	175	ARG	2.6
40	2i	66	ARG	2.6
41	1j	29	ARG	2.6
8	2I	38	LEU	2.6
21	2Z	33	LEU	2.6
33	1b	165	VAL	2.6
39	2h	53	VAL	2.6
40	2i	99	LEU	2.6
42	1k	14	VAL	2.6
1	1A	2115	G	2.6
1	2A	1533	G	2.6
54	2w	72	C	2.6
40	2i	110	GLU	2.6
7	2H	145	ALA	2.6
26	24	52	THR	2.6
34	2c	67	THR	2.6
34	2c	200	ALA	2.6
38	2g	2	ALA	2.6
38	2g	152	ALA	2.6
45	2n	30	ALA	2.6
40	2i	95	LYS	2.6
44	1m	27	LYS	2.6
21	1Z	136	PHE	2.6
21	2Z	68	PRO	2.6
33	2b	152	PHE	2.6
40	2i	101	PHE	2.6
51	1t	98	PRO	2.6
11	2P	79	ARG	2.6
21	2Z	122	ARG	2.6
41	2j	88	LEU	2.6
50	2s	5	LEU	2.6
50	2s	53	ASN	2.6
12	2Q	109	VAL	2.6
33	2b	86	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
38	2g	9	VAL	2.6
48	2q	23	VAL	2.6
1	1A	1069	A	2.6
53	2v	13	A	2.6
6	2G	50	ALA	2.6
15	2T	131	ALA	2.6
36	2e	94	ALA	2.6
45	2n	13	THR	2.6
1	1A	1091	G	2.6
1	1A	2116	G	2.6
32	1a	1030(C)	G	2.6
38	2g	151	TYR	2.6
41	2j	62	HIS	2.6
54	1y	18	G	2.6
54	2y	18	G	2.6
31	29	37	GLY	2.6
40	1i	67	GLY	2.6
50	2s	68	GLY	2.6
1	2A	2132	U	2.6
41	1j	75	ILE	2.6
41	1j	79	ARG	2.6
45	2n	35	ARG	2.6
45	2n	54	PRO	2.6
8	2I	109	ILE	2.6
16	2U	62	ILE	2.6
33	2b	101	MET	2.6
33	2b	185	ILE	2.6
33	2b	211	ILE	2.6
45	2n	57	ARG	2.6
34	2c	142	MET	2.6
41	2j	54	PHE	2.6
34	2c	47	LEU	2.6
40	1i	56	LEU	2.6
51	1t	24	LEU	2.6
40	1i	108	VAL	2.6
41	2j	94	VAL	2.6
21	1Z	66	SER	2.6
33	2b	113	HIS	2.6
40	1i	7	THR	2.6
44	1m	105	THR	2.6
44	2m	33	ALA	2.6
32	1a	1005	A	2.6

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Mol	Chain	Res	Type	RSRZ
44	2m	92	HIS	2.6
53	2v	24	A	2.6
1	1A	154(A)	C	2.6
1	1A	2142	C	2.6
1	1A	2143	C	2.6
44	2m	87	TYR	2.6
52	1u	18	TYR	2.6
11	2P	37	GLY	2.6
26	24	61	ARG	2.6
35	1d	3	ARG	2.6
39	2h	4	ASP	2.6
40	2i	9	ARG	2.6
40	2i	69	GLY	2.6
40	2i	98	PRO	2.6
44	2m	104	ARG	2.6
7	2H	41	MET	2.6
33	1b	185	ILE	2.6
33	1b	222	ILE	2.6
21	2Z	104	PHE	2.6
32	1a	1000	U	2.6
41	1j	11	PHE	2.6
21	2Z	105	VAL	2.6
39	2h	51	VAL	2.6
50	2s	19	VAL	2.6
33	1b	40	HIS	2.6
33	2b	19	HIS	2.6
33	2b	40	HIS	2.6
36	1e	21	ALA	2.6
41	2j	13	HIS	2.6
11	2P	76	LYS	2.6
1	1A	2137	C	2.5
26	24	68	ARG	2.5
32	2a	1149	C	2.5
40	2i	128	ARG	2.5
47	1p	72	ARG	2.5
34	2c	73	PRO	2.5
41	2j	86	MET	2.5
52	1u	16	GLY	2.5
1	1A	2156	G	2.5
1	2A	2168	G	2.5
33	2b	129	GLU	2.5
1	2A	895	U	2.5

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Mol	Chain	Res	Type	RSRZ
20	2Y	90	LEU	2.5
44	2m	66	LEU	2.5
15	1T	123	GLN	2.5
24	22	70	GLN	2.5
34	1c	3	ASN	2.5
35	1d	170	VAL	2.5
40	2i	108	VAL	2.5
46	2o	60	VAL	2.5
48	2q	9	VAL	2.5
33	1b	225	ALA	2.5
33	2b	29	ALA	2.5
34	2c	92	ALA	2.5
41	2j	26	ALA	2.5
47	1p	43	LYS	2.5
33	2b	131	PRO	2.5
34	1c	25	GLY	2.5
35	1d	29	PRO	2.5
1	2A	2143	C	2.5
40	1i	8	GLY	2.5
40	1i	39	GLY	2.5
54	2y	56	C	2.5
12	2Q	65	PHE	2.5
1	1A	2166	G	2.5
1	2A	2124	G	2.5
1	2A	2153	G	2.5
1	2A	2318	G	2.5
33	2b	154	LEU	2.5
1	1A	1066	U	2.5
1	2A	2172	U	2.5
32	2a	1040	U	2.5
34	1c	107	GLN	2.5
20	1Y	92	ASN	2.5
26	14	69	LYS	2.5
33	2b	140	HIS	2.5
34	2c	116	VAL	2.5
51	2t	74	LYS	2.5
35	1d	89	THR	2.5
41	2j	100	THR	2.5
38	1g	4	ARG	2.5
41	2j	70	ARG	2.5
33	2b	92	TYR	2.5
34	2c	109	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	1A	229	A	2.5
1	1A	1070	A	2.5
4	2E	29	GLY	2.5
45	1n	55	GLY	2.5
33	1b	134	GLU	2.5
37	1f	81	ILE	2.5
1	2A	898	C	2.5
32	2a	1007	C	2.5
33	2b	44	LEU	2.5
33	2b	149	LEU	2.5
35	2d	176	LEU	2.5
51	1t	62	LEU	2.5
34	1c	26	LYS	2.5
45	2n	50	LYS	2.5
50	2s	18	LYS	2.5
52	2u	3	LYS	2.5
8	2I	15	VAL	2.5
34	1c	106	VAL	2.5
42	2k	105	VAL	2.5
32	2a	1048	G	2.5
54	1w	71	G	2.5
54	2y	44	G	2.5
15	2T	129	ARG	2.5
34	2c	50	ALA	2.5
40	2i	84	ALA	2.5
42	1k	60	ALA	2.5
43	2l	61	THR	2.5
45	1n	60	SER	2.5
21	2Z	28	MET	2.5
6	1G	146	TYR	2.5
21	1Z	169	GLU	2.5
40	2i	4	TYR	2.5
33	2b	200	ILE	2.5
50	2s	12	ASP	2.5
1	1A	1046	A	2.5
1	1A	2801(A)	A	2.5
1	2A	652(A)	A	2.5
1	2A	2171	A	2.5
32	2a	1447	A	2.5
26	24	9	LEU	2.5
43	2l	126	LYS	2.5
45	2n	9	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
45	2n	47	LEU	2.5
48	2q	100	LYS	2.5
50	2s	71	LEU	2.5
21	2Z	89	PHE	2.5
40	1i	18	PHE	2.5
1	1A	1080	C	2.5
1	1A	2164	C	2.5
1	1A	2791	C	2.5
21	2Z	71	VAL	2.5
34	2c	66	VAL	2.5
34	2c	130	VAL	2.5
34	2c	151	VAL	2.5
51	1t	9	ASN	2.5
1	1A	1097	U	2.5
1	1A	2167	U	2.5
42	1k	89	ALA	2.5
1	2A	2151	G	2.5
1	2A	2319	G	2.5
13	1R	14	SER	2.5
24	22	1	MET	2.5
38	1g	77	SER	2.5
47	2p	45	THR	2.5
32	2a	630	G	2.5
32	2a	1017	G	2.5
32	2a	1023	G	2.5
33	1b	131	PRO	2.4
35	1d	2	GLY	2.4
38	1g	130	GLY	2.4
44	1m	6	GLY	2.4
50	2s	84	GLY	2.4
20	2Y	107	ASP	2.4
33	1b	22	LYS	2.4
33	2b	41	ILE	2.4
40	2i	5	TYR	2.4
44	2m	4	ILE	2.4
48	1q	36	ILE	2.4
44	2m	48	LEU	2.4
1	1A	1509(A)	A	2.4
1	1A	2135	A	2.4
1	1A	2170	A	2.4
1	2A	2892	A	2.4
34	2c	162	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
21	2Z	151	HIS	2.4
37	1f	60	PHE	2.4
40	2i	37	PHE	2.4
5	2F	62	ARG	2.4
44	2m	88	ARG	2.4
7	2H	169	VAL	2.4
34	2c	153	VAL	2.4
44	2m	15	VAL	2.4
4	2E	204	ALA	2.4
7	2H	102	ALA	2.4
34	2c	146	ALA	2.4
45	2n	20	ALA	2.4
34	2c	192	THR	2.4
45	2n	22	THR	2.4
17	2V	73	SER	2.4
26	24	29	PRO	2.4
25	23	60	GLU	2.4
32	2a	1026	G	2.4
34	2c	145	GLY	2.4
36	2e	35	GLY	2.4
41	1j	31	GLY	2.4
41	1j	93	GLY	2.4
44	2m	65	LYS	2.4
51	2t	101	GLY	2.4
54	2y	15	G	2.4
12	2Q	66	ILE	2.4
34	2c	77	ILE	2.4
33	2b	115	LEU	2.4
21	2Z	131	ARG	2.4
33	1b	163	PHE	2.4
33	2b	144	ARG	2.4
36	2e	18	ARG	2.4
38	1g	78	ARG	2.4
38	2g	32	ARG	2.4
1	1A	1177	A	2.4
1	1A	2173	A	2.4
1	2A	6	A	2.4
1	2A	1847	A	2.4
1	2A	2158	A	2.4
54	1y	36	A	2.4
21	2Z	74	VAL	2.4
33	2b	164	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
35	1d	178	VAL	2.4
35	2d	154	ASN	2.4
37	1f	88	VAL	2.4
42	1k	117	ASN	2.4
32	2a	1223	C	2.4
32	2a	1249	C	2.4
33	1b	62	ALA	2.4
34	1c	92	ALA	2.4
34	2c	137	ALA	2.4
1	1A	2109	U	2.4
1	2A	9	U	2.4
1	2A	2130	U	2.4
7	2H	12	PRO	2.4
20	2Y	91	GLU	2.4
33	1b	234	PRO	2.4
35	1d	83	SER	2.4
33	1b	133	LYS	2.4
51	1t	68	LYS	2.4
11	1P	44	GLY	2.4
6	2G	157	ILE	2.4
8	1I	109	ILE	2.4
16	2U	88	ILE	2.4
33	1b	201	ILE	2.4
41	2j	38	ILE	2.4
1	1A	2206	G	2.4
1	1A	2893	G	2.4
1	2A	100	G	2.4
8	1I	38	LEU	2.4
32	2a	1024	G	2.4
36	1e	151	LEU	2.4
54	1y	19	G	2.4
7	2H	42	ARG	2.4
33	1b	130	ARG	2.4
35	1d	153	ARG	2.4
41	2j	56	HIS	2.4
45	2n	49	HIS	2.4
21	2Z	88	PHE	2.4
33	1b	55	PHE	2.4
5	2F	183	VAL	2.4
6	2G	5	VAL	2.4
40	1i	41	VAL	2.4
1	1A	1508	A	2.4

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Mol	Chain	Res	Type	RSRZ
32	2a	1183	A	2.4
5	2F	21	ALA	2.4
19	2X	91	ALA	2.4
33	1b	173	ALA	2.4
4	1E	56	PRO	2.4
7	2H	8	PRO	2.4
7	2H	21	PRO	2.4
12	2Q	112	GLU	2.4
33	2b	22	LYS	2.4
36	2e	120	THR	2.4
21	2Z	92	SER	2.4
32	2a	992	U	2.4
32	2a	1025	U	2.4
32	2a	1196	U	2.4
32	2a	1260	C	2.4
35	1d	189	PRO	2.4
41	1j	35	SER	2.4
50	2s	35	SER	2.4
54	2w	45	U	2.4
6	2G	24	GLY	2.4
34	2c	51	GLY	2.4
26	24	31	ILE	2.4
33	2b	201	ILE	2.4
34	2c	202	ILE	2.4
44	1m	4	ILE	2.4
6	1G	181	ARG	2.4
6	2G	147	ASP	2.4
11	2P	68	GLN	2.4
14	2S	97	ARG	2.4
36	2e	20	GLN	2.4
36	2e	25	ARG	2.4
38	1g	5	ARG	2.4
38	1g	115	ARG	2.4
39	1h	2	LEU	2.4
45	1n	57	ARG	2.4
1	1A	2125	G	2.4
33	1b	70	PHE	2.4
45	2n	16	PHE	2.4
47	1p	38	TYR	2.4
5	1F	89	VAL	2.4
21	2Z	139	VAL	2.4
47	2p	2	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
33	1b	8	LYS	2.4
44	2m	31	LYS	2.4
1	1A	2171	A	2.4
1	2A	878	A	2.4
3	1D	28	GLU	2.4
26	24	30	GLU	2.4
7	2H	55	PRO	2.3
8	1I	108	THR	2.3
33	1b	24	TRP	2.4
40	2i	12	GLU	2.4
40	2i	90	PRO	2.3
42	1k	42	TRP	2.4
52	2u	8	THR	2.3
1	1A	2139	C	2.3
1	1A	2146	C	2.3
7	2H	14	GLY	2.3
26	24	45	GLY	2.3
32	1a	1008	C	2.3
32	2a	1116	C	2.3
33	1b	66	GLY	2.3
40	2i	39	GLY	2.3
40	2i	67	GLY	2.3
5	1F	12	LEU	2.3
6	2G	39	ILE	2.3
35	1d	76	ARG	2.3
39	2h	100	ILE	2.3
40	1i	20	ARG	2.3
40	2i	104	ARG	2.3
6	2G	175	LEU	2.3
8	2I	68	LEU	2.3
33	1b	44	LEU	2.3
33	1b	140	HIS	2.3
38	2g	153	HIS	2.3
45	2n	44	LEU	2.3
47	1p	74	LEU	2.3
51	2t	10	LEU	2.3
7	2H	37	VAL	2.3
7	2H	49	VAL	2.3
21	1Z	42	VAL	2.3
27	15	60	VAL	2.3
43	2l	39	VAL	2.3
50	2s	41	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
32	1a	79	G	2.3
32	1a	1009	G	2.3
32	1a	1021	G	2.3
41	1j	78	ASN	2.3
44	2m	106	ASN	2.3
35	1d	195	ALA	2.3
38	1g	83	ALA	2.3
40	1i	15	ALA	2.3
45	1n	59	ALA	2.3
50	2s	48	THR	2.3
1	2A	229	A	2.3
32	1a	143	A	2.3
32	1a	162	A	2.3
3	2D	262	ARG	2.3
34	1c	79	ARG	2.3
41	2j	36	GLY	2.3
1	1A	2172	U	2.3
1	2A	614(A)	U	2.3
16	1U	117	GLN	2.3
16	2U	71	GLN	2.3
32	1a	203	U	2.3
33	2b	42	ILE	2.3
34	1c	77	ILE	2.3
36	1e	20	GLN	2.3
39	2h	70	GLN	2.3
37	2f	21	LEU	2.3
39	2h	39	LEU	2.3
42	2k	103	LEU	2.3
50	2s	47	HIS	2.3
1	1A	1072	C	2.3
32	2a	1060	C	2.3
15	2T	28	VAL	2.3
15	2T	30	VAL	2.3
20	2Y	45	VAL	2.3
33	1b	31	TYR	2.3
33	2b	230	VAL	2.3
34	2c	86	VAL	2.3
43	2l	69	TYR	2.3
45	2n	21	TYR	2.3
33	1b	129	GLU	2.3
38	2g	37	ASN	2.3
12	2Q	136	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
33	2b	186	ALA	2.3
34	2c	187	ALA	2.3
51	2t	94	ALA	2.3
1	2A	881	G	2.3
1	2A	1042	G	2.3
1	2A	2160	G	2.3
1	2A	2207	G	2.3
17	2V	92	THR	2.3
22	20	43	THR	2.3
15	2T	115	ARG	2.3
25	23	29	ARG	2.3
32	2a	1011	G	2.3
50	2s	63	THR	2.3
45	1n	29	ARG	2.3
49	1r	87	ARG	2.3
51	1t	8	ARG	2.3
1	2A	528	A	2.3
6	2G	29	TRP	2.3
19	2X	94	GLY	2.3
21	2Z	160	GLY	2.3
34	2c	185	GLY	2.3
35	1d	180	GLY	2.3
38	2g	110	GLN	2.3
41	1j	68	HIS	2.3
7	2H	9	ILE	2.3
22	10	84	LEU	2.3
34	2c	39	ILE	2.3
36	2e	80	ILE	2.3
39	1h	112	LEU	2.3
40	2i	79	LEU	2.3
41	1j	40	LEU	2.3
32	2a	997	U	2.3
1	1A	1075	C	2.3
1	1A	2111	C	2.3
1	2A	2474	C	2.3
3	2D	5	LYS	2.3
11	2P	2	LYS	2.3
32	1a	1132	C	2.3
45	1n	36	PHE	2.3
6	2G	31	VAL	2.3
8	2I	7	GLU	2.3
33	2b	170	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
34	2c	138	VAL	2.3
38	1g	8	GLU	2.3
7	2H	83	TYR	2.3
26	24	67	TYR	2.3
47	1p	62	VAL	2.3
50	2s	11	VAL	2.3
7	2H	29	PRO	2.3
18	2W	60	ASN	2.3
50	2s	24	ALA	2.3
7	2H	95	ARG	2.3
7	2H	170	ARG	2.3
14	2S	3	ARG	2.3
8	1I	17	GLN	2.3
33	1b	72	GLY	2.3
34	1c	78	GLY	2.3
34	2c	205	GLY	2.3
36	2e	22	GLY	2.3
40	2i	115	GLY	2.3
5	2F	24	LEU	2.3
8	1I	5	LEU	2.3
32	1a	181	G	2.3
32	2a	485	G	2.3
34	2c	22	TRP	2.3
34	2c	167	TRP	2.3
50	1s	5	LEU	2.3
1	2A	1460	A	2.3
1	2A	2135	A	2.3
21	2Z	1	MET	2.3
13	2R	69	ASP	2.3
33	2b	156	LYS	2.3
50	1s	12	ASP	2.3
32	2a	204	U	2.3
1	2A	1043	C	2.3
14	2S	29	PHE	2.3
21	1Z	168	GLU	2.3
22	20	45	PHE	2.3
32	1a	470	C	2.3
33	2b	55	PHE	2.3
34	2c	10	PHE	2.3
40	2i	18	PHE	2.3
41	2j	64	GLU	2.3
44	2m	60	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
7	2H	3	ARG	2.3
33	2b	137	ARG	2.3
33	2b	199	TYR	2.3
34	2c	21	ARG	2.3
33	1b	207	ALA	2.2
46	1o	69	TYR	2.3
42	1k	87	THR	2.2
34	2c	170	GLN	2.2
40	2i	124	GLN	2.2
50	1s	8	GLY	2.2
7	2H	71	LEU	2.2
33	2b	108	ILE	2.2
33	2b	215	LEU	2.2
38	2g	144	MET	2.2
41	1j	6	ILE	2.2
42	2k	29	ILE	2.2
45	2n	11	LYS	2.2
1	1A	1085	A	2.2
1	2A	899	A	2.2
32	2a	1225	A	2.2
1	1A	2131	G	2.2
1	1A	2133	G	2.2
1	2A	1537	G	2.2
54	1w	1	G	2.2
1	1A	2118	U	2.2
1	2A	2167	U	2.2
1	2A	2895	U	2.2
8	2I	122	GLU	2.2
5	1F	17	ARG	2.2
1	2A	893	C	2.2
1	2A	2174	C	2.2
8	2I	107	VAL	2.2
12	2Q	106	VAL	2.2
20	2Y	53	PRO	2.2
21	2Z	58	VAL	2.2
33	2b	229	VAL	2.2
34	1c	76	VAL	2.2
34	2c	64	VAL	2.2
40	1i	9	ARG	2.2
41	2j	53	PRO	2.2
50	2s	51	VAL	2.2
52	2u	9	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
52	2u	22	ARG	2.2
32	1a	92	C	2.2
32	1a	1037	C	2.2
7	2H	146	ALA	2.2
33	2b	188	ALA	2.2
40	2i	45	ALA	2.2
40	2i	62	TYR	2.2
40	2i	117	HIS	2.2
41	1j	62	HIS	2.2
47	2p	76	GLN	2.2
48	1q	7	THR	2.2
5	1F	207	GLY	2.2
14	2S	83	LYS	2.2
20	2Y	88	LYS	2.2
34	1c	158	GLY	2.2
43	1l	91	LYS	2.2
44	2m	27	LYS	2.2
45	1n	4	LYS	2.2
45	2n	58	LYS	2.2
40	2i	56	LEU	2.2
33	1b	172	ILE	2.2
33	2b	39	ILE	2.2
40	1i	74	ILE	2.2
21	2Z	94	GLU	2.2
32	2a	1324	A	2.2
41	1j	64	GLU	2.2
45	2n	8	GLU	2.2
54	2y	58	A	2.2
1	1A	895	U	2.2
1	1A	1055	G	2.2
1	2A	1114	G	2.2
15	1T	125	ARG	2.2
32	2a	1202	G	2.2
38	1g	3	ARG	2.2
33	2b	105	PHE	2.2
21	2Z	128	VAL	2.2
41	2j	44	VAL	2.2
1	1A	1092	C	2.2
1	1A	1100	C	2.2
1	2A	34	C	2.2
1	2A	2163	C	2.2
6	2G	163	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
14	2S	61	ASN	2.2
44	2m	12	ASN	2.2
45	2n	59	ALA	2.2
55	2x	71	C	2.2
21	2Z	99	TYR	2.2
33	2b	147	LYS	2.2
37	1f	63	TYR	2.2
45	2n	15	LYS	2.2
50	2s	28	LYS	2.2
39	2h	3	THR	2.2
50	2s	77	THR	2.2
34	2c	41	GLY	2.2
51	1t	96	GLY	2.2
21	2Z	133	ILE	2.2
33	2b	223	ILE	2.2
34	1c	14	ILE	2.2
41	2j	82	ILE	2.2
5	2F	161	GLU	2.2
27	25	59	GLU	2.2
34	2c	90	GLU	2.2
12	2Q	6	ARG	2.2
12	2Q	60	ARG	2.2
14	2S	20	ARG	2.2
34	2c	59	ARG	2.2
46	1o	88	ARG	2.2
32	2a	969	A	2.2
21	2Z	15	PRO	2.2
33	2b	91	PRO	2.2
21	2Z	27	VAL	2.2
34	2c	99	VAL	2.2
49	1r	86	VAL	2.2
1	1A	1099	G	2.2
1	1A	2154	G	2.2
1	1A	2190	G	2.2
20	2Y	4	LYS	2.2
33	2b	8	LYS	2.2
41	2j	27	ALA	2.2
42	1k	74	ALA	2.2
43	2l	68	ALA	2.2
51	1t	14	LYS	2.2
54	2w	44	G	2.2
33	2b	16	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
34	2c	168	ALA	2.2
12	2Q	7	MET	2.2
42	1k	13	GLN	2.2
1	2A	645	C	2.2
1	2A	897	C	2.2
1	2A	2142	C	2.2
6	2G	146	TYR	2.2
7	2H	103	LEU	2.2
7	2H	174	GLY	2.2
11	2P	118	GLY	2.2
14	2S	58	LEU	2.2
21	2Z	76	LEU	2.2
27	25	58	LEU	2.2
32	2a	470	C	2.2
44	2m	23	TYR	2.2
44	2m	37	THR	2.2
34	2c	34	LEU	2.2
34	2c	42	LEU	2.2
39	2h	135	CYS	2.2
41	2j	98	ILE	2.2
33	1b	124	SER	2.2
35	1d	137	SER	2.2
36	2e	5	ASP	2.2
40	1i	12	GLU	2.2
21	1Z	103	ARG	2.2
21	1Z	131	ARG	2.2
21	2Z	72	ARG	2.2
21	2Z	81	ARG	2.2
22	20	11	ARG	2.2
35	1d	118	ARG	2.2
39	2h	18	ARG	2.2
42	2k	91	ARG	2.2
50	2s	78	ARG	2.2
4	2E	56	PRO	2.2
34	1c	18	TRP	2.2
35	1d	7	PRO	2.2
47	2p	48	TRP	2.2
3	2D	15	PHE	2.2
1	1A	278	A	2.1
1	1A	1175	U	2.2
1	2A	271(L)	U	2.2
7	2H	138	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
20	2Y	94	LYS	2.2
5	2F	132	VAL	2.1
29	17	46	VAL	2.1
32	1a	160	A	2.1
32	1a	161	A	2.1
32	1a	1040	U	2.2
32	2a	84	U	2.2
32	2a	1126	U	2.2
33	1b	122	PHE	2.2
42	1k	51	LYS	2.2
50	2s	74	PHE	2.2
40	2i	41	VAL	2.1
54	1y	45	U	2.2
55	1x	47	U	2.2
21	2Z	21	ALA	2.1
33	2b	13	ALA	2.1
33	2b	135	GLN	2.1
34	1c	60	ALA	2.1
34	2c	117	ALA	2.1
35	1d	111	ALA	2.1
38	1g	147	ALA	2.1
44	2m	101	GLN	2.1
1	2A	2131	G	2.1
4	2E	63	LEU	2.1
15	1T	37	GLY	2.1
34	1c	13	GLY	2.1
35	1d	16	GLY	2.1
35	1d	155	LEU	2.1
38	2g	38	LEU	2.1
40	2i	8	GLY	2.1
50	2s	26	GLY	2.1
50	2s	46	GLY	2.1
50	2s	79	THR	2.1
51	2t	102	GLY	2.1
54	2w	5	G	2.1
55	1x	46	G	2.1
12	2Q	47	ILE	2.1
41	2j	75	ILE	2.1
50	2s	52	TYR	2.1
1	1A	1052	C	2.1
1	2A	2161	C	2.1
32	2a	1066	C	2.1

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Mol	Chain	Res	Type	RSRZ
32	2a	1114	C	2.1
32	2a	1244	C	2.1
7	2H	40	GLU	2.1
7	2H	58	GLU	2.1
10	1O	108	GLU	2.1
35	2d	73	ARG	2.1
40	2i	120	ARG	2.1
42	1k	36	ASP	2.1
21	1Z	159	PRO	2.1
12	2Q	102	VAL	2.1
25	13	59	VAL	2.1
44	2m	64	TRP	2.1
1	1A	2132	U	2.1
1	2A	1113	U	2.1
7	2H	61	HIS	2.1
6	1G	26	GLN	2.1
32	1a	182	U	2.1
11	2P	140	ALA	2.1
32	2a	983	A	2.1
32	2a	994	A	2.1
33	1b	45	GLN	2.1
33	2b	95	GLN	2.1
34	2c	28	GLN	2.1
40	2i	73	GLN	2.1
44	1m	106	ASN	2.1
6	2G	42	GLY	2.1
8	2I	35	LEU	2.1
21	2Z	163	LEU	2.1
26	24	44	THR	2.1
33	2b	138	LEU	2.1
35	1d	188	LEU	2.1
39	2h	2	LEU	2.1
40	2i	40	LEU	2.1
7	2H	148	ILE	2.1
41	1j	98	ILE	2.1
51	1t	41	ILE	2.1
52	2u	13	ILE	2.1
6	2G	12	TYR	2.1
7	2H	94	TYR	2.1
14	2S	36	TYR	2.1
21	2Z	29	TYR	2.1
1	1A	2153	G	2.1

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Mol	Chain	Res	Type	RSRZ
1	1A	2165	G	2.1
1	2A	2141	G	2.1
8	2I	64	GLU	2.1
21	2Z	97	GLU	2.1
26	24	48	ARG	2.1
33	2b	126	GLU	2.1
34	2c	140	ARG	2.1
35	1d	73	ARG	2.1
41	2j	66	ARG	2.1
45	2n	41	ARG	2.1
48	2q	42	TYR	2.1
32	2a	1061	G	2.1
45	2n	40	CYS	2.1
1	1A	2108	C	2.1
21	2Z	140	ASP	2.1
32	2a	1263	C	2.1
37	1f	83	ASP	2.1
7	2H	13	LYS	2.1
6	2G	142	PRO	2.1
35	1d	37	PRO	2.1
6	2G	23	PHE	2.1
45	1n	37	PHE	2.1
47	1p	16	HIS	2.1
20	2Y	57	GLN	2.1
26	14	46	GLN	2.1
38	1g	9	VAL	2.1
38	2g	86	GLN	2.1
5	2F	130	ALA	2.1
20	2Y	65	ALA	2.1
6	2G	123	ASN	2.1
15	1T	38	ASN	2.1
32	2a	1000	U	2.1
32	2a	1285	A	2.1
35	1d	87	GLY	2.1
35	1d	171	GLY	2.1
37	1f	48	LEU	2.1
40	2i	50	LEU	2.1
41	2j	16	LEU	2.1
46	1o	66	LEU	2.1
51	1t	99	LEU	2.1
15	2T	112	ARG	2.1
38	2g	4	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
39	2h	30	ARG	2.1
46	2o	88	ARG	2.1
21	1Z	120	ILE	2.1
35	1d	156	GLU	2.1
48	2q	96	GLU	2.1
34	1c	23	TYR	2.1
34	2c	29	TYR	2.1
39	2h	58	TYR	2.1
21	2Z	16	SER	2.1
21	2Z	87	ASP	2.1
40	1i	95	LYS	2.1
44	2m	13	LYS	2.1
33	1b	210	SER	2.1
45	2n	60	SER	2.1
50	2s	38	SER	2.1
52	2u	5	ASP	2.1
1	1A	2162	G	2.1
32	1a	216	G	2.1
32	2a	1224	G	2.1
32	2a	1258	G	2.1
1	1A	645	C	2.1
32	1a	1006	C	2.1
32	1a	1019	C	2.1
4	1E	1	MET	2.1
47	1p	1	MET	2.1
6	1G	80	PHE	2.1
6	1G	149	VAL	2.1
12	2Q	29	PHE	2.1
38	1g	13	GLN	2.1
21	1Z	165	VAL	2.1
21	2Z	56	VAL	2.1
34	1c	70	VAL	2.1
35	1d	140	VAL	2.1
40	2i	86	VAL	2.1
47	1p	21	VAL	2.1
21	2Z	7	ALA	2.1
34	2c	180	ALA	2.1
38	1g	2	ALA	2.1
1	1A	362	U	2.1
1	1A	1083	U	2.1
28	26	11	LEU	2.1
32	1a	90	U	2.1

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Mol	Chain	Res	Type	RSRZ
32	2a	5	U	2.1
32	2a	1150	U	2.1
33	2b	24	TRP	2.1
33	1b	153	ARG	2.1
34	2c	79	ARG	2.1
34	2c	204	LEU	2.1
40	1i	102	LEU	2.1
41	2j	43	ARG	2.1
44	2m	96	LEU	2.1
45	2n	53	LEU	2.1
54	1w	47	U	2.1
12	2Q	15	GLY	2.1
6	2G	64	THR	2.1
7	2H	47	GLU	2.1
26	14	57	GLU	2.1
1	2A	1508	A	2.1
32	2a	965	A	2.1
32	2a	1251	A	2.1
32	2a	1256	A	2.1
33	1b	80	ILE	2.1
12	2Q	63	LYS	2.1
14	2S	19	LYS	2.1
34	2c	135	LYS	2.1
34	2c	147	LYS	2.1
38	2g	88	PRO	2.1
39	2h	67	PRO	2.1
35	1d	181	MET	2.1
1	1A	2124	G	2.0
1	2A	271(I)	G	2.0
1	2A	2175	C	2.1
32	1a	144	G	2.0
32	1a	1137	C	2.1
32	2a	970	C	2.1
41	2j	68	HIS	2.1
32	2a	1009	G	2.0
32	2a	1190	G	2.0
54	1w	18	G	2.0
54	2w	19	G	2.0
54	2y	13	C	2.1
35	1d	201	GLN	2.0
38	2g	11	GLN	2.0
20	2Y	7	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
21	2Z	48	PHE	2.0
33	2b	15	VAL	2.0
34	1c	86	VAL	2.0
36	2e	34	VAL	2.0
36	2e	69	VAL	2.0
7	2H	20	ALA	2.0
12	1Q	10	ARG	2.0
14	2S	55	ALA	2.0
33	1b	226	ARG	2.0
34	1c	83	ARG	2.0
35	2d	195	ALA	2.0
38	1g	6	ARG	2.0
38	2g	40	ALA	2.0
44	2m	3	ARG	2.0
50	2s	3	ARG	2.0
8	1I	68	LEU	2.0
8	2I	75	LEU	2.0
33	1b	221	LEU	2.0
39	2h	112	LEU	2.0
7	2H	32	GLU	2.0
33	1b	38	GLY	2.0
34	2c	74	GLY	2.0
39	2h	71	GLY	2.0
40	1i	6	GLY	2.0
40	1i	115	GLY	2.0
41	2j	83	GLU	2.0
51	1t	101	GLY	2.0
5	2F	175	THR	2.0
32	2a	203	U	2.0
20	2Y	75	ILE	2.0
22	20	49	LYS	2.0
33	1b	190	THR	2.0
34	1c	202	ILE	2.0
34	2c	152	ILE	2.0
35	1d	158	ILE	2.0
40	2i	7	THR	2.0
40	2i	118	LYS	2.0
45	1n	17	LYS	2.0
46	2o	5	LYS	2.0
47	2p	33	ILE	2.0
50	1s	79	THR	2.0
55	2x	47	U	2.0

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Mol	Chain	Res	Type	RSRZ
1	1A	1174	A	2.0
1	2A	655	A	2.0
10	2O	7	TYR	2.0
12	2Q	26	TYR	2.0
21	1Z	154	ASP	2.0
39	2h	72	PRO	2.0
42	2k	50	TYR	2.0
5	1F	15	SER	2.0
7	2H	38	SER	2.0
44	2m	97	PRO	2.0
9	2N	1	MET	2.0
33	2b	83	MET	2.0
9	2N	101	HIS	2.0
40	2i	38	GLN	2.0
6	2G	180	PHE	2.0
11	1P	15	ARG	2.0
12	1Q	5	ARG	2.0
14	2S	28	VAL	2.0
17	2V	51	VAL	2.0
20	2Y	2	ARG	2.0
26	24	50	VAL	2.0
32	1a	1007	C	2.0
34	1c	75	VAL	2.0
34	2c	75	VAL	2.0
36	2e	84	PHE	2.0
37	1f	90	VAL	2.0
40	1i	121	ARG	2.0
40	2i	44	VAL	2.0
49	2r	54	ARG	2.0
51	1t	23	ARG	2.0
52	2u	7	ARG	2.0
1	1A	10	G	2.0
1	1A	881	G	2.0
1	1A	2157	G	2.0
1	2A	10	G	2.0
32	2a	976	G	2.0
32	2a	1010	G	2.0
32	2a	1042	G	2.0
33	1b	215	LEU	2.0
34	2c	24	ALA	2.0
34	2c	133	ALA	2.0
35	1d	21	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
38	2g	7	ALA	2.0
40	2i	61	ALA	2.0
51	1t	12	ALA	2.0
54	2w	15	G	2.0
12	1Q	112	GLU	2.0
25	13	60	GLU	2.0
49	2r	66	LEU	2.0
5	2F	208	GLY	2.0
7	2H	78	GLY	2.0
36	1e	22	GLY	2.0
36	2e	23	GLY	2.0
40	2i	29	ASN	2.0
41	1j	55	LYS	2.0
41	2j	55	LYS	2.0
43	2l	29	GLY	2.0
6	2G	161	THR	2.0
7	2H	121	ILE	2.0
7	2H	129	THR	2.0
12	2Q	75	THR	2.0
36	2e	116	THR	2.0
41	2j	23	ILE	2.0
47	1p	22	THR	2.0
1	1A	1090	U	2.0
1	1A	1105	U	2.0
1	2A	362	U	2.0
32	2a	961	U	2.0
32	2a	1065	U	2.0
1	1A	2169	A	2.0
21	2Z	63	ASP	2.0
32	2a	975	A	2.0
32	2a	1357	A	2.0
33	2b	125	PRO	2.0
41	2j	39	PRO	2.0
19	1X	69	TYR	2.0
31	29	6	SER	2.0
34	1c	69	HIS	2.0

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

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	0.46	0.17	96,101,110,117	0
54	G7M	2w	46	24/25	0.58	0.16	86,98,107,118	0
54	4SU	2y	8	20/21	0.61	0.15	94,99,103,117	0
54	5MU	1y	54	21/22	0.61	0.15	88,94,106,116	0
54	G7M	2y	46	24/25	0.64	0.16	96,99,105,124	0
54	G7M	1y	46	24/25	0.65	0.17	91,97,103,117	0
54	G7M	1w	46	24/25	0.65	0.16	72,89,108,125	0
54	5MU	2y	54	21/22	0.67	0.15	93,98,108,122	0
54	PSU	1y	55	20/21	0.68	0.13	91,98,108,119	0
54	MIA	2y	37	22/30	0.69	0.16	83,93,104,117	0
54	4SU	1y	8	20/21	0.69	0.14	92,96,103,107	0
54	PSU	2y	32	20/21	0.72	0.17	86,92,101,110	0
54	PSU	2w	55	20/21	0.77	0.13	82,89,98,101	0
54	4SU	2w	8	20/21	0.78	0.14	92,97,102,108	0
54	PSU	1y	39	20/21	0.79	0.14	84,87,98,100	0
54	MIA	1y	37	22/30	0.80	0.15	81,88,95,103	0
54	PSU	2y	39	20/21	0.84	0.13	84,89,97,104	0
54	5MU	2w	54	21/22	0.85	0.12	78,82,89,93	0
32	2MG	2a	1207	24/25	0.86	0.13	76,86,89,90	0
54	PSU	1w	55	20/21	0.86	0.11	68,79,86,88	0
54	PSU	1y	32	20/21	0.87	0.13	80,88,92,96	0
54	MIA	2w	37	25/30	0.87	0.15	61,76,87,107	0
54	PSU	2w	32	20/21	0.88	0.13	76,85,97,99	0
55	PSU	2x	55	20/21	0.89	0.11	69,75,83,89	0
55	5MU	2x	54	21/22	0.89	0.12	69,79,83,86	0
54	MIA	1w	37	29/30	0.90	0.15	52,60,77,90	0
54	4SU	1w	8	20/21	0.90	0.11	80,85,90,92	0
32	G7M	2a	527	24/25	0.91	0.14	57,66,70,74	0
55	PSU	1x	55	20/21	0.91	0.10	56,62,72,77	0
55	4SU	2x	8	20/21	0.91	0.11	73,81,85,85	0
43	0TD	1l	92	10/11	0.92	0.11	48,53,57,74	0
32	5MC	2a	967	21/22	0.92	0.14	63,70,81,84	0
55	5MU	1x	54	21/22	0.92	0.10	58,64,73,74	0
32	5MC	2a	1400	21/22	0.92	0.15	65,70,73,77	0
1	5MU	2A	1915	21/22	0.92	0.11	65,69,75,76	0
32	M2G	2a	966	25/26	0.93	0.15	61,68,80,84	0
54	PSU	1w	32	20/21	0.93	0.11	63,71,81,82	0
55	5MC	2x	32	21/22	0.93	0.12	68,71,77,79	0
1	PSU	2A	1917	20/21	0.93	0.10	57,62,73,75	0
54	5MU	1w	54	21/22	0.93	0.10	57,70,73,78	0
32	5MC	2a	1404	21/22	0.93	0.11	48,54,59,63	0
1	PSU	2A	1911	20/21	0.94	0.09	59,62,67,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
55	5MC	1x	32	21/22	0.94	0.13	54,59,63,71	0
32	4OC	2a	1402	22/23	0.94	0.10	54,61,67,68	0
32	M2G	1a	966	25/26	0.94	0.12	45,53,63,69	0
1	OMC	2A	1920	21/22	0.94	0.10	54,62,64,65	0
1	MA6	2A	2058	24/25	0.94	0.11	38,49,57,59	0
32	PSU	2a	516	20/21	0.94	0.10	64,72,76,82	0
54	PSU	2w	39	20/21	0.94	0.10	65,81,87,87	0
32	2MG	1a	1207	24/25	0.94	0.10	67,74,77,79	0
32	G7M	1a	527	24/25	0.94	0.10	48,53,59,63	0
55	4SU	1x	8	20/21	0.94	0.09	55,63,67,67	0
32	UR3	2a	1498	21/22	0.95	0.11	53,59,63,68	0
32	MA6	2a	1518	24/25	0.95	0.12	51,64,71,75	0
43	0TD	2l	92	10/11	0.95	0.11	65,68,71,74	0
32	5MC	1a	967	21/22	0.95	0.12	47,54,62,67	0
1	5MU	1A	1915	21/22	0.95	0.09	50,56,59,61	0
32	PSU	1a	516	20/21	0.95	0.08	50,60,64,65	0
32	5MC	2a	1407	21/22	0.95	0.10	48,55,60,66	0
55	31H	2x	76	32/33	0.96	0.09	41,47,60,65	0
1	5MC	2A	1962	21/22	0.96	0.09	39,50,58,68	0
32	MA6	2a	1519	24/25	0.96	0.13	54,61,69,72	0
55	31H	1x	76	32/33	0.96	0.09	24,31,38,47	10
1	PSU	1A	1917	20/21	0.96	0.08	46,52,57,58	0
54	PSU	1w	39	20/21	0.96	0.08	56,68,73,81	0
1	MA6	1A	2058	24/25	0.96	0.11	25,38,41,42	0
1	5MC	2A	1942	21/22	0.96	0.08	53,59,63,63	0
1	5MC	1A	1962	21/22	0.97	0.07	31,39,43,52	0
1	2MA	2A	2503	23/24	0.97	0.09	37,41,44,45	0
1	OMU	2A	2552	21/22	0.97	0.08	39,46,51,55	0
1	PSU	2A	2605	20/21	0.97	0.08	37,41,49,50	0
32	5MC	1a	1400	21/22	0.97	0.08	48,53,57,60	0
32	4OC	1a	1402	22/23	0.97	0.08	43,49,51,54	0
32	5MC	1a	1404	21/22	0.97	0.07	34,43,47,48	0
32	5MC	1a	1407	21/22	0.97	0.08	36,44,46,49	0
32	MA6	1a	1519	24/25	0.97	0.09	41,46,50,53	0
1	5MU	2A	1939	21/22	0.97	0.08	33,39,46,50	0
1	PSU	1A	1911	20/21	0.97	0.07	40,48,54,54	0
1	5MC	1A	1942	21/22	0.97	0.09	36,41,47,51	0
1	OMG	2A	2251	24/25	0.98	0.07	39,44,48,50	0
1	OMG	1A	2251	24/25	0.98	0.05	24,27,32,32	0
32	UR3	1a	1498	21/22	0.98	0.07	40,44,48,54	0
32	MA6	1a	1518	24/25	0.98	0.08	38,42,47,47	0
1	2MA	1A	2503	23/24	0.98	0.06	23,27,29,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	OMU	1A	2552	21/22	0.98	0.07	27,32,34,38	0
1	PSU	1A	2605	20/21	0.98	0.06	24,29,36,37	0
1	5MU	1A	1939	21/22	0.98	0.07	27,32,37,38	0
1	OMC	1A	1920	21/22	0.98	0.06	41,46,48,48	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	2A	3643	1/1	0.44	0.30	85,85,85,85	0
56	MG	2a	1801	1/1	0.48	0.30	89,89,89,89	0
56	MG	1A	4061	1/1	0.49	0.25	79,79,79,79	0
56	MG	1A	4090	1/1	0.50	0.27	85,85,85,85	0
56	MG	1A	4073	1/1	0.52	0.28	86,86,86,86	0
56	MG	1a	1793	1/1	0.52	0.29	83,83,83,83	0
56	MG	1A	3703	1/1	0.53	0.28	56,56,56,56	0
56	MG	2a	1753	1/1	0.54	0.18	92,92,92,92	0
56	MG	1A	4007	1/1	0.56	0.16	69,69,69,69	0
56	MG	1A	4024	1/1	0.56	0.19	62,62,62,62	0
56	MG	2A	3085	1/1	0.56	0.18	87,87,87,87	0
56	MG	1A	3966	1/1	0.57	0.24	82,82,82,82	0
56	MG	1Y	202	1/1	0.59	0.21	79,79,79,79	0
56	MG	1A	4072	1/1	0.59	0.27	78,78,78,78	0
56	MG	2a	1827	1/1	0.59	0.27	81,81,81,81	0
56	MG	2a	1811	1/1	0.60	0.29	82,82,82,82	0
56	MG	2A	3532	1/1	0.60	0.23	69,69,69,69	0
56	MG	2A	3714	1/1	0.61	0.23	82,82,82,82	0
56	MG	2d	302	1/1	0.61	0.29	68,68,68,68	0
56	MG	2A	3295	1/1	0.62	0.23	79,79,79,79	0
56	MG	1B	229	1/1	0.62	0.20	87,87,87,87	0
56	MG	1A	4056	1/1	0.62	0.17	65,65,65,65	0
56	MG	1A	3349	1/1	0.63	0.22	64,64,64,64	0
56	MG	2a	1769	1/1	0.63	0.24	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	1622	1/1	0.63	0.17	73,73,73,73	0
56	MG	2A	3620	1/1	0.64	0.21	78,78,78,78	0
56	MG	2A	3244	1/1	0.64	0.35	79,79,79,79	0
56	MG	1A	3808	1/1	0.64	0.24	73,73,73,73	0
56	MG	2a	1820	1/1	0.64	0.23	74,74,74,74	0
56	MG	2A	3379	1/1	0.64	0.22	64,64,64,64	0
56	MG	1A	4012	1/1	0.64	0.16	80,80,80,80	0
56	MG	2a	1734	1/1	0.65	0.27	67,67,67,67	0
56	MG	1B	233	1/1	0.65	0.23	68,68,68,68	0
56	MG	2A	3732	1/1	0.65	0.31	72,72,72,72	0
56	MG	2A	3297	1/1	0.65	0.32	84,84,84,84	0
56	MG	1A	4076	1/1	0.66	0.17	76,76,76,76	0
56	MG	2j	201	1/1	0.66	0.18	85,85,85,85	0
56	MG	2a	1804	1/1	0.67	0.32	79,79,79,79	0
56	MG	2B	211	1/1	0.67	0.28	79,79,79,79	0
56	MG	1a	1721	1/1	0.67	0.34	88,88,88,88	0
56	MG	1A	3982	1/1	0.68	0.23	69,69,69,69	0
56	MG	2A	3615	1/1	0.69	0.24	60,60,60,60	0
56	MG	2v	102	1/1	0.69	0.39	83,83,83,83	0
56	MG	2a	1624	1/1	0.70	0.26	84,84,84,84	0
56	MG	1A	3802	1/1	0.70	0.21	62,62,62,62	0
56	MG	2A	3345	1/1	0.70	0.21	76,76,76,76	0
56	MG	2a	1755	1/1	0.70	0.20	84,84,84,84	0
56	MG	1A	3293	1/1	0.70	0.51	85,85,85,85	0
56	MG	2A	3058	1/1	0.70	0.30	85,85,85,85	0
56	MG	1A	3088	1/1	0.70	0.22	58,58,58,58	0
56	MG	2A	3163	1/1	0.70	0.27	77,77,77,77	0
56	MG	2A	3169	1/1	0.70	0.16	66,66,66,66	0
56	MG	2A	3188	1/1	0.70	0.33	68,68,68,68	0
56	MG	1A	3094	1/1	0.70	0.18	81,81,81,81	0
56	MG	2A	3273	1/1	0.70	0.36	77,77,77,77	0
56	MG	1a	1635	1/1	0.70	0.31	68,68,68,68	0
56	MG	2A	3195	1/1	0.71	0.17	74,74,74,74	0
56	MG	2A	3336	1/1	0.71	0.43	78,78,78,78	0
56	MG	2A	3205	1/1	0.71	0.33	78,78,78,78	0
56	MG	2a	1781	1/1	0.71	0.28	79,79,79,79	0
56	MG	2a	1797	1/1	0.71	0.23	83,83,83,83	0
56	MG	2A	3046	1/1	0.71	0.24	74,74,74,74	0
56	MG	2A	3794	1/1	0.71	0.18	58,58,58,58	0
56	MG	2A	3502	1/1	0.71	0.26	63,63,63,63	0
56	MG	1A	3875	1/1	0.71	0.19	35,35,35,35	0
56	MG	2a	1822	1/1	0.71	0.39	77,77,77,77	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	0.71	0.28	64,64,64,64	0
56	MG	2a	1646	1/1	0.71	0.40	79,79,79,79	0
56	MG	2a	1722	1/1	0.71	0.47	72,72,72,72	0
56	MG	1A	3765	1/1	0.71	0.14	24,24,24,24	0
56	MG	2A	3770	1/1	0.72	0.23	78,78,78,78	0
56	MG	1A	3830	1/1	0.72	0.20	66,66,66,66	0
56	MG	1A	4041	1/1	0.72	0.26	75,75,75,75	0
56	MG	2a	1603	1/1	0.72	0.28	85,85,85,85	0
56	MG	2a	1616	1/1	0.72	0.29	77,77,77,77	0
56	MG	2A	3530	1/1	0.72	0.21	78,78,78,78	0
56	MG	1A	3794	1/1	0.72	0.18	66,66,66,66	0
56	MG	1a	1662	1/1	0.72	0.31	66,66,66,66	0
56	MG	2a	1670	1/1	0.73	0.31	76,76,76,76	0
56	MG	2a	1690	1/1	0.73	0.24	80,80,80,80	0
56	MG	2a	1716	1/1	0.73	0.24	72,72,72,72	0
56	MG	1A	4040	1/1	0.73	0.15	69,69,69,69	0
56	MG	2A	3057	1/1	0.73	0.27	66,66,66,66	0
56	MG	1O	206	1/1	0.73	0.24	70,70,70,70	0
56	MG	2A	3671	1/1	0.73	0.20	72,72,72,72	0
56	MG	1A	3993	1/1	0.73	0.14	67,67,67,67	0
56	MG	1A	4046	1/1	0.73	0.27	47,47,47,47	0
56	MG	1A	4087	1/1	0.73	0.25	68,68,68,68	0
56	MG	2A	3771	1/1	0.73	0.14	68,68,68,68	0
56	MG	1A	4019	1/1	0.73	0.14	45,45,45,45	0
56	MG	2A	3383	1/1	0.73	0.22	66,66,66,66	0
56	MG	2A	3455	1/1	0.73	0.21	79,79,79,79	0
56	MG	1a	1761	1/1	0.73	0.23	83,83,83,83	0
56	MG	1A	3512	1/1	0.73	0.17	64,64,64,64	0
56	MG	2A	3211	1/1	0.73	0.26	76,76,76,76	0
56	MG	2A	3240	1/1	0.73	0.40	84,84,84,84	0
56	MG	2a	1649	1/1	0.73	0.26	77,77,77,77	0
56	MG	2A	3158	1/1	0.74	0.38	79,79,79,79	0
56	MG	1A	4018	1/1	0.74	0.26	64,64,64,64	0
56	MG	1a	1679	1/1	0.74	0.36	69,69,69,69	0
56	MG	2a	1621	1/1	0.74	0.23	83,83,83,83	0
56	MG	1A	3892	1/1	0.74	0.15	57,57,57,57	0
56	MG	2a	1796	1/1	0.74	0.26	67,67,67,67	0
56	MG	2A	3729	1/1	0.74	0.18	63,63,63,63	0
56	MG	2A	3730	1/1	0.74	0.15	80,80,80,80	0
56	MG	2a	1647	1/1	0.74	0.43	83,83,83,83	0
56	MG	1a	1760	1/1	0.74	0.25	66,66,66,66	0
56	MG	2a	1654	1/1	0.74	0.28	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3292	1/1	0.74	0.27	55,55,55,55	0
56	MG	2a	1676	1/1	0.74	0.27	66,66,66,66	0
56	MG	2A	3337	1/1	0.74	0.16	76,76,76,76	0
56	MG	2A	3773	1/1	0.74	0.18	67,67,67,67	0
56	MG	2A	3086	1/1	0.74	0.28	72,72,72,72	0
56	MG	2a	1749	1/1	0.75	0.14	80,80,80,80	0
56	MG	2a	1752	1/1	0.75	0.23	90,90,90,90	0
56	MG	1A	3898	1/1	0.75	0.14	48,48,48,48	0
56	MG	2A	3687	1/1	0.75	0.21	51,51,51,51	0
56	MG	1B	230	1/1	0.75	0.11	81,81,81,81	0
56	MG	2a	1771	1/1	0.75	0.35	70,70,70,70	0
56	MG	2a	1634	1/1	0.75	0.42	79,79,79,79	0
56	MG	2a	1784	1/1	0.75	0.34	72,72,72,72	0
56	MG	2a	1792	1/1	0.75	0.34	71,71,71,71	0
56	MG	2A	3171	1/1	0.75	0.18	57,57,57,57	0
56	MG	1A	4033	1/1	0.75	0.16	43,43,43,43	0
56	MG	1O	201	1/1	0.75	0.16	72,72,72,72	0
56	MG	1A	3498	1/1	0.75	0.19	65,65,65,65	0
56	MG	2A	3593	1/1	0.75	0.25	83,83,83,83	0
56	MG	2a	1814	1/1	0.75	0.41	81,81,81,81	0
56	MG	2A	3340	1/1	0.75	0.23	72,72,72,72	0
56	MG	1B	222	1/1	0.75	0.26	80,80,80,80	0
56	MG	2a	1701	1/1	0.75	0.19	68,68,68,68	0
56	MG	2A	3624	1/1	0.75	0.24	61,61,61,61	0
56	MG	1a	1774	1/1	0.75	0.25	70,70,70,70	0
56	MG	2A	3666	1/1	0.75	0.25	72,72,72,72	0
56	MG	2y	103	1/1	0.75	0.16	85,85,85,85	0
56	MG	2A	3190	1/1	0.76	0.26	79,79,79,79	0
56	MG	2A	3322	1/1	0.76	0.30	64,64,64,64	0
56	MG	2a	1626	1/1	0.76	0.29	78,78,78,78	0
56	MG	1A	4074	1/1	0.76	0.24	72,72,72,72	0
56	MG	1A	4014	1/1	0.76	0.16	83,83,83,83	0
56	MG	1A	3933	1/1	0.76	0.15	35,35,35,35	0
56	MG	2A	3600	1/1	0.76	0.23	81,81,81,81	0
56	MG	2a	1653	1/1	0.76	0.34	77,77,77,77	0
56	MG	1a	1670	1/1	0.76	0.23	75,75,75,75	0
56	MG	2a	1798	1/1	0.76	0.34	71,71,71,71	0
56	MG	2a	1657	1/1	0.76	0.24	74,74,74,74	0
56	MG	2A	3616	1/1	0.76	0.31	81,81,81,81	0
56	MG	2a	1808	1/1	0.76	0.17	77,77,77,77	0
56	MG	1A	3803	1/1	0.76	0.18	52,52,52,52	0
56	MG	2a	1686	1/1	0.76	0.42	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3797	1/1	0.76	0.18	68,68,68,68	0
56	MG	1a	1694	1/1	0.76	0.31	72,72,72,72	0
56	MG	2F	302	1/1	0.76	0.17	76,76,76,76	0
56	MG	2A	3408	1/1	0.76	0.26	77,77,77,77	0
56	MG	2a	1612	1/1	0.76	0.24	76,76,76,76	0
56	MG	2A	3418	1/1	0.76	0.21	72,72,72,72	0
56	MG	1A	3687	1/1	0.76	0.14	70,70,70,70	0
56	MG	2A	3589	1/1	0.77	0.17	60,60,60,60	0
56	MG	2a	1770	1/1	0.77	0.21	77,77,77,77	0
56	MG	1A	3413	1/1	0.77	0.15	55,55,55,55	0
56	MG	2A	3599	1/1	0.77	0.23	72,72,72,72	0
56	MG	1A	3680	1/1	0.77	0.20	72,72,72,72	0
56	MG	1A	3942	1/1	0.77	0.19	78,78,78,78	0
56	MG	2A	3263	1/1	0.77	0.36	73,73,73,73	0
56	MG	2A	3404	1/1	0.77	0.22	66,66,66,66	0
56	MG	2a	1671	1/1	0.77	0.25	72,72,72,72	0
56	MG	1x	109	1/1	0.77	0.32	76,76,76,76	0
56	MG	2A	3279	1/1	0.77	0.21	76,76,76,76	0
56	MG	2a	1611	1/1	0.77	0.29	81,81,81,81	0
56	MG	2a	1698	1/1	0.77	0.29	77,77,77,77	0
56	MG	2A	3432	1/1	0.77	0.26	75,75,75,75	0
56	MG	2A	3026	1/1	0.77	0.22	79,79,79,79	0
56	MG	2A	3680	1/1	0.77	0.15	69,69,69,69	0
56	MG	1A	3835	1/1	0.77	0.15	73,73,73,73	0
56	MG	1A	3466	1/1	0.77	0.24	67,67,67,67	0
56	MG	1A	3232	1/1	0.77	0.22	66,66,66,66	0
56	MG	1B	221	1/1	0.77	0.14	66,66,66,66	0
56	MG	2a	1636	1/1	0.77	0.23	71,71,71,71	0
56	MG	2a	1745	1/1	0.78	0.29	79,79,79,79	0
56	MG	1A	4091	1/1	0.78	0.19	65,65,65,65	0
56	MG	1A	3939	1/1	0.78	0.14	71,71,71,71	0
56	MG	1A	3404	1/1	0.78	0.23	54,54,54,54	0
56	MG	2a	1754	1/1	0.78	0.14	70,70,70,70	0
56	MG	1a	1677	1/1	0.78	0.32	63,63,63,63	0
56	MG	2a	1763	1/1	0.78	0.23	74,74,74,74	0
56	MG	2A	3080	1/1	0.78	0.23	66,66,66,66	0
56	MG	2A	3245	1/1	0.78	0.21	78,78,78,78	0
56	MG	2a	1630	1/1	0.78	0.36	82,82,82,82	0
56	MG	2A	3692	1/1	0.78	0.18	75,75,75,75	0
56	MG	1A	3862	1/1	0.78	0.18	53,53,53,53	0
56	MG	2a	1785	1/1	0.78	0.21	76,76,76,76	0
56	MG	2A	3725	1/1	0.78	0.15	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3264	1/1	0.78	0.32	78,78,78,78	0
56	MG	1A	3970	1/1	0.78	0.19	71,71,71,71	0
56	MG	2A	3105	1/1	0.78	0.35	73,73,73,73	0
56	MG	2A	3739	1/1	0.78	0.22	70,70,70,70	0
56	MG	2A	3130	1/1	0.78	0.41	78,78,78,78	0
56	MG	2A	3559	1/1	0.78	0.29	70,70,70,70	0
56	MG	1A	3026	1/1	0.78	0.34	68,68,68,68	0
56	MG	2A	3313	1/1	0.78	0.37	74,74,74,74	0
56	MG	2a	1816	1/1	0.78	0.29	75,75,75,75	0
56	MG	1A	3807	1/1	0.78	0.24	76,76,76,76	0
56	MG	1A	3523	1/1	0.78	0.13	59,59,59,59	0
56	MG	2D	303	1/1	0.78	0.18	65,65,65,65	0
56	MG	1A	3350	1/1	0.78	0.30	71,71,71,71	0
56	MG	14	101	1/1	0.78	0.20	81,81,81,81	0
56	MG	2a	1607	1/1	0.78	0.26	79,79,79,79	0
56	MG	1a	1632	1/1	0.78	0.31	83,83,83,83	0
56	MG	1A	3358	1/1	0.79	0.20	59,59,59,59	0
56	MG	1A	3945	1/1	0.79	0.19	69,69,69,69	0
56	MG	1a	1736	1/1	0.79	0.35	81,81,81,81	0
56	MG	2A	3097	1/1	0.79	0.33	68,68,68,68	0
56	MG	1a	1749	1/1	0.79	0.20	74,74,74,74	0
56	MG	1A	3810	1/1	0.79	0.22	65,65,65,65	0
56	MG	2A	3475	1/1	0.79	0.18	70,70,70,70	0
56	MG	1A	3705	1/1	0.79	0.18	58,58,58,58	0
56	MG	2A	3516	1/1	0.79	0.19	55,55,55,55	0
56	MG	1A	3980	1/1	0.79	0.11	33,33,33,33	0
56	MG	2A	3731	1/1	0.79	0.23	69,69,69,69	0
56	MG	1a	1786	1/1	0.79	0.35	64,64,64,64	0
56	MG	2a	1786	1/1	0.79	0.21	77,77,77,77	0
56	MG	2A	3299	1/1	0.79	0.21	68,68,68,68	0
56	MG	1a	1656	1/1	0.79	0.13	61,61,61,61	0
56	MG	2A	3568	1/1	0.79	0.25	47,47,47,47	0
56	MG	1A	3923	1/1	0.79	0.14	65,65,65,65	0
56	MG	1A	3553	1/1	0.79	0.45	78,78,78,78	0
56	MG	2a	1803	1/1	0.79	0.36	66,66,66,66	0
56	MG	1D	310	1/1	0.79	0.21	67,67,67,67	0
56	MG	2a	1805	1/1	0.79	0.27	84,84,84,84	0
56	MG	2A	3798	1/1	0.79	0.23	62,62,62,62	0
56	MG	1A	3784	1/1	0.79	0.29	85,85,85,85	0
56	MG	2A	3206	1/1	0.79	0.26	67,67,67,67	0
56	MG	2a	1694	1/1	0.79	0.29	73,73,73,73	0
56	MG	2E	302	1/1	0.79	0.17	76,76,76,76	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	0.79	0.24	69,69,69,69	0
56	MG	2A	3352	1/1	0.79	0.30	60,60,60,60	0
56	MG	2a	1602	1/1	0.79	0.17	86,86,86,86	0
56	MG	2a	1723	1/1	0.79	0.31	70,70,70,70	0
56	MG	2l	204	1/1	0.79	0.18	77,77,77,77	0
56	MG	2A	3356	1/1	0.79	0.25	62,62,62,62	0
56	MG	2y	101	1/1	0.79	0.13	85,85,85,85	0
56	MG	2y	102	1/1	0.79	0.39	79,79,79,79	0
56	MG	1a	1686	1/1	0.79	0.20	67,67,67,67	0
56	MG	2A	3496	1/1	0.80	0.16	75,75,75,75	0
56	MG	1A	4079	1/1	0.80	0.18	67,67,67,67	0
56	MG	2a	1737	1/1	0.80	0.36	83,83,83,83	0
56	MG	1E	317	1/1	0.80	0.08	37,37,37,37	0
56	MG	2A	3063	1/1	0.80	0.16	61,61,61,61	0
56	MG	2A	3248	1/1	0.80	0.19	72,72,72,72	0
56	MG	2A	3258	1/1	0.80	0.19	82,82,82,82	0
56	MG	2A	3068	1/1	0.80	0.15	63,63,63,63	0
56	MG	1F	312	1/1	0.80	0.21	60,60,60,60	0
56	MG	1A	4085	1/1	0.80	0.25	40,40,40,40	0
56	MG	1a	1727	1/1	0.80	0.23	66,66,66,66	0
56	MG	2A	3595	1/1	0.80	0.13	75,75,75,75	0
56	MG	2A	3598	1/1	0.80	0.26	75,75,75,75	0
56	MG	1A	3584	1/1	0.80	0.22	67,67,67,67	0
56	MG	2A	3100	1/1	0.80	0.23	81,81,81,81	0
56	MG	1a	1742	1/1	0.80	0.21	68,68,68,68	0
56	MG	2A	3109	1/1	0.80	0.26	73,73,73,73	0
56	MG	2A	3617	1/1	0.80	0.18	82,82,82,82	0
56	MG	1A	3721	1/1	0.80	0.23	62,62,62,62	0
56	MG	2A	3146	1/1	0.80	0.18	64,64,64,64	0
56	MG	1a	1758	1/1	0.80	0.15	70,70,70,70	0
56	MG	2A	3665	1/1	0.80	0.17	76,76,76,76	0
56	MG	2a	1641	1/1	0.80	0.25	73,73,73,73	0
56	MG	1A	4057	1/1	0.80	0.14	25,25,25,25	0
56	MG	1a	1603	1/1	0.80	0.21	68,68,68,68	0
56	MG	2A	3349	1/1	0.80	0.29	63,63,63,63	0
56	MG	1A	3445	1/1	0.80	0.19	69,69,69,69	0
56	MG	2A	3354	1/1	0.80	0.30	54,54,54,54	0
56	MG	1A	3987	1/1	0.80	0.16	30,30,30,30	0
56	MG	1B	228	1/1	0.80	0.15	74,74,74,74	0
56	MG	1x	103	1/1	0.80	0.17	65,65,65,65	0
56	MG	1A	3323	1/1	0.80	0.23	65,65,65,65	0
56	MG	1A	3268	1/1	0.80	0.17	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	3820	1/1	0.80	0.23	58,58,58,58	0
56	MG	2A	3222	1/1	0.80	0.23	67,67,67,67	0
56	MG	2q	202	1/1	0.80	0.21	83,83,83,83	0
56	MG	2A	3236	1/1	0.80	0.33	73,73,73,73	0
56	MG	2A	3468	1/1	0.80	0.21	69,69,69,69	0
56	MG	2A	3237	1/1	0.80	0.18	67,67,67,67	0
56	MG	2A	3792	1/1	0.80	0.19	77,77,77,77	0
56	MG	1A	3400	1/1	0.81	0.19	59,59,59,59	0
56	MG	1A	3164	1/1	0.81	0.20	63,63,63,63	0
56	MG	1A	3728	1/1	0.81	0.18	65,65,65,65	0
56	MG	1A	3734	1/1	0.81	0.15	56,56,56,56	0
56	MG	2A	3270	1/1	0.81	0.19	72,72,72,72	0
56	MG	1b	301	1/1	0.81	0.19	81,81,81,81	0
56	MG	1A	3838	1/1	0.81	0.14	64,64,64,64	0
56	MG	2A	3164	1/1	0.81	0.33	79,79,79,79	0
56	MG	1A	3187	1/1	0.81	0.16	58,58,58,58	0
56	MG	2A	3793	1/1	0.81	0.24	66,66,66,66	0
56	MG	2A	3536	1/1	0.81	0.19	73,73,73,73	0
56	MG	2A	3795	1/1	0.81	0.19	75,75,75,75	0
56	MG	2A	3540	1/1	0.81	0.26	70,70,70,70	0
56	MG	2A	3298	1/1	0.81	0.23	85,85,85,85	0
56	MG	2B	205	1/1	0.81	0.32	72,72,72,72	0
56	MG	1A	4062	1/1	0.81	0.20	70,70,70,70	0
56	MG	2A	3035	1/1	0.81	0.23	74,74,74,74	0
56	MG	1A	3419	1/1	0.81	0.17	58,58,58,58	0
56	MG	2a	1766	1/1	0.81	0.27	83,83,83,83	0
56	MG	2a	1768	1/1	0.81	0.22	78,78,78,78	0
56	MG	1A	3425	1/1	0.81	0.21	71,71,71,71	0
56	MG	2A	3198	1/1	0.81	0.48	77,77,77,77	0
56	MG	2l	101	1/1	0.81	0.17	58,58,58,58	0
56	MG	2A	3338	1/1	0.81	0.17	62,62,62,62	0
56	MG	1a	1703	1/1	0.81	0.30	81,81,81,81	0
56	MG	2a	1604	1/1	0.81	0.22	82,82,82,82	0
56	MG	2a	1605	1/1	0.81	0.28	69,69,69,69	0
56	MG	2A	3342	1/1	0.81	0.14	79,79,79,79	0
56	MG	1A	3644	1/1	0.81	0.15	59,59,59,59	0
56	MG	1A	3907	1/1	0.81	0.15	39,39,39,39	0
56	MG	2a	1615	1/1	0.81	0.45	78,78,78,78	0
56	MG	2a	1800	1/1	0.81	0.31	67,67,67,67	0
56	MG	2A	3217	1/1	0.81	0.24	86,86,86,86	0
56	MG	2a	1802	1/1	0.81	0.17	69,69,69,69	0
56	MG	2A	3219	1/1	0.81	0.24	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3077	1/1	0.81	0.26	63,63,63,63	0
56	MG	2A	3635	1/1	0.81	0.28	74,74,74,74	0
56	MG	2A	3377	1/1	0.81	0.34	64,64,64,64	0
56	MG	2a	1809	1/1	0.81	0.29	77,77,77,77	0
56	MG	2A	3656	1/1	0.81	0.17	52,52,52,52	0
56	MG	1A	3369	1/1	0.81	0.39	66,66,66,66	0
56	MG	1A	3804	1/1	0.81	0.12	55,55,55,55	0
56	MG	2a	1637	1/1	0.81	0.33	61,61,61,61	0
56	MG	2A	3390	1/1	0.81	0.37	62,62,62,62	0
56	MG	2A	3391	1/1	0.81	0.30	76,76,76,76	0
56	MG	1l	102	1/1	0.81	0.22	49,49,49,49	0
56	MG	1A	3385	1/1	0.81	0.29	48,48,48,48	0
56	MG	2A	3701	1/1	0.81	0.22	72,72,72,72	0
56	MG	2A	3707	1/1	0.81	0.22	79,79,79,79	0
56	MG	2A	3709	1/1	0.81	0.32	76,76,76,76	0
56	MG	2w	104	1/1	0.81	0.34	81,81,81,81	0
56	MG	2a	1668	1/1	0.81	0.31	66,66,66,66	0
56	MG	2A	3413	1/1	0.81	0.14	65,65,65,65	0
56	MG	1A	3467	1/1	0.81	0.17	72,72,72,72	0
56	MG	2A	3425	1/1	0.82	0.21	63,63,63,63	0
56	MG	1A	3839	1/1	0.82	0.14	69,69,69,69	0
56	MG	2A	3254	1/1	0.82	0.22	66,66,66,66	0
56	MG	2a	1707	1/1	0.82	0.24	79,79,79,79	0
56	MG	1A	3856	1/1	0.82	0.15	63,63,63,63	0
56	MG	1A	3860	1/1	0.82	0.14	57,57,57,57	0
56	MG	2A	3478	1/1	0.82	0.24	65,65,65,65	0
56	MG	2a	1733	1/1	0.82	0.26	79,79,79,79	0
56	MG	2A	3484	1/1	0.82	0.13	42,42,42,42	0
56	MG	1A	3971	1/1	0.82	0.21	66,66,66,66	0
56	MG	2A	3112	1/1	0.82	0.27	63,63,63,63	0
56	MG	1A	3426	1/1	0.82	0.17	57,57,57,57	0
56	MG	1a	1782	1/1	0.82	0.14	66,66,66,66	0
56	MG	2A	3287	1/1	0.82	0.21	55,55,55,55	0
56	MG	1A	3874	1/1	0.82	0.15	43,43,43,43	0
56	MG	2A	3800	1/1	0.82	0.28	74,74,74,74	0
56	MG	1A	3676	1/1	0.82	0.17	64,64,64,64	0
56	MG	1A	3742	1/1	0.82	0.25	65,65,65,65	0
56	MG	2A	3547	1/1	0.82	0.22	64,64,64,64	0
56	MG	2A	3552	1/1	0.82	0.14	39,39,39,39	0
56	MG	1w	104	1/1	0.82	0.24	75,75,75,75	0
56	MG	1x	102	1/1	0.82	0.22	68,68,68,68	0
56	MG	2a	1774	1/1	0.82	0.21	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3320	1/1	0.82	0.29	77,77,77,77	0
56	MG	2a	1783	1/1	0.82	0.16	60,60,60,60	0
56	MG	1A	3526	1/1	0.82	0.28	59,59,59,59	0
56	MG	2A	3325	1/1	0.82	0.18	67,67,67,67	0
56	MG	2A	3326	1/1	0.82	0.27	80,80,80,80	0
56	MG	2a	1789	1/1	0.82	0.29	77,77,77,77	0
56	MG	2A	3327	1/1	0.82	0.34	54,54,54,54	0
56	MG	1A	3306	1/1	0.82	0.35	63,63,63,63	0
56	MG	2A	3604	1/1	0.82	0.17	67,67,67,67	0
56	MG	2A	3612	1/1	0.82	0.14	58,58,58,58	0
56	MG	2A	3193	1/1	0.82	0.28	72,72,72,72	0
56	MG	1x	113	1/1	0.82	0.19	85,85,85,85	0
56	MG	2A	3197	1/1	0.82	0.12	65,65,65,65	0
56	MG	1A	3583	1/1	0.82	0.25	54,54,54,54	0
56	MG	2A	3203	1/1	0.82	0.17	73,73,73,73	0
56	MG	2A	3625	1/1	0.82	0.15	57,57,57,57	0
56	MG	1A	3833	1/1	0.82	0.25	66,66,66,66	0
56	MG	1A	3327	1/1	0.82	0.31	64,64,64,64	0
56	MG	2A	3644	1/1	0.82	0.32	71,71,71,71	0
56	MG	2A	3049	1/1	0.82	0.25	71,71,71,71	0
56	MG	2A	3213	1/1	0.82	0.16	49,49,49,49	0
56	MG	2A	3215	1/1	0.82	0.45	59,59,59,59	0
56	MG	1a	1705	1/1	0.82	0.11	70,70,70,70	0
56	MG	1a	1718	1/1	0.82	0.15	75,75,75,75	0
56	MG	2A	3682	1/1	0.82	0.18	40,40,40,40	0
56	MG	2A	3389	1/1	0.82	0.29	78,78,78,78	0
56	MG	1O	205	1/1	0.82	0.18	73,73,73,73	0
56	MG	1A	3606	1/1	0.82	0.12	37,37,37,37	0
56	MG	2r	101	1/1	0.82	0.23	82,82,82,82	0
56	MG	1a	1735	1/1	0.82	0.11	70,70,70,70	0
56	MG	1T	201	1/1	0.82	0.19	61,61,61,61	0
56	MG	1A	4086	1/1	0.82	0.20	54,54,54,54	0
56	MG	1a	1748	1/1	0.82	0.17	69,69,69,69	0
56	MG	2A	3420	1/1	0.82	0.28	77,77,77,77	0
56	MG	2A	3083	1/1	0.83	0.16	63,63,63,63	0
56	MG	1A	3958	1/1	0.83	0.17	53,53,53,53	0
56	MG	1A	3846	1/1	0.83	0.13	76,76,76,76	0
56	MG	2A	3096	1/1	0.83	0.30	79,79,79,79	0
56	MG	2A	3429	1/1	0.83	0.14	52,52,52,52	0
56	MG	2a	1689	1/1	0.83	0.29	71,71,71,71	0
56	MG	1a	1725	1/1	0.83	0.21	82,82,82,82	0
56	MG	2A	3433	1/1	0.83	0.24	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1B	234	1/1	0.83	0.18	74,74,74,74	0
56	MG	2A	3715	1/1	0.83	0.18	77,77,77,77	0
56	MG	1A	4050	1/1	0.83	0.09	37,37,37,37	0
56	MG	2A	3274	1/1	0.83	0.26	69,69,69,69	0
56	MG	1E	314	1/1	0.83	0.17	69,69,69,69	0
56	MG	1A	3101	1/1	0.83	0.14	66,66,66,66	0
56	MG	2a	1728	1/1	0.83	0.23	67,67,67,67	0
56	MG	1A	3530	1/1	0.83	0.36	72,72,72,72	0
56	MG	2A	3296	1/1	0.83	0.41	84,84,84,84	0
56	MG	2A	3742	1/1	0.83	0.21	52,52,52,52	0
56	MG	2A	3757	1/1	0.83	0.25	69,69,69,69	0
56	MG	2A	3758	1/1	0.83	0.21	49,49,49,49	0
56	MG	1A	3698	1/1	0.83	0.18	59,59,59,59	0
56	MG	2A	3521	1/1	0.83	0.13	62,62,62,62	0
56	MG	1A	3294	1/1	0.83	0.17	55,55,55,55	0
56	MG	2A	3782	1/1	0.83	0.14	69,69,69,69	0
56	MG	1A	3256	1/1	0.83	0.11	41,41,41,41	0
56	MG	2A	3305	1/1	0.83	0.18	61,61,61,61	0
56	MG	2A	3539	1/1	0.83	0.21	70,70,70,70	0
56	MG	2A	3307	1/1	0.83	0.24	68,68,68,68	0
56	MG	1A	3889	1/1	0.83	0.26	49,49,49,49	0
56	MG	1A	3995	1/1	0.83	0.17	56,56,56,56	0
56	MG	1A	3708	1/1	0.83	0.24	60,60,60,60	0
56	MG	2B	203	1/1	0.83	0.28	66,66,66,66	0
56	MG	1A	4008	1/1	0.83	0.11	69,69,69,69	0
56	MG	2B	206	1/1	0.83	0.27	67,67,67,67	0
56	MG	1A	4080	1/1	0.83	0.18	66,66,66,66	0
56	MG	1a	1622	1/1	0.83	0.27	75,75,75,75	0
56	MG	1A	4011	1/1	0.83	0.17	77,77,77,77	0
56	MG	1A	3497	1/1	0.83	0.13	80,80,80,80	0
56	MG	1a	1642	1/1	0.83	0.23	67,67,67,67	0
56	MG	1a	1649	1/1	0.83	0.23	65,65,65,65	0
56	MG	1a	1652	1/1	0.83	0.35	69,69,69,69	0
56	MG	2A	3602	1/1	0.83	0.18	75,75,75,75	0
56	MG	1A	4013	1/1	0.83	0.12	60,60,60,60	0
56	MG	2A	3609	1/1	0.83	0.16	63,63,63,63	0
56	MG	1A	4088	1/1	0.83	0.16	63,63,63,63	0
56	MG	2A	3043	1/1	0.83	0.30	65,65,65,65	0
56	MG	1A	3586	1/1	0.83	0.28	64,64,64,64	0
56	MG	1A	3024	1/1	0.83	0.29	70,70,70,70	0
56	MG	2A	3374	1/1	0.83	0.36	66,66,66,66	0
56	MG	1B	212	1/1	0.83	0.30	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	1a	1680	1/1	0.83	0.32	63,63,63,63	0
56	MG	2A	3628	1/1	0.83	0.25	71,71,71,71	0
56	MG	1A	3638	1/1	0.83	0.21	70,70,70,70	0
56	MG	2A	3638	1/1	0.83	0.22	67,67,67,67	0
56	MG	2A	3065	1/1	0.83	0.19	60,60,60,60	0
56	MG	2a	1828	1/1	0.83	0.29	79,79,79,79	0
56	MG	2A	3238	1/1	0.83	0.22	75,75,75,75	0
56	MG	2A	3651	1/1	0.83	0.22	65,65,65,65	0
56	MG	1A	3371	1/1	0.83	0.28	62,62,62,62	0
56	MG	2a	1645	1/1	0.83	0.34	72,72,72,72	0
56	MG	2A	3396	1/1	0.83	0.20	66,66,66,66	0
56	MG	1A	3099	1/1	0.83	0.17	69,69,69,69	0
56	MG	1A	3786	1/1	0.83	0.21	61,61,61,61	0
56	MG	2A	3673	1/1	0.83	0.10	78,78,78,78	0
56	MG	2A	3677	1/1	0.83	0.22	69,69,69,69	0
56	MG	2A	3679	1/1	0.83	0.19	82,82,82,82	0
56	MG	1A	3412	1/1	0.84	0.15	65,65,65,65	0
56	MG	1A	3180	1/1	0.84	0.24	56,56,56,56	0
56	MG	1A	3959	1/1	0.84	0.20	65,65,65,65	0
56	MG	1A	3965	1/1	0.84	0.14	74,74,74,74	0
56	MG	2A	3089	1/1	0.84	0.14	48,48,48,48	0
56	MG	2A	3695	1/1	0.84	0.23	69,69,69,69	0
56	MG	2A	3095	1/1	0.84	0.14	73,73,73,73	0
56	MG	1A	3329	1/1	0.84	0.12	47,47,47,47	0
56	MG	2A	3483	1/1	0.84	0.22	66,66,66,66	0
56	MG	1A	3370	1/1	0.84	0.19	59,59,59,59	0
56	MG	1A	3334	1/1	0.84	0.12	53,53,53,53	0
56	MG	2A	3104	1/1	0.84	0.24	75,75,75,75	0
56	MG	2a	1693	1/1	0.84	0.27	72,72,72,72	0
56	MG	2A	3513	1/1	0.84	0.22	76,76,76,76	0
56	MG	2a	1697	1/1	0.84	0.30	74,74,74,74	0
56	MG	1A	3720	1/1	0.84	0.21	73,73,73,73	0
56	MG	10	108	1/1	0.84	0.24	67,67,67,67	0
56	MG	2A	3528	1/1	0.84	0.19	59,59,59,59	0
56	MG	2a	1708	1/1	0.84	0.23	78,78,78,78	0
56	MG	1A	3573	1/1	0.84	0.23	46,46,46,46	0
56	MG	11	104	1/1	0.84	0.17	77,77,77,77	0
56	MG	2A	3145	1/1	0.84	0.34	63,63,63,63	0
56	MG	2a	1726	1/1	0.84	0.30	79,79,79,79	0
56	MG	1A	3984	1/1	0.84	0.18	49,49,49,49	0
56	MG	2A	3147	1/1	0.84	0.21	69,69,69,69	0
56	MG	2A	3153	1/1	0.84	0.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3546	1/1	0.84	0.29	74,74,74,74	0
56	MG	2a	1739	1/1	0.84	0.43	79,79,79,79	0
56	MG	2a	1743	1/1	0.84	0.21	78,78,78,78	0
56	MG	1a	1777	1/1	0.84	0.22	69,69,69,69	0
56	MG	1a	1602	1/1	0.84	0.28	70,70,70,70	0
56	MG	2A	3553	1/1	0.84	0.14	40,40,40,40	0
56	MG	1A	3438	1/1	0.84	0.17	50,50,50,50	0
56	MG	1a	1788	1/1	0.84	0.19	84,84,84,84	0
56	MG	1a	1791	1/1	0.84	0.13	76,76,76,76	0
56	MG	1A	3376	1/1	0.84	0.24	64,64,64,64	0
56	MG	1A	3994	1/1	0.84	0.15	75,75,75,75	0
56	MG	2B	201	1/1	0.84	0.34	78,78,78,78	0
56	MG	1l	202	1/1	0.84	0.17	67,67,67,67	0
56	MG	1A	3465	1/1	0.84	0.32	76,76,76,76	0
56	MG	1A	3594	1/1	0.84	0.14	62,62,62,62	0
56	MG	2B	208	1/1	0.84	0.25	73,73,73,73	0
56	MG	1A	3598	1/1	0.84	0.28	59,59,59,59	0
56	MG	2B	212	1/1	0.84	0.35	78,78,78,78	0
56	MG	2A	3347	1/1	0.84	0.17	57,57,57,57	0
56	MG	2D	306	1/1	0.84	0.29	59,59,59,59	0
56	MG	2A	3199	1/1	0.84	0.32	52,52,52,52	0
56	MG	2A	3350	1/1	0.84	0.31	54,54,54,54	0
56	MG	2a	1791	1/1	0.84	0.23	77,77,77,77	0
56	MG	1A	3348	1/1	0.84	0.21	66,66,66,66	0
56	MG	2a	1795	1/1	0.84	0.22	74,74,74,74	0
56	MG	2G	201	1/1	0.84	0.17	75,75,75,75	0
56	MG	1A	3634	1/1	0.84	0.20	58,58,58,58	0
56	MG	25	101	1/1	0.84	0.28	68,68,68,68	0
56	MG	2A	3015	1/1	0.84	0.24	65,65,65,65	0
56	MG	2A	3362	1/1	0.84	0.38	64,64,64,64	0
56	MG	1A	4093	1/1	0.84	0.17	65,65,65,65	0
56	MG	2A	3212	1/1	0.84	0.17	58,58,58,58	0
56	MG	2a	1606	1/1	0.84	0.31	81,81,81,81	0
56	MG	1a	1665	1/1	0.84	0.26	71,71,71,71	0
56	MG	2A	3633	1/1	0.84	0.22	56,56,56,56	0
56	MG	2A	3634	1/1	0.84	0.19	55,55,55,55	0
56	MG	2a	1613	1/1	0.84	0.41	81,81,81,81	0
56	MG	1A	3895	1/1	0.84	0.22	47,47,47,47	0
56	MG	2A	3637	1/1	0.84	0.18	74,74,74,74	0
56	MG	1A	3245	1/1	0.84	0.19	72,72,72,72	0
56	MG	2A	3641	1/1	0.84	0.09	35,35,35,35	0
56	MG	2a	1623	1/1	0.84	0.38	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3047	1/1	0.84	0.15	51,51,51,51	0
56	MG	1A	3496	1/1	0.84	0.16	81,81,81,81	0
56	MG	2A	3234	1/1	0.84	0.13	59,59,59,59	0
56	MG	1A	3651	1/1	0.84	0.16	53,53,53,53	0
56	MG	2a	1635	1/1	0.84	0.23	79,79,79,79	0
56	MG	1A	3401	1/1	0.84	0.12	51,51,51,51	0
56	MG	1A	3934	1/1	0.84	0.14	65,65,65,65	0
56	MG	2w	101	1/1	0.84	0.14	80,80,80,80	0
56	MG	2a	1639	1/1	0.84	0.34	76,76,76,76	0
56	MG	2x	105	1/1	0.84	0.16	70,70,70,70	0
56	MG	1A	3678	1/1	0.84	0.09	45,45,45,45	0
56	MG	1A	3195	1/1	0.84	0.36	73,73,73,73	0
56	MG	1A	4043	1/1	0.84	0.17	57,57,57,57	0
56	MG	2A	3431	1/1	0.85	0.14	57,57,57,57	0
56	MG	1A	3382	1/1	0.85	0.31	73,73,73,73	0
56	MG	2A	3252	1/1	0.85	0.20	72,72,72,72	0
56	MG	2A	3088	1/1	0.85	0.34	61,61,61,61	0
56	MG	2a	1659	1/1	0.85	0.22	70,70,70,70	0
56	MG	2A	3699	1/1	0.85	0.19	48,48,48,48	0
56	MG	1A	3733	1/1	0.85	0.10	46,46,46,46	0
56	MG	2A	3260	1/1	0.85	0.19	80,80,80,80	0
56	MG	2A	3092	1/1	0.85	0.17	80,80,80,80	0
56	MG	2a	1677	1/1	0.85	0.23	67,67,67,67	0
56	MG	2a	1682	1/1	0.85	0.19	68,68,68,68	0
56	MG	1a	1737	1/1	0.85	0.12	80,80,80,80	0
56	MG	2a	1688	1/1	0.85	0.36	72,72,72,72	0
56	MG	1a	1741	1/1	0.85	0.26	77,77,77,77	0
56	MG	2A	3722	1/1	0.85	0.17	68,68,68,68	0
56	MG	1A	4051	1/1	0.85	0.15	69,69,69,69	0
56	MG	2A	3499	1/1	0.85	0.20	49,49,49,49	0
56	MG	2a	1696	1/1	0.85	0.20	69,69,69,69	0
56	MG	1A	3968	1/1	0.85	0.11	70,70,70,70	0
56	MG	2A	3503	1/1	0.85	0.16	65,65,65,65	0
56	MG	2a	1699	1/1	0.85	0.18	78,78,78,78	0
56	MG	1A	3845	1/1	0.85	0.16	75,75,75,75	0
56	MG	1a	1750	1/1	0.85	0.14	72,72,72,72	0
56	MG	2A	3740	1/1	0.85	0.22	59,59,59,59	0
56	MG	2A	3520	1/1	0.85	0.17	58,58,58,58	0
56	MG	2a	1718	1/1	0.85	0.17	80,80,80,80	0
56	MG	2A	3752	1/1	0.85	0.18	66,66,66,66	0
56	MG	1A	3423	1/1	0.85	0.19	63,63,63,63	0
56	MG	1A	3976	1/1	0.85	0.12	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3120	1/1	0.85	0.11	66,66,66,66	0
56	MG	1A	4064	1/1	0.85	0.15	39,39,39,39	0
56	MG	1A	3850	1/1	0.85	0.17	59,59,59,59	0
56	MG	1A	3006	1/1	0.85	0.35	74,74,74,74	0
56	MG	1A	3744	1/1	0.85	0.12	42,42,42,42	0
56	MG	2A	3542	1/1	0.85	0.35	84,84,84,84	0
56	MG	2A	3309	1/1	0.85	0.33	72,72,72,72	0
56	MG	1A	4075	1/1	0.85	0.13	59,59,59,59	0
56	MG	2A	3315	1/1	0.85	0.11	76,76,76,76	0
56	MG	1A	3387	1/1	0.85	0.11	57,57,57,57	0
56	MG	1A	3989	1/1	0.85	0.33	35,35,35,35	0
56	MG	2A	3555	1/1	0.85	0.16	61,61,61,61	0
56	MG	2a	1756	1/1	0.85	0.29	74,74,74,74	0
56	MG	2a	1762	1/1	0.85	0.19	72,72,72,72	0
56	MG	2A	3556	1/1	0.85	0.24	55,55,55,55	0
56	MG	1a	1620	1/1	0.85	0.33	74,74,74,74	0
56	MG	1A	3359	1/1	0.85	0.16	56,56,56,56	0
56	MG	1A	3065	1/1	0.85	0.22	62,62,62,62	0
56	MG	2A	3184	1/1	0.85	0.27	80,80,80,80	0
56	MG	1A	3181	1/1	0.85	0.24	55,55,55,55	0
56	MG	2A	3596	1/1	0.85	0.20	70,70,70,70	0
56	MG	1A	3797	1/1	0.85	0.09	23,23,23,23	0
56	MG	1A	3410	1/1	0.85	0.34	75,75,75,75	0
56	MG	1x	106	1/1	0.85	0.25	64,64,64,64	0
56	MG	1A	3578	1/1	0.85	0.33	63,63,63,63	0
56	MG	2F	303	1/1	0.85	0.33	74,74,74,74	0
56	MG	1A	3580	1/1	0.85	0.34	62,62,62,62	0
56	MG	2W	201	1/1	0.85	0.15	69,69,69,69	0
56	MG	2A	3005	1/1	0.85	0.15	62,62,62,62	0
56	MG	2A	3200	1/1	0.85	0.20	73,73,73,73	0
56	MG	1a	1660	1/1	0.85	0.21	67,67,67,67	0
56	MG	2A	3353	1/1	0.85	0.29	58,58,58,58	0
56	MG	1A	3291	1/1	0.85	0.14	47,47,47,47	0
56	MG	1B	211	1/1	0.85	0.15	61,61,61,61	0
56	MG	2A	3360	1/1	0.85	0.14	53,53,53,53	0
56	MG	1A	3470	1/1	0.85	0.38	69,69,69,69	0
56	MG	2a	1610	1/1	0.85	0.21	66,66,66,66	0
56	MG	1A	3707	1/1	0.85	0.09	69,69,69,69	0
56	MG	1a	1678	1/1	0.85	0.33	57,57,57,57	0
56	MG	2A	3378	1/1	0.85	0.21	70,70,70,70	0
56	MG	1A	3476	1/1	0.85	0.38	58,58,58,58	0
56	MG	1B	223	1/1	0.85	0.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1812	1/1	0.85	0.20	73,73,73,73	0
56	MG	2a	1619	1/1	0.85	0.18	79,79,79,79	0
56	MG	1A	3717	1/1	0.85	0.12	63,63,63,63	0
56	MG	2A	3062	1/1	0.85	0.38	74,74,74,74	0
56	MG	2a	1821	1/1	0.85	0.32	76,76,76,76	0
56	MG	2A	3230	1/1	0.85	0.25	73,73,73,73	0
56	MG	1A	3831	1/1	0.85	0.15	55,55,55,55	0
56	MG	2A	3398	1/1	0.85	0.12	71,71,71,71	0
56	MG	2a	1829	1/1	0.85	0.28	64,64,64,64	0
56	MG	2A	3652	1/1	0.85	0.13	56,56,56,56	0
56	MG	2a	1633	1/1	0.85	0.40	70,70,70,70	0
56	MG	2l	202	1/1	0.85	0.10	70,70,70,70	0
56	MG	2A	3654	1/1	0.85	0.15	61,61,61,61	0
56	MG	1A	3950	1/1	0.85	0.14	57,57,57,57	0
56	MG	1A	3488	1/1	0.85	0.15	65,65,65,65	0
56	MG	1A	4042	1/1	0.85	0.07	19,19,19,19	0
56	MG	1A	3233	1/1	0.85	0.13	56,56,56,56	0
56	MG	2w	102	1/1	0.85	0.21	83,83,83,83	0
56	MG	1D	311	1/1	0.85	0.25	42,42,42,42	0
56	MG	1E	309	1/1	0.85	0.22	63,63,63,63	0
56	MG	2A	3426	1/1	0.85	0.23	61,61,61,61	0
56	MG	2A	3247	1/1	0.85	0.30	68,68,68,68	0
56	MG	2a	1648	1/1	0.85	0.26	80,80,80,80	0
56	MG	1A	3983	1/1	0.86	0.15	66,66,66,66	0
56	MG	1A	3183	1/1	0.86	0.11	81,81,81,81	0
56	MG	1E	310	1/1	0.86	0.14	59,59,59,59	0
56	MG	2A	3778	1/1	0.86	0.19	63,63,63,63	0
56	MG	1A	4063	1/1	0.86	0.12	60,60,60,60	0
56	MG	1A	3505	1/1	0.86	0.17	66,66,66,66	0
56	MG	2a	1700	1/1	0.86	0.10	64,64,64,64	0
56	MG	2A	3208	1/1	0.86	0.25	66,66,66,66	0
56	MG	2A	3582	1/1	0.86	0.15	54,54,54,54	0
56	MG	2A	3584	1/1	0.86	0.20	67,67,67,67	0
56	MG	1A	4065	1/1	0.86	0.25	55,55,55,55	0
56	MG	2A	3590	1/1	0.86	0.30	72,72,72,72	0
56	MG	2A	3591	1/1	0.86	0.34	65,65,65,65	0
56	MG	1A	4068	1/1	0.86	0.29	65,65,65,65	0
56	MG	2B	202	1/1	0.86	0.17	60,60,60,60	0
56	MG	1A	3906	1/1	0.86	0.12	26,26,26,26	0
56	MG	2a	1731	1/1	0.86	0.33	69,69,69,69	0
56	MG	2A	3357	1/1	0.86	0.39	68,68,68,68	0
56	MG	1A	3506	1/1	0.86	0.19	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3908	1/1	0.86	0.16	42,42,42,42	0
56	MG	2A	3369	1/1	0.86	0.40	70,70,70,70	0
56	MG	2A	3373	1/1	0.86	0.34	73,73,73,73	0
56	MG	2A	3074	1/1	0.86	0.26	62,62,62,62	0
56	MG	2A	3376	1/1	0.86	0.30	66,66,66,66	0
56	MG	1A	3916	1/1	0.86	0.11	31,31,31,31	0
56	MG	1Z	302	1/1	0.86	0.08	69,69,69,69	0
56	MG	2A	3231	1/1	0.86	0.20	59,59,59,59	0
56	MG	1A	3999	1/1	0.86	0.14	41,41,41,41	0
56	MG	2A	3385	1/1	0.86	0.27	67,67,67,67	0
56	MG	1A	4006	1/1	0.86	0.10	52,52,52,52	0
56	MG	1a	1747	1/1	0.86	0.21	65,65,65,65	0
56	MG	1A	3605	1/1	0.86	0.13	59,59,59,59	0
56	MG	2a	1601	1/1	0.86	0.14	61,61,61,61	0
56	MG	2A	3393	1/1	0.86	0.15	56,56,56,56	0
56	MG	1A	3267	1/1	0.86	0.32	72,72,72,72	0
56	MG	1a	1601	1/1	0.86	0.11	53,53,53,53	0
56	MG	1a	1757	1/1	0.86	0.16	75,75,75,75	0
56	MG	2A	3246	1/1	0.86	0.16	76,76,76,76	0
56	MG	1A	3516	1/1	0.86	0.20	82,82,82,82	0
56	MG	2a	1608	1/1	0.86	0.25	73,73,73,73	0
56	MG	1A	3837	1/1	0.86	0.15	62,62,62,62	0
56	MG	1A	3517	1/1	0.86	0.19	60,60,60,60	0
56	MG	1a	1621	1/1	0.86	0.30	57,57,57,57	0
56	MG	1A	3944	1/1	0.86	0.17	59,59,59,59	0
56	MG	2A	3428	1/1	0.86	0.23	76,76,76,76	0
56	MG	2a	1794	1/1	0.86	0.15	63,63,63,63	0
56	MG	2A	3108	1/1	0.86	0.43	74,74,74,74	0
56	MG	2a	1617	1/1	0.86	0.23	77,77,77,77	0
56	MG	1A	3403	1/1	0.86	0.16	54,54,54,54	0
56	MG	1A	3947	1/1	0.86	0.14	54,54,54,54	0
56	MG	2A	3668	1/1	0.86	0.15	67,67,67,67	0
56	MG	2A	3115	1/1	0.86	0.25	88,88,88,88	0
56	MG	2A	3442	1/1	0.86	0.35	66,66,66,66	0
56	MG	2a	1625	1/1	0.86	0.29	74,74,74,74	0
56	MG	1a	1636	1/1	0.86	0.24	69,69,69,69	0
56	MG	1a	1789	1/1	0.86	0.35	82,82,82,82	0
56	MG	2a	1806	1/1	0.86	0.29	71,71,71,71	0
56	MG	2A	3133	1/1	0.86	0.22	64,64,64,64	0
56	MG	2A	3139	1/1	0.86	0.36	78,78,78,78	0
56	MG	2A	3291	1/1	0.86	0.18	67,67,67,67	0
56	MG	2A	3140	1/1	0.86	0.27	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1813	1/1	0.86	0.24	84,84,84,84	0
56	MG	1a	1638	1/1	0.86	0.27	70,70,70,70	0
56	MG	2a	1815	1/1	0.86	0.25	66,66,66,66	0
56	MG	1A	3525	1/1	0.86	0.24	57,57,57,57	0
56	MG	1a	1644	1/1	0.86	0.21	70,70,70,70	0
56	MG	2A	3704	1/1	0.86	0.19	66,66,66,66	0
56	MG	2A	3706	1/1	0.86	0.24	65,65,65,65	0
56	MG	1l	201	1/1	0.86	0.10	78,78,78,78	0
56	MG	1A	3144	1/1	0.86	0.25	46,46,46,46	0
56	MG	1A	3158	1/1	0.86	0.13	63,63,63,63	0
56	MG	1A	3540	1/1	0.86	0.13	69,69,69,69	0
56	MG	2e	201	1/1	0.86	0.10	78,78,78,78	0
56	MG	2A	3168	1/1	0.86	0.28	75,75,75,75	0
56	MG	2A	3522	1/1	0.86	0.21	76,76,76,76	0
56	MG	1A	3046	1/1	0.86	0.09	38,38,38,38	0
56	MG	1a	1661	1/1	0.86	0.27	65,65,65,65	0
56	MG	1A	3029	1/1	0.86	0.13	41,41,41,41	0
56	MG	2A	3185	1/1	0.86	0.33	74,74,74,74	0
56	MG	1A	3418	1/1	0.86	0.20	69,69,69,69	0
56	MG	1A	3040	1/1	0.86	0.20	66,66,66,66	0
56	MG	1A	3881	1/1	0.86	0.11	49,49,49,49	0
56	MG	1A	3248	1/1	0.86	0.13	63,63,63,63	0
56	MG	1A	3389	1/1	0.86	0.29	42,42,42,42	0
56	MG	2A	3039	1/1	0.86	0.33	77,77,77,77	0
56	MG	2A	3766	1/1	0.86	0.13	67,67,67,67	0
56	MG	1a	1755	1/1	0.87	0.26	72,72,72,72	0
56	MG	1A	3311	1/1	0.87	0.34	65,65,65,65	0
56	MG	1A	3312	1/1	0.87	0.26	64,64,64,64	0
56	MG	1a	1759	1/1	0.87	0.13	46,46,46,46	0
56	MG	13	104	1/1	0.87	0.23	62,62,62,62	0
56	MG	2A	3605	1/1	0.87	0.26	73,73,73,73	0
56	MG	2A	3606	1/1	0.87	0.16	52,52,52,52	0
56	MG	2A	3341	1/1	0.87	0.16	78,78,78,78	0
56	MG	2A	3610	1/1	0.87	0.14	69,69,69,69	0
56	MG	2A	3611	1/1	0.87	0.19	40,40,40,40	0
56	MG	1A	3997	1/1	0.87	0.09	25,25,25,25	0
56	MG	2A	3613	1/1	0.87	0.10	71,71,71,71	0
56	MG	1a	1762	1/1	0.87	0.14	67,67,67,67	0
56	MG	1a	1765	1/1	0.87	0.21	73,73,73,73	0
56	MG	15	108	1/1	0.87	0.12	62,62,62,62	0
56	MG	1A	3450	1/1	0.87	0.23	50,50,50,50	0
56	MG	1A	4005	1/1	0.87	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	3460	1/1	0.87	0.22	73,73,73,73	0
56	MG	1a	1604	1/1	0.87	0.11	66,66,66,66	0
56	MG	1a	1617	1/1	0.87	0.20	52,52,52,52	0
56	MG	1A	3657	1/1	0.87	0.12	52,52,52,52	0
56	MG	1A	3363	1/1	0.87	0.19	60,60,60,60	0
56	MG	2A	3189	1/1	0.87	0.20	60,60,60,60	0
56	MG	2A	3365	1/1	0.87	0.19	66,66,66,66	0
56	MG	2A	3366	1/1	0.87	0.26	72,72,72,72	0
56	MG	1a	1794	1/1	0.87	0.28	68,68,68,68	0
56	MG	2a	1662	1/1	0.87	0.27	67,67,67,67	0
56	MG	2A	3192	1/1	0.87	0.36	71,71,71,71	0
56	MG	1A	3927	1/1	0.87	0.18	63,63,63,63	0
56	MG	2A	3375	1/1	0.87	0.31	62,62,62,62	0
56	MG	1e	3100	1/1	0.87	0.12	76,76,76,76	0
56	MG	1a	1624	1/1	0.87	0.25	63,63,63,63	0
56	MG	2a	1678	1/1	0.87	0.20	63,63,63,63	0
56	MG	2A	3661	1/1	0.87	0.15	52,52,52,52	0
56	MG	1A	3315	1/1	0.87	0.37	75,75,75,75	0
56	MG	1n	101	1/1	0.87	0.17	59,59,59,59	0
56	MG	1n	102	1/1	0.87	0.23	66,66,66,66	0
56	MG	1A	3406	1/1	0.87	0.29	72,72,72,72	0
56	MG	2A	3387	1/1	0.87	0.30	64,64,64,64	0
56	MG	1A	4097	1/1	0.87	0.28	58,58,58,58	0
56	MG	1A	3469	1/1	0.87	0.21	73,73,73,73	0
56	MG	1A	3020	1/1	0.87	0.19	55,55,55,55	0
56	MG	1A	3555	1/1	0.87	0.12	56,56,56,56	0
56	MG	1A	4022	1/1	0.87	0.13	59,59,59,59	0
56	MG	2A	3397	1/1	0.87	0.18	71,71,71,71	0
56	MG	1A	3572	1/1	0.87	0.17	49,49,49,49	0
56	MG	1A	3706	1/1	0.87	0.25	62,62,62,62	0
56	MG	2A	3405	1/1	0.87	0.18	59,59,59,59	0
56	MG	2a	1711	1/1	0.87	0.40	74,74,74,74	0
56	MG	2A	3406	1/1	0.87	0.32	71,71,71,71	0
56	MG	2A	3020	1/1	0.87	0.34	69,69,69,69	0
56	MG	2a	1721	1/1	0.87	0.30	84,84,84,84	0
56	MG	1A	3948	1/1	0.87	0.10	48,48,48,48	0
56	MG	2A	3415	1/1	0.87	0.14	59,59,59,59	0
56	MG	2A	3221	1/1	0.87	0.18	70,70,70,70	0
56	MG	2A	3027	1/1	0.87	0.19	50,50,50,50	0
56	MG	2A	3224	1/1	0.87	0.18	73,73,73,73	0
56	MG	2A	3225	1/1	0.87	0.16	73,73,73,73	0
56	MG	2A	3028	1/1	0.87	0.14	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	3172	1/1	0.87	0.09	45,45,45,45	0
56	MG	2A	3233	1/1	0.87	0.21	54,54,54,54	0
56	MG	2a	1742	1/1	0.87	0.35	68,68,68,68	0
56	MG	2A	3036	1/1	0.87	0.16	57,57,57,57	0
56	MG	2A	3733	1/1	0.87	0.11	79,79,79,79	0
56	MG	2A	3735	1/1	0.87	0.12	62,62,62,62	0
56	MG	1A	3956	1/1	0.87	0.14	60,60,60,60	0
56	MG	2A	3434	1/1	0.87	0.16	69,69,69,69	0
56	MG	2A	3437	1/1	0.87	0.19	60,60,60,60	0
56	MG	1A	3574	1/1	0.87	0.15	44,44,44,44	0
56	MG	2A	3447	1/1	0.87	0.29	69,69,69,69	0
56	MG	1A	3575	1/1	0.87	0.13	49,49,49,49	0
56	MG	2A	3764	1/1	0.87	0.35	86,86,86,86	0
56	MG	2A	3239	1/1	0.87	0.14	60,60,60,60	0
56	MG	1A	3576	1/1	0.87	0.16	57,57,57,57	0
56	MG	1E	307	1/1	0.87	0.22	57,57,57,57	0
56	MG	2A	3772	1/1	0.87	0.22	55,55,55,55	0
56	MG	2A	3481	1/1	0.87	0.16	64,64,64,64	0
56	MG	2A	3052	1/1	0.87	0.25	72,72,72,72	0
56	MG	2a	1775	1/1	0.87	0.20	55,55,55,55	0
56	MG	2a	1778	1/1	0.87	0.34	67,67,67,67	0
56	MG	2a	1780	1/1	0.87	0.18	73,73,73,73	0
56	MG	1A	3004	1/1	0.87	0.09	28,28,28,28	0
56	MG	2A	3786	1/1	0.87	0.18	77,77,77,77	0
56	MG	1A	3495	1/1	0.87	0.14	62,62,62,62	0
56	MG	1a	1684	1/1	0.87	0.24	72,72,72,72	0
56	MG	1A	3104	1/1	0.87	0.33	53,53,53,53	0
56	MG	1a	1691	1/1	0.87	0.25	62,62,62,62	0
56	MG	1A	3058	1/1	0.87	0.14	49,49,49,49	0
56	MG	1a	1695	1/1	0.87	0.19	53,53,53,53	0
56	MG	2A	3261	1/1	0.87	0.29	70,70,70,70	0
56	MG	2A	3803	1/1	0.87	0.17	61,61,61,61	0
56	MG	2A	3804	1/1	0.87	0.20	73,73,73,73	0
56	MG	2A	3262	1/1	0.87	0.29	70,70,70,70	0
56	MG	1a	1698	1/1	0.87	0.33	63,63,63,63	0
56	MG	2A	3524	1/1	0.87	0.13	63,63,63,63	0
56	MG	1A	3861	1/1	0.87	0.23	49,49,49,49	0
56	MG	1G	204	1/1	0.87	0.23	69,69,69,69	0
56	MG	1a	1710	1/1	0.87	0.23	68,68,68,68	0
56	MG	2B	209	1/1	0.87	0.32	75,75,75,75	0
56	MG	2A	3533	1/1	0.87	0.29	66,66,66,66	0
56	MG	1A	3740	1/1	0.87	0.25	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	2B	215	1/1	0.87	0.31	70,70,70,70	0
56	MG	2A	3538	1/1	0.87	0.17	68,68,68,68	0
56	MG	1O	204	1/1	0.87	0.18	58,58,58,58	0
56	MG	1A	3098	1/1	0.87	0.15	55,55,55,55	0
56	MG	2A	3091	1/1	0.87	0.24	67,67,67,67	0
56	MG	1A	3500	1/1	0.87	0.25	70,70,70,70	0
56	MG	1a	1730	1/1	0.87	0.18	70,70,70,70	0
56	MG	1a	1734	1/1	0.87	0.25	66,66,66,66	0
56	MG	2a	1817	1/1	0.87	0.25	78,78,78,78	0
56	MG	2N	201	1/1	0.87	0.15	83,83,83,83	0
56	MG	2P	201	1/1	0.87	0.18	61,61,61,61	0
56	MG	2T	201	1/1	0.87	0.18	71,71,71,71	0
56	MG	1P	205	1/1	0.87	0.21	48,48,48,48	0
56	MG	20	101	1/1	0.87	0.25	72,72,72,72	0
56	MG	2A	3099	1/1	0.87	0.19	68,68,68,68	0
56	MG	2a	1830	1/1	0.87	0.21	77,77,77,77	0
56	MG	1Q	204	1/1	0.87	0.15	72,72,72,72	0
56	MG	27	102	1/1	0.87	0.28	72,72,72,72	0
56	MG	2A	3306	1/1	0.87	0.15	69,69,69,69	0
56	MG	1S	202	1/1	0.87	0.18	60,60,60,60	0
56	MG	1A	3752	1/1	0.87	0.16	57,57,57,57	0
56	MG	2A	3580	1/1	0.87	0.17	46,46,46,46	0
56	MG	1V	206	1/1	0.87	0.25	68,68,68,68	0
56	MG	2v	101	1/1	0.87	0.31	75,75,75,75	0
56	MG	1A	3503	1/1	0.87	0.11	57,57,57,57	0
56	MG	2A	3316	1/1	0.87	0.21	56,56,56,56	0
56	MG	1A	3264	1/1	0.87	0.17	67,67,67,67	0
56	MG	2A	3321	1/1	0.87	0.34	69,69,69,69	0
56	MG	2A	3592	1/1	0.87	0.16	75,75,75,75	0
56	MG	1A	3397	1/1	0.87	0.12	47,47,47,47	0
56	MG	10	109	1/1	0.87	0.12	58,58,58,58	0
56	MG	1a	1751	1/1	0.87	0.21	67,67,67,67	0
56	MG	1N	201	1/1	0.88	0.18	64,64,64,64	0
56	MG	2A	3136	1/1	0.88	0.14	50,50,50,50	0
56	MG	2a	1618	1/1	0.88	0.20	71,71,71,71	0
56	MG	1a	1743	1/1	0.88	0.17	64,64,64,64	0
56	MG	1A	3471	1/1	0.88	0.12	54,54,54,54	0
56	MG	2A	3144	1/1	0.88	0.21	62,62,62,62	0
56	MG	2A	3614	1/1	0.88	0.20	67,67,67,67	0
56	MG	1A	3407	1/1	0.88	0.16	58,58,58,58	0
56	MG	1A	3479	1/1	0.88	0.25	51,51,51,51	0
56	MG	1A	3205	1/1	0.88	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	2a	1627	1/1	0.88	0.29	77,77,77,77	0
56	MG	1A	4031	1/1	0.88	0.10	51,51,51,51	0
56	MG	1A	3582	1/1	0.88	0.23	61,61,61,61	0
56	MG	2A	3160	1/1	0.88	0.16	48,48,48,48	0
56	MG	2A	3162	1/1	0.88	0.15	68,68,68,68	0
56	MG	1R	208	1/1	0.88	0.29	45,45,45,45	0
56	MG	1A	3411	1/1	0.88	0.21	50,50,50,50	0
56	MG	2A	3166	1/1	0.88	0.23	78,78,78,78	0
56	MG	2A	3636	1/1	0.88	0.11	60,60,60,60	0
56	MG	1A	3751	1/1	0.88	0.14	58,58,58,58	0
56	MG	1A	3909	1/1	0.88	0.32	66,66,66,66	0
56	MG	1Y	201	1/1	0.88	0.29	66,66,66,66	0
56	MG	2A	3642	1/1	0.88	0.15	73,73,73,73	0
56	MG	2A	3372	1/1	0.88	0.24	68,68,68,68	0
56	MG	1A	3911	1/1	0.88	0.13	69,69,69,69	0
56	MG	1A	3914	1/1	0.88	0.10	68,68,68,68	0
56	MG	1A	3143	1/1	0.88	0.17	56,56,56,56	0
56	MG	1A	3920	1/1	0.88	0.11	50,50,50,50	0
56	MG	2a	1661	1/1	0.88	0.44	74,74,74,74	0
56	MG	1a	1780	1/1	0.88	0.23	59,59,59,59	0
56	MG	2a	1663	1/1	0.88	0.19	59,59,59,59	0
56	MG	2A	3657	1/1	0.88	0.09	65,65,65,65	0
56	MG	1A	4053	1/1	0.88	0.14	54,54,54,54	0
56	MG	1A	3753	1/1	0.88	0.10	22,22,22,22	0
56	MG	2a	1674	1/1	0.88	0.25	60,60,60,60	0
56	MG	1A	3001	1/1	0.88	0.17	46,46,46,46	0
56	MG	1A	3782	1/1	0.88	0.11	51,51,51,51	0
56	MG	2A	3669	1/1	0.88	0.15	67,67,67,67	0
56	MG	1A	3286	1/1	0.88	0.16	52,52,52,52	0
56	MG	2a	1685	1/1	0.88	0.14	79,79,79,79	0
56	MG	1A	3935	1/1	0.88	0.15	73,73,73,73	0
56	MG	2A	3675	1/1	0.88	0.15	64,64,64,64	0
56	MG	1A	3054	1/1	0.88	0.13	48,48,48,48	0
56	MG	2A	3202	1/1	0.88	0.25	62,62,62,62	0
56	MG	2a	1691	1/1	0.88	0.41	73,73,73,73	0
56	MG	2a	1692	1/1	0.88	0.29	66,66,66,66	0
56	MG	1a	1795	1/1	0.88	0.35	55,55,55,55	0
56	MG	1A	3501	1/1	0.88	0.15	53,53,53,53	0
56	MG	1A	3246	1/1	0.88	0.29	64,64,64,64	0
56	MG	1a	1611	1/1	0.88	0.29	69,69,69,69	0
56	MG	2A	3401	1/1	0.88	0.20	66,66,66,66	0
56	MG	2A	3210	1/1	0.88	0.18	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	3622	1/1	0.88	0.16	59,59,59,59	0
56	MG	1A	3103	1/1	0.88	0.33	44,44,44,44	0
56	MG	2a	1706	1/1	0.88	0.32	76,76,76,76	0
56	MG	1A	3637	1/1	0.88	0.14	57,57,57,57	0
56	MG	1A	3806	1/1	0.88	0.15	61,61,61,61	0
56	MG	2A	3708	1/1	0.88	0.12	67,67,67,67	0
56	MG	2a	1714	1/1	0.88	0.33	68,68,68,68	0
56	MG	1a	1623	1/1	0.88	0.28	61,61,61,61	0
56	MG	1A	3951	1/1	0.88	0.09	28,28,28,28	0
56	MG	2A	3419	1/1	0.88	0.38	64,64,64,64	0
56	MG	2A	3716	1/1	0.88	0.30	74,74,74,74	0
56	MG	2A	3717	1/1	0.88	0.14	80,80,80,80	0
56	MG	1a	1626	1/1	0.88	0.32	67,67,67,67	0
56	MG	1A	4078	1/1	0.88	0.19	59,59,59,59	0
56	MG	2a	1730	1/1	0.88	0.28	70,70,70,70	0
56	MG	1A	3068	1/1	0.88	0.15	60,60,60,60	0
56	MG	1x	115	1/1	0.88	0.29	70,70,70,70	0
56	MG	1A	3642	1/1	0.88	0.09	31,31,31,31	0
56	MG	1A	3809	1/1	0.88	0.15	41,41,41,41	0
56	MG	1A	3390	1/1	0.88	0.14	71,71,71,71	0
56	MG	1A	3811	1/1	0.88	0.22	31,31,31,31	0
56	MG	1A	3816	1/1	0.88	0.10	37,37,37,37	0
56	MG	1a	1651	1/1	0.88	0.21	64,64,64,64	0
56	MG	2a	1747	1/1	0.88	0.12	72,72,72,72	0
56	MG	1A	3301	1/1	0.88	0.27	50,50,50,50	0
56	MG	2A	3445	1/1	0.88	0.22	59,59,59,59	0
56	MG	1a	1654	1/1	0.88	0.09	56,56,56,56	0
56	MG	2A	3453	1/1	0.88	0.14	38,38,38,38	0
56	MG	2A	3762	1/1	0.88	0.14	54,54,54,54	0
56	MG	2A	3454	1/1	0.88	0.25	65,65,65,65	0
56	MG	1A	3398	1/1	0.88	0.12	54,54,54,54	0
56	MG	2A	3458	1/1	0.88	0.12	26,26,26,26	0
56	MG	2A	3241	1/1	0.88	0.16	58,58,58,58	0
56	MG	2A	3243	1/1	0.88	0.16	80,80,80,80	0
56	MG	1a	1659	1/1	0.88	0.22	71,71,71,71	0
56	MG	2A	3044	1/1	0.88	0.19	59,59,59,59	0
56	MG	1A	3974	1/1	0.88	0.23	64,64,64,64	0
56	MG	1A	4095	1/1	0.88	0.24	57,57,57,57	0
56	MG	2A	3788	1/1	0.88	0.13	62,62,62,62	0
56	MG	2A	3489	1/1	0.88	0.22	46,46,46,46	0
56	MG	1A	3673	1/1	0.88	0.19	57,57,57,57	0
56	MG	1a	1663	1/1	0.88	0.30	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3053	1/1	0.88	0.16	68,68,68,68	0
56	MG	2A	3256	1/1	0.88	0.24	69,69,69,69	0
56	MG	1A	3519	1/1	0.88	0.12	57,57,57,57	0
56	MG	1A	3457	1/1	0.88	0.14	69,69,69,69	0
56	MG	2A	3801	1/1	0.88	0.25	74,74,74,74	0
56	MG	2A	3059	1/1	0.88	0.15	81,81,81,81	0
56	MG	1a	1674	1/1	0.88	0.31	73,73,73,73	0
56	MG	2A	3808	1/1	0.88	0.12	74,74,74,74	0
56	MG	1B	215	1/1	0.88	0.23	64,64,64,64	0
56	MG	1B	218	1/1	0.88	0.13	52,52,52,52	0
56	MG	1A	3458	1/1	0.88	0.20	57,57,57,57	0
56	MG	1A	3459	1/1	0.88	0.27	50,50,50,50	0
56	MG	1A	3690	1/1	0.88	0.10	39,39,39,39	0
56	MG	2A	3277	1/1	0.88	0.24	74,74,74,74	0
56	MG	1a	1685	1/1	0.88	0.37	65,65,65,65	0
56	MG	2A	3282	1/1	0.88	0.15	70,70,70,70	0
56	MG	2A	3286	1/1	0.88	0.19	67,67,67,67	0
56	MG	2B	213	1/1	0.88	0.26	67,67,67,67	0
56	MG	1B	226	1/1	0.88	0.15	58,58,58,58	0
56	MG	2A	3289	1/1	0.88	0.40	72,72,72,72	0
56	MG	1a	1689	1/1	0.88	0.33	63,63,63,63	0
56	MG	2E	301	1/1	0.88	0.29	73,73,73,73	0
56	MG	1B	227	1/1	0.88	0.14	50,50,50,50	0
56	MG	1A	3528	1/1	0.88	0.30	58,58,58,58	0
56	MG	2A	3551	1/1	0.88	0.20	70,70,70,70	0
56	MG	1A	3529	1/1	0.88	0.33	65,65,65,65	0
56	MG	1A	3399	1/1	0.88	0.11	51,51,51,51	0
56	MG	1A	3853	1/1	0.88	0.13	49,49,49,49	0
56	MG	2O	201	1/1	0.88	0.25	66,66,66,66	0
56	MG	2A	3304	1/1	0.88	0.41	76,76,76,76	0
56	MG	1A	3855	1/1	0.88	0.16	56,56,56,56	0
56	MG	2V	201	1/1	0.88	0.34	54,54,54,54	0
56	MG	1D	308	1/1	0.88	0.20	50,50,50,50	0
56	MG	2X	101	1/1	0.88	0.12	77,77,77,77	0
56	MG	1a	1712	1/1	0.88	0.16	64,64,64,64	0
56	MG	1A	3463	1/1	0.88	0.14	59,59,59,59	0
56	MG	1A	3355	1/1	0.88	0.18	57,57,57,57	0
56	MG	2A	3314	1/1	0.88	0.32	78,78,78,78	0
56	MG	1A	3303	1/1	0.88	0.28	61,61,61,61	0
56	MG	1A	3715	1/1	0.88	0.14	41,41,41,41	0
56	MG	2A	3317	1/1	0.88	0.19	79,79,79,79	0
56	MG	2A	3318	1/1	0.88	0.18	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2t	201	1/1	0.88	0.15	54,54,54,54	0
56	MG	1A	3869	1/1	0.88	0.16	52,52,52,52	0
56	MG	1A	3872	1/1	0.88	0.10	37,37,37,37	0
56	MG	1A	3257	1/1	0.88	0.10	46,46,46,46	0
56	MG	2A	3324	1/1	0.88	0.27	70,70,70,70	0
56	MG	2w	103	1/1	0.88	0.14	77,77,77,77	0
56	MG	2A	3114	1/1	0.88	0.16	44,44,44,44	0
56	MG	1A	3362	1/1	0.88	0.24	64,64,64,64	0
56	MG	1F	313	1/1	0.88	0.23	63,63,63,63	0
56	MG	2A	3125	1/1	0.88	0.16	68,68,68,68	0
56	MG	1A	3263	1/1	0.88	0.15	59,59,59,59	0
56	MG	2A	3021	1/1	0.89	0.19	67,67,67,67	0
56	MG	2A	3025	1/1	0.89	0.31	55,55,55,55	0
56	MG	2A	3726	1/1	0.89	0.19	69,69,69,69	0
56	MG	1A	3179	1/1	0.89	0.20	35,35,35,35	0
56	MG	2A	3525	1/1	0.89	0.28	67,67,67,67	0
56	MG	1U	203	1/1	0.89	0.15	59,59,59,59	0
56	MG	1A	3207	1/1	0.89	0.10	59,59,59,59	0
56	MG	2A	3531	1/1	0.89	0.20	73,73,73,73	0
56	MG	2a	1680	1/1	0.89	0.21	55,55,55,55	0
56	MG	1V	207	1/1	0.89	0.15	62,62,62,62	0
56	MG	2a	1684	1/1	0.89	0.37	68,68,68,68	0
56	MG	2A	3328	1/1	0.89	0.37	62,62,62,62	0
56	MG	2A	3335	1/1	0.89	0.22	62,62,62,62	0
56	MG	1A	3910	1/1	0.89	0.14	45,45,45,45	0
56	MG	2A	3748	1/1	0.89	0.26	58,58,58,58	0
56	MG	2A	3038	1/1	0.89	0.30	64,64,64,64	0
56	MG	1A	4083	1/1	0.89	0.08	43,43,43,43	0
56	MG	1A	3308	1/1	0.89	0.13	63,63,63,63	0
56	MG	2A	3761	1/1	0.89	0.13	56,56,56,56	0
56	MG	10	106	1/1	0.89	0.14	52,52,52,52	0
56	MG	2A	3545	1/1	0.89	0.18	64,64,64,64	0
56	MG	2A	3204	1/1	0.89	0.16	59,59,59,59	0
56	MG	2A	3344	1/1	0.89	0.13	72,72,72,72	0
56	MG	2A	3550	1/1	0.89	0.16	66,66,66,66	0
56	MG	1a	1717	1/1	0.89	0.16	66,66,66,66	0
56	MG	1A	3595	1/1	0.89	0.28	66,66,66,66	0
56	MG	2a	1705	1/1	0.89	0.16	62,62,62,62	0
56	MG	2A	3048	1/1	0.89	0.22	70,70,70,70	0
56	MG	1A	3915	1/1	0.89	0.11	59,59,59,59	0
56	MG	1A	3475	1/1	0.89	0.25	41,41,41,41	0
56	MG	2A	3558	1/1	0.89	0.16	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1712	1/1	0.89	0.28	74,74,74,74	0
56	MG	1l	103	1/1	0.89	0.10	47,47,47,47	0
56	MG	2A	3055	1/1	0.89	0.17	56,56,56,56	0
56	MG	2A	3574	1/1	0.89	0.16	58,58,58,58	0
56	MG	2a	1720	1/1	0.89	0.19	58,58,58,58	0
56	MG	2A	3355	1/1	0.89	0.23	44,44,44,44	0
56	MG	1A	3821	1/1	0.89	0.14	52,52,52,52	0
56	MG	1A	3922	1/1	0.89	0.12	63,63,63,63	0
56	MG	2a	1725	1/1	0.89	0.23	60,60,60,60	0
56	MG	2A	3585	1/1	0.89	0.10	55,55,55,55	0
56	MG	2a	1727	1/1	0.89	0.29	85,85,85,85	0
56	MG	1A	4092	1/1	0.89	0.20	62,62,62,62	0
56	MG	2a	1729	1/1	0.89	0.44	57,57,57,57	0
56	MG	2A	3060	1/1	0.89	0.25	60,60,60,60	0
56	MG	1A	3285	1/1	0.89	0.11	57,57,57,57	0
56	MG	18	101	1/1	0.89	0.22	66,66,66,66	0
56	MG	18	104	1/1	0.89	0.21	53,53,53,53	0
56	MG	2A	3594	1/1	0.89	0.12	63,63,63,63	0
56	MG	19	101	1/1	0.89	0.15	51,51,51,51	0
56	MG	2a	1740	1/1	0.89	0.31	72,72,72,72	0
56	MG	2A	3069	1/1	0.89	0.18	71,71,71,71	0
56	MG	1A	4094	1/1	0.89	0.10	62,62,62,62	0
56	MG	1A	3527	1/1	0.89	0.22	48,48,48,48	0
56	MG	1A	3832	1/1	0.89	0.09	44,44,44,44	0
56	MG	1B	207	1/1	0.89	0.20	73,73,73,73	0
56	MG	2A	3084	1/1	0.89	0.16	61,61,61,61	0
56	MG	1A	3609	1/1	0.89	0.22	55,55,55,55	0
56	MG	2A	3382	1/1	0.89	0.35	64,64,64,64	0
56	MG	2A	3608	1/1	0.89	0.19	58,58,58,58	0
56	MG	1a	1612	1/1	0.89	0.14	71,71,71,71	0
56	MG	1A	4015	1/1	0.89	0.15	57,57,57,57	0
56	MG	2A	3242	1/1	0.89	0.26	74,74,74,74	0
56	MG	1A	3732	1/1	0.89	0.09	65,65,65,65	0
56	MG	1A	3936	1/1	0.89	0.12	58,58,58,58	0
56	MG	1A	3210	1/1	0.89	0.15	50,50,50,50	0
56	MG	1A	3313	1/1	0.89	0.08	47,47,47,47	0
56	MG	1A	4026	1/1	0.89	0.16	65,65,65,65	0
56	MG	1A	4029	1/1	0.89	0.12	55,55,55,55	0
56	MG	2A	3249	1/1	0.89	0.12	67,67,67,67	0
56	MG	2Q	203	1/1	0.89	0.12	66,66,66,66	0
56	MG	2A	3400	1/1	0.89	0.30	67,67,67,67	0
56	MG	2A	3250	1/1	0.89	0.17	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	4030	1/1	0.89	0.10	47,47,47,47	0
56	MG	2W	203	1/1	0.89	0.28	72,72,72,72	0
56	MG	2A	3631	1/1	0.89	0.11	68,68,68,68	0
56	MG	1a	1769	1/1	0.89	0.16	64,64,64,64	0
56	MG	2a	1788	1/1	0.89	0.41	75,75,75,75	0
56	MG	1A	3738	1/1	0.89	0.11	50,50,50,50	0
56	MG	2A	3407	1/1	0.89	0.17	61,61,61,61	0
56	MG	25	103	1/1	0.89	0.22	62,62,62,62	0
56	MG	2a	1793	1/1	0.89	0.21	74,74,74,74	0
56	MG	1A	3494	1/1	0.89	0.09	65,65,65,65	0
56	MG	2A	3410	1/1	0.89	0.21	67,67,67,67	0
56	MG	2A	3259	1/1	0.89	0.11	78,78,78,78	0
56	MG	2A	3640	1/1	0.89	0.20	58,58,58,58	0
56	MG	2A	3106	1/1	0.89	0.17	42,42,42,42	0
56	MG	1a	1779	1/1	0.89	0.13	81,81,81,81	0
56	MG	1A	3531	1/1	0.89	0.37	57,57,57,57	0
56	MG	1a	1781	1/1	0.89	0.17	65,65,65,65	0
56	MG	2A	3421	1/1	0.89	0.18	64,64,64,64	0
56	MG	1A	3641	1/1	0.89	0.11	39,39,39,39	0
56	MG	1A	3533	1/1	0.89	0.20	49,49,49,49	0
56	MG	2A	3655	1/1	0.89	0.10	57,57,57,57	0
56	MG	1B	235	1/1	0.89	0.19	73,73,73,73	0
56	MG	1A	3287	1/1	0.89	0.30	69,69,69,69	0
56	MG	1A	3456	1/1	0.89	0.25	61,61,61,61	0
56	MG	2A	3662	1/1	0.89	0.11	66,66,66,66	0
56	MG	1A	3761	1/1	0.89	0.16	35,35,35,35	0
56	MG	2A	3135	1/1	0.89	0.29	66,66,66,66	0
56	MG	1A	3762	1/1	0.89	0.14	47,47,47,47	0
56	MG	1A	3960	1/1	0.89	0.19	59,59,59,59	0
56	MG	1A	3654	1/1	0.89	0.09	29,29,29,29	0
56	MG	1A	3864	1/1	0.89	0.07	44,44,44,44	0
56	MG	2A	3674	1/1	0.89	0.17	69,69,69,69	0
56	MG	2A	3293	1/1	0.89	0.17	65,65,65,65	0
56	MG	2a	1826	1/1	0.89	0.20	66,66,66,66	0
56	MG	1A	4058	1/1	0.89	0.12	55,55,55,55	0
56	MG	2a	1629	1/1	0.89	0.11	93,93,93,93	0
56	MG	1A	3655	1/1	0.89	0.11	29,29,29,29	0
56	MG	1A	3223	1/1	0.89	0.23	51,51,51,51	0
56	MG	1a	1666	1/1	0.89	0.31	70,70,70,70	0
56	MG	2A	3684	1/1	0.89	0.11	58,58,58,58	0
56	MG	2A	3155	1/1	0.89	0.39	74,74,74,74	0
56	MG	2A	3691	1/1	0.89	0.11	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	2l	203	1/1	0.89	0.14	74,74,74,74	0
56	MG	2A	3302	1/1	0.89	0.15	65,65,65,65	0
56	MG	1A	3224	1/1	0.89	0.15	52,52,52,52	0
56	MG	2a	1643	1/1	0.89	0.18	68,68,68,68	0
56	MG	1A	3260	1/1	0.89	0.27	74,74,74,74	0
56	MG	1A	3133	1/1	0.89	0.12	52,52,52,52	0
56	MG	1A	3337	1/1	0.89	0.21	43,43,43,43	0
56	MG	1A	3340	1/1	0.89	0.30	73,73,73,73	0
56	MG	1A	3344	1/1	0.89	0.26	55,55,55,55	0
56	MG	1x	114	1/1	0.89	0.18	74,74,74,74	0
56	MG	1A	3508	1/1	0.89	0.27	41,41,41,41	0
56	MG	2x	104	1/1	0.89	0.34	78,78,78,78	0
56	MG	1A	3062	1/1	0.89	0.34	69,69,69,69	0
56	MG	2A	3013	1/1	0.89	0.34	70,70,70,70	0
56	MG	1A	3468	1/1	0.89	0.19	66,66,66,66	0
56	MG	1A	4077	1/1	0.89	0.10	62,62,62,62	0
58	ZN	24	501	1/1	0.89	0.15	132,132,132,132	0
60	K	2x	101	1/1	0.89	0.28	81,81,81,81	0
56	MG	2A	3174	1/1	0.90	0.12	62,62,62,62	0
56	MG	2A	3182	1/1	0.90	0.22	67,67,67,67	0
56	MG	1S	201	1/1	0.90	0.34	51,51,51,51	0
56	MG	2A	3004	1/1	0.90	0.14	49,49,49,49	0
56	MG	2a	1675	1/1	0.90	0.34	70,70,70,70	0
56	MG	2A	3187	1/1	0.90	0.19	64,64,64,64	0
56	MG	1A	3541	1/1	0.90	0.10	69,69,69,69	0
56	MG	1a	1688	1/1	0.90	0.35	68,68,68,68	0
56	MG	2A	3332	1/1	0.90	0.18	71,71,71,71	0
56	MG	1S	203	1/1	0.90	0.08	73,73,73,73	0
56	MG	1a	1690	1/1	0.90	0.13	57,57,57,57	0
56	MG	1A	3551	1/1	0.90	0.18	41,41,41,41	0
56	MG	2A	3194	1/1	0.90	0.14	62,62,62,62	0
56	MG	1A	3428	1/1	0.90	0.16	49,49,49,49	0
56	MG	1A	3792	1/1	0.90	0.13	46,46,46,46	0
56	MG	1A	3656	1/1	0.90	0.08	26,26,26,26	0
56	MG	2A	3343	1/1	0.90	0.09	70,70,70,70	0
56	MG	1A	3182	1/1	0.90	0.17	65,65,65,65	0
56	MG	2A	3032	1/1	0.90	0.12	40,40,40,40	0
56	MG	1a	1704	1/1	0.90	0.20	71,71,71,71	0
56	MG	2a	1695	1/1	0.90	0.20	58,58,58,58	0
56	MG	2A	3554	1/1	0.90	0.18	40,40,40,40	0
56	MG	1A	3660	1/1	0.90	0.09	27,27,27,27	0
56	MG	1a	1708	1/1	0.90	0.17	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	3567	1/1	0.90	0.24	32,32,32,32	0
56	MG	1A	3444	1/1	0.90	0.18	46,46,46,46	0
56	MG	2A	3560	1/1	0.90	0.14	51,51,51,51	0
56	MG	2A	3780	1/1	0.90	0.10	47,47,47,47	0
56	MG	1A	3351	1/1	0.90	0.20	66,66,66,66	0
56	MG	1A	3446	1/1	0.90	0.17	71,71,71,71	0
56	MG	2A	3787	1/1	0.90	0.27	65,65,65,65	0
56	MG	2a	1710	1/1	0.90	0.26	71,71,71,71	0
56	MG	1A	3353	1/1	0.90	0.19	66,66,66,66	0
56	MG	2A	3791	1/1	0.90	0.14	53,53,53,53	0
56	MG	1A	3208	1/1	0.90	0.10	69,69,69,69	0
56	MG	2A	3359	1/1	0.90	0.20	38,38,38,38	0
56	MG	1B	203	1/1	0.90	0.14	59,59,59,59	0
56	MG	2A	3588	1/1	0.90	0.14	51,51,51,51	0
56	MG	1A	3249	1/1	0.90	0.18	57,57,57,57	0
56	MG	2A	3363	1/1	0.90	0.45	74,74,74,74	0
56	MG	1a	1731	1/1	0.90	0.24	76,76,76,76	0
56	MG	1A	3314	1/1	0.90	0.18	52,52,52,52	0
56	MG	2A	3802	1/1	0.90	0.17	74,74,74,74	0
56	MG	2A	3367	1/1	0.90	0.30	57,57,57,57	0
56	MG	1A	3254	1/1	0.90	0.18	72,72,72,72	0
56	MG	2A	3805	1/1	0.90	0.29	74,74,74,74	0
56	MG	1B	213	1/1	0.90	0.27	67,67,67,67	0
56	MG	1A	3819	1/1	0.90	0.07	40,40,40,40	0
56	MG	1a	1740	1/1	0.90	0.14	63,63,63,63	0
56	MG	2A	3227	1/1	0.90	0.21	78,78,78,78	0
56	MG	1A	3053	1/1	0.90	0.09	56,56,56,56	0
56	MG	1A	3462	1/1	0.90	0.14	58,58,58,58	0
56	MG	2A	3232	1/1	0.90	0.12	72,72,72,72	0
56	MG	1A	3829	1/1	0.90	0.09	52,52,52,52	0
56	MG	1a	1746	1/1	0.90	0.14	68,68,68,68	0
56	MG	2A	3607	1/1	0.90	0.31	69,69,69,69	0
56	MG	1A	3515	1/1	0.90	0.11	74,74,74,74	0
56	MG	1A	3710	1/1	0.90	0.14	60,60,60,60	0
56	MG	2A	3386	1/1	0.90	0.45	69,69,69,69	0
56	MG	2A	3076	1/1	0.90	0.21	62,62,62,62	0
56	MG	1A	3587	1/1	0.90	0.14	35,35,35,35	0
56	MG	2A	3078	1/1	0.90	0.17	54,54,54,54	0
56	MG	2E	305	1/1	0.90	0.22	66,66,66,66	0
56	MG	2a	1760	1/1	0.90	0.15	66,66,66,66	0
56	MG	1A	3035	1/1	0.90	0.11	52,52,52,52	0
56	MG	2F	301	1/1	0.90	0.11	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	3082	1/1	0.90	0.16	65,65,65,65	0
56	MG	1A	3194	1/1	0.90	0.34	42,42,42,42	0
56	MG	2F	304	1/1	0.90	0.10	52,52,52,52	0
56	MG	1A	3596	1/1	0.90	0.17	42,42,42,42	0
56	MG	2A	3618	1/1	0.90	0.10	48,48,48,48	0
56	MG	2A	3619	1/1	0.90	0.23	62,62,62,62	0
56	MG	1A	4044	1/1	0.90	0.12	69,69,69,69	0
56	MG	1A	3727	1/1	0.90	0.12	67,67,67,67	0
56	MG	1A	3333	1/1	0.90	0.11	63,63,63,63	0
56	MG	2T	203	1/1	0.90	0.26	65,65,65,65	0
56	MG	2U	201	1/1	0.90	0.17	59,59,59,59	0
56	MG	2A	3626	1/1	0.90	0.16	55,55,55,55	0
56	MG	2A	3627	1/1	0.90	0.12	53,53,53,53	0
56	MG	1A	3844	1/1	0.90	0.27	55,55,55,55	0
56	MG	1A	3295	1/1	0.90	0.11	55,55,55,55	0
56	MG	1A	3226	1/1	0.90	0.18	58,58,58,58	0
56	MG	1a	1763	1/1	0.90	0.21	61,61,61,61	0
56	MG	1A	3416	1/1	0.90	0.19	56,56,56,56	0
56	MG	1a	1767	1/1	0.90	0.10	62,62,62,62	0
56	MG	2A	3411	1/1	0.90	0.20	57,57,57,57	0
56	MG	1a	1768	1/1	0.90	0.09	70,70,70,70	0
56	MG	1A	3851	1/1	0.90	0.36	44,44,44,44	0
56	MG	1A	3621	1/1	0.90	0.12	57,57,57,57	0
56	MG	1a	1639	1/1	0.90	0.18	68,68,68,68	0
56	MG	2a	1799	1/1	0.90	0.19	71,71,71,71	0
56	MG	1E	311	1/1	0.90	0.11	27,27,27,27	0
56	MG	1A	3739	1/1	0.90	0.08	29,29,29,29	0
56	MG	2A	3650	1/1	0.90	0.12	54,54,54,54	0
56	MG	1A	3049	1/1	0.90	0.07	26,26,26,26	0
56	MG	2a	1609	1/1	0.90	0.41	77,77,77,77	0
56	MG	2A	3110	1/1	0.90	0.49	77,77,77,77	0
56	MG	1E	318	1/1	0.90	0.17	45,45,45,45	0
56	MG	1F	311	1/1	0.90	0.13	54,54,54,54	0
56	MG	2A	3275	1/1	0.90	0.36	58,58,58,58	0
56	MG	2a	1810	1/1	0.90	0.13	69,69,69,69	0
56	MG	1a	1653	1/1	0.90	0.25	73,73,73,73	0
56	MG	1A	3198	1/1	0.90	0.18	49,49,49,49	0
56	MG	1A	3635	1/1	0.90	0.12	26,26,26,26	0
56	MG	2A	3435	1/1	0.90	0.31	74,74,74,74	0
56	MG	1A	3422	1/1	0.90	0.14	59,59,59,59	0
56	MG	1I	201	1/1	0.90	0.14	67,67,67,67	0
56	MG	1A	3307	1/1	0.90	0.22	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	3865	1/1	0.90	0.19	39,39,39,39	0
56	MG	1d	301	1/1	0.90	0.15	78,78,78,78	0
56	MG	1A	3168	1/1	0.90	0.25	39,39,39,39	0
56	MG	2a	1825	1/1	0.90	0.30	63,63,63,63	0
56	MG	1A	3486	1/1	0.90	0.13	57,57,57,57	0
56	MG	1A	3392	1/1	0.90	0.34	74,74,74,74	0
56	MG	2A	3678	1/1	0.90	0.20	59,59,59,59	0
56	MG	2A	3459	1/1	0.90	0.31	65,65,65,65	0
56	MG	1m	3002	1/1	0.90	0.24	69,69,69,69	0
56	MG	1A	3650	1/1	0.90	0.11	60,60,60,60	0
56	MG	2A	3301	1/1	0.90	0.29	62,62,62,62	0
56	MG	2A	3686	1/1	0.90	0.33	53,53,53,53	0
56	MG	1a	1672	1/1	0.90	0.26	65,65,65,65	0
56	MG	2a	1638	1/1	0.90	0.40	78,78,78,78	0
56	MG	1r	101	1/1	0.90	0.30	69,69,69,69	0
56	MG	1Q	201	1/1	0.90	0.27	44,44,44,44	0
56	MG	2a	1642	1/1	0.90	0.33	70,70,70,70	0
56	MG	2A	3159	1/1	0.90	0.23	61,61,61,61	0
56	MG	1A	3778	1/1	0.90	0.08	69,69,69,69	0
56	MG	1R	202	1/1	0.90	0.33	64,64,64,64	0
56	MG	2v	103	1/1	0.90	0.26	59,59,59,59	0
56	MG	2A	3310	1/1	0.90	0.20	72,72,72,72	0
56	MG	1R	205	1/1	0.90	0.26	58,58,58,58	0
56	MG	1x	107	1/1	0.90	0.22	71,71,71,71	0
56	MG	2a	1651	1/1	0.90	0.15	74,74,74,74	0
56	MG	2x	103	1/1	0.90	0.11	72,72,72,72	0
56	MG	1R	206	1/1	0.90	0.18	35,35,35,35	0
56	MG	2A	3517	1/1	0.90	0.17	51,51,51,51	0
56	MG	2A	3167	1/1	0.90	0.22	62,62,62,62	0
56	MG	1x	112	1/1	0.90	0.21	76,76,76,76	0
56	MG	1a	1682	1/1	0.90	0.31	66,66,66,66	0
56	MG	1A	3887	1/1	0.90	0.13	69,69,69,69	0
56	MG	2A	3719	1/1	0.90	0.12	62,62,62,62	0
56	MG	2a	1631	1/1	0.91	0.28	55,55,55,55	0
56	MG	2a	1632	1/1	0.91	0.29	56,56,56,56	0
56	MG	1A	3482	1/1	0.91	0.20	60,60,60,60	0
56	MG	1W	201	1/1	0.91	0.12	53,53,53,53	0
56	MG	1A	4070	1/1	0.91	0.26	69,69,69,69	0
56	MG	1A	3554	1/1	0.91	0.30	58,58,58,58	0
56	MG	1A	3940	1/1	0.91	0.11	58,58,58,58	0
56	MG	10	102	1/1	0.91	0.13	59,59,59,59	0
56	MG	2A	3676	1/1	0.91	0.21	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3266	1/1	0.91	0.31	74,74,74,74	0
56	MG	10	105	1/1	0.91	0.24	68,68,68,68	0
56	MG	2A	3272	1/1	0.91	0.18	62,62,62,62	0
56	MG	1A	3483	1/1	0.91	0.20	60,60,60,60	0
56	MG	2A	3443	1/1	0.91	0.29	67,67,67,67	0
56	MG	1A	3564	1/1	0.91	0.10	42,42,42,42	0
56	MG	1A	3169	1/1	0.91	0.22	64,64,64,64	0
56	MG	2A	3448	1/1	0.91	0.11	57,57,57,57	0
56	MG	2A	3690	1/1	0.91	0.24	64,64,64,64	0
56	MG	1A	3570	1/1	0.91	0.27	64,64,64,64	0
56	MG	1A	3694	1/1	0.91	0.22	61,61,61,61	0
56	MG	2a	1655	1/1	0.91	0.34	72,72,72,72	0
56	MG	2A	3693	1/1	0.91	0.12	69,69,69,69	0
56	MG	2A	3280	1/1	0.91	0.18	62,62,62,62	0
56	MG	2A	3696	1/1	0.91	0.18	61,61,61,61	0
56	MG	2A	3456	1/1	0.91	0.14	38,38,38,38	0
56	MG	2A	3107	1/1	0.91	0.21	56,56,56,56	0
56	MG	2A	3283	1/1	0.91	0.19	65,65,65,65	0
56	MG	2A	3284	1/1	0.91	0.10	60,60,60,60	0
56	MG	1A	3427	1/1	0.91	0.09	55,55,55,55	0
56	MG	1A	3090	1/1	0.91	0.27	61,61,61,61	0
56	MG	2A	3479	1/1	0.91	0.14	54,54,54,54	0
56	MG	2A	3710	1/1	0.91	0.11	64,64,64,64	0
56	MG	2A	3713	1/1	0.91	0.14	63,63,63,63	0
56	MG	2A	3480	1/1	0.91	0.26	60,60,60,60	0
56	MG	1A	3952	1/1	0.91	0.09	69,69,69,69	0
56	MG	2a	1681	1/1	0.91	0.32	63,63,63,63	0
56	MG	1A	3825	1/1	0.91	0.12	67,67,67,67	0
56	MG	2A	3292	1/1	0.91	0.13	63,63,63,63	0
56	MG	1A	3828	1/1	0.91	0.10	37,37,37,37	0
56	MG	1A	3432	1/1	0.91	0.18	57,57,57,57	0
56	MG	2A	3724	1/1	0.91	0.13	54,54,54,54	0
56	MG	2A	3119	1/1	0.91	0.10	50,50,50,50	0
56	MG	1A	3434	1/1	0.91	0.12	76,76,76,76	0
56	MG	2A	3727	1/1	0.91	0.12	66,66,66,66	0
56	MG	1A	3234	1/1	0.91	0.11	56,56,56,56	0
56	MG	2A	3512	1/1	0.91	0.17	64,64,64,64	0
56	MG	2A	3126	1/1	0.91	0.19	78,78,78,78	0
56	MG	1a	1772	1/1	0.91	0.14	64,64,64,64	0
56	MG	1A	3261	1/1	0.91	0.17	62,62,62,62	0
56	MG	2A	3734	1/1	0.91	0.18	59,59,59,59	0
56	MG	1A	3321	1/1	0.91	0.18	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	3713	1/1	0.91	0.22	52,52,52,52	0
56	MG	1A	3244	1/1	0.91	0.26	54,54,54,54	0
56	MG	2A	3741	1/1	0.91	0.17	45,45,45,45	0
56	MG	2a	1703	1/1	0.91	0.31	68,68,68,68	0
56	MG	1A	3356	1/1	0.91	0.16	66,66,66,66	0
56	MG	2A	3744	1/1	0.91	0.09	37,37,37,37	0
56	MG	2A	3747	1/1	0.91	0.10	46,46,46,46	0
56	MG	2A	3141	1/1	0.91	0.18	63,63,63,63	0
56	MG	2a	1709	1/1	0.91	0.19	77,77,77,77	0
56	MG	1A	3975	1/1	0.91	0.10	29,29,29,29	0
56	MG	2A	3311	1/1	0.91	0.09	63,63,63,63	0
56	MG	1B	202	1/1	0.91	0.31	62,62,62,62	0
56	MG	1A	3719	1/1	0.91	0.11	54,54,54,54	0
56	MG	2a	1715	1/1	0.91	0.14	69,69,69,69	0
56	MG	1B	204	1/1	0.91	0.27	67,67,67,67	0
56	MG	1A	3455	1/1	0.91	0.14	50,50,50,50	0
56	MG	1A	3357	1/1	0.91	0.11	66,66,66,66	0
56	MG	1A	3326	1/1	0.91	0.16	60,60,60,60	0
56	MG	1a	1627	1/1	0.91	0.30	66,66,66,66	0
56	MG	1A	3849	1/1	0.91	0.10	39,39,39,39	0
56	MG	2A	3543	1/1	0.91	0.20	75,75,75,75	0
56	MG	1A	3593	1/1	0.91	0.11	45,45,45,45	0
56	MG	2A	3779	1/1	0.91	0.12	69,69,69,69	0
56	MG	1B	216	1/1	0.91	0.09	68,68,68,68	0
56	MG	1A	3731	1/1	0.91	0.15	58,58,58,58	0
56	MG	2A	3785	1/1	0.91	0.18	57,57,57,57	0
56	MG	1A	3992	1/1	0.91	0.13	66,66,66,66	0
56	MG	2a	1732	1/1	0.91	0.45	67,67,67,67	0
56	MG	1A	3511	1/1	0.91	0.28	39,39,39,39	0
56	MG	1a	1643	1/1	0.91	0.17	63,63,63,63	0
56	MG	2A	3790	1/1	0.91	0.22	66,66,66,66	0
56	MG	2A	3330	1/1	0.91	0.11	71,71,71,71	0
56	MG	1A	3297	1/1	0.91	0.31	52,52,52,52	0
56	MG	2a	1741	1/1	0.91	0.11	76,76,76,76	0
56	MG	1A	3513	1/1	0.91	0.12	66,66,66,66	0
56	MG	2A	3172	1/1	0.91	0.25	65,65,65,65	0
56	MG	1A	3736	1/1	0.91	0.11	24,24,24,24	0
56	MG	2a	1746	1/1	0.91	0.15	62,62,62,62	0
56	MG	2A	3176	1/1	0.91	0.18	53,53,53,53	0
56	MG	2A	3339	1/1	0.91	0.26	72,72,72,72	0
56	MG	1A	3737	1/1	0.91	0.11	37,37,37,37	0
56	MG	1A	3360	1/1	0.91	0.14	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3571	1/1	0.91	0.11	59,59,59,59	0
56	MG	2A	3572	1/1	0.91	0.25	70,70,70,70	0
56	MG	1A	3863	1/1	0.91	0.10	35,35,35,35	0
56	MG	2a	1759	1/1	0.91	0.14	59,59,59,59	0
56	MG	2A	3579	1/1	0.91	0.14	48,48,48,48	0
56	MG	2A	3806	1/1	0.91	0.20	69,69,69,69	0
56	MG	1B	231	1/1	0.91	0.09	58,58,58,58	0
56	MG	2A	3581	1/1	0.91	0.11	55,55,55,55	0
56	MG	2a	1767	1/1	0.91	0.11	72,72,72,72	0
56	MG	1x	108	1/1	0.91	0.34	76,76,76,76	0
56	MG	1a	1657	1/1	0.91	0.18	67,67,67,67	0
56	MG	2A	3346	1/1	0.91	0.17	59,59,59,59	0
56	MG	2A	3586	1/1	0.91	0.24	69,69,69,69	0
56	MG	2B	207	1/1	0.91	0.12	72,72,72,72	0
56	MG	1A	3361	1/1	0.91	0.24	56,56,56,56	0
56	MG	2a	1777	1/1	0.91	0.16	56,56,56,56	0
56	MG	1A	3093	1/1	0.91	0.23	57,57,57,57	0
56	MG	2B	210	1/1	0.91	0.33	68,68,68,68	0
56	MG	1A	4010	1/1	0.91	0.10	64,64,64,64	0
56	MG	1D	302	1/1	0.91	0.22	44,44,44,44	0
56	MG	2A	3003	1/1	0.91	0.24	57,57,57,57	0
56	MG	2B	214	1/1	0.91	0.29	67,67,67,67	0
56	MG	1D	304	1/1	0.91	0.10	43,43,43,43	0
56	MG	1A	3330	1/1	0.91	0.26	60,60,60,60	0
56	MG	1A	3870	1/1	0.91	0.20	43,43,43,43	0
56	MG	1a	1668	1/1	0.91	0.28	64,64,64,64	0
56	MG	2A	3019	1/1	0.91	0.19	51,51,51,51	0
56	MG	1a	1669	1/1	0.91	0.11	47,47,47,47	0
56	MG	1A	3743	1/1	0.91	0.13	42,42,42,42	0
56	MG	2E	308	1/1	0.91	0.15	49,49,49,49	0
56	MG	1A	3610	1/1	0.91	0.22	57,57,57,57	0
56	MG	1A	3747	1/1	0.91	0.15	52,52,52,52	0
56	MG	1A	3878	1/1	0.91	0.14	33,33,33,33	0
56	MG	1A	3749	1/1	0.91	0.10	41,41,41,41	0
56	MG	2A	3368	1/1	0.91	0.35	68,68,68,68	0
56	MG	1A	3368	1/1	0.91	0.14	54,54,54,54	0
56	MG	1A	3120	1/1	0.91	0.16	42,42,42,42	0
56	MG	1A	3131	1/1	0.91	0.10	65,65,65,65	0
56	MG	1F	310	1/1	0.91	0.17	55,55,55,55	0
56	MG	2R	201	1/1	0.91	0.12	53,53,53,53	0
56	MG	1A	4027	1/1	0.91	0.11	56,56,56,56	0
56	MG	2T	202	1/1	0.91	0.12	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	3042	1/1	0.91	0.14	58,58,58,58	0
56	MG	2T	204	1/1	0.91	0.22	72,72,72,72	0
56	MG	1A	3756	1/1	0.91	0.13	25,25,25,25	0
56	MG	1A	3897	1/1	0.91	0.17	70,70,70,70	0
56	MG	2V	202	1/1	0.91	0.18	64,64,64,64	0
56	MG	1A	3414	1/1	0.91	0.18	66,66,66,66	0
56	MG	1A	3335	1/1	0.91	0.20	57,57,57,57	0
56	MG	1A	3372	1/1	0.91	0.25	54,54,54,54	0
56	MG	2A	3384	1/1	0.91	0.24	57,57,57,57	0
56	MG	20	102	1/1	0.91	0.18	61,61,61,61	0
56	MG	2A	3229	1/1	0.91	0.10	78,78,78,78	0
56	MG	2A	3621	1/1	0.91	0.22	61,61,61,61	0
56	MG	2a	1823	1/1	0.91	0.32	62,62,62,62	0
56	MG	1A	3770	1/1	0.91	0.11	70,70,70,70	0
56	MG	2A	3051	1/1	0.91	0.18	77,77,77,77	0
56	MG	2A	3388	1/1	0.91	0.31	63,63,63,63	0
56	MG	1O	203	1/1	0.91	0.20	63,63,63,63	0
56	MG	1A	3774	1/1	0.91	0.13	42,42,42,42	0
56	MG	1A	3777	1/1	0.91	0.12	30,30,30,30	0
56	MG	1A	3375	1/1	0.91	0.14	42,42,42,42	0
56	MG	1A	4045	1/1	0.91	0.14	61,61,61,61	0
56	MG	1A	3912	1/1	0.91	0.12	53,53,53,53	0
56	MG	2I	201	1/1	0.91	0.18	72,72,72,72	0
56	MG	1A	3474	1/1	0.91	0.23	50,50,50,50	0
56	MG	1Q	205	1/1	0.91	0.15	60,60,60,60	0
56	MG	1A	3027	1/1	0.91	0.23	82,82,82,82	0
56	MG	2A	3402	1/1	0.91	0.15	72,72,72,72	0
56	MG	1A	3649	1/1	0.91	0.14	51,51,51,51	0
56	MG	1A	3919	1/1	0.91	0.10	46,46,46,46	0
56	MG	1A	3534	1/1	0.91	0.24	56,56,56,56	0
56	MG	1A	3538	1/1	0.91	0.12	53,53,53,53	0
56	MG	1a	1729	1/1	0.91	0.16	58,58,58,58	0
56	MG	1A	3250	1/1	0.91	0.15	68,68,68,68	0
56	MG	1A	3230	1/1	0.91	0.10	56,56,56,56	0
56	MG	2a	1620	1/1	0.91	0.10	65,65,65,65	0
56	MG	1A	3542	1/1	0.91	0.26	64,64,64,64	0
56	MG	1T	202	1/1	0.91	0.15	69,69,69,69	0
56	MG	2A	3251	1/1	0.91	0.28	68,68,68,68	0
56	MG	1A	3549	1/1	0.91	0.39	61,61,61,61	0
56	MG	1U	204	1/1	0.91	0.27	40,40,40,40	0
56	MG	1V	202	1/1	0.91	0.23	43,43,43,43	0
56	MG	2A	3664	1/1	0.91	0.13	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3422	1/1	0.91	0.12	44,44,44,44	0
56	MG	1A	3480	1/1	0.91	0.10	60,60,60,60	0
56	MG	1A	3082	1/1	0.92	0.28	52,52,52,52	0
56	MG	1A	3967	1/1	0.92	0.15	48,48,48,48	0
56	MG	1a	1637	1/1	0.92	0.28	63,63,63,63	0
56	MG	1A	3824	1/1	0.92	0.19	60,60,60,60	0
56	MG	1A	3558	1/1	0.92	0.27	46,46,46,46	0
56	MG	2A	3207	1/1	0.92	0.16	64,64,64,64	0
56	MG	1a	1640	1/1	0.92	0.16	61,61,61,61	0
56	MG	2A	3392	1/1	0.92	0.13	62,62,62,62	0
56	MG	1x	111	1/1	0.92	0.17	37,37,37,37	0
56	MG	1B	219	1/1	0.92	0.21	52,52,52,52	0
56	MG	1A	3691	1/1	0.92	0.10	36,36,36,36	0
56	MG	1A	3481	1/1	0.92	0.10	57,57,57,57	0
56	MG	2A	3667	1/1	0.92	0.12	71,71,71,71	0
56	MG	1A	3415	1/1	0.92	0.35	69,69,69,69	0
56	MG	1A	3700	1/1	0.92	0.10	31,31,31,31	0
56	MG	1A	3978	1/1	0.92	0.08	21,21,21,21	0
56	MG	1A	3702	1/1	0.92	0.12	36,36,36,36	0
56	MG	2A	3011	1/1	0.92	0.11	44,44,44,44	0
56	MG	2a	1644	1/1	0.92	0.12	83,83,83,83	0
56	MG	2A	3223	1/1	0.92	0.17	61,61,61,61	0
56	MG	1A	3568	1/1	0.92	0.13	72,72,72,72	0
56	MG	1A	3704	1/1	0.92	0.07	61,61,61,61	0
56	MG	2A	3226	1/1	0.92	0.20	69,69,69,69	0
56	MG	1A	3056	1/1	0.92	0.27	54,54,54,54	0
56	MG	1A	3485	1/1	0.92	0.17	51,51,51,51	0
56	MG	1A	3274	1/1	0.92	0.09	46,46,46,46	0
56	MG	2A	3683	1/1	0.92	0.12	66,66,66,66	0
56	MG	1A	3364	1/1	0.92	0.23	48,48,48,48	0
56	MG	2a	1656	1/1	0.92	0.18	82,82,82,82	0
56	MG	1A	3492	1/1	0.92	0.16	51,51,51,51	0
56	MG	1A	3365	1/1	0.92	0.15	62,62,62,62	0
56	MG	2a	1660	1/1	0.92	0.09	59,59,59,59	0
56	MG	1a	1664	1/1	0.92	0.28	71,71,71,71	0
56	MG	2A	3235	1/1	0.92	0.11	64,64,64,64	0
56	MG	1A	3848	1/1	0.92	0.12	25,25,25,25	0
56	MG	2a	1666	1/1	0.92	0.34	74,74,74,74	0
56	MG	1A	3714	1/1	0.92	0.10	47,47,47,47	0
56	MG	1A	3366	1/1	0.92	0.18	50,50,50,50	0
56	MG	2A	3037	1/1	0.92	0.24	65,65,65,65	0
56	MG	2a	1672	1/1	0.92	0.19	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	3697	1/1	0.92	0.11	47,47,47,47	0
56	MG	1A	4001	1/1	0.92	0.07	44,44,44,44	0
56	MG	1A	3324	1/1	0.92	0.22	52,52,52,52	0
56	MG	2A	3040	1/1	0.92	0.15	58,58,58,58	0
56	MG	2A	3705	1/1	0.92	0.10	55,55,55,55	0
56	MG	2A	3041	1/1	0.92	0.23	73,73,73,73	0
56	MG	1A	3149	1/1	0.92	0.19	35,35,35,35	0
56	MG	1a	1673	1/1	0.92	0.33	68,68,68,68	0
56	MG	1A	3089	1/1	0.92	0.16	51,51,51,51	0
56	MG	1a	1675	1/1	0.92	0.30	63,63,63,63	0
56	MG	1E	312	1/1	0.92	0.13	68,68,68,68	0
56	MG	1A	3202	1/1	0.92	0.07	45,45,45,45	0
56	MG	1A	3857	1/1	0.92	0.14	63,63,63,63	0
56	MG	2A	3451	1/1	0.92	0.12	55,55,55,55	0
56	MG	2A	3452	1/1	0.92	0.09	58,58,58,58	0
56	MG	1A	3289	1/1	0.92	0.11	57,57,57,57	0
56	MG	1a	1681	1/1	0.92	0.31	55,55,55,55	0
56	MG	1F	309	1/1	0.92	0.10	52,52,52,52	0
56	MG	1A	3374	1/1	0.92	0.19	42,42,42,42	0
56	MG	1A	3247	1/1	0.92	0.25	46,46,46,46	0
56	MG	1A	3439	1/1	0.92	0.28	42,42,42,42	0
56	MG	2A	3460	1/1	0.92	0.18	45,45,45,45	0
56	MG	2A	3463	1/1	0.92	0.15	58,58,58,58	0
56	MG	1a	1687	1/1	0.92	0.22	61,61,61,61	0
56	MG	1A	3443	1/1	0.92	0.12	65,65,65,65	0
56	MG	2A	3477	1/1	0.92	0.10	68,68,68,68	0
56	MG	2A	3061	1/1	0.92	0.37	66,66,66,66	0
56	MG	1A	3018	1/1	0.92	0.08	47,47,47,47	0
56	MG	1A	3379	1/1	0.92	0.13	51,51,51,51	0
56	MG	2A	3265	1/1	0.92	0.19	69,69,69,69	0
56	MG	1A	3601	1/1	0.92	0.12	62,62,62,62	0
56	MG	2A	3267	1/1	0.92	0.33	70,70,70,70	0
56	MG	2A	3487	1/1	0.92	0.17	51,51,51,51	0
56	MG	2A	3746	1/1	0.92	0.18	63,63,63,63	0
56	MG	2A	3488	1/1	0.92	0.07	51,51,51,51	0
56	MG	2A	3269	1/1	0.92	0.35	60,60,60,60	0
56	MG	1N	203	1/1	0.92	0.10	51,51,51,51	0
56	MG	2A	3755	1/1	0.92	0.11	51,51,51,51	0
56	MG	1A	3108	1/1	0.92	0.30	34,34,34,34	0
56	MG	2A	3071	1/1	0.92	0.23	46,46,46,46	0
56	MG	2A	3759	1/1	0.92	0.12	60,60,60,60	0
56	MG	1A	4025	1/1	0.92	0.06	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	3505	1/1	0.92	0.10	38,38,38,38	0
56	MG	2A	3506	1/1	0.92	0.14	64,64,64,64	0
56	MG	2A	3765	1/1	0.92	0.16	66,66,66,66	0
56	MG	2A	3509	1/1	0.92	0.11	34,34,34,34	0
56	MG	1A	3002	1/1	0.92	0.10	52,52,52,52	0
56	MG	1A	3608	1/1	0.92	0.10	37,37,37,37	0
56	MG	1A	3451	1/1	0.92	0.21	69,69,69,69	0
56	MG	2A	3079	1/1	0.92	0.08	54,54,54,54	0
56	MG	1A	3879	1/1	0.92	0.10	44,44,44,44	0
56	MG	1A	3339	1/1	0.92	0.15	70,70,70,70	0
56	MG	1A	3882	1/1	0.92	0.14	30,30,30,30	0
56	MG	1a	1713	1/1	0.92	0.12	52,52,52,52	0
56	MG	1A	3886	1/1	0.92	0.08	21,21,21,21	0
56	MG	2A	3288	1/1	0.92	0.14	57,57,57,57	0
56	MG	1R	201	1/1	0.92	0.13	57,57,57,57	0
56	MG	2A	3290	1/1	0.92	0.11	58,58,58,58	0
56	MG	2A	3789	1/1	0.92	0.17	69,69,69,69	0
56	MG	1a	1719	1/1	0.92	0.16	53,53,53,53	0
56	MG	1a	1720	1/1	0.92	0.20	64,64,64,64	0
56	MG	1A	3616	1/1	0.92	0.14	62,62,62,62	0
56	MG	2A	3294	1/1	0.92	0.19	68,68,68,68	0
56	MG	1A	3888	1/1	0.92	0.08	44,44,44,44	0
56	MG	1A	3620	1/1	0.92	0.16	45,45,45,45	0
56	MG	2A	3541	1/1	0.92	0.08	41,41,41,41	0
56	MG	1A	3252	1/1	0.92	0.14	35,35,35,35	0
56	MG	1A	3341	1/1	0.92	0.23	50,50,50,50	0
56	MG	1A	3896	1/1	0.92	0.26	35,35,35,35	0
56	MG	1A	3253	1/1	0.92	0.10	62,62,62,62	0
56	MG	1A	3393	1/1	0.92	0.14	64,64,64,64	0
56	MG	1A	3347	1/1	0.92	0.29	73,73,73,73	0
56	MG	1A	3760	1/1	0.92	0.08	29,29,29,29	0
56	MG	1A	3123	1/1	0.92	0.19	56,56,56,56	0
56	MG	2A	3807	1/1	0.92	0.13	72,72,72,72	0
56	MG	1A	3124	1/1	0.92	0.24	39,39,39,39	0
56	MG	1A	3764	1/1	0.92	0.08	34,34,34,34	0
56	MG	2a	1773	1/1	0.92	0.10	69,69,69,69	0
56	MG	1A	3305	1/1	0.92	0.11	51,51,51,51	0
56	MG	1A	3126	1/1	0.92	0.29	40,40,40,40	0
56	MG	2A	3312	1/1	0.92	0.16	68,68,68,68	0
56	MG	1X	104	1/1	0.92	0.41	53,53,53,53	0
56	MG	2a	1779	1/1	0.92	0.24	78,78,78,78	0
56	MG	1A	3771	1/1	0.92	0.08	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	3117	1/1	0.92	0.28	65,65,65,65	0
56	MG	2A	3564	1/1	0.92	0.14	63,63,63,63	0
56	MG	2A	3565	1/1	0.92	0.16	54,54,54,54	0
56	MG	1A	3258	1/1	0.92	0.16	51,51,51,51	0
56	MG	1A	3354	1/1	0.92	0.17	68,68,68,68	0
56	MG	2A	3122	1/1	0.92	0.13	67,67,67,67	0
56	MG	1Z	303	1/1	0.92	0.23	57,57,57,57	0
56	MG	2a	1790	1/1	0.92	0.14	67,67,67,67	0
56	MG	1a	1752	1/1	0.92	0.14	77,77,77,77	0
56	MG	1a	1753	1/1	0.92	0.19	62,62,62,62	0
56	MG	1A	3535	1/1	0.92	0.20	61,61,61,61	0
56	MG	2A	3134	1/1	0.92	0.21	50,50,50,50	0
56	MG	1A	3652	1/1	0.92	0.13	40,40,40,40	0
56	MG	2E	303	1/1	0.92	0.30	64,64,64,64	0
56	MG	1A	3653	1/1	0.92	0.07	27,27,27,27	0
56	MG	2E	306	1/1	0.92	0.10	38,38,38,38	0
56	MG	1A	3259	1/1	0.92	0.14	66,66,66,66	0
56	MG	2A	3329	1/1	0.92	0.35	72,72,72,72	0
56	MG	1A	3790	1/1	0.92	0.13	31,31,31,31	0
56	MG	1A	3932	1/1	0.92	0.11	30,30,30,30	0
56	MG	2A	3334	1/1	0.92	0.11	65,65,65,65	0
56	MG	1A	3791	1/1	0.92	0.10	25,25,25,25	0
56	MG	1A	3539	1/1	0.92	0.12	66,66,66,66	0
56	MG	13	103	1/1	0.92	0.20	58,58,58,58	0
56	MG	1A	3309	1/1	0.92	0.28	58,58,58,58	0
56	MG	2A	3149	1/1	0.92	0.10	45,45,45,45	0
56	MG	1A	3795	1/1	0.92	0.09	44,44,44,44	0
56	MG	15	103	1/1	0.92	0.14	42,42,42,42	0
56	MG	1a	1771	1/1	0.92	0.15	81,81,81,81	0
56	MG	1A	3409	1/1	0.92	0.19	46,46,46,46	0
56	MG	1A	3658	1/1	0.92	0.09	43,43,43,43	0
56	MG	1a	1776	1/1	0.92	0.14	78,78,78,78	0
56	MG	18	102	1/1	0.92	0.24	53,53,53,53	0
56	MG	1A	3011	1/1	0.92	0.11	56,56,56,56	0
56	MG	2a	1818	1/1	0.92	0.21	64,64,64,64	0
56	MG	2a	1819	1/1	0.92	0.25	65,65,65,65	0
56	MG	18	105	1/1	0.92	0.17	52,52,52,52	0
56	MG	1A	3943	1/1	0.92	0.09	55,55,55,55	0
56	MG	2W	202	1/1	0.92	0.43	56,56,56,56	0
56	MG	2A	3351	1/1	0.92	0.27	47,47,47,47	0
56	MG	1A	3664	1/1	0.92	0.08	34,34,34,34	0
56	MG	1A	3668	1/1	0.92	0.06	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3228	1/1	0.92	0.15	40,40,40,40	0
56	MG	20	104	1/1	0.92	0.15	58,58,58,58	0
56	MG	1A	3017	1/1	0.92	0.20	65,65,65,65	0
56	MG	1A	3949	1/1	0.92	0.06	38,38,38,38	0
56	MG	2A	3175	1/1	0.92	0.21	68,68,68,68	0
56	MG	25	104	1/1	0.92	0.14	53,53,53,53	0
56	MG	1A	3477	1/1	0.92	0.20	67,67,67,67	0
56	MG	2A	3178	1/1	0.92	0.30	64,64,64,64	0
56	MG	2A	3179	1/1	0.92	0.10	51,51,51,51	0
56	MG	1a	1614	1/1	0.92	0.18	60,60,60,60	0
56	MG	2A	3364	1/1	0.92	0.28	63,63,63,63	0
56	MG	2A	3623	1/1	0.92	0.28	74,74,74,74	0
56	MG	1A	3140	1/1	0.92	0.17	43,43,43,43	0
56	MG	1a	1796	1/1	0.92	0.15	72,72,72,72	0
56	MG	1a	1619	1/1	0.92	0.35	71,71,71,71	0
56	MG	1A	3683	1/1	0.92	0.12	37,37,37,37	0
56	MG	1B	201	1/1	0.92	0.21	56,56,56,56	0
56	MG	2A	3371	1/1	0.92	0.35	62,62,62,62	0
56	MG	1f	3101	1/1	0.92	0.20	55,55,55,55	0
56	MG	2A	3191	1/1	0.92	0.11	48,48,48,48	0
56	MG	1A	3812	1/1	0.92	0.08	50,50,50,50	0
56	MG	1A	3813	1/1	0.92	0.07	42,42,42,42	0
56	MG	1A	3684	1/1	0.92	0.17	30,30,30,30	0
56	MG	1A	3685	1/1	0.92	0.09	24,24,24,24	0
56	MG	2A	3196	1/1	0.92	0.19	63,63,63,63	0
56	MG	1A	3962	1/1	0.92	0.18	65,65,65,65	0
56	MG	1a	1631	1/1	0.92	0.23	75,75,75,75	0
56	MG	1A	3686	1/1	0.92	0.10	29,29,29,29	0
56	MG	1w	105	1/1	0.92	0.29	67,67,67,67	0
56	MG	2a	1652	1/1	0.93	0.13	62,62,62,62	0
56	MG	2A	3519	1/1	0.93	0.20	43,43,43,43	0
56	MG	1A	3643	1/1	0.93	0.07	33,33,33,33	0
56	MG	1U	202	1/1	0.93	0.23	46,46,46,46	0
56	MG	1A	3440	1/1	0.93	0.12	48,48,48,48	0
56	MG	1A	3442	1/1	0.93	0.17	42,42,42,42	0
56	MG	1A	4084	1/1	0.93	0.09	32,32,32,32	0
56	MG	1V	203	1/1	0.93	0.38	35,35,35,35	0
56	MG	1A	3552	1/1	0.93	0.28	65,65,65,65	0
56	MG	1A	3491	1/1	0.93	0.18	38,38,38,38	0
56	MG	1a	1696	1/1	0.93	0.09	49,49,49,49	0
56	MG	1a	1697	1/1	0.93	0.37	57,57,57,57	0
56	MG	2A	3737	1/1	0.93	0.06	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	3745	1/1	0.93	0.12	52,52,52,52	0
56	MG	1a	1702	1/1	0.93	0.39	66,66,66,66	0
56	MG	1W	203	1/1	0.93	0.25	47,47,47,47	0
56	MG	1A	3237	1/1	0.93	0.11	47,47,47,47	0
56	MG	1A	4089	1/1	0.93	0.09	56,56,56,56	0
56	MG	1A	3969	1/1	0.93	0.17	66,66,66,66	0
56	MG	1Y	203	1/1	0.93	0.35	53,53,53,53	0
56	MG	1A	3269	1/1	0.93	0.08	47,47,47,47	0
56	MG	2a	1679	1/1	0.93	0.28	66,66,66,66	0
56	MG	2A	3749	1/1	0.93	0.09	57,57,57,57	0
56	MG	1A	3316	1/1	0.93	0.22	38,38,38,38	0
56	MG	1A	3130	1/1	0.93	0.13	44,44,44,44	0
56	MG	2a	1683	1/1	0.93	0.16	53,53,53,53	0
56	MG	10	104	1/1	0.93	0.18	48,48,48,48	0
56	MG	1A	3858	1/1	0.93	0.07	27,27,27,27	0
56	MG	1A	3447	1/1	0.93	0.08	51,51,51,51	0
56	MG	2A	3209	1/1	0.93	0.37	48,48,48,48	0
56	MG	1A	3449	1/1	0.93	0.17	47,47,47,47	0
56	MG	1A	3402	1/1	0.93	0.12	47,47,47,47	0
56	MG	1A	3162	1/1	0.93	0.35	34,34,34,34	0
56	MG	2A	3054	1/1	0.93	0.20	58,58,58,58	0
56	MG	2A	3557	1/1	0.93	0.12	47,47,47,47	0
56	MG	1A	3452	1/1	0.93	0.09	58,58,58,58	0
56	MG	1A	3050	1/1	0.93	0.16	30,30,30,30	0
56	MG	1A	3986	1/1	0.93	0.10	55,55,55,55	0
56	MG	2A	3775	1/1	0.93	0.07	48,48,48,48	0
56	MG	2A	3777	1/1	0.93	0.13	46,46,46,46	0
56	MG	2A	3561	1/1	0.93	0.11	68,68,68,68	0
56	MG	2A	3361	1/1	0.93	0.08	52,52,52,52	0
56	MG	1B	208	1/1	0.93	0.24	62,62,62,62	0
56	MG	2A	3567	1/1	0.93	0.10	61,61,61,61	0
56	MG	2A	3783	1/1	0.93	0.12	61,61,61,61	0
56	MG	1B	209	1/1	0.93	0.11	55,55,55,55	0
56	MG	1A	3866	1/1	0.93	0.14	39,39,39,39	0
56	MG	1A	3867	1/1	0.93	0.26	39,39,39,39	0
56	MG	1A	3200	1/1	0.93	0.14	44,44,44,44	0
56	MG	2A	3576	1/1	0.93	0.07	45,45,45,45	0
56	MG	1A	3766	1/1	0.93	0.07	57,57,57,57	0
56	MG	2A	3066	1/1	0.93	0.17	50,50,50,50	0
56	MG	2a	1713	1/1	0.93	0.15	59,59,59,59	0
56	MG	1A	3288	1/1	0.93	0.12	65,65,65,65	0
56	MG	1A	3873	1/1	0.93	0.07	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	1744	1/1	0.93	0.12	70,70,70,70	0
56	MG	1A	3165	1/1	0.93	0.17	40,40,40,40	0
56	MG	1A	3579	1/1	0.93	0.12	44,44,44,44	0
56	MG	1A	3016	1/1	0.93	0.25	54,54,54,54	0
56	MG	1A	3581	1/1	0.93	0.31	72,72,72,72	0
56	MG	1B	225	1/1	0.93	0.11	57,57,57,57	0
56	MG	2a	1724	1/1	0.93	0.36	62,62,62,62	0
56	MG	1a	1605	1/1	0.93	0.16	53,53,53,53	0
56	MG	2A	3081	1/1	0.93	0.08	57,57,57,57	0
56	MG	2A	3380	1/1	0.93	0.20	48,48,48,48	0
56	MG	2A	3381	1/1	0.93	0.13	44,44,44,44	0
56	MG	1A	3331	1/1	0.93	0.33	64,64,64,64	0
56	MG	1A	3134	1/1	0.93	0.10	42,42,42,42	0
56	MG	1a	1754	1/1	0.93	0.13	73,73,73,73	0
56	MG	1A	3251	1/1	0.93	0.13	52,52,52,52	0
56	MG	1A	3787	1/1	0.93	0.10	56,56,56,56	0
56	MG	1A	3464	1/1	0.93	0.15	61,61,61,61	0
56	MG	2B	204	1/1	0.93	0.14	74,74,74,74	0
56	MG	1A	3170	1/1	0.93	0.16	54,54,54,54	0
56	MG	1A	3890	1/1	0.93	0.13	52,52,52,52	0
56	MG	1A	3588	1/1	0.93	0.15	33,33,33,33	0
56	MG	2A	3093	1/1	0.93	0.12	56,56,56,56	0
56	MG	1A	3520	1/1	0.93	0.21	44,44,44,44	0
56	MG	1A	3171	1/1	0.93	0.10	55,55,55,55	0
56	MG	2A	3394	1/1	0.93	0.10	66,66,66,66	0
56	MG	2A	3395	1/1	0.93	0.25	45,45,45,45	0
56	MG	1A	3524	1/1	0.93	0.26	50,50,50,50	0
56	MG	2a	1750	1/1	0.93	0.12	74,74,74,74	0
56	MG	1A	3338	1/1	0.93	0.20	47,47,47,47	0
56	MG	2A	3253	1/1	0.93	0.18	52,52,52,52	0
56	MG	1a	1628	1/1	0.93	0.21	59,59,59,59	0
56	MG	1A	3219	1/1	0.93	0.17	54,54,54,54	0
56	MG	1A	3298	1/1	0.93	0.22	55,55,55,55	0
56	MG	1a	1634	1/1	0.93	0.15	70,70,70,70	0
56	MG	1A	3221	1/1	0.93	0.12	58,58,58,58	0
56	MG	2a	1761	1/1	0.93	0.13	71,71,71,71	0
56	MG	1A	3136	1/1	0.93	0.15	48,48,48,48	0
56	MG	1A	4028	1/1	0.93	0.08	37,37,37,37	0
56	MG	2A	3622	1/1	0.93	0.14	57,57,57,57	0
56	MG	1A	3607	1/1	0.93	0.08	53,53,53,53	0
56	MG	1A	3079	1/1	0.93	0.10	58,58,58,58	0
56	MG	1A	3711	1/1	0.93	0.15	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1E	315	1/1	0.93	0.20	44,44,44,44	0
56	MG	1A	3063	1/1	0.93	0.36	61,61,61,61	0
56	MG	2a	1772	1/1	0.93	0.22	70,70,70,70	0
56	MG	2A	3416	1/1	0.93	0.31	70,70,70,70	0
56	MG	2A	3629	1/1	0.93	0.12	77,77,77,77	0
56	MG	2A	3268	1/1	0.93	0.17	68,68,68,68	0
56	MG	2a	1776	1/1	0.93	0.16	58,58,58,58	0
56	MG	2A	3632	1/1	0.93	0.08	66,66,66,66	0
56	MG	1A	4036	1/1	0.93	0.07	52,52,52,52	0
56	MG	1a	1645	1/1	0.93	0.21	70,70,70,70	0
56	MG	2R	202	1/1	0.93	0.24	55,55,55,55	0
56	MG	2A	3271	1/1	0.93	0.14	64,64,64,64	0
56	MG	2a	1782	1/1	0.93	0.23	55,55,55,55	0
56	MG	1A	3087	1/1	0.93	0.13	35,35,35,35	0
56	MG	2A	3424	1/1	0.93	0.19	45,45,45,45	0
56	MG	2A	3123	1/1	0.93	0.23	66,66,66,66	0
56	MG	1a	1650	1/1	0.93	0.10	48,48,48,48	0
56	MG	1A	3615	1/1	0.93	0.11	31,31,31,31	0
56	MG	2A	3276	1/1	0.93	0.23	58,58,58,58	0
56	MG	2A	3430	1/1	0.93	0.24	67,67,67,67	0
56	MG	1A	3814	1/1	0.93	0.10	28,28,28,28	0
56	MG	2A	3648	1/1	0.93	0.13	35,35,35,35	0
56	MG	2W	205	1/1	0.93	0.12	56,56,56,56	0
56	MG	2A	3649	1/1	0.93	0.10	43,43,43,43	0
56	MG	2A	3278	1/1	0.93	0.23	75,75,75,75	0
56	MG	1A	3148	1/1	0.93	0.22	39,39,39,39	0
56	MG	1A	3817	1/1	0.93	0.09	41,41,41,41	0
56	MG	2A	3281	1/1	0.93	0.29	73,73,73,73	0
56	MG	1A	3718	1/1	0.93	0.14	55,55,55,55	0
56	MG	25	102	1/1	0.93	0.19	56,56,56,56	0
56	MG	2A	3441	1/1	0.93	0.18	47,47,47,47	0
56	MG	1A	3430	1/1	0.93	0.18	55,55,55,55	0
56	MG	2A	3137	1/1	0.93	0.15	46,46,46,46	0
56	MG	28	101	1/1	0.93	0.33	61,61,61,61	0
56	MG	28	102	1/1	0.93	0.16	59,59,59,59	0
56	MG	2A	3285	1/1	0.93	0.16	61,61,61,61	0
56	MG	2a	1807	1/1	0.93	0.13	67,67,67,67	0
56	MG	1A	3928	1/1	0.93	0.09	37,37,37,37	0
56	MG	1A	3537	1/1	0.93	0.29	61,61,61,61	0
56	MG	1N	205	1/1	0.93	0.23	54,54,54,54	0
56	MG	2A	3142	1/1	0.93	0.21	42,42,42,42	0
56	MG	1A	3822	1/1	0.93	0.22	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	1O	202	1/1	0.93	0.17	60,60,60,60	0
56	MG	1A	3431	1/1	0.93	0.20	55,55,55,55	0
56	MG	1A	3722	1/1	0.93	0.14	57,57,57,57	0
56	MG	2A	3457	1/1	0.93	0.19	55,55,55,55	0
56	MG	1A	3723	1/1	0.93	0.13	61,61,61,61	0
56	MG	2A	3151	1/1	0.93	0.15	55,55,55,55	0
56	MG	2A	3152	1/1	0.93	0.16	68,68,68,68	0
56	MG	2a	1614	1/1	0.93	0.22	61,61,61,61	0
56	MG	2A	3462	1/1	0.93	0.14	64,64,64,64	0
56	MG	1A	3724	1/1	0.93	0.08	52,52,52,52	0
56	MG	2A	3464	1/1	0.93	0.14	75,75,75,75	0
56	MG	2A	3467	1/1	0.93	0.10	47,47,47,47	0
56	MG	2A	3154	1/1	0.93	0.11	64,64,64,64	0
56	MG	2A	3470	1/1	0.93	0.13	57,57,57,57	0
56	MG	2A	3685	1/1	0.93	0.09	42,42,42,42	0
56	MG	2A	3474	1/1	0.93	0.16	64,64,64,64	0
56	MG	1A	3626	1/1	0.93	0.06	42,42,42,42	0
56	MG	2d	301	1/1	0.93	0.41	67,67,67,67	0
56	MG	1A	3629	1/1	0.93	0.12	61,61,61,61	0
56	MG	1x	104	1/1	0.93	0.25	70,70,70,70	0
56	MG	1a	1671	1/1	0.93	0.15	68,68,68,68	0
56	MG	2A	3161	1/1	0.93	0.17	53,53,53,53	0
56	MG	1A	3633	1/1	0.93	0.09	41,41,41,41	0
56	MG	1A	3262	1/1	0.93	0.12	58,58,58,58	0
56	MG	1Q	207	1/1	0.93	0.15	45,45,45,45	0
56	MG	2A	3165	1/1	0.93	0.17	71,71,71,71	0
56	MG	2A	3700	1/1	0.93	0.10	68,68,68,68	0
56	MG	1x	110	1/1	0.93	0.09	60,60,60,60	0
56	MG	1A	3128	1/1	0.93	0.24	38,38,38,38	0
56	MG	1A	3836	1/1	0.93	0.07	70,70,70,70	0
56	MG	2A	3498	1/1	0.93	0.15	40,40,40,40	0
56	MG	1A	3184	1/1	0.93	0.13	40,40,40,40	0
56	MG	1A	3151	1/1	0.93	0.19	40,40,40,40	0
56	MG	1A	3543	1/1	0.93	0.22	45,45,45,45	0
56	MG	2A	3504	1/1	0.93	0.21	61,61,61,61	0
56	MG	2A	3002	1/1	0.93	0.28	61,61,61,61	0
56	MG	1A	3840	1/1	0.93	0.14	56,56,56,56	0
56	MG	1A	3841	1/1	0.93	0.12	66,66,66,66	0
56	MG	1a	1683	1/1	0.93	0.32	64,64,64,64	0
56	MG	1A	3843	1/1	0.93	0.11	24,24,24,24	0
56	MG	2A	3180	1/1	0.93	0.24	62,62,62,62	0
56	MG	2A	3720	1/1	0.93	0.11	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	3545	1/1	0.93	0.16	60,60,60,60	0
56	MG	1A	4002	1/1	0.94	0.12	42,42,42,42	0
56	MG	2A	3745	1/1	0.94	0.13	53,53,53,53	0
56	MG	1A	3532	1/1	0.94	0.08	26,26,26,26	0
56	MG	1A	3328	1/1	0.94	0.13	53,53,53,53	0
56	MG	1A	3105	1/1	0.94	0.15	38,38,38,38	0
56	MG	1A	3107	1/1	0.94	0.31	46,46,46,46	0
56	MG	1A	3611	1/1	0.94	0.07	26,26,26,26	0
56	MG	2A	3370	1/1	0.94	0.37	68,68,68,68	0
56	MG	2A	3756	1/1	0.94	0.20	73,73,73,73	0
56	MG	1A	3893	1/1	0.94	0.15	52,52,52,52	0
56	MG	1A	3612	1/1	0.94	0.06	32,32,32,32	0
56	MG	1a	1607	1/1	0.94	0.09	56,56,56,56	0
56	MG	2A	3760	1/1	0.94	0.10	46,46,46,46	0
56	MG	1a	1610	1/1	0.94	0.13	67,67,67,67	0
56	MG	1A	3613	1/1	0.94	0.14	32,32,32,32	0
56	MG	1A	3239	1/1	0.94	0.08	35,35,35,35	0
56	MG	1A	3241	1/1	0.94	0.35	43,43,43,43	0
56	MG	1A	3900	1/1	0.94	0.09	53,53,53,53	0
56	MG	2A	3768	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	3901	1/1	0.94	0.09	45,45,45,45	0
56	MG	2A	3569	1/1	0.94	0.17	65,65,65,65	0
56	MG	1B	236	1/1	0.94	0.09	40,40,40,40	0
56	MG	1A	3902	1/1	0.94	0.11	35,35,35,35	0
56	MG	2A	3774	1/1	0.94	0.07	41,41,41,41	0
56	MG	1A	3031	1/1	0.94	0.20	46,46,46,46	0
56	MG	1A	3112	1/1	0.94	0.10	38,38,38,38	0
56	MG	1A	3381	1/1	0.94	0.13	54,54,54,54	0
56	MG	1A	3625	1/1	0.94	0.06	33,33,33,33	0
56	MG	1E	303	1/1	0.94	0.15	42,42,42,42	0
56	MG	1A	3437	1/1	0.94	0.14	61,61,61,61	0
56	MG	1A	3336	1/1	0.94	0.11	66,66,66,66	0
56	MG	2A	3101	1/1	0.94	0.16	57,57,57,57	0
56	MG	1A	3818	1/1	0.94	0.06	39,39,39,39	0
56	MG	2A	3587	1/1	0.94	0.16	45,45,45,45	0
56	MG	1A	3150	1/1	0.94	0.19	37,37,37,37	0
56	MG	2a	1704	1/1	0.94	0.27	70,70,70,70	0
56	MG	1A	3490	1/1	0.94	0.14	36,36,36,36	0
56	MG	1a	1775	1/1	0.94	0.08	62,62,62,62	0
56	MG	2A	3255	1/1	0.94	0.21	62,62,62,62	0
56	MG	1A	4034	1/1	0.94	0.08	32,32,32,32	0
56	MG	2A	3257	1/1	0.94	0.10	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	1A	3117	1/1	0.94	0.25	34,34,34,34	0
56	MG	1A	4038	1/1	0.94	0.18	53,53,53,53	0
56	MG	1A	3091	1/1	0.94	0.12	62,62,62,62	0
56	MG	1F	305	1/1	0.94	0.11	41,41,41,41	0
56	MG	1A	3122	1/1	0.94	0.16	48,48,48,48	0
56	MG	1a	1783	1/1	0.94	0.09	66,66,66,66	0
56	MG	2A	3601	1/1	0.94	0.20	68,68,68,68	0
56	MG	1A	3729	1/1	0.94	0.09	54,54,54,54	0
56	MG	1a	1787	1/1	0.94	0.26	62,62,62,62	0
56	MG	2A	3121	1/1	0.94	0.27	62,62,62,62	0
56	MG	1A	3827	1/1	0.94	0.17	47,47,47,47	0
56	MG	1A	3639	1/1	0.94	0.14	25,25,25,25	0
56	MG	1A	3092	1/1	0.94	0.14	28,28,28,28	0
56	MG	1G	202	1/1	0.94	0.27	65,65,65,65	0
56	MG	2A	3414	1/1	0.94	0.13	41,41,41,41	0
56	MG	2A	3129	1/1	0.94	0.10	57,57,57,57	0
56	MG	1G	203	1/1	0.94	0.08	66,66,66,66	0
56	MG	1A	3343	1/1	0.94	0.22	43,43,43,43	0
56	MG	1A	4048	1/1	0.94	0.06	27,27,27,27	0
56	MG	1A	4049	1/1	0.94	0.08	56,56,56,56	0
56	MG	1A	3396	1/1	0.94	0.30	46,46,46,46	0
56	MG	1A	3735	1/1	0.94	0.08	62,62,62,62	0
56	MG	2A	3423	1/1	0.94	0.20	63,63,63,63	0
56	MG	1N	206	1/1	0.94	0.21	61,61,61,61	0
56	MG	2a	1738	1/1	0.94	0.17	62,62,62,62	0
56	MG	1A	3563	1/1	0.94	0.11	46,46,46,46	0
56	MG	1A	3647	1/1	0.94	0.08	45,45,45,45	0
56	MG	2A	3427	1/1	0.94	0.15	53,53,53,53	0
56	MG	1A	3047	1/1	0.94	0.10	39,39,39,39	0
56	MG	1A	3499	1/1	0.94	0.16	45,45,45,45	0
56	MG	2a	1744	1/1	0.94	0.15	76,76,76,76	0
56	MG	1A	4060	1/1	0.94	0.12	62,62,62,62	0
56	MG	1A	3941	1/1	0.94	0.12	58,58,58,58	0
56	MG	1A	3448	1/1	0.94	0.22	70,70,70,70	0
56	MG	1a	1667	1/1	0.94	0.20	63,63,63,63	0
56	MG	2E	304	1/1	0.94	0.13	45,45,45,45	0
56	MG	2A	3150	1/1	0.94	0.08	40,40,40,40	0
56	MG	1A	3299	1/1	0.94	0.15	37,37,37,37	0
56	MG	2A	3436	1/1	0.94	0.09	44,44,44,44	0
56	MG	1A	3166	1/1	0.94	0.21	45,45,45,45	0
56	MG	2A	3438	1/1	0.94	0.32	65,65,65,65	0
56	MG	2a	1758	1/1	0.94	0.21	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	3440	1/1	0.94	0.33	64,64,64,64	0
56	MG	1A	3167	1/1	0.94	0.06	38,38,38,38	0
56	MG	1x	105	1/1	0.94	0.13	51,51,51,51	0
56	MG	2F	307	1/1	0.94	0.24	49,49,49,49	0
56	MG	1Q	206	1/1	0.94	0.12	50,50,50,50	0
56	MG	2A	3156	1/1	0.94	0.15	57,57,57,57	0
56	MG	2A	3157	1/1	0.94	0.13	43,43,43,43	0
56	MG	1A	4067	1/1	0.94	0.14	44,44,44,44	0
56	MG	2Q	202	1/1	0.94	0.23	54,54,54,54	0
56	MG	1A	3213	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3454	1/1	0.94	0.27	62,62,62,62	0
56	MG	2A	3645	1/1	0.94	0.14	69,69,69,69	0
56	MG	2A	3646	1/1	0.94	0.18	61,61,61,61	0
56	MG	1A	3509	1/1	0.94	0.50	47,47,47,47	0
56	MG	1A	3750	1/1	0.94	0.10	58,58,58,58	0
56	MG	1R	207	1/1	0.94	0.10	53,53,53,53	0
56	MG	1A	3214	1/1	0.94	0.12	52,52,52,52	0
56	MG	2A	3303	1/1	0.94	0.34	56,56,56,56	0
56	MG	2A	3653	1/1	0.94	0.17	62,62,62,62	0
56	MG	1A	3216	1/1	0.94	0.21	42,42,42,42	0
56	MG	1A	3955	1/1	0.94	0.10	54,54,54,54	0
56	MG	2A	3001	1/1	0.94	0.25	54,54,54,54	0
56	MG	1A	3034	1/1	0.94	0.22	35,35,35,35	0
56	MG	2A	3659	1/1	0.94	0.10	67,67,67,67	0
56	MG	2A	3308	1/1	0.94	0.17	54,54,54,54	0
56	MG	1A	3220	1/1	0.94	0.09	45,45,45,45	0
56	MG	1A	3669	1/1	0.94	0.12	31,31,31,31	0
56	MG	1A	3095	1/1	0.94	0.21	46,46,46,46	0
56	MG	2A	3173	1/1	0.94	0.23	67,67,67,67	0
56	MG	2A	3471	1/1	0.94	0.08	42,42,42,42	0
56	MG	2A	3472	1/1	0.94	0.11	61,61,61,61	0
56	MG	2A	3473	1/1	0.94	0.09	41,41,41,41	0
56	MG	1A	3129	1/1	0.94	0.21	57,57,57,57	0
56	MG	27	103	1/1	0.94	0.09	52,52,52,52	0
56	MG	2A	3672	1/1	0.94	0.11	61,61,61,61	0
56	MG	1A	3964	1/1	0.94	0.15	66,66,66,66	0
56	MG	28	103	1/1	0.94	0.32	56,56,56,56	0
56	MG	1U	209	1/1	0.94	0.19	39,39,39,39	0
56	MG	2A	3177	1/1	0.94	0.10	43,43,43,43	0
56	MG	2A	3016	1/1	0.94	0.07	38,38,38,38	0
56	MG	1A	3060	1/1	0.94	0.15	30,30,30,30	0
56	MG	2A	3319	1/1	0.94	0.37	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	3083	1/1	0.94	0.20	40,40,40,40	0
56	MG	1A	3522	1/1	0.94	0.31	47,47,47,47	0
56	MG	2A	3486	1/1	0.94	0.09	42,42,42,42	0
56	MG	2A	3022	1/1	0.94	0.17	67,67,67,67	0
56	MG	1A	3061	1/1	0.94	0.10	54,54,54,54	0
56	MG	1A	3102	1/1	0.94	0.05	34,34,34,34	0
56	MG	2A	3492	1/1	0.94	0.25	57,57,57,57	0
56	MG	2A	3495	1/1	0.94	0.15	46,46,46,46	0
56	MG	2A	3689	1/1	0.94	0.20	71,71,71,71	0
56	MG	1A	3320	1/1	0.94	0.08	51,51,51,51	0
56	MG	1W	204	1/1	0.94	0.15	55,55,55,55	0
56	MG	1X	102	1/1	0.94	0.15	45,45,45,45	0
56	MG	2A	3500	1/1	0.94	0.11	54,54,54,54	0
56	MG	1A	3776	1/1	0.94	0.13	63,63,63,63	0
56	MG	1X	105	1/1	0.94	0.13	56,56,56,56	0
56	MG	1A	3231	1/1	0.94	0.20	51,51,51,51	0
56	MG	2A	3698	1/1	0.94	0.12	43,43,43,43	0
56	MG	2A	3333	1/1	0.94	0.18	69,69,69,69	0
56	MG	1A	3322	1/1	0.94	0.17	59,59,59,59	0
56	MG	1a	1707	1/1	0.94	0.30	70,70,70,70	0
56	MG	1A	3780	1/1	0.94	0.06	36,36,36,36	0
56	MG	1a	1709	1/1	0.94	0.15	61,61,61,61	0
56	MG	2A	3515	1/1	0.94	0.12	69,69,69,69	0
56	MG	1A	3868	1/1	0.94	0.22	35,35,35,35	0
56	MG	1a	1711	1/1	0.94	0.17	55,55,55,55	0
56	MG	1A	3025	1/1	0.94	0.20	42,42,42,42	0
56	MG	1A	3692	1/1	0.94	0.10	29,29,29,29	0
56	MG	1A	3871	1/1	0.94	0.16	63,63,63,63	0
56	MG	1A	3785	1/1	0.94	0.14	56,56,56,56	0
56	MG	2f	202	1/1	0.94	0.10	65,65,65,65	0
56	MG	2A	3523	1/1	0.94	0.09	26,26,26,26	0
56	MG	1A	3693	1/1	0.94	0.10	23,23,23,23	0
56	MG	1A	3600	1/1	0.94	0.10	36,36,36,36	0
56	MG	2A	3718	1/1	0.94	0.07	38,38,38,38	0
56	MG	2A	3526	1/1	0.94	0.17	64,64,64,64	0
56	MG	2q	201	1/1	0.94	0.36	74,74,74,74	0
56	MG	1A	3988	1/1	0.94	0.08	18,18,18,18	0
56	MG	1A	3696	1/1	0.94	0.07	30,30,30,30	0
56	MG	1B	210	1/1	0.94	0.11	61,61,61,61	0
56	MG	1A	3272	1/1	0.94	0.09	49,49,49,49	0
56	MG	1l	105	1/1	0.94	0.08	49,49,49,49	0
56	MG	1A	3604	1/1	0.94	0.08	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3537	1/1	0.94	0.20	56,56,56,56	0
56	MG	1a	1732	1/1	0.94	0.20	49,49,49,49	0
56	MG	2A	3214	1/1	0.94	0.17	48,48,48,48	0
56	MG	1a	1733	1/1	0.94	0.10	54,54,54,54	0
56	MG	2x	102	1/1	0.94	0.28	72,72,72,72	0
56	MG	2A	3216	1/1	0.94	0.21	47,47,47,47	0
56	MG	1A	3793	1/1	0.94	0.08	47,47,47,47	0
56	MG	1B	214	1/1	0.94	0.12	37,37,37,37	0
56	MG	1A	3022	1/1	0.94	0.07	47,47,47,47	0
56	MG	1A	3883	1/1	0.94	0.08	32,32,32,32	0
56	MG	1A	3885	1/1	0.94	0.08	33,33,33,33	0
56	MG	1A	3279	1/1	0.94	0.13	31,31,31,31	0
56	MG	2A	3548	1/1	0.94	0.10	72,72,72,72	0
56	MG	1A	3823	1/1	0.95	0.28	65,65,65,65	0
56	MG	1A	3996	1/1	0.95	0.07	33,33,33,33	0
56	MG	2A	3769	1/1	0.95	0.06	26,26,26,26	0
56	MG	1A	3421	1/1	0.95	0.12	40,40,40,40	0
56	MG	2a	1673	1/1	0.95	0.14	62,62,62,62	0
56	MG	1A	3188	1/1	0.95	0.28	41,41,41,41	0
56	MG	1A	3386	1/1	0.95	0.10	31,31,31,31	0
56	MG	2A	3597	1/1	0.95	0.09	61,61,61,61	0
56	MG	1A	3325	1/1	0.95	0.18	45,45,45,45	0
56	MG	1A	4003	1/1	0.95	0.09	50,50,50,50	0
56	MG	2A	3776	1/1	0.95	0.07	45,45,45,45	0
56	MG	1A	3903	1/1	0.95	0.20	38,38,38,38	0
56	MG	1A	3681	1/1	0.95	0.06	33,33,33,33	0
56	MG	1y	101	1/1	0.95	0.17	43,43,43,43	0
56	MG	1A	3544	1/1	0.95	0.16	33,33,33,33	0
56	MG	1a	1693	1/1	0.95	0.19	44,44,44,44	0
56	MG	1Z	301	1/1	0.95	0.20	59,59,59,59	0
56	MG	2A	3784	1/1	0.95	0.12	60,60,60,60	0
56	MG	1A	3191	1/1	0.95	0.20	56,56,56,56	0
56	MG	1B	217	1/1	0.95	0.17	55,55,55,55	0
56	MG	2A	3007	1/1	0.95	0.24	65,65,65,65	0
56	MG	1A	4009	1/1	0.95	0.09	59,59,59,59	0
56	MG	1A	3504	1/1	0.95	0.24	50,50,50,50	0
56	MG	1A	3005	1/1	0.95	0.13	50,50,50,50	0
56	MG	2A	3300	1/1	0.95	0.09	76,76,76,76	0
56	MG	1A	3754	1/1	0.95	0.17	45,45,45,45	0
56	MG	1A	3152	1/1	0.95	0.14	45,45,45,45	0
56	MG	1A	3913	1/1	0.95	0.06	44,44,44,44	0
56	MG	1a	1706	1/1	0.95	0.34	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	2A	3796	1/1	0.95	0.07	69,69,69,69	0
56	MG	1A	3300	1/1	0.95	0.13	31,31,31,31	0
56	MG	2A	3023	1/1	0.95	0.17	51,51,51,51	0
56	MG	2A	3799	1/1	0.95	0.09	54,54,54,54	0
56	MG	2A	3449	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	3197	1/1	0.95	0.29	49,49,49,49	0
56	MG	1A	3510	1/1	0.95	0.26	46,46,46,46	0
56	MG	1A	3917	1/1	0.95	0.17	54,54,54,54	0
56	MG	1A	3302	1/1	0.95	0.41	64,64,64,64	0
56	MG	2A	3030	1/1	0.95	0.07	44,44,44,44	0
56	MG	2A	3031	1/1	0.95	0.09	52,52,52,52	0
56	MG	1A	3618	1/1	0.95	0.06	34,34,34,34	0
56	MG	1B	232	1/1	0.95	0.10	58,58,58,58	0
56	MG	1A	3842	1/1	0.95	0.19	49,49,49,49	0
56	MG	2A	3183	1/1	0.95	0.21	67,67,67,67	0
56	MG	1A	3100	1/1	0.95	0.08	53,53,53,53	0
56	MG	17	105	1/1	0.95	0.11	55,55,55,55	0
56	MG	2a	1717	1/1	0.95	0.14	59,59,59,59	0
56	MG	1A	3925	1/1	0.95	0.07	37,37,37,37	0
56	MG	2A	3465	1/1	0.95	0.10	45,45,45,45	0
56	MG	2A	3466	1/1	0.95	0.14	61,61,61,61	0
56	MG	1A	3767	1/1	0.95	0.10	23,23,23,23	0
56	MG	1a	1722	1/1	0.95	0.14	54,54,54,54	0
56	MG	2A	3639	1/1	0.95	0.06	61,61,61,61	0
56	MG	1D	301	1/1	0.95	0.13	43,43,43,43	0
56	MG	2A	3323	1/1	0.95	0.12	43,43,43,43	0
56	MG	1A	3768	1/1	0.95	0.07	27,27,27,27	0
56	MG	18	106	1/1	0.95	0.16	49,49,49,49	0
56	MG	2A	3045	1/1	0.95	0.15	37,37,37,37	0
56	MG	2D	301	1/1	0.95	0.18	51,51,51,51	0
56	MG	2D	302	1/1	0.95	0.17	56,56,56,56	0
56	MG	1A	3930	1/1	0.95	0.11	64,64,64,64	0
56	MG	2D	305	1/1	0.95	0.32	46,46,46,46	0
56	MG	2A	3476	1/1	0.95	0.11	33,33,33,33	0
56	MG	2a	1736	1/1	0.95	0.16	56,56,56,56	0
56	MG	1A	3435	1/1	0.95	0.13	49,49,49,49	0
56	MG	1D	309	1/1	0.95	0.13	32,32,32,32	0
56	MG	1A	3565	1/1	0.95	0.30	39,39,39,39	0
56	MG	2A	3331	1/1	0.95	0.12	67,67,67,67	0
56	MG	2A	3050	1/1	0.95	0.08	65,65,65,65	0
56	MG	2A	3482	1/1	0.95	0.07	42,42,42,42	0
56	MG	1A	3566	1/1	0.95	0.17	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	4037	1/1	0.95	0.07	50,50,50,50	0
56	MG	1a	1606	1/1	0.95	0.32	63,63,63,63	0
56	MG	1A	3775	1/1	0.95	0.12	56,56,56,56	0
56	MG	2A	3658	1/1	0.95	0.10	41,41,41,41	0
56	MG	2a	1748	1/1	0.95	0.21	67,67,67,67	0
56	MG	1A	4039	1/1	0.95	0.10	28,28,28,28	0
56	MG	2F	305	1/1	0.95	0.12	58,58,58,58	0
56	MG	2a	1751	1/1	0.95	0.13	63,63,63,63	0
56	MG	2F	306	1/1	0.95	0.14	55,55,55,55	0
56	MG	2A	3056	1/1	0.95	0.06	49,49,49,49	0
56	MG	2A	3490	1/1	0.95	0.09	39,39,39,39	0
56	MG	1A	3436	1/1	0.95	0.23	43,43,43,43	0
56	MG	1A	3938	1/1	0.95	0.09	53,53,53,53	0
56	MG	1A	3852	1/1	0.95	0.15	55,55,55,55	0
56	MG	2Q	201	1/1	0.95	0.12	63,63,63,63	0
56	MG	2A	3497	1/1	0.95	0.10	43,43,43,43	0
56	MG	1a	1616	1/1	0.95	0.05	54,54,54,54	0
56	MG	1A	3627	1/1	0.95	0.07	22,22,22,22	0
56	MG	2A	3670	1/1	0.95	0.15	43,43,43,43	0
56	MG	2a	1764	1/1	0.95	0.10	53,53,53,53	0
56	MG	2a	1765	1/1	0.95	0.12	80,80,80,80	0
56	MG	1A	3628	1/1	0.95	0.08	23,23,23,23	0
56	MG	1E	316	1/1	0.95	0.12	57,57,57,57	0
56	MG	1A	3225	1/1	0.95	0.20	47,47,47,47	0
56	MG	1A	3632	1/1	0.95	0.14	49,49,49,49	0
56	MG	2A	3348	1/1	0.95	0.14	41,41,41,41	0
56	MG	1A	3273	1/1	0.95	0.13	46,46,46,46	0
56	MG	1A	3859	1/1	0.95	0.10	51,51,51,51	0
56	MG	2A	3511	1/1	0.95	0.08	37,37,37,37	0
56	MG	1a	1625	1/1	0.95	0.10	50,50,50,50	0
56	MG	2A	3218	1/1	0.95	0.16	47,47,47,47	0
56	MG	2A	3514	1/1	0.95	0.07	44,44,44,44	0
56	MG	1A	3709	1/1	0.95	0.05	16,16,16,16	0
56	MG	2A	3220	1/1	0.95	0.21	48,48,48,48	0
56	MG	1A	3160	1/1	0.95	0.22	36,36,36,36	0
56	MG	20	103	1/1	0.95	0.23	69,69,69,69	0
56	MG	1A	3201	1/1	0.95	0.07	33,33,33,33	0
56	MG	1a	1629	1/1	0.95	0.23	74,74,74,74	0
56	MG	23	101	1/1	0.95	0.09	55,55,55,55	0
56	MG	2A	3358	1/1	0.95	0.34	63,63,63,63	0
56	MG	1A	3521	1/1	0.95	0.17	38,38,38,38	0
56	MG	1A	3478	1/1	0.95	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1787	1/1	0.95	0.31	65,65,65,65	0
56	MG	1a	1633	1/1	0.95	0.10	49,49,49,49	0
56	MG	27	101	1/1	0.95	0.29	51,51,51,51	0
56	MG	1A	3281	1/1	0.95	0.29	41,41,41,41	0
56	MG	1A	3953	1/1	0.95	0.17	42,42,42,42	0
56	MG	1A	3954	1/1	0.95	0.06	52,52,52,52	0
56	MG	1A	3640	1/1	0.95	0.08	35,35,35,35	0
56	MG	1N	202	1/1	0.95	0.13	49,49,49,49	0
56	MG	2A	3087	1/1	0.95	0.15	48,48,48,48	0
56	MG	1A	3367	1/1	0.95	0.10	49,49,49,49	0
56	MG	1A	3405	1/1	0.95	0.13	59,59,59,59	0
56	MG	2A	3703	1/1	0.95	0.10	69,69,69,69	0
56	MG	1A	3142	1/1	0.95	0.11	47,47,47,47	0
56	MG	1A	3801	1/1	0.95	0.33	30,30,30,30	0
56	MG	1A	3163	1/1	0.95	0.23	57,57,57,57	0
56	MG	1A	3015	1/1	0.95	0.16	48,48,48,48	0
56	MG	1a	1647	1/1	0.95	0.13	44,44,44,44	0
56	MG	1a	1648	1/1	0.95	0.15	55,55,55,55	0
56	MG	1A	3648	1/1	0.95	0.09	46,46,46,46	0
56	MG	2A	3711	1/1	0.95	0.07	64,64,64,64	0
56	MG	2A	3712	1/1	0.95	0.07	54,54,54,54	0
56	MG	1A	3805	1/1	0.95	0.12	49,49,49,49	0
56	MG	1A	3069	1/1	0.95	0.16	31,31,31,31	0
56	MG	2A	3102	1/1	0.95	0.17	57,57,57,57	0
56	MG	2A	3103	1/1	0.95	0.12	41,41,41,41	0
56	MG	1A	3876	1/1	0.95	0.08	31,31,31,31	0
56	MG	2A	3549	1/1	0.95	0.12	58,58,58,58	0
56	MG	1a	1784	1/1	0.95	0.08	62,62,62,62	0
56	MG	1A	3877	1/1	0.95	0.10	32,32,32,32	0
56	MG	2A	3721	1/1	0.95	0.25	80,80,80,80	0
56	MG	1A	3725	1/1	0.95	0.07	33,33,33,33	0
56	MG	1A	3132	1/1	0.95	0.17	46,46,46,46	0
56	MG	1A	3972	1/1	0.95	0.07	58,58,58,58	0
56	MG	1A	3973	1/1	0.95	0.10	61,61,61,61	0
56	MG	1a	1792	1/1	0.95	0.13	64,64,64,64	0
56	MG	2A	3113	1/1	0.95	0.14	42,42,42,42	0
56	MG	1A	4082	1/1	0.95	0.09	52,52,52,52	0
56	MG	2a	1824	1/1	0.95	0.16	72,72,72,72	0
56	MG	1A	3489	1/1	0.95	0.34	55,55,55,55	0
56	MG	1R	203	1/1	0.95	0.25	38,38,38,38	0
56	MG	2A	3118	1/1	0.95	0.08	57,57,57,57	0
56	MG	2A	3562	1/1	0.95	0.14	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	3373	1/1	0.95	0.10	53,53,53,53	0
56	MG	2A	3736	1/1	0.95	0.06	47,47,47,47	0
56	MG	1A	3346	1/1	0.95	0.15	43,43,43,43	0
56	MG	2A	3738	1/1	0.95	0.08	63,63,63,63	0
56	MG	1A	3884	1/1	0.95	0.12	26,26,26,26	0
56	MG	2f	201	1/1	0.95	0.12	49,49,49,49	0
56	MG	2a	1640	1/1	0.95	0.18	66,66,66,66	0
56	MG	1A	3589	1/1	0.95	0.07	37,37,37,37	0
56	MG	1A	3981	1/1	0.95	0.12	55,55,55,55	0
56	MG	1A	3591	1/1	0.95	0.12	63,63,63,63	0
56	MG	1A	3290	1/1	0.95	0.23	32,32,32,32	0
56	MG	2A	3573	1/1	0.95	0.08	39,39,39,39	0
56	MG	1A	3235	1/1	0.95	0.23	37,37,37,37	0
56	MG	2A	3575	1/1	0.95	0.16	50,50,50,50	0
56	MG	1A	3536	1/1	0.95	0.09	51,51,51,51	0
56	MG	1A	3041	1/1	0.95	0.07	37,37,37,37	0
56	MG	2a	1650	1/1	0.95	0.31	62,62,62,62	0
56	MG	2A	3750	1/1	0.95	0.15	45,45,45,45	0
56	MG	1A	3891	1/1	0.95	0.09	31,31,31,31	0
56	MG	2A	3753	1/1	0.95	0.08	47,47,47,47	0
56	MG	1w	101	1/1	0.95	0.07	48,48,48,48	0
56	MG	1w	102	1/1	0.95	0.08	56,56,56,56	0
56	MG	1A	3597	1/1	0.95	0.12	61,61,61,61	0
56	MG	2A	3138	1/1	0.95	0.15	55,55,55,55	0
56	MG	1U	206	1/1	0.95	0.20	43,43,43,43	0
56	MG	1U	207	1/1	0.95	0.32	39,39,39,39	0
56	MG	1A	3990	1/1	0.95	0.08	26,26,26,26	0
56	MG	1A	3666	1/1	0.95	0.06	29,29,29,29	0
56	MG	1A	3238	1/1	0.95	0.14	37,37,37,37	0
56	MG	2a	1664	1/1	0.95	0.21	62,62,62,62	0
58	ZN	14	102	1/1	0.95	0.10	111,111,111,111	0
56	MG	2a	1665	1/1	0.95	0.14	46,46,46,46	0
60	K	1x	101	1/1	0.95	0.29	75,75,75,75	0
56	MG	1A	3113	1/1	0.95	0.19	40,40,40,40	0
56	MG	2A	3124	1/1	0.96	0.14	51,51,51,51	0
56	MG	1A	3675	1/1	0.96	0.07	32,32,32,32	0
56	MG	2A	3439	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3076	1/1	0.96	0.19	48,48,48,48	0
56	MG	2A	3128	1/1	0.96	0.17	45,45,45,45	0
56	MG	1A	3119	1/1	0.96	0.16	48,48,48,48	0
56	MG	1a	1646	1/1	0.96	0.09	56,56,56,56	0
56	MG	1A	3317	1/1	0.96	0.24	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	2A	3446	1/1	0.96	0.16	68,68,68,68	0
56	MG	1A	3318	1/1	0.96	0.08	61,61,61,61	0
56	MG	1A	4066	1/1	0.96	0.08	37,37,37,37	0
56	MG	1A	3957	1/1	0.96	0.09	30,30,30,30	0
56	MG	2a	1702	1/1	0.96	0.10	67,67,67,67	0
56	MG	2A	3450	1/1	0.96	0.10	61,61,61,61	0
56	MG	1A	3772	1/1	0.96	0.05	32,32,32,32	0
56	MG	1A	3077	1/1	0.96	0.12	38,38,38,38	0
56	MG	1A	3473	1/1	0.96	0.09	52,52,52,52	0
56	MG	1Q	203	1/1	0.96	0.06	44,44,44,44	0
56	MG	1a	1655	1/1	0.96	0.20	53,53,53,53	0
56	MG	1A	3961	1/1	0.96	0.10	55,55,55,55	0
56	MG	1A	3599	1/1	0.96	0.09	30,30,30,30	0
56	MG	1a	1658	1/1	0.96	0.11	55,55,55,55	0
56	MG	1A	3963	1/1	0.96	0.19	61,61,61,61	0
56	MG	1A	3420	1/1	0.96	0.20	38,38,38,38	0
56	MG	2A	3148	1/1	0.96	0.06	55,55,55,55	0
56	MG	1w	103	1/1	0.96	0.13	61,61,61,61	0
56	MG	1A	3121	1/1	0.96	0.32	48,48,48,48	0
56	MG	1A	3602	1/1	0.96	0.12	31,31,31,31	0
56	MG	1A	3781	1/1	0.96	0.04	47,47,47,47	0
56	MG	2a	1719	1/1	0.96	0.19	53,53,53,53	0
56	MG	1A	3603	1/1	0.96	0.11	44,44,44,44	0
56	MG	1A	3078	1/1	0.96	0.11	30,30,30,30	0
56	MG	1A	3271	1/1	0.96	0.17	36,36,36,36	0
56	MG	1A	3227	1/1	0.96	0.12	45,45,45,45	0
56	MG	1A	3695	1/1	0.96	0.10	35,35,35,35	0
56	MG	1A	3032	1/1	0.96	0.21	31,31,31,31	0
56	MG	1A	3185	1/1	0.96	0.06	52,52,52,52	0
56	MG	1A	3277	1/1	0.96	0.11	38,38,38,38	0
56	MG	1A	3701	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3880	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	3153	1/1	0.96	0.09	37,37,37,37	0
56	MG	1A	3154	1/1	0.96	0.23	41,41,41,41	0
56	MG	1U	205	1/1	0.96	0.16	48,48,48,48	0
56	MG	1A	3796	1/1	0.96	0.09	51,51,51,51	0
56	MG	1A	3189	1/1	0.96	0.19	36,36,36,36	0
56	MG	2a	1735	1/1	0.96	0.38	57,57,57,57	0
56	MG	1U	208	1/1	0.96	0.23	42,42,42,42	0
56	MG	1A	3433	1/1	0.96	0.09	64,64,64,64	0
56	MG	1U	210	1/1	0.96	0.40	42,42,42,42	0
56	MG	1A	4096	1/1	0.96	0.08	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	3487	1/1	0.96	0.12	48,48,48,48	0
56	MG	2A	3008	1/1	0.96	0.17	52,52,52,52	0
56	MG	1A	3377	1/1	0.96	0.10	54,54,54,54	0
56	MG	2A	3491	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3617	1/1	0.96	0.11	34,34,34,34	0
56	MG	1A	3157	1/1	0.96	0.10	45,45,45,45	0
56	MG	1A	3380	1/1	0.96	0.11	45,45,45,45	0
56	MG	2R	203	1/1	0.96	0.11	50,50,50,50	0
56	MG	2A	3017	1/1	0.96	0.07	58,58,58,58	0
56	MG	1B	205	1/1	0.96	0.07	51,51,51,51	0
56	MG	2A	3181	1/1	0.96	0.07	56,56,56,56	0
56	MG	1A	3547	1/1	0.96	0.09	35,35,35,35	0
56	MG	2A	3501	1/1	0.96	0.10	41,41,41,41	0
56	MG	1A	3712	1/1	0.96	0.10	53,53,53,53	0
56	MG	1a	1692	1/1	0.96	0.23	63,63,63,63	0
56	MG	1A	3548	1/1	0.96	0.16	34,34,34,34	0
56	MG	1X	107	1/1	0.96	0.10	59,59,59,59	0
56	MG	2a	1757	1/1	0.96	0.06	51,51,51,51	0
56	MG	1A	3193	1/1	0.96	0.43	36,36,36,36	0
56	MG	1A	3550	1/1	0.96	0.14	40,40,40,40	0
56	MG	2A	3510	1/1	0.96	0.09	47,47,47,47	0
56	MG	1A	3236	1/1	0.96	0.19	36,36,36,36	0
56	MG	2A	3029	1/1	0.96	0.09	44,44,44,44	0
56	MG	1A	3493	1/1	0.96	0.30	45,45,45,45	0
56	MG	1a	1700	1/1	0.96	0.17	49,49,49,49	0
56	MG	2A	3694	1/1	0.96	0.07	56,56,56,56	0
56	MG	1A	4000	1/1	0.96	0.07	31,31,31,31	0
56	MG	2A	3033	1/1	0.96	0.10	47,47,47,47	0
56	MG	1A	3080	1/1	0.96	0.10	45,45,45,45	0
56	MG	10	101	1/1	0.96	0.09	48,48,48,48	0
56	MG	1A	3630	1/1	0.96	0.11	32,32,32,32	0
56	MG	1A	3159	1/1	0.96	0.15	33,33,33,33	0
56	MG	1A	3196	1/1	0.96	0.07	47,47,47,47	0
56	MG	2A	3201	1/1	0.96	0.14	48,48,48,48	0
56	MG	1A	3556	1/1	0.96	0.16	35,35,35,35	0
56	MG	1B	220	1/1	0.96	0.08	42,42,42,42	0
56	MG	1A	3388	1/1	0.96	0.38	47,47,47,47	0
56	MG	2A	3527	1/1	0.96	0.09	55,55,55,55	0
56	MG	1A	3636	1/1	0.96	0.09	17,17,17,17	0
56	MG	1A	3561	1/1	0.96	0.28	41,41,41,41	0
56	MG	1A	3081	1/1	0.96	0.20	40,40,40,40	0
56	MG	1a	1715	1/1	0.96	0.14	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	3019	1/1	0.96	0.12	50,50,50,50	0
56	MG	12	101	1/1	0.96	0.12	56,56,56,56	0
56	MG	12	102	1/1	0.96	0.10	48,48,48,48	0
56	MG	13	102	1/1	0.96	0.12	45,45,45,45	0
56	MG	1A	3043	1/1	0.96	0.13	34,34,34,34	0
56	MG	1A	3826	1/1	0.96	0.06	62,62,62,62	0
56	MG	1A	3086	1/1	0.96	0.23	39,39,39,39	0
56	MG	1a	1726	1/1	0.96	0.12	63,63,63,63	0
56	MG	1A	3044	1/1	0.96	0.12	48,48,48,48	0
56	MG	15	104	1/1	0.96	0.21	44,44,44,44	0
56	MG	15	106	1/1	0.96	0.19	40,40,40,40	0
56	MG	1A	3203	1/1	0.96	0.07	25,25,25,25	0
56	MG	16	101	1/1	0.96	0.09	53,53,53,53	0
56	MG	17	103	1/1	0.96	0.14	38,38,38,38	0
56	MG	17	104	1/1	0.96	0.13	54,54,54,54	0
56	MG	1A	3204	1/1	0.96	0.09	36,36,36,36	0
56	MG	1A	3918	1/1	0.96	0.07	47,47,47,47	0
56	MG	2A	3064	1/1	0.96	0.12	36,36,36,36	0
56	MG	1A	4023	1/1	0.96	0.08	51,51,51,51	0
56	MG	2A	3228	1/1	0.96	0.12	62,62,62,62	0
56	MG	1a	1739	1/1	0.96	0.05	52,52,52,52	0
56	MG	2A	3067	1/1	0.96	0.06	53,53,53,53	0
56	MG	2a	1628	1/1	0.96	0.38	62,62,62,62	0
56	MG	1A	3646	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3023	1/1	0.96	0.08	16,16,16,16	0
56	MG	1A	3507	1/1	0.96	0.30	35,35,35,35	0
56	MG	2A	3073	1/1	0.96	0.17	35,35,35,35	0
56	MG	1A	3067	1/1	0.96	0.05	33,33,33,33	0
56	MG	2A	3075	1/1	0.96	0.29	60,60,60,60	0
56	MG	1A	3453	1/1	0.96	0.22	49,49,49,49	0
56	MG	1a	1745	1/1	0.96	0.09	59,59,59,59	0
56	MG	1A	3926	1/1	0.96	0.10	38,38,38,38	0
56	MG	1A	3036	1/1	0.96	0.11	45,45,45,45	0
56	MG	1A	3059	1/1	0.96	0.39	66,66,66,66	0
56	MG	2A	3570	1/1	0.96	0.10	37,37,37,37	0
56	MG	1A	3929	1/1	0.96	0.06	68,68,68,68	0
56	MG	1A	3212	1/1	0.96	0.05	44,44,44,44	0
56	MG	1E	306	1/1	0.96	0.17	37,37,37,37	0
56	MG	1a	1608	1/1	0.96	0.26	55,55,55,55	0
56	MG	1a	1609	1/1	0.96	0.09	27,27,27,27	0
56	MG	1A	4035	1/1	0.96	0.06	39,39,39,39	0
56	MG	2A	3578	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	3255	1/1	0.96	0.16	37,37,37,37	0
56	MG	1a	1756	1/1	0.96	0.07	57,57,57,57	0
56	MG	1A	3514	1/1	0.96	0.07	46,46,46,46	0
56	MG	2A	3403	1/1	0.96	0.31	50,50,50,50	0
56	MG	2A	3090	1/1	0.96	0.07	42,42,42,42	0
56	MG	1a	1613	1/1	0.96	0.13	54,54,54,54	0
56	MG	1A	3075	1/1	0.96	0.06	30,30,30,30	0
56	MG	1A	3115	1/1	0.96	0.10	49,49,49,49	0
56	MG	1E	313	1/1	0.96	0.12	30,30,30,30	0
56	MG	2A	3409	1/1	0.96	0.12	52,52,52,52	0
56	MG	1A	3215	1/1	0.96	0.22	45,45,45,45	0
56	MG	1A	3937	1/1	0.96	0.08	45,45,45,45	0
56	MG	2A	3412	1/1	0.96	0.19	70,70,70,70	0
56	MG	1a	1764	1/1	0.96	0.18	49,49,49,49	0
56	MG	1A	3310	1/1	0.96	0.34	61,61,61,61	0
56	MG	1A	3661	1/1	0.96	0.05	30,30,30,30	0
56	MG	1A	3847	1/1	0.96	0.08	22,22,22,22	0
56	MG	2A	3417	1/1	0.96	0.09	48,48,48,48	0
56	MG	1F	303	1/1	0.96	0.10	55,55,55,55	0
56	MG	2a	1669	1/1	0.96	0.29	84,84,84,84	0
56	MG	1A	3662	1/1	0.96	0.09	26,26,26,26	0
56	MG	1F	306	1/1	0.96	0.13	44,44,44,44	0
56	MG	1F	307	1/1	0.96	0.14	38,38,38,38	0
56	MG	1A	3116	1/1	0.96	0.19	40,40,40,40	0
56	MG	2A	3603	1/1	0.96	0.11	42,42,42,42	0
56	MG	1A	3758	1/1	0.96	0.07	28,28,28,28	0
56	MG	1A	3217	1/1	0.96	0.08	57,57,57,57	0
56	MG	1A	3174	1/1	0.96	0.36	39,39,39,39	0
56	MG	1A	3946	1/1	0.96	0.11	52,52,52,52	0
56	MG	1G	201	1/1	0.96	0.11	36,36,36,36	0
56	MG	1A	3590	1/1	0.96	0.17	32,32,32,32	0
56	MG	1A	4054	1/1	0.96	0.13	17,17,17,17	0
56	MG	2x	106	1/1	0.96	0.18	51,51,51,51	0
56	MG	1A	3854	1/1	0.96	0.11	58,58,58,58	0
56	MG	1a	1785	1/1	0.96	0.06	57,57,57,57	0
56	MG	1A	3763	1/1	0.96	0.12	34,34,34,34	0
56	MG	1A	3671	1/1	0.96	0.05	28,28,28,28	0
56	MG	1A	4059	1/1	0.96	0.07	41,41,41,41	0
58	ZN	2n	501	1/1	0.96	0.06	97,97,97,97	0
56	MG	1A	3178	1/1	0.96	0.06	40,40,40,40	0
56	MG	1a	1790	1/1	0.96	0.15	64,64,64,64	0
56	MG	1A	3147	1/1	0.97	0.07	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	2A	3098	1/1	0.97	0.10	31,31,31,31	0
56	MG	15	102	1/1	0.97	0.25	37,37,37,37	0
56	MG	1A	3074	1/1	0.97	0.09	32,32,32,32	0
56	MG	1F	302	1/1	0.97	0.14	34,34,34,34	0
56	MG	1A	3894	1/1	0.97	0.06	47,47,47,47	0
56	MG	2A	3469	1/1	0.97	0.10	43,43,43,43	0
56	MG	15	107	1/1	0.97	0.18	50,50,50,50	0
56	MG	1A	3977	1/1	0.97	0.12	36,36,36,36	0
56	MG	1A	4069	1/1	0.97	0.21	57,57,57,57	0
56	MG	17	102	1/1	0.97	0.12	32,32,32,32	0
56	MG	1A	3345	1/1	0.97	0.17	38,38,38,38	0
56	MG	1F	308	1/1	0.97	0.14	34,34,34,34	0
56	MG	1A	3042	1/1	0.97	0.23	34,34,34,34	0
56	MG	1a	1699	1/1	0.97	0.13	45,45,45,45	0
56	MG	2A	3111	1/1	0.97	0.16	51,51,51,51	0
56	MG	1A	3051	1/1	0.97	0.15	31,31,31,31	0
56	MG	2A	3754	1/1	0.97	0.06	60,60,60,60	0
56	MG	1A	3125	1/1	0.97	0.17	34,34,34,34	0
56	MG	18	103	1/1	0.97	0.09	46,46,46,46	0
56	MG	1A	3218	1/1	0.97	0.19	42,42,42,42	0
56	MG	2A	3116	1/1	0.97	0.28	68,68,68,68	0
56	MG	1A	3052	1/1	0.97	0.10	49,49,49,49	0
56	MG	2A	3485	1/1	0.97	0.11	50,50,50,50	0
56	MG	1A	3985	1/1	0.97	0.04	46,46,46,46	0
56	MG	1A	3461	1/1	0.97	0.21	44,44,44,44	0
56	MG	1A	3028	1/1	0.97	0.16	36,36,36,36	0
56	MG	1A	3741	1/1	0.97	0.11	60,60,60,60	0
56	MG	1A	3352	1/1	0.97	0.10	43,43,43,43	0
56	MG	1A	3592	1/1	0.97	0.23	43,43,43,43	0
56	MG	1A	3663	1/1	0.97	0.10	37,37,37,37	0
56	MG	1A	3109	1/1	0.97	0.31	37,37,37,37	0
56	MG	1N	204	1/1	0.97	0.06	40,40,40,40	0
56	MG	2A	3630	1/1	0.97	0.06	35,35,35,35	0
56	MG	2A	3127	1/1	0.97	0.08	52,52,52,52	0
56	MG	1a	1716	1/1	0.97	0.12	40,40,40,40	0
56	MG	1A	3746	1/1	0.97	0.05	48,48,48,48	0
56	MG	1A	3222	1/1	0.97	0.11	40,40,40,40	0
56	MG	1A	3408	1/1	0.97	0.07	55,55,55,55	0
56	MG	2A	3009	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3155	1/1	0.97	0.09	41,41,41,41	0
56	MG	1A	3998	1/1	0.97	0.07	33,33,33,33	0
56	MG	1A	3111	1/1	0.97	0.20	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3064	1/1	0.97	0.13	38,38,38,38	0
56	MG	1a	1615	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3674	1/1	0.97	0.05	56,56,56,56	0
56	MG	1a	1728	1/1	0.97	0.07	53,53,53,53	0
56	MG	1P	202	1/1	0.97	0.27	37,37,37,37	0
56	MG	2A	3143	1/1	0.97	0.16	41,41,41,41	0
56	MG	1a	1618	1/1	0.97	0.06	42,42,42,42	0
56	MG	1P	204	1/1	0.97	0.30	32,32,32,32	0
56	MG	1A	3190	1/1	0.97	0.21	41,41,41,41	0
56	MG	1A	3265	1/1	0.97	0.11	43,43,43,43	0
56	MG	2A	3518	1/1	0.97	0.09	43,43,43,43	0
56	MG	1A	3472	1/1	0.97	0.07	45,45,45,45	0
56	MG	1A	3921	1/1	0.97	0.06	15,15,15,15	0
56	MG	1A	3759	1/1	0.97	0.08	38,38,38,38	0
56	MG	1A	3266	1/1	0.97	0.10	50,50,50,50	0
56	MG	1A	3007	1/1	0.97	0.05	47,47,47,47	0
56	MG	1A	3192	1/1	0.97	0.24	37,37,37,37	0
56	MG	1A	3066	1/1	0.97	0.15	37,37,37,37	0
56	MG	2A	3034	1/1	0.97	0.11	27,27,27,27	0
56	MG	1B	206	1/1	0.97	0.10	47,47,47,47	0
56	MG	1R	204	1/1	0.97	0.33	45,45,45,45	0
56	MG	1A	3270	1/1	0.97	0.28	50,50,50,50	0
56	MG	1A	3039	1/1	0.97	0.30	38,38,38,38	0
56	MG	2a	1658	1/1	0.97	0.13	49,49,49,49	0
56	MG	1A	3319	1/1	0.97	0.12	45,45,45,45	0
56	MG	1A	3688	1/1	0.97	0.10	34,34,34,34	0
56	MG	1A	4016	1/1	0.97	0.12	51,51,51,51	0
56	MG	1A	3135	1/1	0.97	0.13	45,45,45,45	0
56	MG	1A	3033	1/1	0.97	0.24	35,35,35,35	0
56	MG	1A	3424	1/1	0.97	0.08	52,52,52,52	0
56	MG	1A	3137	1/1	0.97	0.24	31,31,31,31	0
56	MG	1a	1641	1/1	0.97	0.06	51,51,51,51	0
56	MG	1A	3484	1/1	0.97	0.20	46,46,46,46	0
56	MG	1A	3275	1/1	0.97	0.23	42,42,42,42	0
56	MG	2A	3170	1/1	0.97	0.10	33,33,33,33	0
56	MG	1A	3139	1/1	0.97	0.07	44,44,44,44	0
56	MG	1A	3118	1/1	0.97	0.14	42,42,42,42	0
56	MG	1A	3699	1/1	0.97	0.09	28,28,28,28	0
56	MG	1A	3141	1/1	0.97	0.07	21,21,21,21	0
56	MG	2A	3681	1/1	0.97	0.15	58,58,58,58	0
56	MG	1A	3282	1/1	0.97	0.16	49,49,49,49	0
56	MG	1A	3283	1/1	0.97	0.21	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	1B	224	1/1	0.97	0.15	59,59,59,59	0
56	MG	1A	4032	1/1	0.97	0.11	30,30,30,30	0
56	MG	1A	3783	1/1	0.97	0.09	23,23,23,23	0
56	MG	2D	304	1/1	0.97	0.07	26,26,26,26	0
56	MG	1A	3284	1/1	0.97	0.05	35,35,35,35	0
56	MG	1A	3085	1/1	0.97	0.23	34,34,34,34	0
56	MG	1A	3030	1/1	0.97	0.23	32,32,32,32	0
56	MG	1A	3332	1/1	0.97	0.29	58,58,58,58	0
56	MG	1A	3240	1/1	0.97	0.28	32,32,32,32	0
56	MG	2a	1687	1/1	0.97	0.18	40,40,40,40	0
56	MG	1X	101	1/1	0.97	0.28	46,46,46,46	0
56	MG	1A	3072	1/1	0.97	0.14	33,33,33,33	0
56	MG	1A	3560	1/1	0.97	0.16	37,37,37,37	0
56	MG	1A	3383	1/1	0.97	0.10	46,46,46,46	0
56	MG	2A	3563	1/1	0.97	0.06	33,33,33,33	0
56	MG	1A	3384	1/1	0.97	0.28	33,33,33,33	0
56	MG	1a	1778	1/1	0.97	0.09	67,67,67,67	0
56	MG	2A	3566	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3441	1/1	0.97	0.16	39,39,39,39	0
56	MG	2A	3702	1/1	0.97	0.07	70,70,70,70	0
56	MG	2A	3070	1/1	0.97	0.14	44,44,44,44	0
56	MG	1A	3145	1/1	0.97	0.18	34,34,34,34	0
56	MG	2A	3072	1/1	0.97	0.08	48,48,48,48	0
56	MG	1A	3206	1/1	0.97	0.08	34,34,34,34	0
56	MG	1A	3798	1/1	0.97	0.07	25,25,25,25	0
56	MG	1A	3502	1/1	0.97	0.17	34,34,34,34	0
56	MG	1A	3146	1/1	0.97	0.13	38,38,38,38	0
56	MG	1A	3569	1/1	0.97	0.12	41,41,41,41	0
56	MG	1A	3175	1/1	0.97	0.06	36,36,36,36	0
56	MG	2A	3577	1/1	0.97	0.07	49,49,49,49	0
56	MG	10	103	1/1	0.97	0.08	49,49,49,49	0
56	MG	2A	3444	1/1	0.97	0.08	70,70,70,70	0
56	MG	1E	302	1/1	0.97	0.19	49,49,49,49	0
56	MG	1A	3571	1/1	0.97	0.08	46,46,46,46	0
56	MG	1E	304	1/1	0.97	0.08	37,37,37,37	0
56	MG	2A	3583	1/1	0.97	0.11	36,36,36,36	0
56	MG	1E	305	1/1	0.97	0.19	34,34,34,34	0
56	MG	1a	1676	1/1	0.97	0.20	50,50,50,50	0
56	MG	1A	3209	1/1	0.97	0.06	35,35,35,35	0
56	MG	1A	3176	1/1	0.97	0.14	34,34,34,34	0
56	MG	1A	3391	1/1	0.97	0.12	63,63,63,63	0
56	MG	1A	3645	1/1	0.97	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	3177	1/1	0.97	0.09	21,21,21,21	0
56	MG	1A	3342	1/1	0.97	0.31	40,40,40,40	0
56	MG	2A	3728	1/1	0.97	0.10	62,62,62,62	0
56	MG	1A	3394	1/1	0.97	0.06	35,35,35,35	0
57	WC9	2A	3809	34/34	0.97	0.09	35,43,48,51	0
56	MG	1A	3395	1/1	0.97	0.11	37,37,37,37	0
58	ZN	2Y	501	1/1	0.97	0.05	88,88,88,88	0
56	MG	1A	3730	1/1	0.97	0.05	55,55,55,55	0
56	MG	2A	3094	1/1	0.97	0.09	55,55,55,55	0
56	MG	1A	3815	1/1	0.97	0.07	27,27,27,27	0
56	MG	1m	3001	1/1	0.97	0.10	56,56,56,56	0
56	MG	1A	3296	1/1	0.98	0.06	37,37,37,37	0
56	MG	1A	3243	1/1	0.98	0.07	46,46,46,46	0
56	MG	1A	3757	1/1	0.98	0.05	40,40,40,40	0
56	MG	1A	3084	1/1	0.98	0.14	30,30,30,30	0
56	MG	1A	3577	1/1	0.98	0.14	31,31,31,31	0
56	MG	1A	3073	1/1	0.98	0.07	14,14,14,14	0
56	MG	1a	1723	1/1	0.98	0.06	41,41,41,41	0
56	MG	1a	1724	1/1	0.98	0.07	39,39,39,39	0
56	MG	1A	3417	1/1	0.98	0.08	49,49,49,49	0
56	MG	1A	3659	1/1	0.98	0.07	40,40,40,40	0
56	MG	2a	1667	1/1	0.98	0.06	52,52,52,52	0
56	MG	1A	3008	1/1	0.98	0.12	27,27,27,27	0
56	MG	2A	3743	1/1	0.98	0.10	39,39,39,39	0
56	MG	1A	4052	1/1	0.98	0.07	43,43,43,43	0
56	MG	1A	3619	1/1	0.98	0.11	31,31,31,31	0
56	MG	1A	3038	1/1	0.98	0.21	33,33,33,33	0
56	MG	1l	101	1/1	0.98	0.30	37,37,37,37	0
56	MG	1A	3199	1/1	0.98	0.13	19,19,19,19	0
56	MG	1A	3045	1/1	0.98	0.06	40,40,40,40	0
56	MG	1A	3665	1/1	0.98	0.06	41,41,41,41	0
56	MG	1A	3624	1/1	0.98	0.05	50,50,50,50	0
56	MG	1A	3304	1/1	0.98	0.05	33,33,33,33	0
56	MG	1A	3585	1/1	0.98	0.10	12,12,12,12	0
56	MG	13	101	1/1	0.98	0.09	38,38,38,38	0
56	MG	1A	3773	1/1	0.98	0.06	22,22,22,22	0
56	MG	1A	3670	1/1	0.98	0.06	31,31,31,31	0
56	MG	1A	3138	1/1	0.98	0.30	32,32,32,32	0
56	MG	1A	3672	1/1	0.98	0.05	27,27,27,27	0
56	MG	1P	201	1/1	0.98	0.43	39,39,39,39	0
56	MG	2W	204	1/1	0.98	0.10	43,43,43,43	0
56	MG	1A	4004	1/1	0.98	0.07	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3660	1/1	0.98	0.04	37,37,37,37	0
56	MG	2X	102	1/1	0.98	0.08	54,54,54,54	0
56	MG	2A	3186	1/1	0.98	0.05	65,65,65,65	0
56	MG	1P	203	1/1	0.98	0.10	33,33,33,33	0
56	MG	2A	3663	1/1	0.98	0.06	37,37,37,37	0
56	MG	2A	3006	1/1	0.98	0.08	38,38,38,38	0
56	MG	15	105	1/1	0.98	0.22	33,33,33,33	0
56	MG	1A	3009	1/1	0.98	0.04	25,25,25,25	0
56	MG	1A	3518	1/1	0.98	0.07	56,56,56,56	0
56	MG	2A	3010	1/1	0.98	0.06	40,40,40,40	0
56	MG	1A	3779	1/1	0.98	0.07	47,47,47,47	0
56	MG	2A	3012	1/1	0.98	0.07	46,46,46,46	0
56	MG	1Q	202	1/1	0.98	0.12	34,34,34,34	0
56	MG	2A	3014	1/1	0.98	0.26	49,49,49,49	0
56	MG	17	101	1/1	0.98	0.10	37,37,37,37	0
56	MG	1A	3278	1/1	0.98	0.27	43,43,43,43	0
56	MG	1A	4071	1/1	0.98	0.08	45,45,45,45	0
56	MG	1A	3726	1/1	0.98	0.07	25,25,25,25	0
56	MG	2A	3781	1/1	0.98	0.14	64,64,64,64	0
56	MG	1A	3631	1/1	0.98	0.06	24,24,24,24	0
56	MG	1A	3677	1/1	0.98	0.08	29,29,29,29	0
56	MG	1A	3055	1/1	0.98	0.05	37,37,37,37	0
56	MG	1D	303	1/1	0.98	0.09	18,18,18,18	0
56	MG	2A	3024	1/1	0.98	0.13	38,38,38,38	0
56	MG	1A	3280	1/1	0.98	0.34	39,39,39,39	0
56	MG	1D	305	1/1	0.98	0.20	35,35,35,35	0
56	MG	1D	306	1/1	0.98	0.13	38,38,38,38	0
56	MG	1D	307	1/1	0.98	0.13	52,52,52,52	0
56	MG	1A	3161	1/1	0.98	0.24	35,35,35,35	0
56	MG	1A	3682	1/1	0.98	0.06	29,29,29,29	0
56	MG	2A	3688	1/1	0.98	0.06	58,58,58,58	0
56	MG	1A	3429	1/1	0.98	0.22	43,43,43,43	0
56	MG	1A	4017	1/1	0.98	0.04	48,48,48,48	0
56	MG	1E	301	1/1	0.98	0.17	34,34,34,34	0
56	MG	2A	3493	1/1	0.98	0.09	37,37,37,37	0
56	MG	2A	3494	1/1	0.98	0.06	32,32,32,32	0
56	MG	1a	1770	1/1	0.98	0.08	47,47,47,47	0
56	MG	1A	3557	1/1	0.98	0.07	25,25,25,25	0
56	MG	1A	3010	1/1	0.98	0.04	27,27,27,27	0
56	MG	1A	3559	1/1	0.98	0.15	44,44,44,44	0
56	MG	1A	3106	1/1	0.98	0.04	29,29,29,29	0
56	MG	1A	3057	1/1	0.98	0.06	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3689	1/1	0.98	0.10	47,47,47,47	0
56	MG	1E	308	1/1	0.98	0.12	30,30,30,30	0
56	MG	2A	3131	1/1	0.98	0.18	46,46,46,46	0
56	MG	2A	3132	1/1	0.98	0.14	44,44,44,44	0
56	MG	1A	3562	1/1	0.98	0.07	41,41,41,41	0
56	MG	1A	3186	1/1	0.98	0.09	45,45,45,45	0
56	MG	2A	3507	1/1	0.98	0.07	41,41,41,41	0
56	MG	1A	3799	1/1	0.98	0.05	47,47,47,47	0
56	MG	1A	3800	1/1	0.98	0.05	28,28,28,28	0
56	MG	1V	201	1/1	0.98	0.16	33,33,33,33	0
56	MG	1A	3048	1/1	0.98	0.05	34,34,34,34	0
56	MG	1A	3003	1/1	0.98	0.06	22,22,22,22	0
56	MG	1V	205	1/1	0.98	0.24	54,54,54,54	0
56	MG	1A	3211	1/1	0.98	0.14	36,36,36,36	0
56	MG	1a	1701	1/1	0.98	0.14	41,41,41,41	0
56	MG	1A	3127	1/1	0.98	0.35	41,41,41,41	0
56	MG	1A	3110	1/1	0.98	0.06	38,38,38,38	0
56	MG	1A	3697	1/1	0.98	0.06	15,15,15,15	0
56	MG	1F	301	1/1	0.98	0.10	39,39,39,39	0
56	MG	1A	3012	1/1	0.98	0.03	30,30,30,30	0
56	MG	1A	3096	1/1	0.98	0.06	37,37,37,37	0
56	MG	1X	103	1/1	0.98	0.05	48,48,48,48	0
56	MG	1F	304	1/1	0.98	0.08	36,36,36,36	0
56	MG	2A	3723	1/1	0.98	0.11	41,41,41,41	0
56	MG	1a	1630	1/1	0.98	0.16	33,33,33,33	0
57	WC9	1A	4098	34/34	0.98	0.07	22,27,32,33	0
56	MG	1A	3097	1/1	0.98	0.17	22,22,22,22	0
56	MG	1X	106	1/1	0.98	0.07	37,37,37,37	0
56	MG	1A	3114	1/1	0.98	0.06	37,37,37,37	0
56	MG	2A	3529	1/1	0.98	0.06	45,45,45,45	0
58	ZN	29	501	1/1	0.98	0.04	76,76,76,76	0
56	MG	1a	1714	1/1	0.98	0.04	35,35,35,35	0
59	SF4	1d	302	8/8	0.98	0.05	64,70,73,76	0
56	MG	1A	3242	1/1	0.98	0.08	50,50,50,50	0
56	MG	1A	3924	1/1	0.98	0.09	38,38,38,38	0
56	MG	2A	3508	1/1	0.99	0.06	41,41,41,41	0
56	MG	1U	201	1/1	0.99	0.20	34,34,34,34	0
56	MG	1A	3834	1/1	0.99	0.09	39,39,39,39	0
56	MG	1A	3229	1/1	0.99	0.14	38,38,38,38	0
56	MG	1A	3899	1/1	0.99	0.08	45,45,45,45	0
56	MG	2A	3751	1/1	0.99	0.08	43,43,43,43	0
56	MG	1A	3679	1/1	0.99	0.05	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	10	107	1/1	0.99	0.03	41,41,41,41	0
56	MG	1A	3173	1/1	0.99	0.11	38,38,38,38	0
56	MG	1A	3276	1/1	0.99	0.11	28,28,28,28	0
56	MG	1A	3667	1/1	0.99	0.07	29,29,29,29	0
56	MG	1A	3904	1/1	0.99	0.05	31,31,31,31	0
56	MG	1A	3979	1/1	0.99	0.10	30,30,30,30	0
56	MG	1A	3905	1/1	0.99	0.04	32,32,32,32	0
56	MG	1A	3021	1/1	0.99	0.02	26,26,26,26	0
56	MG	1A	3931	1/1	0.99	0.05	49,49,49,49	0
56	MG	1V	204	1/1	0.99	0.12	32,32,32,32	0
56	MG	2A	3763	1/1	0.99	0.06	35,35,35,35	0
56	MG	1A	3378	1/1	0.99	0.22	24,24,24,24	0
56	MG	1A	3037	1/1	0.99	0.14	25,25,25,25	0
56	MG	1A	3070	1/1	0.99	0.08	14,14,14,14	0
56	MG	2A	3767	1/1	0.99	0.04	62,62,62,62	0
56	MG	1A	3748	1/1	0.99	0.03	26,26,26,26	0
56	MG	2A	3018	1/1	0.99	0.11	29,29,29,29	0
56	MG	1W	202	1/1	0.99	0.18	37,37,37,37	0
56	MG	1a	1766	1/1	0.99	0.05	57,57,57,57	0
56	MG	2A	3399	1/1	0.99	0.11	25,25,25,25	0
56	MG	15	101	1/1	0.99	0.17	34,34,34,34	0
56	MG	1t	201	1/1	0.99	0.04	64,64,64,64	0
56	MG	2A	3534	1/1	0.99	0.04	33,33,33,33	0
56	MG	2A	3535	1/1	0.99	0.02	42,42,42,42	0
56	MG	1A	3546	1/1	0.99	0.12	38,38,38,38	0
56	MG	1A	3071	1/1	0.99	0.12	29,29,29,29	0
56	MG	1A	3156	1/1	0.99	0.23	39,39,39,39	0
56	MG	1A	3769	1/1	0.99	0.03	35,35,35,35	0
56	MG	1A	4047	1/1	0.99	0.03	39,39,39,39	0
56	MG	1a	1773	1/1	0.99	0.04	52,52,52,52	0
56	MG	1A	3991	1/1	0.99	0.05	36,36,36,36	0
56	MG	1A	3788	1/1	0.99	0.06	23,23,23,23	0
56	MG	1A	4081	1/1	0.99	0.04	37,37,37,37	0
56	MG	1A	4020	1/1	0.99	0.02	26,26,26,26	0
56	MG	1a	1738	1/1	0.99	0.06	62,62,62,62	0
56	MG	1A	4021	1/1	0.99	0.05	49,49,49,49	0
58	ZN	1Y	204	1/1	0.99	0.03	63,63,63,63	0
56	MG	1A	3789	1/1	0.99	0.04	27,27,27,27	0
58	ZN	15	109	1/1	0.99	0.03	45,45,45,45	0
58	ZN	1n	103	1/1	0.99	0.04	68,68,68,68	0
56	MG	1A	3013	1/1	0.99	0.13	30,30,30,30	0
56	MG	1A	3623	1/1	0.99	0.06	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	ZN	25	105	1/1	0.99	0.04	60,60,60,60	0
58	ZN	26	501	1/1	0.99	0.03	60,60,60,60	0
56	MG	1A	4055	1/1	0.99	0.09	33,33,33,33	0
56	MG	2A	3461	1/1	0.99	0.06	47,47,47,47	0
56	MG	2A	3647	1/1	0.99	0.04	37,37,37,37	0
59	SF4	2d	303	8/8	0.99	0.05	64,66,74,76	0
56	MG	1A	3014	1/1	0.99	0.05	27,27,27,27	0
56	MG	1A	3755	1/1	0.99	0.06	47,47,47,47	0
58	ZN	19	102	1/1	1.00	0.06	46,46,46,46	0
56	MG	1A	3716	1/1	1.00	0.06	26,26,26,26	0
56	MG	1A	3614	1/1	1.00	0.07	36,36,36,36	0
58	ZN	16	102	1/1	1.00	0.02	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.