



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 11:44 am BST

PDB ID : 6CFJ
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with histidyl-CAM and bound to mRNA and A-, P-, and E-site tRNAs at 2.8Å resolution
Authors : Tereshchenkov, A.G.; Dobosz-Bartoszek, M.; Osterman, I.A.; Marks, J.; Sergeeva, V.A.; Kasatsky, P.; Komarova, E.S.; Stavrianidi, A.N.; Rodin, I.A.; Konevega, A.L.; Sergiev, P.V.; Sumbatyan, N.V.; Mankin, A.S.; Bogdanov, A.A.; Polikanov, Y.S.
Deposited on : 2018-02-15
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

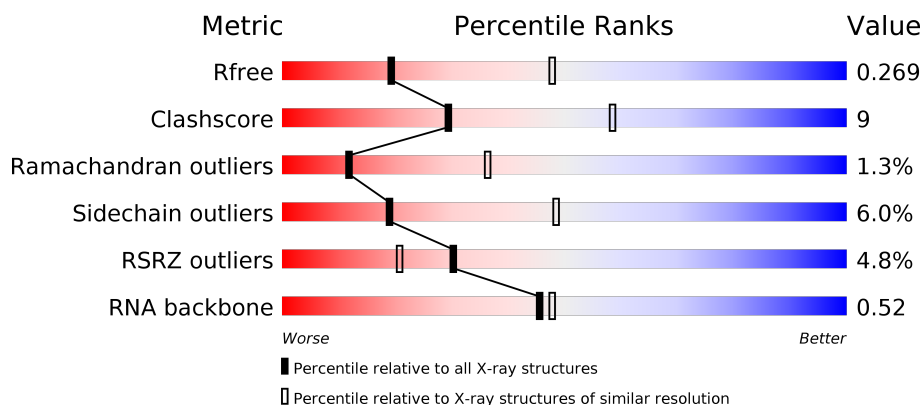
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.











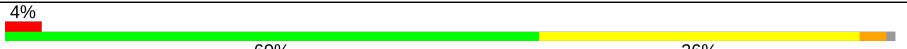

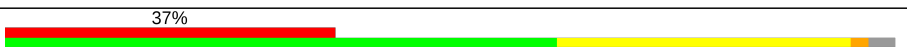





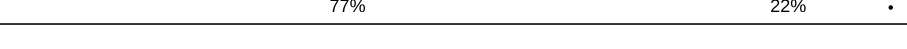


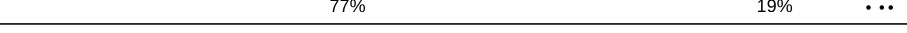





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	<div> <div></div> <div>60% 32% 6% .</div> </div>
1	2A	2915	<div> <div></div> <div>52% 36% 8% .</div> </div>
2	1B	121	<div> <div></div> <div>64% 30% 5% .</div> </div>



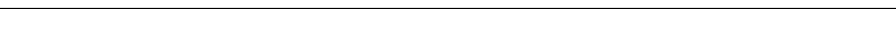
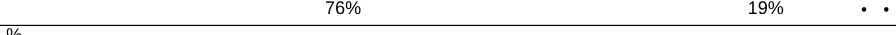


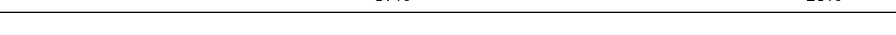



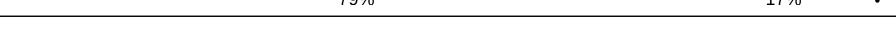


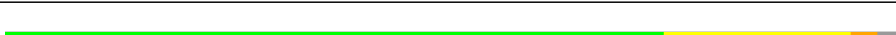




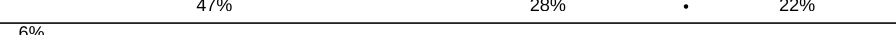


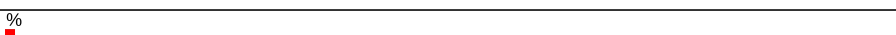



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Mol	Chain	Length	Quality of chain
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	

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Mol	Chain	Length	Quality of chain
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	
27	15	60	

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Mol	Chain	Length	Quality of chain
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	
39	2h	138	

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Mol	Chain	Length	Quality of chain
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	
52	1u	27	

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Mol	Chain	Length	Quality of chain
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
56	MG	1A	3201	-	-	-	X
56	MG	1A	3226	-	-	-	X
56	MG	1B	211	-	-	-	X
56	MG	2W	202	-	-	-	X
56	MG	2v	3002	-	-	-	X

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 299109 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	1273	G	UNK	conflict	GB 37223181
2A	1227	G	UNK	conflict	GB 37223181

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

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

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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			
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			

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

- Molecule 53 is a RNA chain called mRNA.

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1x	8	4SU	G	conflict	GB 205271127
2x	8	4SU	G	conflict	GB 205271127

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	10	Total	Mg	0	0
			10	10		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	17	5	Total 5	Mg 5	0	0
56	2d	2	Total 2	Mg 2	0	0
56	1T	2	Total 2	Mg 2	0	0
56	1N	5	Total 5	Mg 5	0	0
56	20	3	Total 3	Mg 3	0	0
56	18	3	Total 3	Mg 3	0	0
56	2W	3	Total 3	Mg 3	0	0
56	1Y	2	Total 2	Mg 2	0	0
56	13	2	Total 2	Mg 2	0	0
56	1f	1	Total 1	Mg 1	0	0
56	1P	3	Total 3	Mg 3	0	0
56	2B	21	Total 21	Mg 21	0	0
56	2l	4	Total 4	Mg 4	0	0
56	1q	1	Total 1	Mg 1	0	0
56	2a	233	Total 233	Mg 233	0	0
56	1E	13	Total 13	Mg 13	0	0
56	1b	2	Total 2	Mg 2	0	0
56	25	3	Total 3	Mg 3	0	0
56	2F	4	Total 4	Mg 4	0	0
56	16	3	Total 3	Mg 3	0	0
56	28	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2e	1	Total Mg 1 1	0	0
56	1W	5	Total Mg 5 5	0	0
56	1A	1063	Total Mg 1063 1063	0	0
56	1t	1	Total Mg 1 1	0	0
56	1n	2	Total Mg 2 2	0	0
56	2P	1	Total Mg 1 1	0	0
56	1X	6	Total Mg 6 6	0	0
56	12	2	Total Mg 2 2	0	0
56	1y	4	Total Mg 4 4	0	0
56	1S	3	Total Mg 3 3	0	0
56	1p	1	Total Mg 1 1	0	0
56	2T	3	Total Mg 3 3	0	0
56	1D	14	Total Mg 14 14	0	0
56	23	1	Total Mg 1 1	0	0
56	1e	1	Total Mg 1 1	0	0
56	2G	1	Total Mg 1 1	0	0
56	1I	1	Total Mg 1 1	0	0
56	2f	1	Total Mg 1 1	0	0
56	1V	3	Total Mg 3 3	0	0
56	2X	2	Total Mg 2 2	0	0
56	1w	11	Total Mg 11 11	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1a	215	Total Mg 215 215	0	0
56	2Q	3	Total Mg 3 3	0	0
56	15	6	Total Mg 6 6	0	0
56	1x	15	Total Mg 15 15	0	0
56	2j	2	Total Mg 2 2	0	0
56	1R	5	Total Mg 5 5	0	0
56	1s	1	Total Mg 1 1	0	0
56	1m	1	Total Mg 1 1	0	0
56	2U	6	Total Mg 6 6	0	0
56	1G	5	Total Mg 5 5	0	0
56	2O	2	Total Mg 2 2	0	0
56	11	5	Total Mg 5 5	0	0
56	2r	2	Total Mg 2 2	0	0
56	21	1	Total Mg 1 1	0	0
56	2g	1	Total Mg 1 1	0	0
56	2w	9	Total Mg 9 9	0	0
56	1v	1	Total Mg 1 1	0	0
56	2x	5	Total Mg 5 5	0	0
56	2R	4	Total Mg 4 4	0	0
56	1Z	4	Total Mg 4 4	0	0
56	2D	7	Total Mg 7 7	0	0

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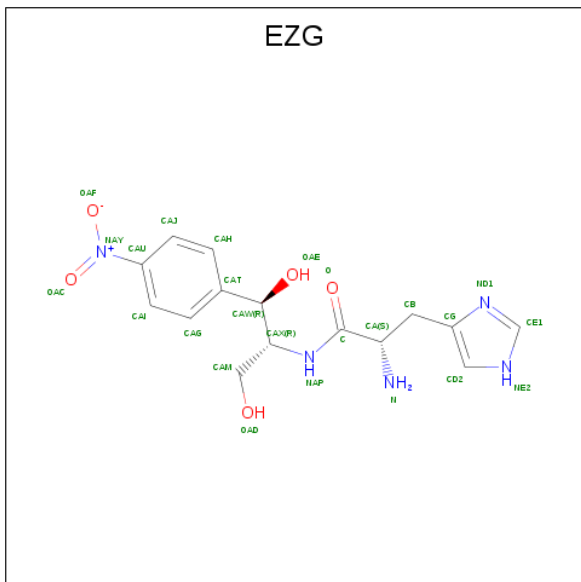
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2q	4	Total Mg 4 4	0	0
56	1U	6	Total Mg 6 6	0	0
56	1O	7	Total Mg 7 7	0	0
56	1r	1	Total Mg 1 1	0	0
56	19	1	Total Mg 1 1	0	0
56	1l	3	Total Mg 3 3	0	0
56	2V	2	Total Mg 2 2	0	0
56	1F	9	Total Mg 9 9	0	0
56	10	5	Total Mg 5 5	0	0
56	2t	1	Total Mg 1 1	0	0
56	1Q	5	Total Mg 5 5	0	0
56	2A	754	Total Mg 754 754	0	0
56	2Z	1	Total Mg 1 1	0	0
56	1B	38	Total Mg 38 38	0	0
56	2y	7	Total Mg 7 7	0	0
56	27	2	Total Mg 2 2	0	0
56	2v	5	Total Mg 5 5	0	0

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 58 is N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]-L-histidinamide (three-letter code: EZG) (formula: C₁₅H₁₉N₅O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1A	1	Total	C	N	O	0	0
			25	15	5	5		
58	2A	1	Total	C	N	O	0	0
			25	15	5	5		

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

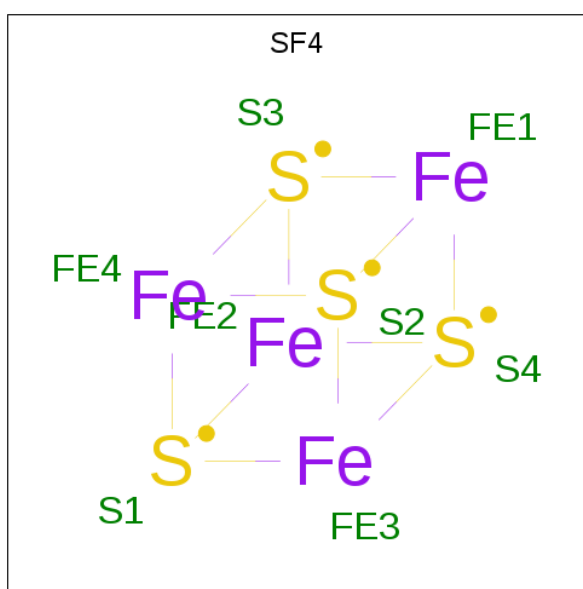
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	29	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		

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

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	1433	Total	O	0	0
			1433	1433		
61	1B	65	Total	O	0	0
			65	65		
61	1D	24	Total	O	0	0
			24	24		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1E	30	Total 30	O 30	0	0
61	1F	10	Total 10	O 10	0	0
61	1G	8	Total 8	O 8	0	0
61	1H	1	Total 1	O 1	0	0
61	1I	2	Total 2	O 2	0	0
61	1N	6	Total 6	O 6	0	0
61	1O	8	Total 8	O 8	0	0
61	1P	18	Total 18	O 18	0	0
61	1Q	12	Total 12	O 12	0	0
61	1R	12	Total 12	O 12	0	0
61	1S	4	Total 4	O 4	0	0
61	1T	7	Total 7	O 7	0	0
61	1U	9	Total 9	O 9	0	0
61	1V	8	Total 8	O 8	0	0
61	1W	8	Total 8	O 8	0	0
61	1X	8	Total 8	O 8	0	0
61	1Y	2	Total 2	O 2	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	10	Total 10	O 10	0	0
61	11	7	Total 7	O 7	0	0
61	12	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	4	Total 4	O 4	0	0
61	15	5	Total 5	O 5	0	0
61	16	2	Total 2	O 2	0	0
61	17	9	Total 9	O 9	0	0
61	18	7	Total 7	O 7	0	0
61	1a	315	Total 315	O 315	0	0
61	1b	1	Total 1	O 1	0	0
61	1e	1	Total 1	O 1	0	0
61	1f	1	Total 1	O 1	0	0
61	1g	1	Total 1	O 1	0	0
61	1j	1	Total 1	O 1	0	0
61	1l	6	Total 6	O 6	0	0
61	1m	1	Total 1	O 1	0	0
61	1n	1	Total 1	O 1	0	0
61	1q	3	Total 3	O 3	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	6	Total 6	O 6	0	0
61	1w	20	Total 20	O 20	0	0
61	1x	14	Total 14	O 14	0	0
61	1y	2	Total 2	O 2	0	0
61	2A	885	Total 885	O 885	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2B	26	Total 26	O 26	0	0
61	2D	18	Total 18	O 18	0	0
61	2E	14	Total 14	O 14	0	0
61	2F	18	Total 18	O 18	0	0
61	2I	4	Total 4	O 4	0	0
61	2N	1	Total 1	O 1	0	0
61	2P	12	Total 12	O 12	0	0
61	2Q	2	Total 2	O 2	0	0
61	2R	2	Total 2	O 2	0	0
61	2T	6	Total 6	O 6	0	0
61	2U	3	Total 3	O 3	0	0
61	2V	1	Total 1	O 1	0	0
61	2W	3	Total 3	O 3	0	0
61	2X	1	Total 1	O 1	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	2	Total 2	O 2	0	0
61	20	4	Total 4	O 4	0	0
61	21	8	Total 8	O 8	0	0
61	22	1	Total 1	O 1	0	0
61	23	1	Total 1	O 1	0	0
61	25	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	26	1	Total 1	O 1	0	0
61	27	4	Total 4	O 4	0	0
61	28	4	Total 4	O 4	0	0
61	29	1	Total 1	O 1	0	0
61	2a	258	Total 258	O 258	0	0
61	2c	1	Total 1	O 1	0	0
61	2d	3	Total 3	O 3	0	0
61	2e	1	Total 1	O 1	0	0
61	2g	1	Total 1	O 1	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	4	Total 4	O 4	0	0
61	2l	6	Total 6	O 6	0	0
61	2o	1	Total 1	O 1	0	0
61	2p	2	Total 2	O 2	0	0
61	2q	1	Total 1	O 1	0	0
61	2r	1	Total 1	O 1	0	0
61	2t	5	Total 5	O 5	0	0
61	2u	1	Total 1	O 1	0	0
61	2v	2	Total 2	O 2	0	0
61	2w	2	Total 2	O 2	0	0
61	2x	6	Total 6	O 6	0	0

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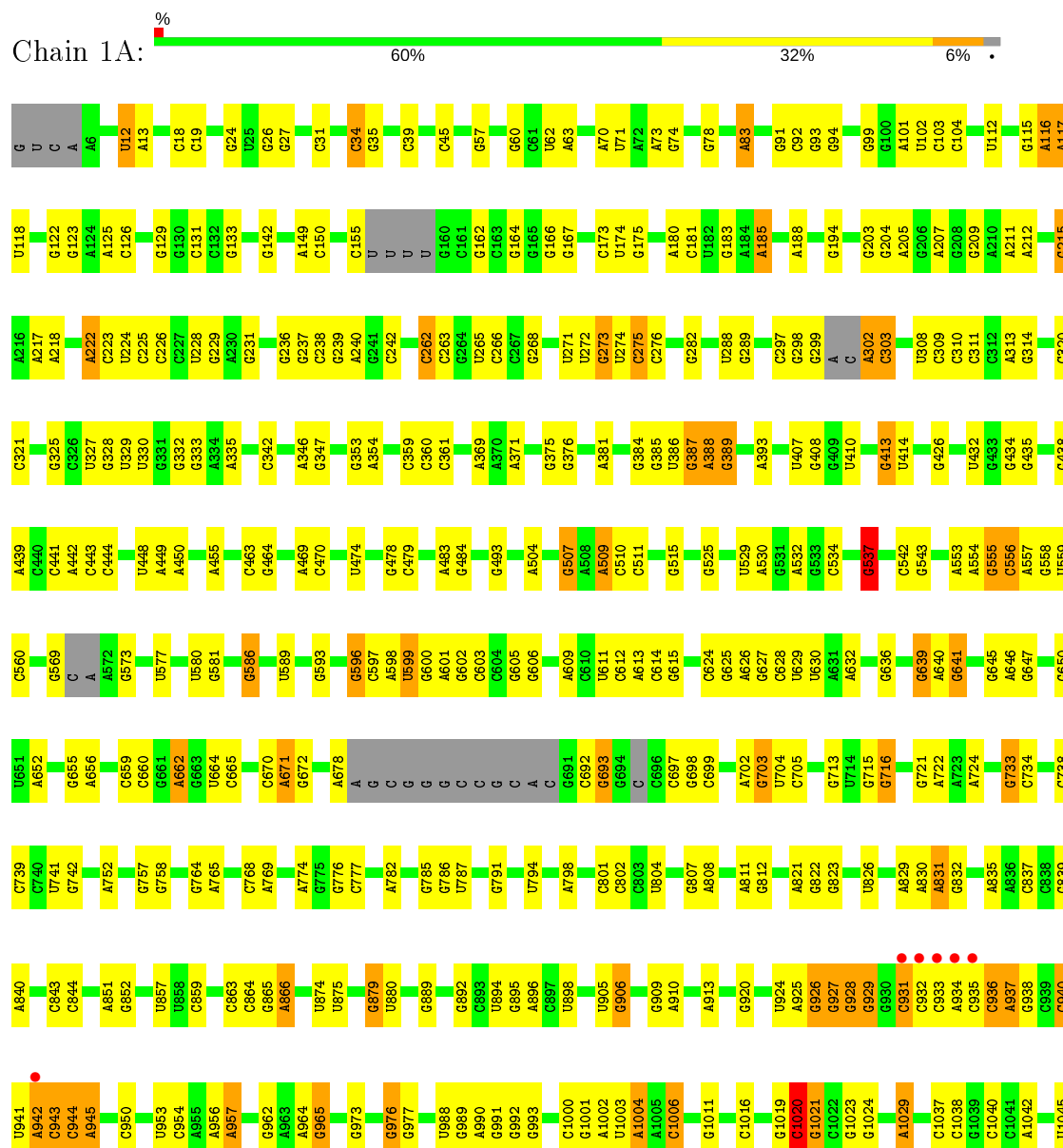
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2y	18	Total	O	0	0
			18	18		

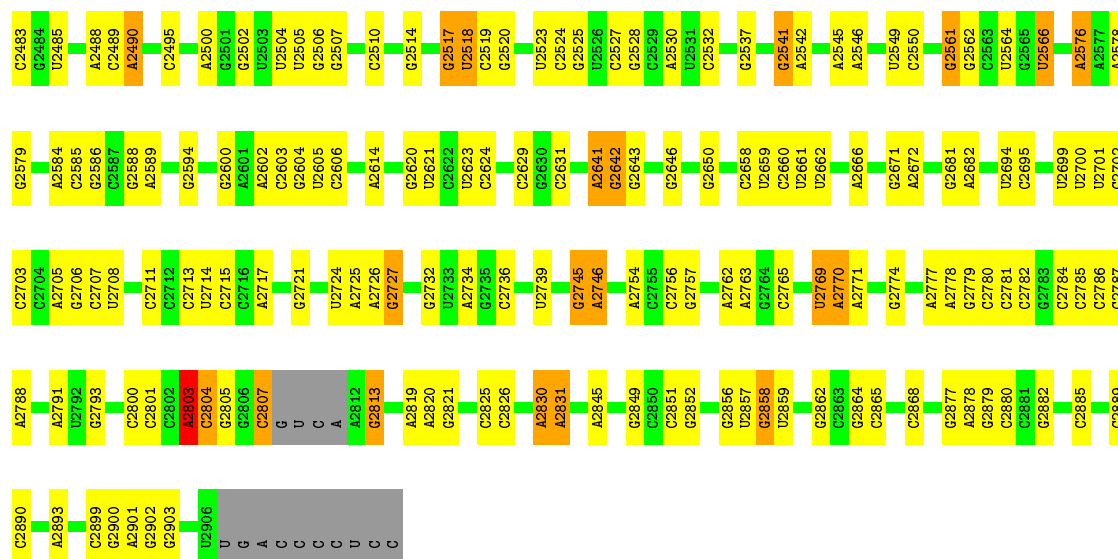
3 Residue-property plots

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

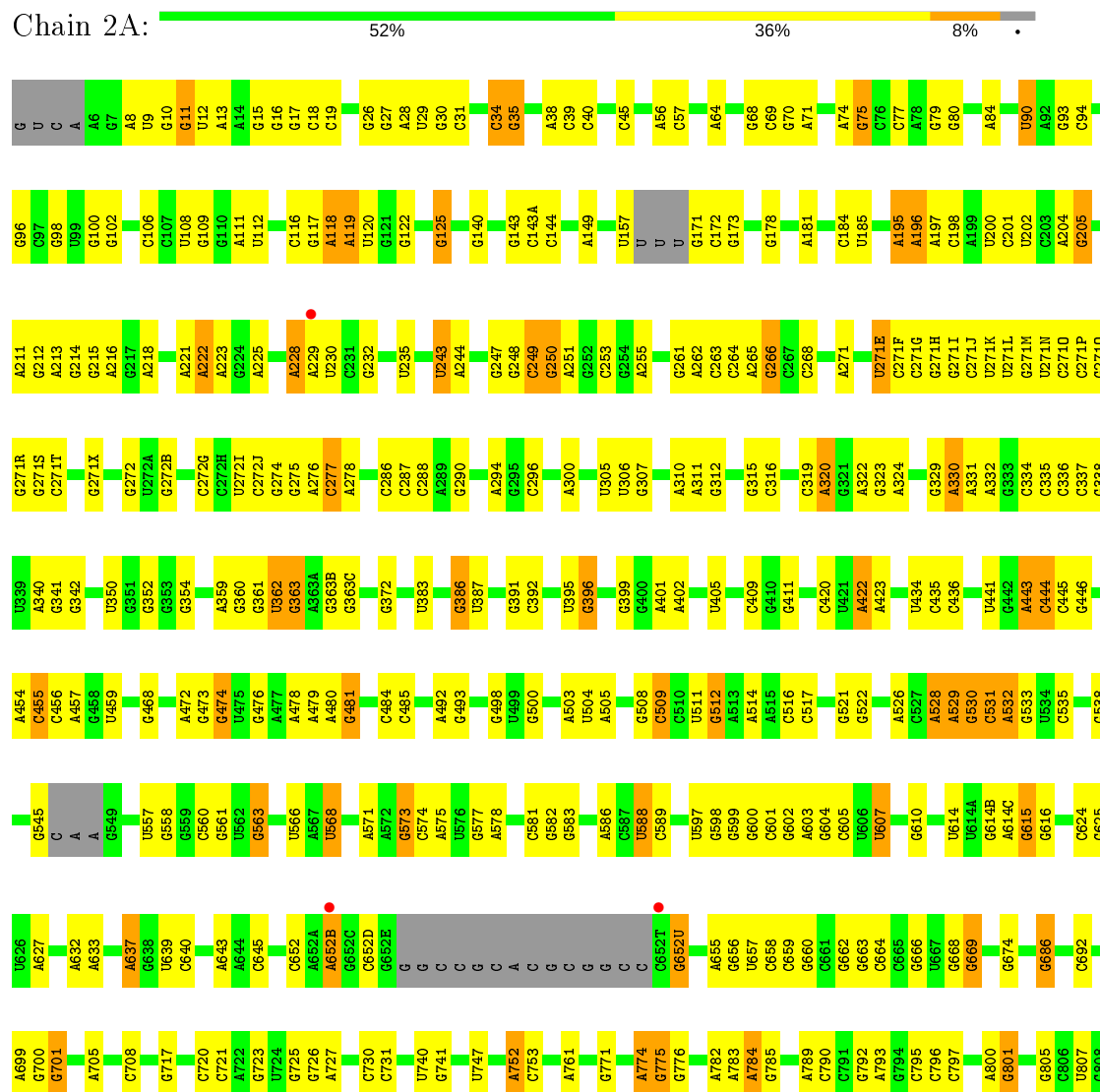
• Molecule 1: 23S Ribosomal RNA



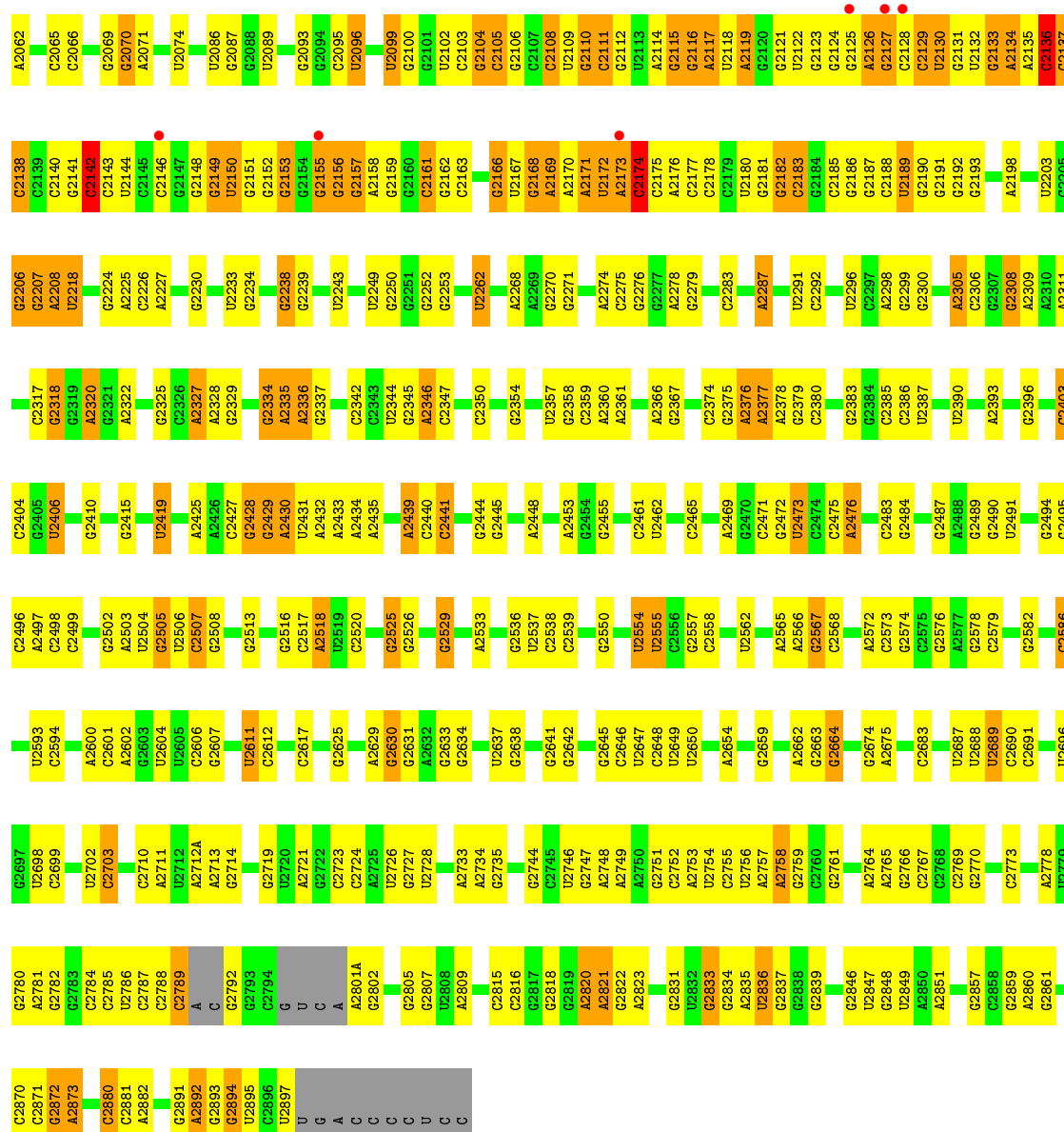




• Molecule 1: 23S Ribosomal RNA

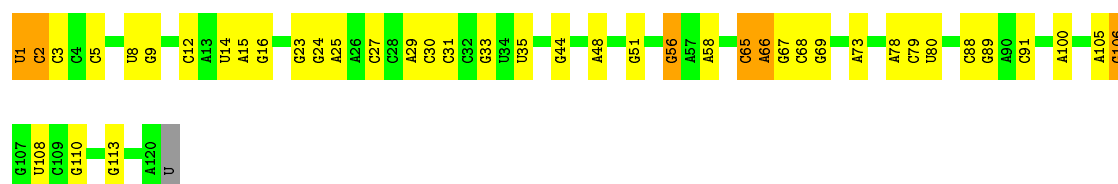


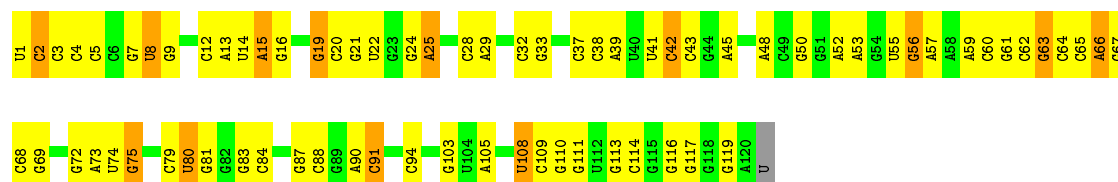
A1966	C1830	A1722	C1617	C1530	G1442	G1347	A1247	G1169	A	C1038	G956	C884	G809
C1967	G1831	U1739	G1622	C1531	A1445	U1352	G1248	G1170	G	G1039	A957	C885	U810
A1970	G1835	G1740	G1626	C1532	G1446	U1353	U1249	G1171	C	C1040	U958	C886	U811
A1971	C1836	G1746	G1627	G1533	G1448	A1354	G1250	G	U	C1041	A959	A887	C812
A1972	C1837	C1751	G1628	U	A1449	A1355	G1251	U	C	G1042	A960	C888	C816
C1973	G1838	C1751	U1629	C1536	G1450	A1359	A1252	A	A	G1043	A961	C889	C816
C1983	G1839	C1754	G1629	G1537	C1450A	A1360	A1253	U	C	G	A962	A890	C816
C1983	C1839	C1754	G1629	G1538	C1451	A1360	U1254	A	U	G	G966	A892	A819
A1847	C1840	C1755	C1636	G1539	G1455	C1363	G1256	C1178	U	A	G966	C893	A820
A1848	C1841	A1755	A1637	G1540	G1456	G1364	G1257	C1179	U	A	G974	C894	A821
A1991	C1842	A1756	C1638	A1542	G1457	A1365	G1258	C1180	U	A	C975	U895	A821
C1992	C1843	U1757	U1639	C1543	G1460	A1366	A1259	C1181	C	C	A980	C896	A824
U1993	G1857	A1759	C1640	C1544	G1461	A1367	A1260	A1182	G	A	A980	C897	A824
C1996	C1866	A1762	G1647	C1546	C1462	C1370	G1261	G1183	A	G	A983	C898	U826
G1997	A1876	G1763	C1648	C1547	G1463	U1371	U1262	G1184	G	C	A983	A899	U827
C1998	G1877	G1764	C1649	C1548	C1464	U1372	A1263	G1185	C	C	A983	A900	U828
C1999	G1878	G1765	C1650	C1549	G1465	U1373	A1264	G1186	G	A	C987	A901	A829
A2001	C1879	G1766	G1651	C1550	C1466	A1379	A1265	G1187	G	A	C987	C902	U833
G2002	C1880	G1767	G1652	C1551	G1467	U1380	U1266	G1188	A	G	A990	C903	U833
G2010	C1881	G1768	G1653	C1552	G1468	G1381	U1267	G1189	G	A	C991	C904	G836
G2011	A1882	A1773	A1654	C1553	G1469	U1382	A1268	U1198	U	G	C992	U907	U839
G2012	C1883	G1774	C1655	C1554	G1470	A1384	G1270	U1199	U	G	G993	U907	C840
A2013	C1884	G1775	G1656	C1555	G1471	G1385	G1271	U1200	U	U	C994	C908	C840
A2014	C1885	G1776	C1657	C1556	G1472	U1386	A1272	G1201	G	G	C995	A910	G848
C1989	G1886	G1777	G1658	C1557	G1473	U1387	U1273	C1202	C	C	A996	A911	A849
A1900	C1887	A1778	A1659	C1558	G1474	G1388	A1274	U1203	U	U	U999	C912	C850
A1901	C1888	G1779	C1660	C1559	G1475	U1389	U1275	U1204	A	A	U999	C913	C850
A2019	C1889	G1780	G1661	C1560	G1476	A1390	U1276	U1205	U	U	A1000	C914	U851
A2020	C1890	G1781	A1662	C1561	G1477	U1391	U1277	U1206	A	A	A1001	C915	G852
G2021	C1891	G1782	C1663	C1562	G1478	U1392	A1278	G1207	G	G	A1002	C916	G853
G2022	C1892	G1783	G1664	C1563	G1479	U1393	U1279	G1208	A	A	G1003	A917	G854
G2023	C1893	A1784	A1665	C1564	G1480	U1394	U1280	U1209	G	G	C1007	C919	C856
G2024	C1894	G1785	C1666	C1565	G1481	U1395	U1281	U1210	C	C	A1010	C920	U858
C2025	C1895	G1786	G1667	C1566	G1482	U1396	U1282	U1211	C	C	A1011	C921	U859
C2026	C1896	G1787	C1668	C1567	G1483	U1397	U1283	U1212	A	A	U1012	C922	U860
A2031	C1897	G1788	A1669	C1568	G1484	U1398	U1284	U1213	G	G	U1013	C923	U861
C2032	C1898	G1789	G1670	C1569	G1485	U1399	U1285	U1214	C	C	G1016	C924	A863
A2033	C1899	G1790	C1671	C1570	G1486	U1400	U1286	U1215	C	C	U1017	C925	A864
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G2035	C1901	G1792	C1673	C1572	G1488	U1402	U1288	U1217	U	U	U1019	C927	A866
C2036	C1902	G1793	G1674	C1573	G1489	U1403	U1289	U1218	U	U	A1020	C928	U868
G2037	C1903	G1794	C1675	C1574	G1490	U1404	U1290	U1219	C	C	A1021	C929	G869
C2038	C1904	G1795	G1676	C1575	G1491	U1405	U1291	U1220	A	A	G1022	C930	A870
C2039	C1905	G1796	C1677	C1576	G1492	U1406	U1292	U1221	G	G	U1023	C931	A871
C2040	C1906	G1797	G1678	C1577	G1493	U1407	U1293	U1222	C	C	G1024	C932	U871
U2041	C1907	G1798	C1679	C1578	G1494	U1408	U1294	U1223	A	A	U1025	C933	G874
A2042	C1908	G1799	G1680	C1579	G1495	U1409	U1295	U1224	C	C	U1026	C934	G875
C2043	C1909	G1800	C1681	C1580	G1496	U1410	U1296	U1225	U	U	A1027	C935	C876
C2044	C1910	G1801	G1682	C1581	G1497	U1411	U1297	U1226	C	C	A1028	C936	U877
U1946	C1911	G1802	C1683	C1582	G1498	U1412	U1298	U1227	A	A	U1029	C937	A878
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	C1946	G1837	C1718	C1617	G1538	U1447	U1333	U1262	A	A	U1064	C972	G913
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	C1950	G1841	C1722	C1621	G1542	U1451	U1337	U1266	A	A	U1068	C976	G917
	C1951	G1842	G1723	C1622	G1543	U1452	U1338	U1267	C	C	U1069	C977	G918
	C1952	G1843	C1724	C1623	G1544	U1453	U1339	U1268	A	A	U1070	C978	G919
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	C1954	G1845	C1726	C1625	G1546	U1455	U1341	U1270	A	A	U1072	C980	G921
	C1955	G1846	G1727	C1626	G1547	U1456	U1342	U1271	C	C	U1073	C981	G922
	C1956	G1847	C1728	C1627	G1548	U1457	U1343	U1272	A	A	U1074	C982	G923
	C1957	G1848	G1729	C1628	G1549	U1458	U1344	U1273	C	C	U1075	C983	G924
	C1958	G1849	C1730	C1629	G1550	U1459	U1345	U1274	A	A	U1076	C984	G925
	C1959	G1850	G1731	C1630	G1551	U1460	U1346	U1275	C	C	U1077	C985	G926
	C1960	G1851	C1732	C1631	G1552	U1461	U1347	U1276	A	A	U1078	C986	G927
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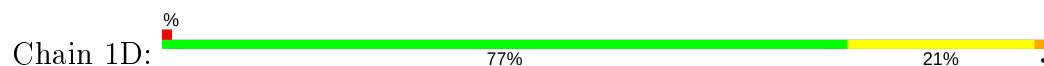
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 64% 30% 5%

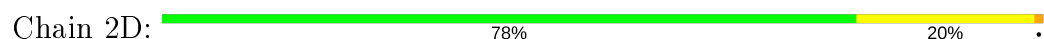




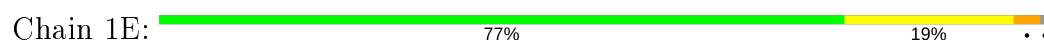
- Molecule 3: 50S ribosomal protein L2



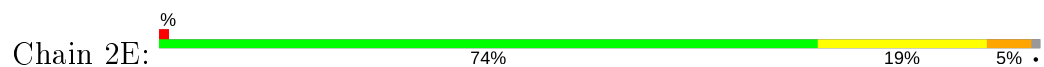
- Molecule 3: 50S ribosomal protein L2



- Molecule 4: 50S ribosomal protein L3

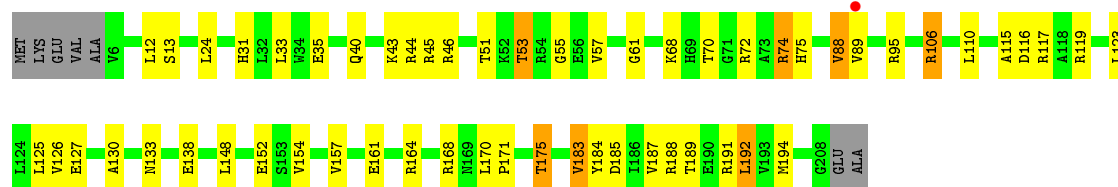


- Molecule 4: 50S ribosomal protein L3



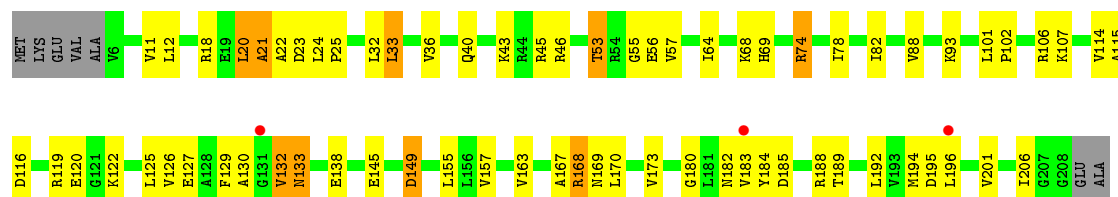
- Molecule 5: 50S ribosomal protein L4

Chain 1F:  70% 23%



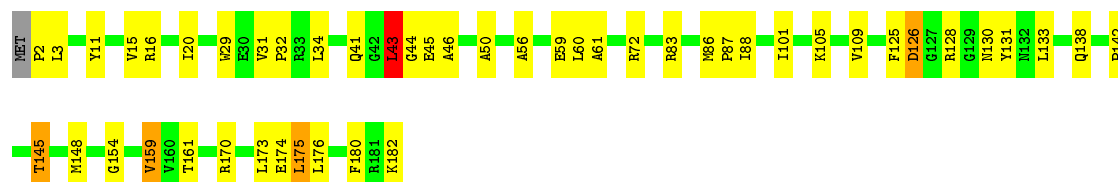
- Molecule 5: 50S ribosomal protein L4

Chain 2F:  64% 29%



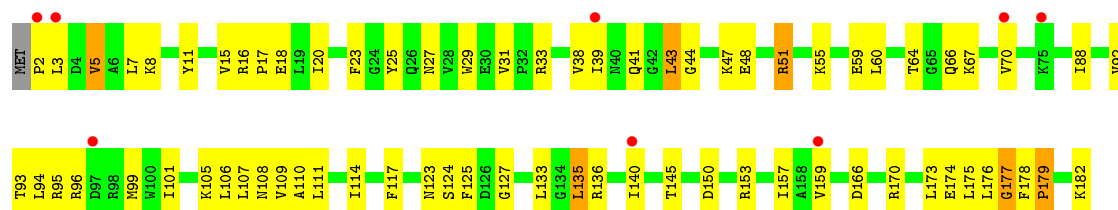
- Molecule 6: 50S ribosomal protein L5

Chain 1G:  73% 24%




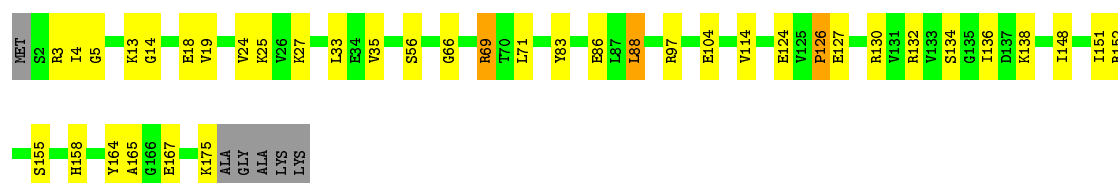
- Molecule 6: 50S ribosomal protein L5

Chain 2G:  60% 36%

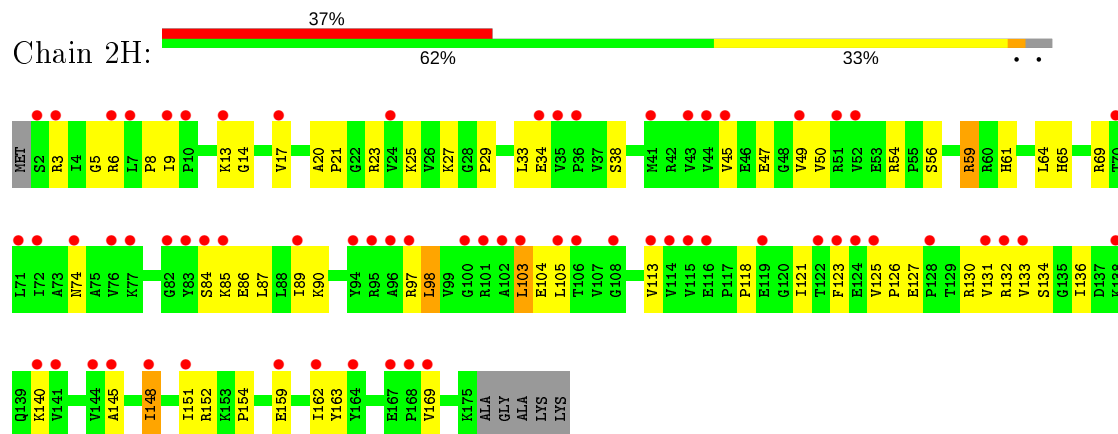


- Molecule 7: 50S ribosomal protein L6

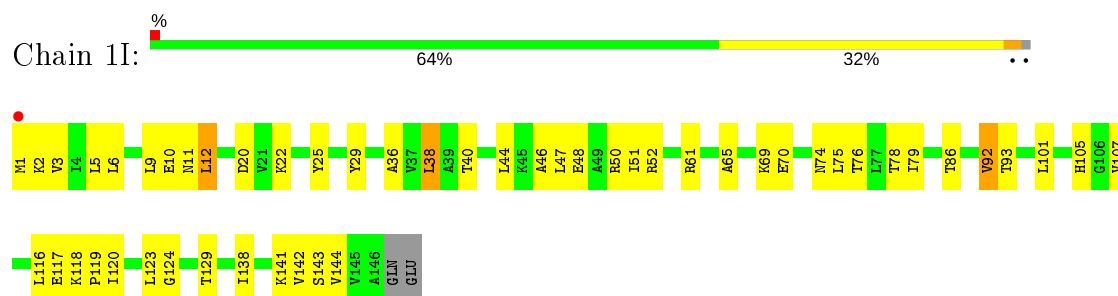
Chain 1H:  75% 20%



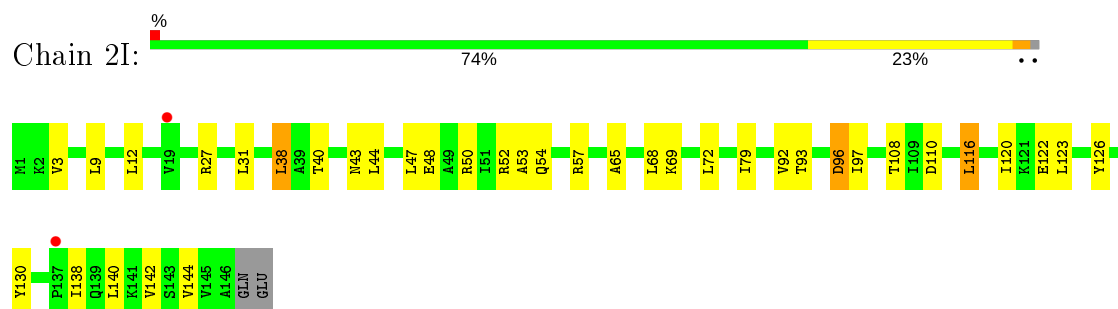
- Molecule 7: 50S ribosomal protein L6



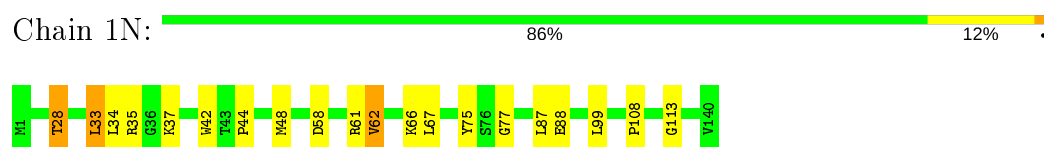
- Molecule 8: 50S ribosomal protein L9



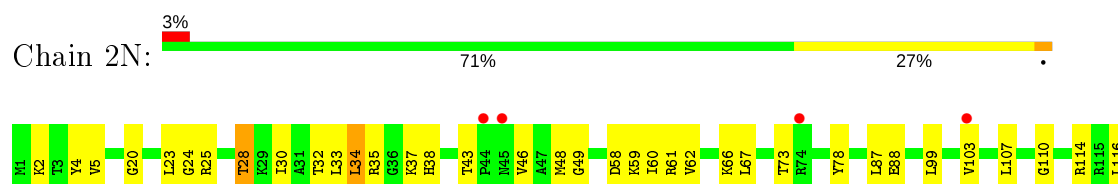
- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



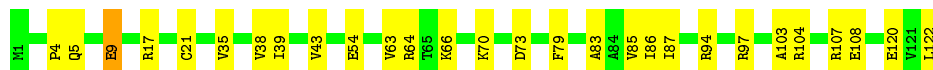
- Molecule 9: 50S ribosomal protein L13





- Molecule 10: 50S ribosomal protein L14

Chain 1O: 77% 22%



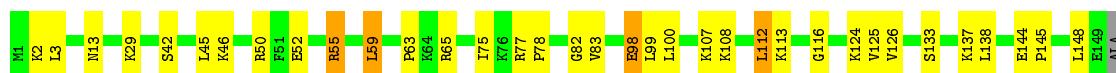
- Molecule 10: 50S ribosomal protein L14

Chain 2O: 75% 23%



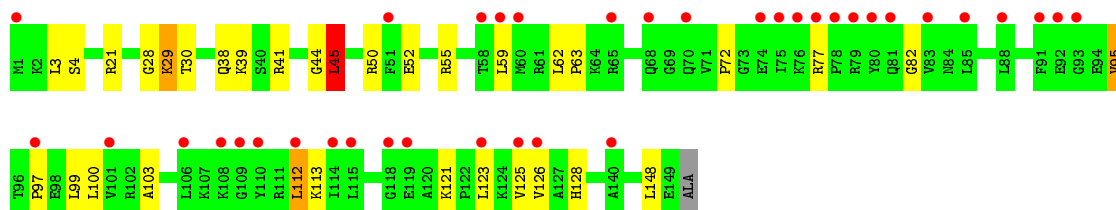
- Molecule 11: 50S ribosomal protein L15

Chain 1P: 76% 21%



- Molecule 11: 50S ribosomal protein L15

Chain 2P: 25% 77% 19%



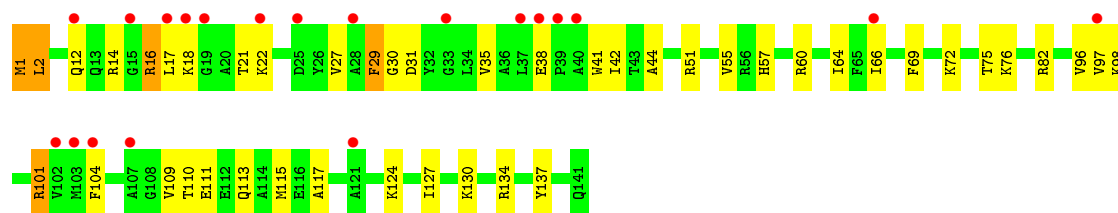
- Molecule 12: 50S ribosomal protein L16

Chain 1Q: 72% 27%



- Molecule 12: 50S ribosomal protein L16

Chain 2Q: 14% 68% 28%



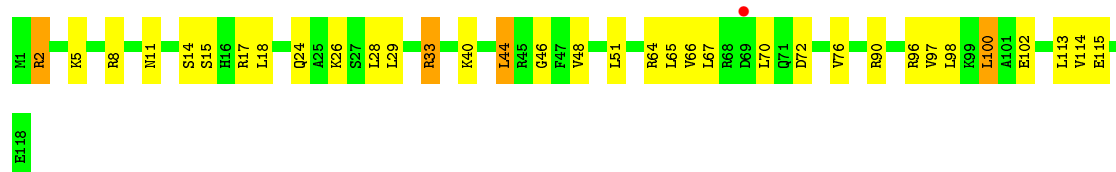
- Molecule 13: 50S ribosomal protein L17

Chain 1R: 75% 19% 6%



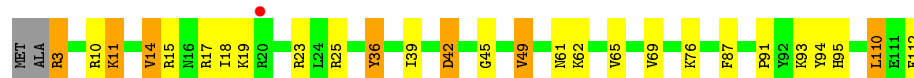
- Molecule 13: 50S ribosomal protein L17

Chain 2R: 71% 25% 4%



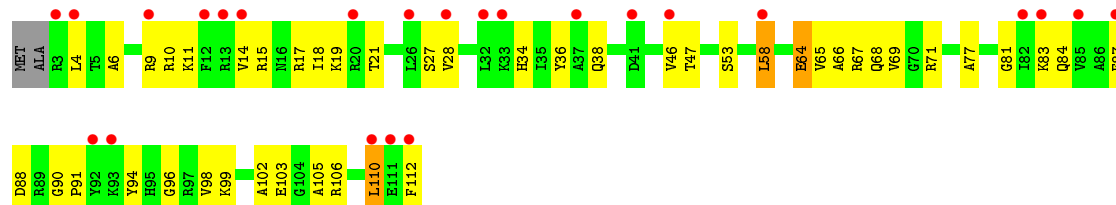
- Molecule 14: 50S ribosomal protein L18

Chain 1S: 74% 18% 6%



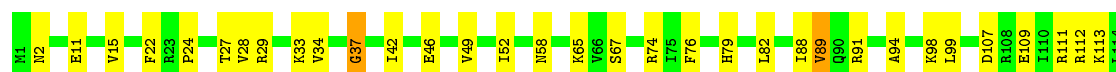
- Molecule 14: 50S ribosomal protein L18

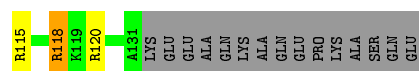
Chain 2S: 58% 38% 4%



- Molecule 15: 50S ribosomal protein L19

Chain 1T: 65% 23% 10%





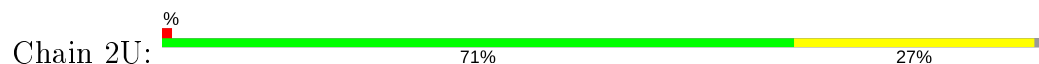
- Molecule 15: 50S ribosomal protein L19



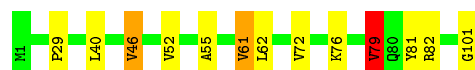
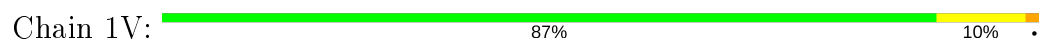
- Molecule 16: 50S ribosomal protein L20



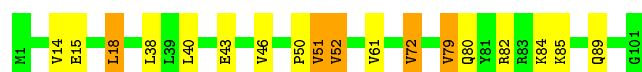
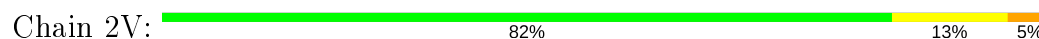
- Molecule 16: 50S ribosomal protein L20



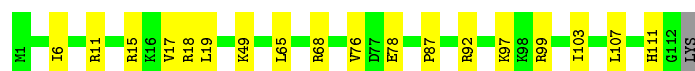
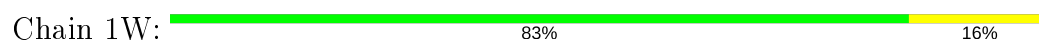
- Molecule 17: 50S ribosomal protein L21



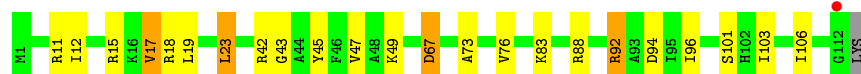
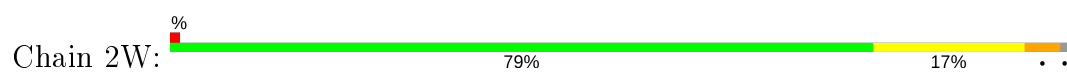
- Molecule 17: 50S ribosomal protein L21



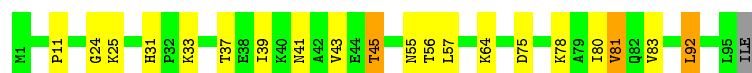
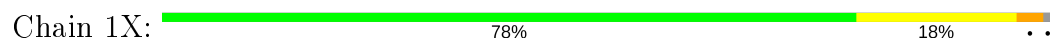
- Molecule 18: 50S ribosomal protein L22



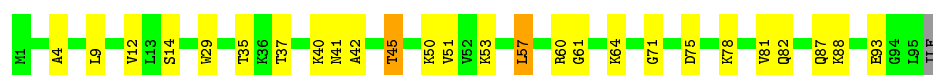
- Molecule 18: 50S ribosomal protein L22



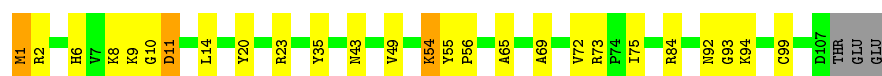
- Molecule 19: 50S ribosomal protein L23



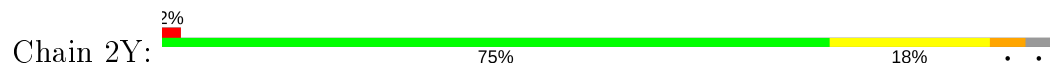
- Molecule 19: 50S ribosomal protein L23



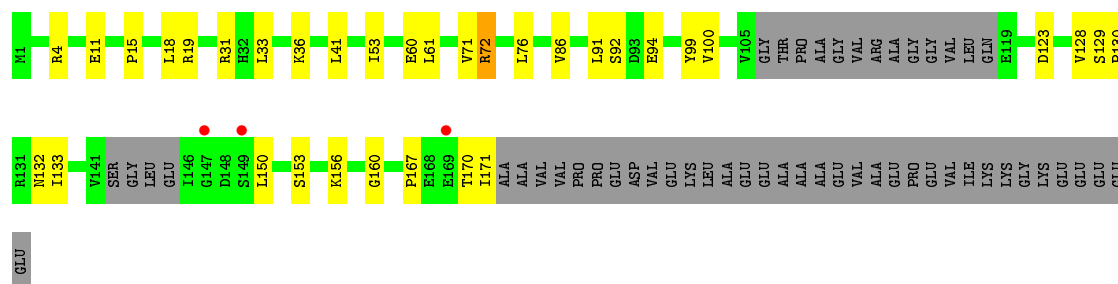
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

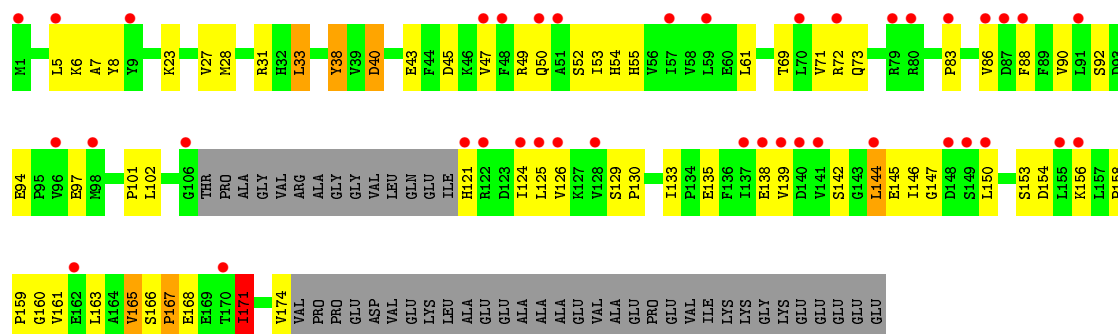


- Molecule 21: 50S ribosomal protein L25

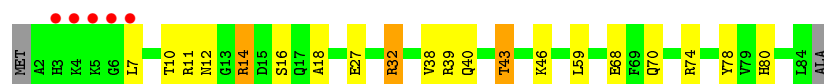
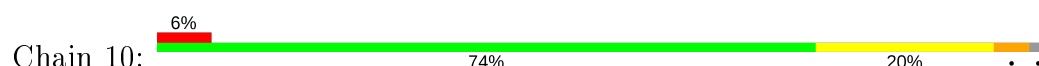


- Molecule 21: 50S ribosomal protein L25





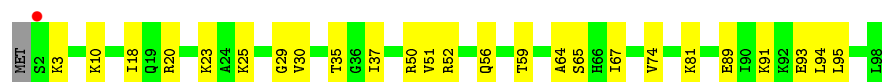
- Molecule 22: 50S ribosomal protein L27



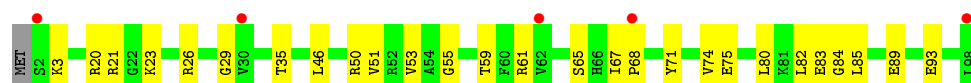
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28



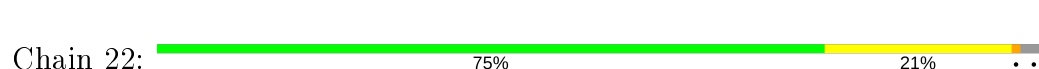
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29

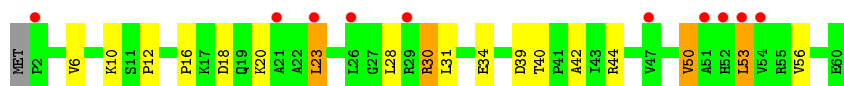




- Molecule 25: 50S ribosomal protein L30



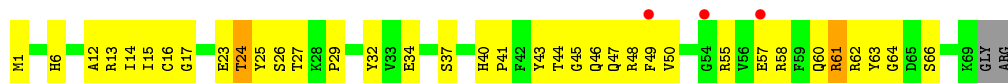
- Molecule 25: 50S ribosomal protein L30



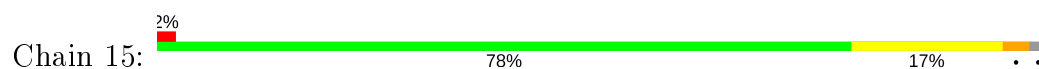
- Molecule 26: 50S ribosomal protein L31



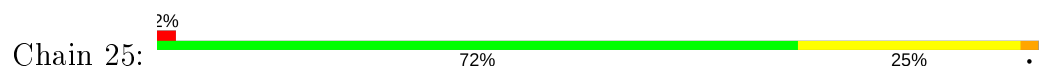
- Molecule 26: 50S ribosomal protein L31



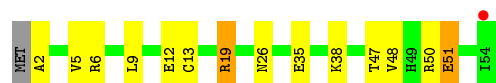
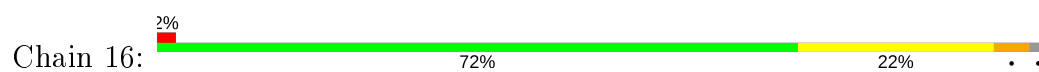
- Molecule 27: 50S ribosomal protein L32



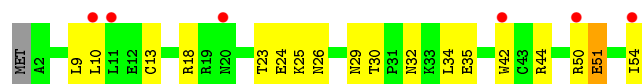
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



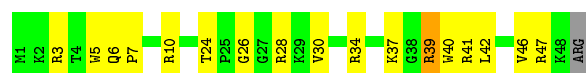
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



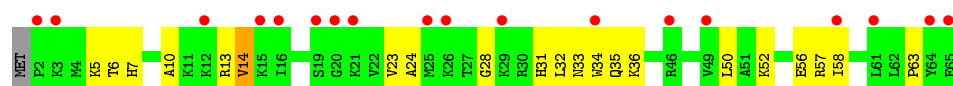
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



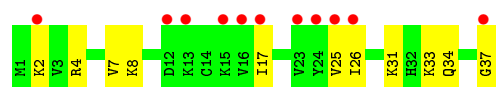
- Molecule 30: 50S ribosomal protein L35



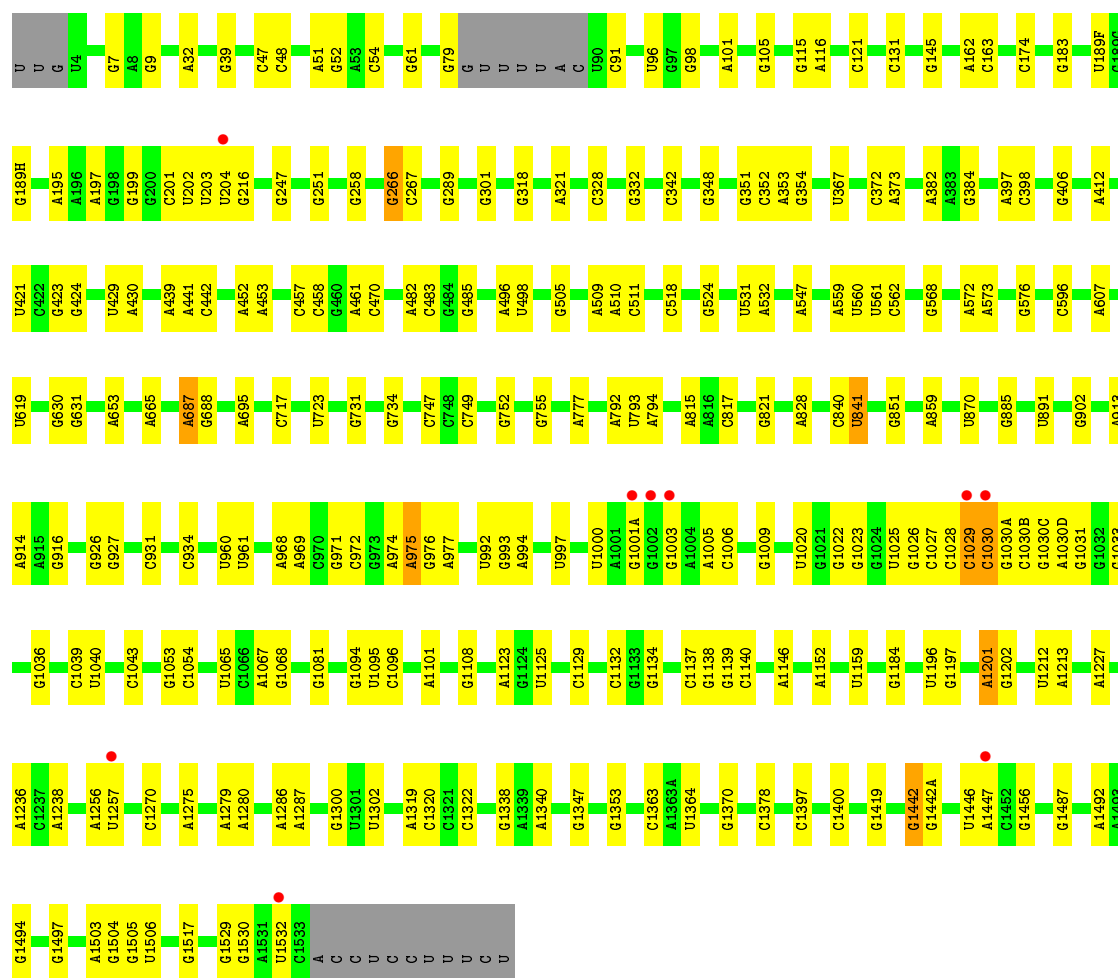
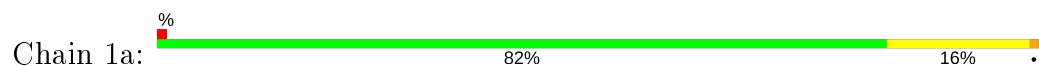
- Molecule 31: 50S ribosomal protein L36



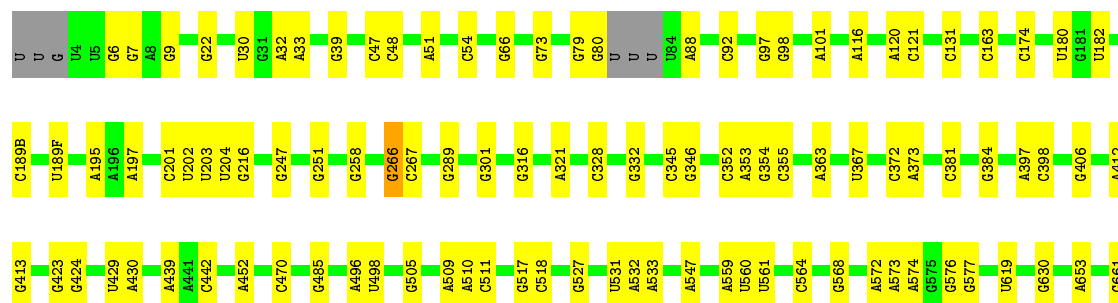
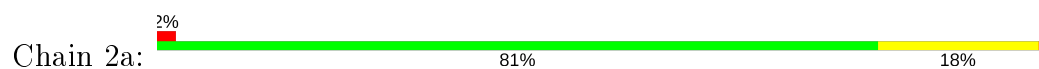
- Molecule 31: 50S ribosomal protein L36

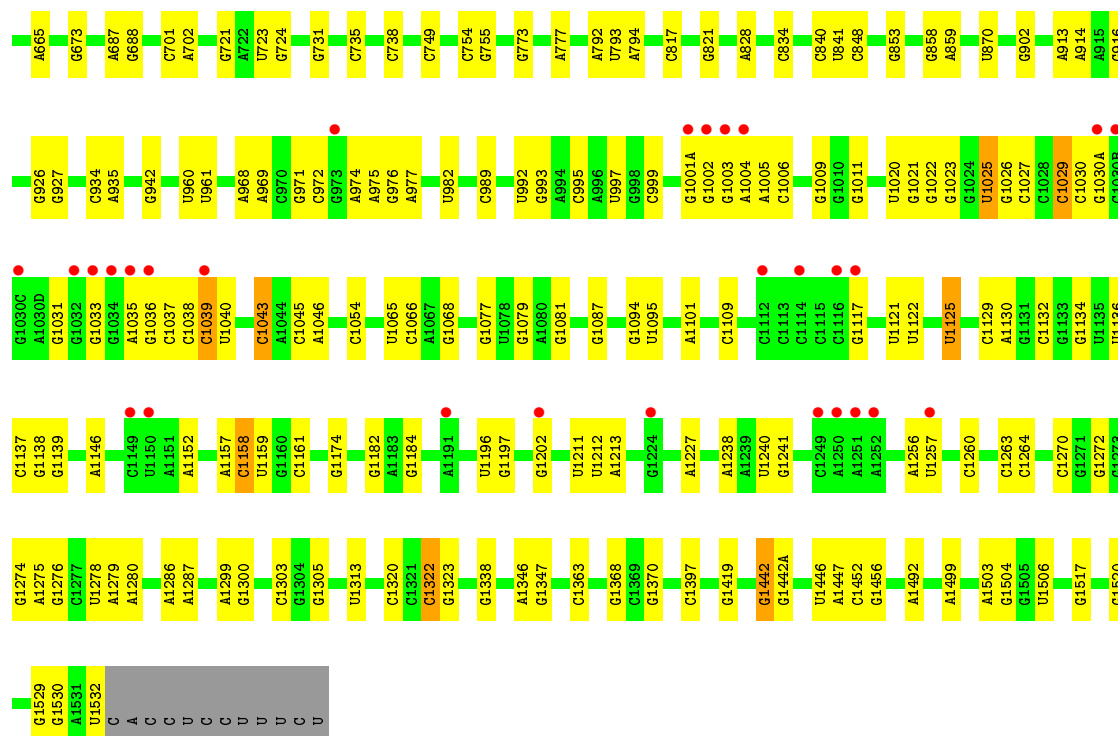


• Molecule 32: 16S Ribosomal RNA

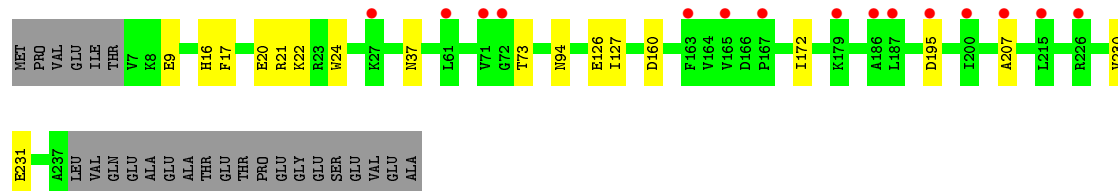
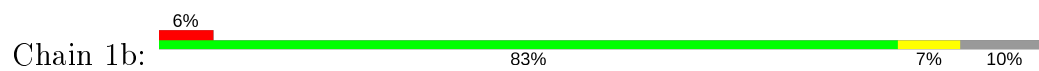


• Molecule 32: 16S Ribosomal RNA

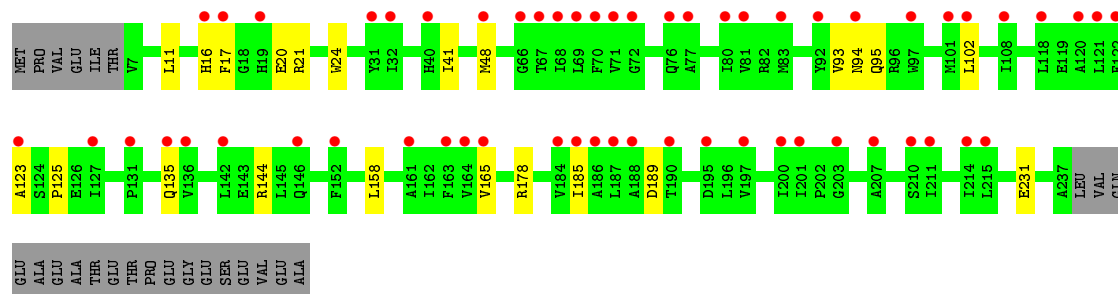
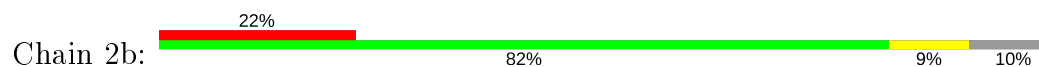




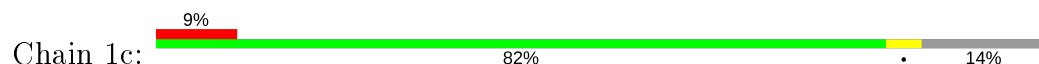
• Molecule 33: 30S ribosomal protein S2



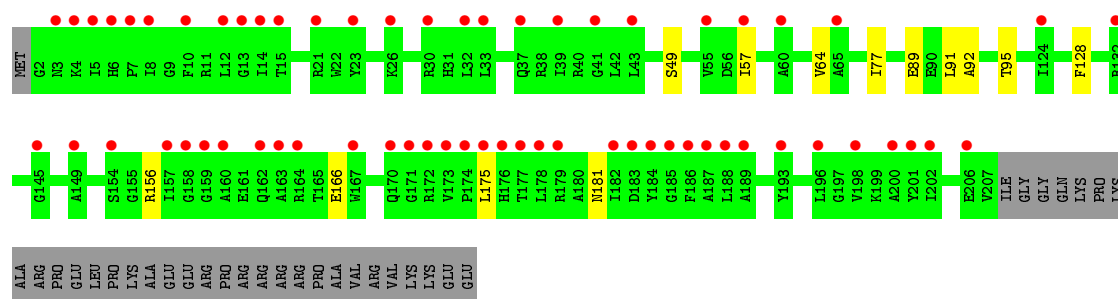
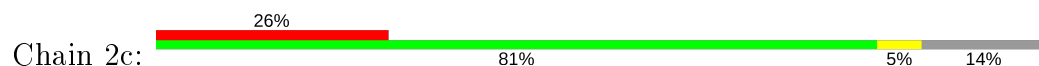
• Molecule 33: 30S ribosomal protein S2



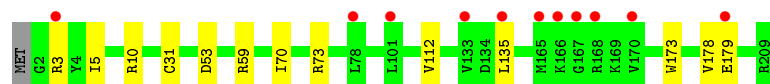
• Molecule 34: 30S ribosomal protein S3



- Molecule 34: 30S ribosomal protein S3



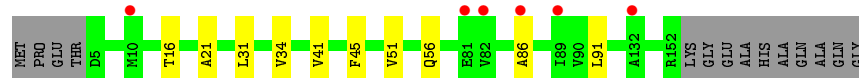
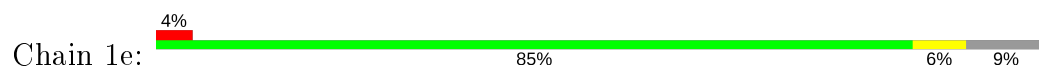
- Molecule 35: 30S ribosomal protein S4



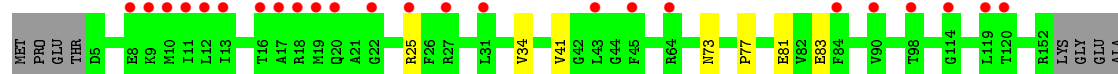
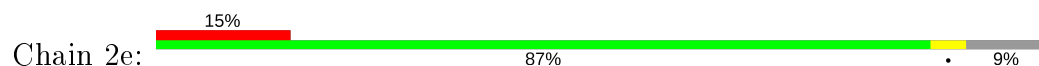
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



HIS
ALA
GLN
ALA
GLN
GLY

- Molecule 37: 30S ribosomal protein S6

Chain 1f:  96% ..

H1
V72
N73
S93
H100
ALA

- Molecule 37: 30S ribosomal protein S6

Chain 2f:  96% ..

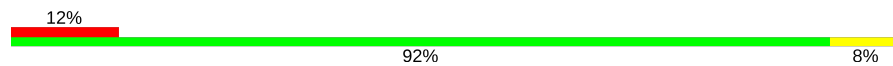
H1
L10
R28
Y59
L75
H100
ALA

- Molecule 38: 30S ribosomal protein S7

Chain 1g:  94% 5% ..

MET
A2
R3
R4
R5
R6
L12
L16
T24
S77
R78
R79
R80
R81
R82
R83
R84
R85
R86
E90
R94
H153
Y154
R155
W156

- Molecule 38: 30S ribosomal protein S7

Chain 2g:  92% 8% ..

MET
A2
R3
R4
V9
D15
L16
T24
L27
R32
L42
G55
R78
R79
V80
G81
G82
A83
R84
Y85
Q86
R95
S98
L104
E113
R114
R115
Y154
R155
W156

- Molecule 39: 30S ribosomal protein S8

Chain 1h:  94% ..

MET
L2
D25
S29
E49
I83
R84
R85
V95
L112
L119
L133
W138

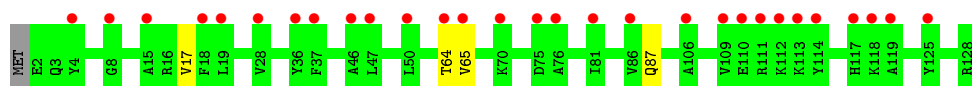
- Molecule 39: 30S ribosomal protein S8

Chain 2h:  93% 5% ..

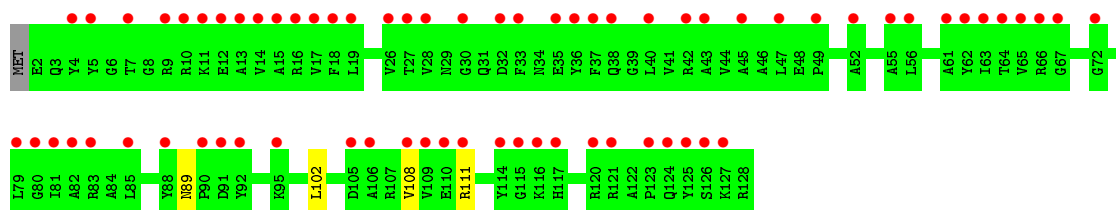
MET
L2
T3
N9
L10
T11
R12
N15
A16
T17
R18
V19
Y20
K21
D25
R68
D73
L80
R83
R84
S87
R91
Y111
L112
L133
W138

- Molecule 40: 30S ribosomal protein S9

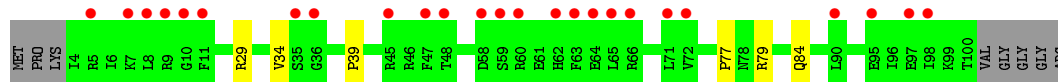
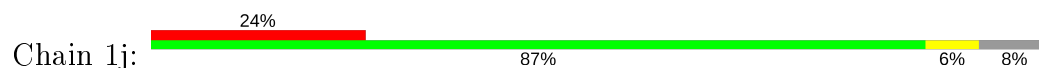
Chain 1i:  96% ..



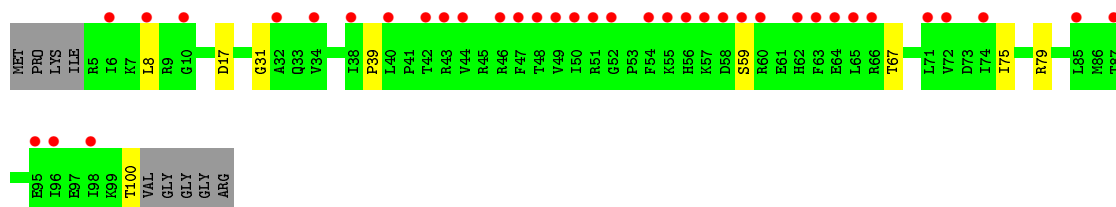
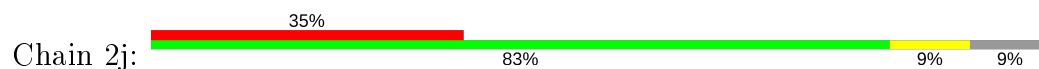
- Molecule 40: 30S ribosomal protein S9



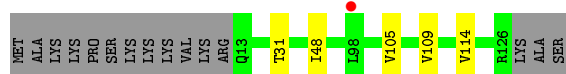
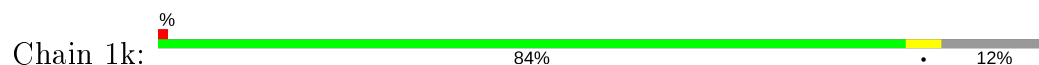
- Molecule 41: 30S ribosomal protein S10



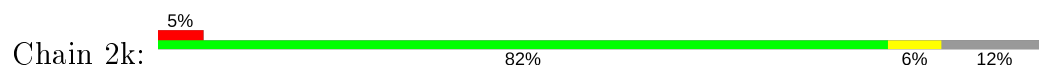
- Molecule 41: 30S ribosomal protein S10




- Molecule 42: 30S ribosomal protein S11

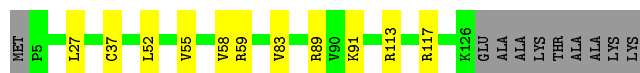


- Molecule 42: 30S ribosomal protein S11




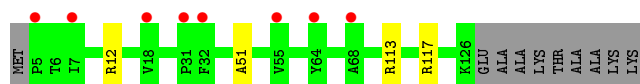
- Molecule 43: 30S ribosomal protein S12

Chain 1l: 



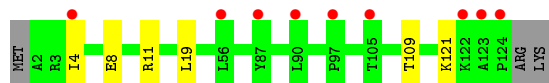
- Molecule 43: 30S ribosomal protein S12

Chain 2l: 



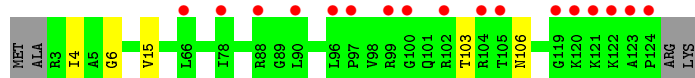
- Molecule 44: 30S ribosomal protein S13

Chain 1m: 




- Molecule 44: 30S ribosomal protein S13

Chain 2m: 




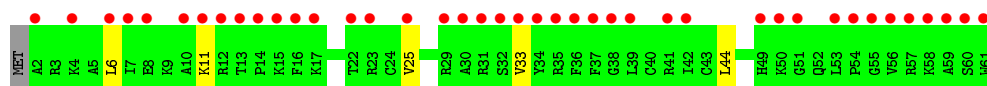
- Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n: 



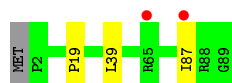
- Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n: 

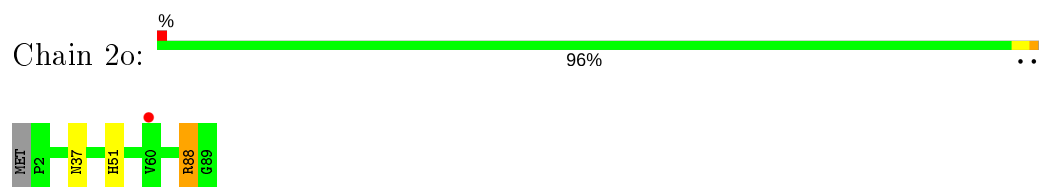


- Molecule 46: 30S ribosomal protein S15

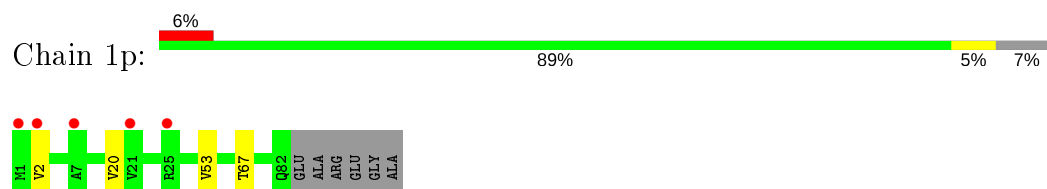
Chain 1o: 



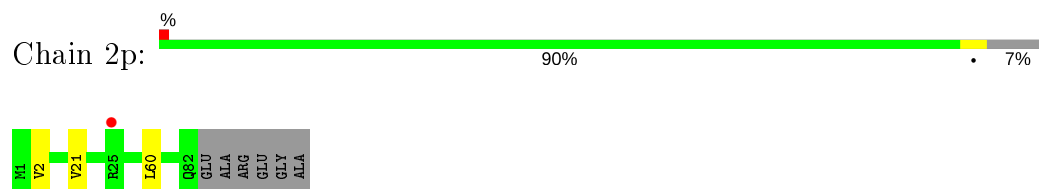
- Molecule 46: 30S ribosomal protein S15



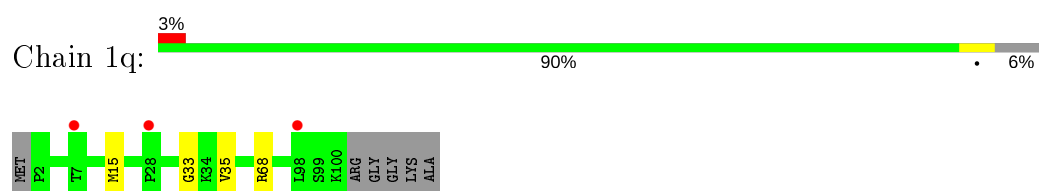
- Molecule 47: 30S ribosomal protein S16



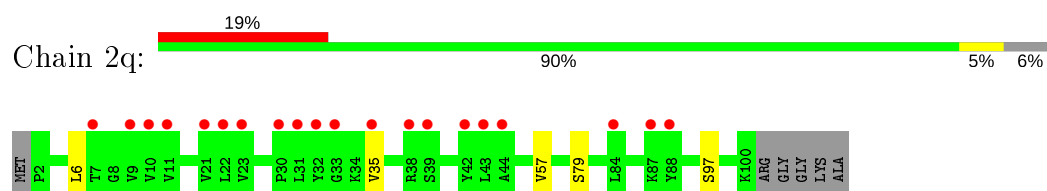
- Molecule 47: 30S ribosomal protein S16



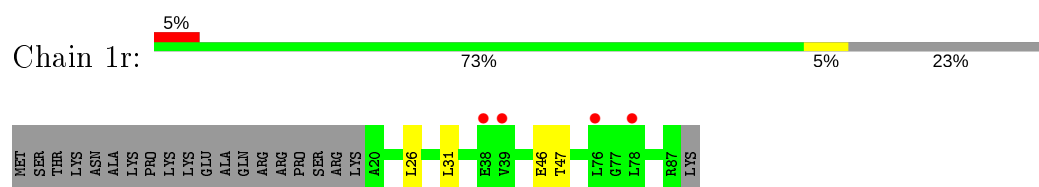
- Molecule 48: 30S ribosomal protein S17



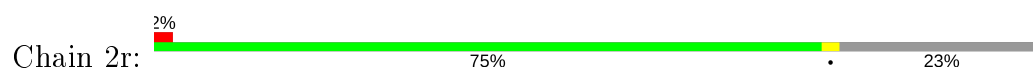
- Molecule 48: 30S ribosomal protein S17

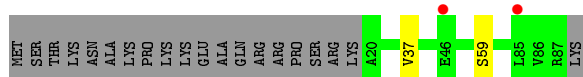


- Molecule 49: 30S ribosomal protein S18

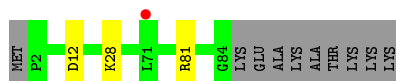
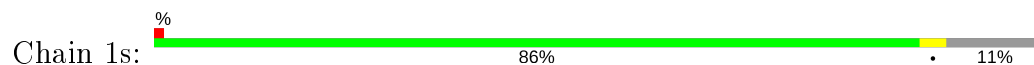


- Molecule 49: 30S ribosomal protein S18

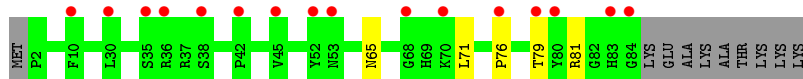
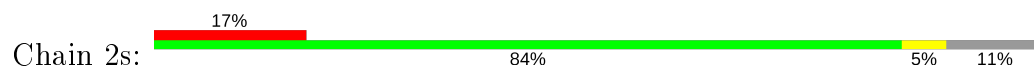




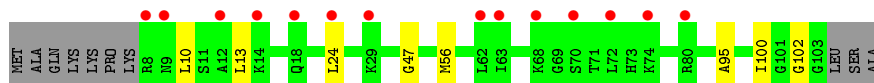
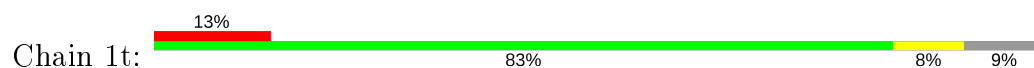
- Molecule 50: 30S ribosomal protein S19



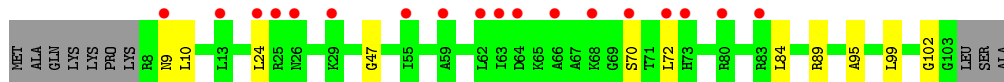
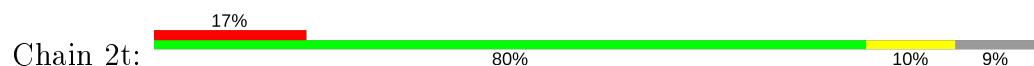
- Molecule 50: 30S ribosomal protein S19



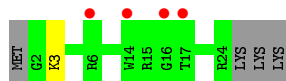
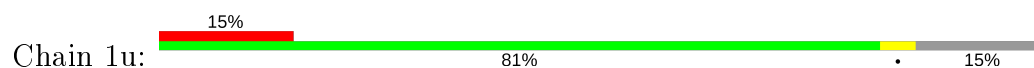
- Molecule 51: 30S ribosomal protein S20



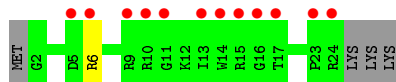
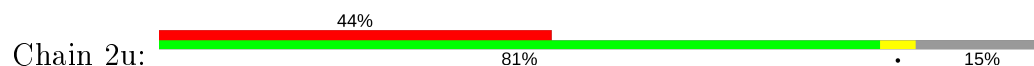
- Molecule 51: 30S ribosomal protein S20



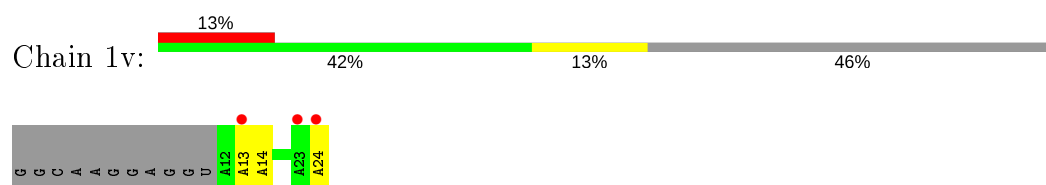
- Molecule 52: 30S ribosomal protein Thx



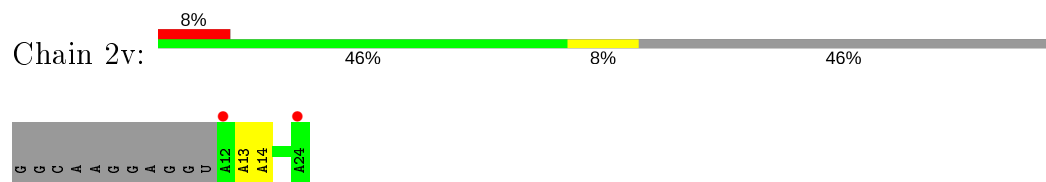
- Molecule 52: 30S ribosomal protein Thx



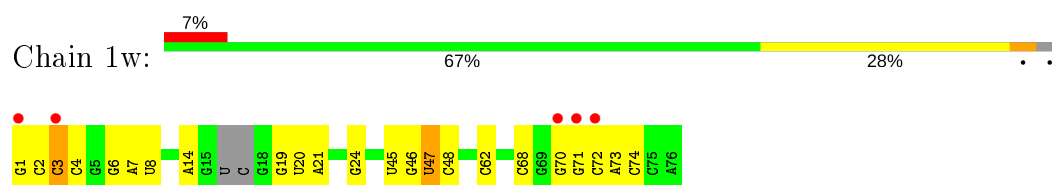
- Molecule 53: mRNA



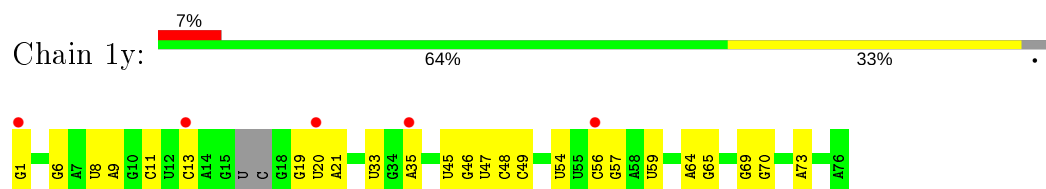
- Molecule 53: mRNA



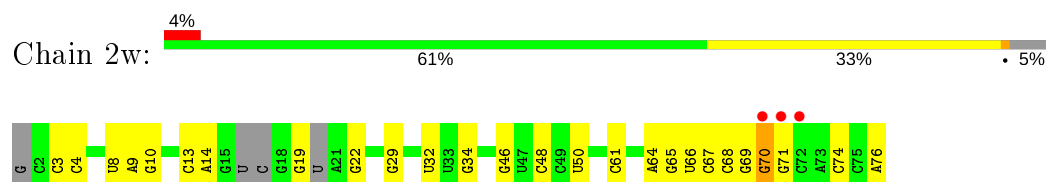
- Molecule 54: A-site and E-site tRNAs



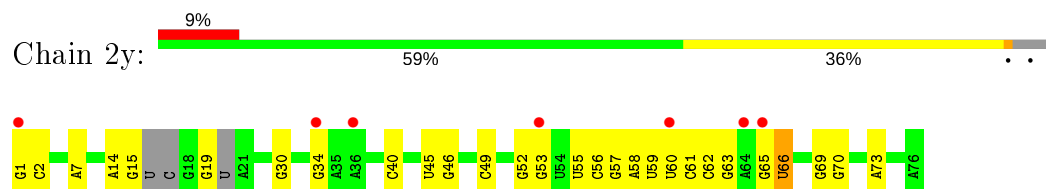
- Molecule 54: A-site and E-site tRNAs



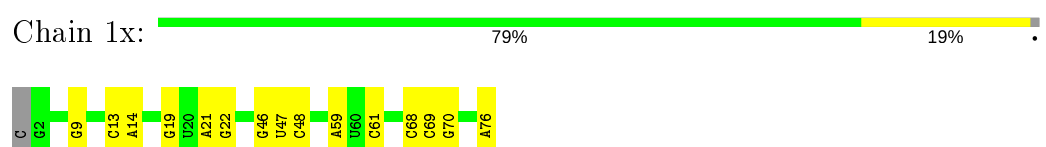
- Molecule 54: A-site and E-site tRNAs



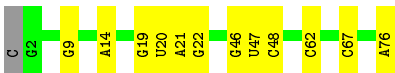
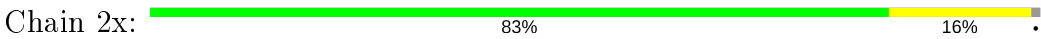
- Molecule 54: A-site and E-site tRNAs



- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.78Å 449.83Å 622.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.54 – 2.80 181.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.0 (152.54-2.80) 94.0 (181.84-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.214 , 0.269 0.214 , 0.269	Depositor DCC
R_{free} test set	67418 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	299109	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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: 5MU, ZN, 4SU, OMG, 2MU, MIA, SF4, 0TD, MG, 2MA, M2G, 2MG, 5MC, UR3, MA6, 4OC, EZG, 7MG, K, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.50	0/69009	0.96	49/107712 (0.0%)
1	2A	0.39	0/67293	0.89	43/105034 (0.0%)
2	1B	0.45	1/2882 (0.0%)	0.88	0/4494
2	2B	0.40	1/2879 (0.0%)	0.92	2/4487 (0.0%)
3	1D	0.35	0/2186	0.55	0/2944
3	2D	0.34	0/2186	0.55	0/2944
4	1E	0.35	0/1592	0.56	0/2149
4	2E	0.30	0/1592	0.51	0/2149
5	1F	0.33	0/1619	0.53	0/2193
5	2F	0.31	0/1615	0.50	0/2188
6	1G	0.30	0/1448	0.49	0/1957
6	2G	0.29	0/1453	0.48	1/1963 (0.1%)
7	1H	0.33	0/1356	0.51	0/1834
7	2H	0.31	0/1356	0.49	1/1834 (0.1%)
8	1I	0.29	0/1112	0.48	0/1514
8	2I	0.28	0/1079	0.47	0/1475
9	1N	0.34	0/1144	0.50	0/1543
9	2N	0.28	0/1144	0.47	0/1543
10	1O	0.36	0/943	0.55	0/1269
10	2O	0.31	0/943	0.52	0/1269
11	1P	0.35	0/1152	0.55	0/1533
11	2P	0.31	0/1152	0.53	0/1533
12	1Q	0.33	0/1143	0.51	0/1527
12	2Q	0.29	0/1143	0.49	0/1527
13	1R	0.32	0/982	0.53	0/1312
13	2R	0.28	0/982	0.49	0/1312
14	1S	0.31	0/883	0.52	0/1176
14	2S	0.29	0/880	0.49	0/1172
15	1T	0.32	0/1105	0.51	0/1477
15	2T	0.28	0/1097	0.47	0/1468
16	1U	0.36	0/977	0.51	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.29	0/977	0.43	0/1301
17	1V	0.34	0/782	0.56	0/1049
17	2V	0.29	0/782	0.53	0/1049
18	1W	0.34	0/897	0.54	0/1205
18	2W	0.30	0/897	0.51	0/1205
19	1X	0.35	0/764	0.56	0/1025
19	2X	0.30	0/764	0.54	1/1025 (0.1%)
20	1Y	0.34	0/819	0.54	0/1095
20	2Y	0.32	0/819	0.51	0/1095
21	1Z	0.32	0/1267	0.52	0/1717
21	2Z	0.30	0/1299	0.51	0/1763
22	10	0.35	0/662	0.55	0/881
22	20	0.32	0/662	0.49	0/881
23	11	0.34	0/762	0.52	0/1014
23	21	0.31	0/762	0.54	0/1014
24	12	0.33	0/590	0.46	0/781
24	22	0.27	0/590	0.43	0/781
25	13	0.33	0/474	0.50	0/635
25	23	0.28	0/469	0.46	0/630
26	14	0.35	0/565	0.59	0/761
26	24	0.30	0/545	0.50	0/737
27	15	0.36	0/469	0.54	0/635
27	25	0.32	0/469	0.50	0/635
28	16	0.35	0/460	0.53	0/613
28	26	0.31	0/456	0.51	0/608
29	17	0.34	0/426	0.55	0/561
29	27	0.32	0/426	0.54	0/561
30	18	0.34	0/525	0.56	0/691
30	28	0.31	0/525	0.49	0/691
31	19	0.34	0/310	0.53	0/407
31	29	0.30	0/310	0.51	0/407
32	1a	0.36	0/35795	0.88	25/55864 (0.0%)
32	2a	0.36	2/35886 (0.0%)	0.90	38/56005 (0.1%)
33	1b	0.29	0/1881	0.47	0/2542
33	2b	0.30	0/1860	0.50	0/2518
34	1c	0.29	0/1572	0.47	0/2126
34	2c	0.29	0/1566	0.47	0/2119
35	1d	0.29	0/1685	0.46	0/2262
35	2d	0.29	0/1704	0.47	0/2284
36	1e	0.30	0/1145	0.49	0/1543
36	2e	0.29	0/1149	0.52	0/1548
37	1f	0.29	0/823	0.48	0/1115
37	2f	0.30	0/829	0.48	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.30	0/1250	0.46	0/1679
38	2g	0.28	0/1254	0.43	0/1683
39	1h	0.29	0/1108	0.47	0/1494
39	2h	0.28	0/1108	0.47	0/1494
40	1i	0.29	0/1002	0.47	0/1346
40	2i	0.29	0/997	0.49	0/1343
41	1j	0.27	0/722	0.47	0/982
41	2j	0.29	0/727	0.50	0/988
42	1k	0.27	0/844	0.47	0/1145
42	2k	0.27	0/848	0.47	0/1149
43	1l	0.31	0/937	0.52	0/1260
43	2l	0.30	0/937	0.55	0/1260
44	1m	0.28	0/969	0.46	0/1302
44	2m	0.28	0/961	0.49	0/1291
45	1n	0.31	0/501	0.47	0/664
45	2n	0.33	0/501	0.50	0/664
46	1o	0.27	0/739	0.42	0/985
46	2o	0.28	0/739	0.46	0/985
47	1p	0.28	0/697	0.50	0/939
47	2p	0.27	0/693	0.47	0/935
48	1q	0.28	0/836	0.48	0/1117
48	2q	0.29	0/836	0.47	0/1117
49	1r	0.30	0/560	0.46	0/746
49	2r	0.28	0/560	0.46	0/746
50	1s	0.29	0/667	0.52	0/900
50	2s	0.30	0/661	0.56	0/893
51	1t	0.28	0/730	0.48	0/965
51	2t	0.27	0/729	0.42	0/965
52	1u	0.28	0/203	0.50	0/266
52	2u	0.30	0/203	0.50	0/266
53	1v	0.38	0/310	0.88	0/480
53	2v	0.49	0/310	0.94	0/480
54	1w	0.51	1/1606 (0.1%)	1.05	5/2497 (0.2%)
54	1y	0.53	1/1606 (0.1%)	1.14	7/2497 (0.3%)
54	2w	0.47	0/1556	1.17	4/2418 (0.2%)
54	2y	0.54	1/1583 (0.1%)	1.09	2/2459 (0.1%)
55	1x	0.48	0/1725	1.09	12/2689 (0.4%)
55	2x	0.45	0/1725	1.09	10/2689 (0.4%)
All	All	0.40	7/316686 (0.0%)	0.83	200/474113 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	1	G	OP3-P	-10.33	1.48	1.61
54	1y	1	G	OP3-P	-10.31	1.48	1.61
54	2y	1	G	OP3-P	-10.09	1.49	1.61
2	1B	1	U	OP3-P	-10.05	1.49	1.61
2	2B	1	U	OP3-P	-10.04	1.49	1.61
32	2a	1272	G	C6-N1	-8.32	1.33	1.39
32	2a	1272	G	N1-C2	-7.58	1.31	1.37

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	C5-C6-O6	19.26	140.16	128.60
32	2a	1263	C	N1-C2-O2	17.07	129.14	118.90
32	2a	1272	G	N1-C2-N2	-15.02	102.68	116.20
32	2a	1272	G	N3-C2-N2	14.88	130.32	119.90
32	2a	1272	G	N1-C6-O6	-12.36	112.48	119.90
32	2a	1263	C	C2-N3-C4	12.03	125.92	119.90
32	2a	1263	C	N3-C2-O2	-10.82	114.32	121.90
1	2A	2136	C	N1-C2-O2	10.74	125.34	118.90
1	1A	1121	C	N1-C2-O2	10.30	125.08	118.90
32	1a	1025	U	N1-C2-O2	10.04	129.83	122.80
55	1x	46	G	C6-N1-C2	-9.76	119.25	125.10
55	2x	46	G	C6-N1-C2	-9.39	119.46	125.10
1	1A	1109	G	C5-C6-O6	9.36	134.22	128.60
2	2B	80	U	O4'-C1'-N1	9.05	115.44	108.20
32	2a	1263	C	C5-C4-N4	8.83	126.38	120.20
32	2a	1039	C	N1-C2-O2	8.79	124.18	118.90
1	1A	1121	C	C2-N3-C4	8.59	124.19	119.90
1	1A	537	G	O4'-C1'-N9	8.48	114.99	108.20
54	1y	64	A	N1-C6-N6	-8.42	113.55	118.60
1	2A	2136	C	N3-C2-O2	-8.36	116.05	121.90
32	2a	1272	G	C5-C6-N1	-8.29	107.35	111.50
1	2A	2473	U	C2-N1-C1'	8.26	127.61	117.70
32	2a	1272	G	C6-N1-C2	8.08	129.95	125.10
55	2x	14	A	C4-C5-C6	8.08	121.04	117.00
54	1y	33	U	C2-N1-C1'	7.97	127.26	117.70
54	1w	47	U	C2-N1-C1'	7.93	127.22	117.70
1	2A	2149	G	N3-C4-N9	7.93	130.76	126.00
1	1A	1045	U	O5'-P-OP2	-7.86	98.63	105.70
54	1y	64	A	C5-C6-N6	7.76	129.91	123.70
32	2a	1263	C	C6-N1-C2	-7.74	117.20	120.30
32	2a	1025	U	N1-C2-O2	7.71	128.19	122.80
32	2a	79	G	C5-C6-O6	7.69	133.21	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	C2-N3-C4	-7.57	108.11	111.90
1	1A	12	U	C2-N1-C1'	7.47	126.66	117.70
55	2x	22	G	C5-N7-C8	-7.39	100.60	104.30
1	1A	1686	U	O5'-P-OP2	-7.38	99.06	105.70
32	1a	1030(B)	C	C2-N1-C1'	7.32	126.85	118.80
1	1A	2158	C	C2-N1-C1'	7.23	126.75	118.80
32	2a	1263	C	C5-C6-N1	7.23	124.61	121.00
32	1a	1025	U	N3-C2-O2	-7.21	117.15	122.20
55	2x	14	A	C5-N7-C8	7.20	107.50	103.90
55	1x	14	A	C4-C5-C6	7.03	120.51	117.00
54	1y	56	C	N1-C2-O2	7.01	123.11	118.90
32	1a	1030	C	N1-C2-O2	6.95	123.07	118.90
55	1x	22	G	N1-C6-O6	-6.93	115.74	119.90
32	2a	1272	G	C4-N9-C1'	6.89	135.46	126.50
32	1a	1025	U	C2-N1-C1'	6.83	125.90	117.70
55	1x	46	G	C5-C6-N1	6.79	114.90	111.50
1	1A	1109	G	C6-N1-C2	6.78	129.17	125.10
32	2a	1001(A)	G	N3-C2-N2	6.76	124.63	119.90
1	1A	2177	G	C5-C6-O6	-6.74	124.56	128.60
32	1a	1036	G	N3-C2-N2	-6.68	115.22	119.90
1	2A	801	G	O5'-P-OP2	-6.65	99.72	105.70
32	2a	1263	C	N3-C4-N4	-6.62	113.36	118.00
1	2A	1313	U	C2-N1-C1'	6.60	125.62	117.70
32	2a	1029	C	N1-C2-O2	6.57	122.84	118.90
32	1a	1027	C	N3-C4-C5	-6.53	119.29	121.90
55	2x	14	A	C5-C6-N1	-6.52	114.44	117.70
1	1A	2189	U	C2-N1-C1'	6.51	125.51	117.70
55	1x	14	A	C5-C6-N1	-6.49	114.45	117.70
1	2A	2142	C	C2-N1-C1'	6.43	125.88	118.80
55	2x	22	G	C4-C5-C6	-6.39	114.97	118.80
32	2a	754	C	C2-N1-C1'	6.37	125.81	118.80
55	1x	22	G	C5-N7-C8	-6.35	101.12	104.30
1	2A	504	U	C2-N1-C1'	6.35	125.32	117.70
1	1A	1121	C	C5-C4-N4	6.34	124.64	120.20
1	2A	2149	G	N9-C4-C5	-6.34	102.86	105.40
1	1A	2252	C	N1-C2-O2	6.32	122.69	118.90
55	2x	46	G	C5-C6-N1	6.30	114.65	111.50
1	1A	2177	G	N1-C6-O6	6.29	123.67	119.90
1	2A	1698	A	O4'-C1'-N9	6.26	113.21	108.20
1	1A	1359	U	C2-N1-C1'	6.25	125.20	117.70
55	1x	14	A	C5-N7-C8	6.21	107.01	103.90
32	2a	754	C	N1-C2-O2	6.21	122.63	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1109	G	N3-C2-N2	6.21	124.25	119.90
32	1a	1030(B)	C	N1-C2-O2	6.19	122.61	118.90
1	1A	2014	G	P-O3'-C3'	6.18	127.11	119.70
32	1a	1030	C	C2-N3-C4	6.14	122.97	119.90
1	1A	2158	C	N1-C2-O2	6.13	122.58	118.90
32	2a	1272	G	C8-N9-C1'	-6.13	119.03	127.00
55	1x	22	G	C4-C5-C6	-6.11	115.14	118.80
1	1A	894	U	C2-N1-C1'	6.09	125.00	117.70
1	2A	1614	A	O5'-P-OP1	-6.06	100.24	105.70
32	1a	1030(B)	C	C6-N1-C2	-6.05	117.88	120.30
32	2a	1025	U	N3-C2-O2	-6.03	117.98	122.20
54	1y	33	U	N1-C2-O2	6.03	127.02	122.80
1	1A	1121	C	N3-C2-O2	-6.02	117.68	121.90
1	1A	2858	G	O4'-C1'-N9	6.00	113.00	108.20
1	1A	599	U	O5'-P-OP1	-5.98	100.32	105.70
1	2A	2149	G	C8-N9-C1'	-5.93	119.29	127.00
1	2A	90	U	C2-N1-C1'	5.85	124.72	117.70
32	2a	1001(A)	G	N9-C4-C5	-5.82	103.07	105.40
1	1A	1321	A	N1-C6-N6	5.82	122.09	118.60
32	1a	1029	C	C2-N3-C4	5.82	122.81	119.90
1	1A	2189	U	N1-C2-O2	5.80	126.86	122.80
1	2A	2473	U	N1-C2-O2	5.80	126.86	122.80
1	1A	2158	C	C6-N1-C1'	-5.79	113.85	120.80
32	2a	1043	C	N1-C2-O2	5.79	122.38	118.90
1	2A	2149	G	C4-N9-C1'	5.79	134.03	126.50
32	2a	1039	C	C2-N3-C4	5.78	122.79	119.90
55	1x	22	G	C5-C6-N1	5.77	114.38	111.50
1	1A	1295	U	O5'-P-OP1	-5.76	100.51	105.70
1	1A	1219	A	OP1-P-O3'	5.76	117.88	105.20
32	1a	841	U	C5-C6-N1	5.75	125.57	122.70
1	1A	215	G	O4'-C1'-N9	5.74	112.79	108.20
55	2x	22	G	N3-C4-N9	-5.72	122.56	126.00
32	2a	1001(A)	G	N3-C4-N9	5.72	129.43	126.00
54	2w	67	C	C5-C4-N4	5.70	124.19	120.20
1	2A	614	U	N3-C2-O2	-5.70	118.21	122.20
2	2B	1	U	C2-N1-C1'	5.70	124.54	117.70
1	1A	2001	C	C6-N1-C2	-5.69	118.02	120.30
1	1A	892	G	O4'-C1'-N9	5.68	112.75	108.20
1	2A	2149	G	C6-C5-N7	-5.68	126.99	130.40
1	1A	1311	A	O5'-P-OP2	-5.67	100.60	105.70
32	1a	266	G	P-O3'-C3'	5.65	126.48	119.70
1	1A	1109	G	N1-C6-O6	-5.64	116.51	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1786	A	O4'-C1'-N9	5.64	112.72	108.20
32	2a	1030	C	N1-C2-O2	5.64	122.28	118.90
32	1a	1025	U	C6-N1-C1'	-5.63	113.32	121.20
55	2x	22	G	N3-C4-C5	5.59	131.40	128.60
32	1a	1067	A	P-O3'-C3'	5.58	126.40	119.70
54	2w	70	G	N3-C2-N2	-5.56	116.01	119.90
32	2a	266	G	N3-C4-C5	-5.55	125.83	128.60
54	1y	33	U	C6-N1-C1'	-5.54	113.44	121.20
1	2A	2136	C	C2-N1-C1'	5.52	124.87	118.80
1	2A	2473	U	C6-N1-C1'	-5.52	113.48	121.20
1	1A	2189	U	N3-C2-O2	-5.51	118.34	122.20
1	1A	1388	A	O5'-P-OP2	-5.51	100.74	105.70
55	1x	14	A	C4-N9-C1'	5.46	136.13	126.30
1	1A	840	A	O5'-P-OP2	-5.45	100.79	105.70
55	1x	14	A	C8-N9-C1'	-5.43	117.92	127.70
1	1A	1302	G	N9-C4-C5	-5.43	103.23	105.40
32	2a	1158	C	C2-N1-C1'	5.42	124.77	118.80
7	2H	98	LEU	CA-CB-CG	5.41	127.74	115.30
1	2A	928	G	C6-C5-N7	-5.41	127.16	130.40
1	1A	410	U	C2-N1-C1'	-5.40	111.22	117.70
1	2A	945	A	N1-C6-N6	5.40	121.84	118.60
54	1w	47	U	C5-C6-N1	5.39	125.40	122.70
1	1A	12	U	C5-C6-N1	5.39	125.39	122.70
54	1w	47	U	C6-N1-C1'	-5.38	113.66	121.20
1	2A	228	A	P-O3'-C3'	5.38	126.15	119.70
54	1w	3	C	C2-N1-C1'	5.37	124.71	118.80
1	2A	2142	C	N1-C2-O2	5.37	122.12	118.90
1	2A	2096	U	N1-C2-O2	5.37	126.56	122.80
54	1y	33	U	C5-C6-N1	5.37	125.38	122.70
1	2A	1992	G	P-O3'-C3'	5.36	126.13	119.70
55	2x	22	G	C8-N9-C1'	5.35	133.96	127.00
1	1A	1302	G	C8-N9-C1'	-5.34	120.05	127.00
6	2G	177	GLY	C-N-CA	-5.34	108.34	121.70
1	2A	383	U	O4'-C1'-N1	5.33	112.47	108.20
32	1a	687	A	P-O3'-C3'	5.32	126.09	119.70
1	2A	2335	A	O4'-C1'-N9	5.32	112.45	108.20
1	2A	928	G	N1-C6-O6	5.29	123.07	119.90
32	1a	975	A	O4'-C1'-N9	-5.29	103.97	108.20
1	2A	2149	G	C4-C5-N7	5.28	112.91	110.80
1	2A	2155	G	N9-C4-C5	-5.28	103.29	105.40
32	1a	115	G	P-O3'-C3'	5.27	126.03	119.70
1	2A	2163	C	C6-N1-C2	-5.27	118.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	7	A	C6-N1-C2	-5.26	115.44	118.60
32	1a	1065	U	P-O3'-C3'	5.26	126.01	119.70
1	2A	2174	C	N1-C2-O2	5.26	122.06	118.90
54	2y	66	U	C5-C4-O4	-5.26	122.74	125.90
1	2A	2848	G	O4'-C1'-N9	5.26	112.41	108.20
1	1A	1807	G	O5'-P-OP2	-5.24	100.98	105.70
32	1a	1030(B)	C	N3-C2-O2	-5.24	118.24	121.90
1	2A	1698	A	C6-C5-N7	-5.23	128.64	132.30
32	1a	1201	A	P-O3'-C3'	5.23	125.98	119.70
32	2a	266	G	P-O3'-C3'	5.23	125.97	119.70
1	1A	2803	A	C2-N3-C4	5.23	113.21	110.60
1	2A	2473	U	N3-C2-O2	-5.23	118.54	122.20
32	2a	1132	C	C2-N1-C1'	5.21	124.53	118.80
1	1A	2485	U	N3-C2-O2	-5.20	118.56	122.20
1	2A	986	C	C6-N1-C2	-5.19	118.22	120.30
32	1a	1036	G	C6-N1-C2	-5.18	121.99	125.10
1	1A	507	G	O4'-C1'-N9	5.18	112.34	108.20
1	2A	528	A	P-O3'-C3'	5.17	125.91	119.70
1	2A	901	A	N7-C8-N9	5.17	116.39	113.80
32	1a	1442	G	N3-C4-C5	-5.17	126.02	128.60
1	1A	1132	A	N1-C6-N6	-5.16	115.50	118.60
32	2a	1272	G	N1-C2-N3	5.16	127.00	123.90
32	1a	1027	C	C6-N1-C1'	5.14	126.97	120.80
54	2w	70	G	N9-C4-C5	5.13	107.45	105.40
1	2A	195	A	P-O3'-C3'	5.12	125.84	119.70
54	2w	10	G	C4-N9-C1'	5.11	133.15	126.50
1	1A	1359	U	N3-C2-O2	-5.11	118.63	122.20
1	1A	12	U	C6-N1-C1'	-5.09	114.07	121.20
1	2A	512	G	O4'-C1'-N9	5.09	112.27	108.20
1	1A	1700	G	C8-N9-C4	-5.09	104.36	106.40
32	2a	1125	U	C2-N1-C1'	5.08	123.80	117.70
54	1w	47	U	N1-C2-O2	5.07	126.35	122.80
32	2a	913	A	P-O3'-C3'	5.07	125.79	119.70
32	2a	1322	C	N1-C2-O2	-5.07	115.86	118.90
55	1x	46	G	N9-C4-C5	5.07	107.43	105.40
19	2X	57	LEU	CA-CB-CG	5.06	126.94	115.30
1	1A	1020	C	N1-C2-O2	-5.05	115.87	118.90
1	2A	2318	G	N3-C4-C5	-5.05	126.08	128.60
1	2A	504	U	N1-C2-O2	5.04	126.33	122.80
1	1A	2561	G	N1-C6-O6	5.03	122.92	119.90
32	2a	1442	G	P-O3'-C3'	5.02	125.72	119.70
32	1a	913	A	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31192	701	0
1	2A	60322	0	30423	818	0
2	1B	2577	0	1305	26	0
2	2B	2575	0	1303	44	0
3	1D	2136	0	2218	48	0
3	2D	2136	0	2218	50	0
4	1E	1559	0	1618	28	0
4	2E	1559	0	1618	39	0
5	1F	1584	0	1625	37	0
5	2F	1580	0	1619	45	0
6	1G	1423	0	1436	29	0
6	2G	1428	0	1438	45	0
7	1H	1330	0	1407	24	0
7	2H	1330	0	1407	44	0
8	1I	1097	0	1140	32	0
8	2I	1064	0	1082	22	0
9	1N	1117	0	1184	14	0
9	2N	1117	0	1184	23	0
10	1O	933	0	996	20	0
10	2O	933	0	996	23	0
11	1P	1135	0	1212	29	0
11	2P	1135	0	1212	37	0
12	1Q	1122	0	1179	27	0
12	2Q	1122	0	1179	32	0
13	1R	968	0	1033	20	0
13	2R	968	0	1033	22	0
14	1S	873	0	927	23	0
14	2S	870	0	923	37	0
15	1T	1091	0	1151	22	0
15	2T	1083	0	1136	27	0
16	1U	959	0	1019	18	0
16	2U	959	0	1019	26	0
17	1V	771	0	830	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	2V	771	0	830	10	0
18	1W	886	0	940	15	0
18	2W	886	0	940	14	0
19	1X	750	0	814	15	0
19	2X	750	0	814	18	0
20	1Y	806	0	881	15	0
20	2Y	806	0	881	15	0
21	1Z	1240	0	1240	16	0
21	2Z	1271	0	1273	39	0
22	10	653	0	674	19	0
22	20	653	0	674	19	0
23	11	755	0	826	15	0
23	21	755	0	826	23	0
24	12	588	0	643	9	0
24	22	588	0	643	13	0
25	13	469	0	518	13	0
25	23	464	0	514	12	0
26	14	552	0	533	13	0
26	24	532	0	503	23	0
27	15	455	0	465	9	0
27	25	455	0	465	14	0
28	16	453	0	473	9	0
28	26	449	0	469	9	0
29	17	418	0	467	9	0
29	27	418	0	467	18	0
30	18	517	0	582	18	0
30	28	517	0	582	19	0
31	19	307	0	335	7	0
31	29	307	0	335	8	0
32	1a	32246	0	16295	0	0
32	2a	32327	0	16339	0	0
33	1b	1846	0	1867	0	0
33	2b	1825	0	1828	0	0
34	1c	1548	0	1535	0	0
34	2c	1542	0	1517	0	0
35	1d	1655	0	1672	0	0
35	2d	1674	0	1714	0	0
36	1e	1129	0	1184	0	0
36	2e	1133	0	1191	0	0
37	1f	810	0	804	0	0
37	2f	816	0	808	0	0
38	1g	1231	0	1238	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	2g	1235	0	1249	0	0
39	1h	1088	0	1126	0	0
39	2h	1088	0	1126	0	0
40	1i	983	0	986	0	0
40	2i	978	0	966	0	0
41	1j	709	0	650	0	0
41	2j	714	0	672	0	0
42	1k	829	0	825	0	0
42	2k	833	0	836	0	0
43	1l	932	0	981	0	0
43	2l	932	0	981	0	0
44	1m	958	0	1002	0	0
44	2m	950	0	988	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0
46	1o	728	0	760	0	0
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	677	0	686	0	0
48	1q	823	0	891	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	652	0	662	0	0
50	2s	646	0	644	0	0
51	1t	728	0	798	0	0
51	2t	727	0	796	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1v	277	0	140	0	0
53	2v	277	0	140	0	0
54	1w	1592	0	819	0	0
54	1y	1585	0	804	0	0
54	2w	1544	0	788	0	0
54	2y	1565	0	795	0	0
55	1x	1625	0	827	0	0
55	2x	1625	0	828	0	0
56	10	5	0	0	0	0
56	11	5	0	0	0	0
56	12	2	0	0	0	0
56	13	2	0	0	0	0
56	15	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	16	3	0	0	0	0
56	17	5	0	0	0	0
56	18	3	0	0	0	0
56	19	1	0	0	0	0
56	1A	1063	0	0	0	0
56	1B	38	0	0	0	0
56	1D	14	0	0	0	0
56	1E	13	0	0	0	0
56	1F	9	0	0	0	0
56	1G	5	0	0	0	0
56	1I	1	0	0	0	0
56	1N	5	0	0	0	0
56	1O	7	0	0	0	0
56	1P	3	0	0	0	0
56	1Q	5	0	0	0	0
56	1R	5	0	0	0	0
56	1S	3	0	0	0	0
56	1T	2	0	0	0	0
56	1U	6	0	0	0	0
56	1V	3	0	0	0	0
56	1W	5	0	0	0	0
56	1X	6	0	0	0	0
56	1Y	2	0	0	0	0
56	1Z	4	0	0	0	0
56	1a	215	0	0	0	0
56	1b	2	0	0	0	0
56	1e	1	0	0	0	0
56	1f	1	0	0	0	0
56	1l	3	0	0	0	0
56	1m	1	0	0	0	0
56	1n	2	0	0	0	0
56	1p	1	0	0	0	0
56	1q	1	0	0	0	0
56	1r	1	0	0	0	0
56	1s	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	1	0	0	0	0
56	1w	11	0	0	0	0
56	1x	15	0	0	0	0
56	1y	4	0	0	0	0
56	20	3	0	0	0	0
56	21	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	23	1	0	0	0	0
56	25	3	0	0	0	0
56	27	2	0	0	0	0
56	28	2	0	0	0	0
56	2A	754	0	0	0	0
56	2B	21	0	0	0	0
56	2D	7	0	0	0	0
56	2E	10	0	0	0	0
56	2F	4	0	0	0	0
56	2G	1	0	0	0	0
56	2O	2	0	0	0	0
56	2P	1	0	0	0	0
56	2Q	3	0	0	0	0
56	2R	4	0	0	0	0
56	2T	3	0	0	0	0
56	2U	6	0	0	0	0
56	2V	2	0	0	0	0
56	2W	3	0	0	0	0
56	2X	2	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	233	0	0	0	0
56	2d	2	0	0	0	0
56	2e	1	0	0	0	0
56	2f	1	0	0	0	0
56	2g	1	0	0	0	0
56	2j	2	0	0	0	0
56	2l	4	0	0	0	0
56	2q	4	0	0	0	0
56	2r	2	0	0	0	0
56	2t	1	0	0	0	0
56	2v	5	0	0	0	0
56	2w	9	0	0	0	0
56	2x	5	0	0	0	0
56	2y	7	0	0	0	0
57	1A	2	0	0	0	0
57	2A	2	0	0	0	0
58	1A	25	0	0	2	0
58	2A	25	0	0	1	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	0	0
61	10	10	0	0	0	0
61	11	7	0	0	0	0
61	12	2	0	0	0	0
61	13	4	0	0	0	0
61	15	5	0	0	1	0
61	16	2	0	0	0	0
61	17	9	0	0	1	0
61	18	7	0	0	1	0
61	1A	1433	0	0	74	0
61	1B	65	0	0	2	0
61	1D	24	0	0	0	0
61	1E	30	0	0	4	0
61	1F	10	0	0	4	0
61	1G	8	0	0	2	0
61	1H	1	0	0	0	0
61	1I	2	0	0	0	0
61	1N	6	0	0	1	0
61	1O	8	0	0	0	0
61	1P	18	0	0	1	0
61	1Q	12	0	0	0	0
61	1R	12	0	0	0	0
61	1S	4	0	0	0	0
61	1T	7	0	0	0	0
61	1U	9	0	0	0	0
61	1V	8	0	0	0	0
61	1W	8	0	0	0	0
61	1X	8	0	0	1	0
61	1Y	2	0	0	0	0
61	1Z	1	0	0	0	0
61	1a	315	0	0	0	0
61	1b	1	0	0	0	0
61	1e	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6l	1f	1	0	0	0	0
6l	1g	1	0	0	0	0
6l	1j	1	0	0	0	0
6l	1l	6	0	0	0	0
6l	1m	1	0	0	0	0
6l	1n	1	0	0	0	0
6l	1q	3	0	0	0	0
6l	1u	1	0	0	0	0
6l	1v	6	0	0	0	0
6l	1w	20	0	0	0	0
6l	1x	14	0	0	0	0
6l	1y	2	0	0	0	0
6l	20	4	0	0	0	0
6l	21	8	0	0	0	0
6l	22	1	0	0	0	0
6l	23	1	0	0	0	0
6l	25	4	0	0	0	0
6l	26	1	0	0	0	0
6l	27	4	0	0	0	0
6l	28	4	0	0	0	0
6l	29	1	0	0	0	0
6l	2A	885	0	0	53	0
6l	2B	26	0	0	0	0
6l	2D	18	0	0	4	0
6l	2E	14	0	0	2	0
6l	2F	18	0	0	0	0
6l	2I	4	0	0	0	0
6l	2N	1	0	0	0	0
6l	2P	12	0	0	1	0
6l	2Q	2	0	0	0	0
6l	2R	2	0	0	0	0
6l	2T	6	0	0	0	0
6l	2U	3	0	0	0	0
6l	2V	1	0	0	0	0
6l	2W	3	0	0	0	0
6l	2X	1	0	0	0	0
6l	2Y	1	0	0	1	0
6l	2Z	2	0	0	0	0
6l	2a	258	0	0	0	0
6l	2c	1	0	0	0	0
6l	2d	3	0	0	0	0
6l	2e	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2g	1	0	0	0	0
61	2i	1	0	0	0	0
61	2j	4	0	0	0	0
61	2l	6	0	0	0	0
61	2o	1	0	0	0	0
61	2p	2	0	0	0	0
61	2q	1	0	0	0	0
61	2r	1	0	0	0	0
61	2t	5	0	0	0	0
61	2u	1	0	0	0	0
61	2v	2	0	0	0	0
61	2w	2	0	0	0	0
61	2x	6	0	0	0	0
61	2y	18	0	0	0	0
All	All	299109	0	196685	2479	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 9.

All (2479) 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:2158:C:N4	1:1A:2177:G:H1	1.36	1.21
1:2A:2136:C:N4	1:2A:2155:G:H1	1.46	1.12
1:2A:2129:C:N4	1:2A:2159:G:H1	1.49	1.10
1:1A:1128:U:H3	1:1A:1132:A:N6	1.48	1.09
1:1A:2149:G:H1	1:1A:2183:C:N4	1.54	1.05
1:2A:2138:C:N4	1:2A:2153:G:H1	1.56	1.03
1:2A:1002:G:H1	1:2A:1038:C:N4	42.97	1.02
1:2A:2129:C:H42	1:2A:2159:G:H1	1.04	0.97
1:1A:1128:U:O4	1:1A:1132:A:N1	1.99	0.95
1:2A:2114:A:N6	1:2A:2119:A:N7	2.15	0.95
1:1A:1100:A:N6	1:1A:1151:U:H3	1.65	0.94
1:2A:1002:G:H1	1:2A:1038:C:H42	43.27	0.94
1:2A:2129:C:N3	1:2A:2159:G:N2	2.17	0.92
11:2P:39:LYS:HB2	11:2P:45:LEU:HG	1.50	0.90
1:1A:1100:A:H61	1:1A:1151:U:H3	1.16	0.89
1:1A:2158:C:N3	1:1A:2177:G:N2	2.20	0.89
1:1A:2149:G:H1	1:1A:2183:C:H42	0.88	0.88
1:2A:2143:C:H42	1:2A:2148:G:H1	1.20	0.87
1:2A:2807:G:N1	1:2A:2893:G:O6	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1004:A:N6	1:1A:1037:C:N3	55.45	0.86
1:2A:2136:C:N4	1:2A:2155:G:N1	2.23	0.86
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.09	0.85
1:2A:2138:C:H42	1:2A:2153:G:H1	0.86	0.85
1:1A:1111:U:O2	1:1A:1119:A:N6	2.08	0.85
29:17:24:THR:HG22	29:17:27:GLY:H	1.39	0.85
1:2A:2108:C:H42	1:2A:2181:G:H1	1.19	0.85
1:2A:1422:G:H5''	10:2O:48:PRO:HB3	99.35	0.85
1:1A:656:A:OP1	11:1P:65:ARG:NH1	2.09	0.85
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.58	0.84
20:1Y:92:ASN:HB3	20:1Y:94:LYS:H	1.42	0.84
8:2I:93:THR:H	8:2I:96:ASP:HB2	1.42	0.84
1:2A:2308:G:O6	1:2A:2311:A:N6	2.12	0.83
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.12	0.83
1:2A:2136:C:N3	1:2A:2155:G:N2	2.26	0.83
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.60	0.82
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.14	0.82
1:1A:1118:C:O2	1:1A:1138:C:N4	2.12	0.82
1:1A:1140:U:H1'	1:1A:1143:U:H5	1.44	0.82
1:1A:1117:G:O6	1:1A:1146:C:N4	2.13	0.82
25:13:6:VAL:HG13	25:13:54:VAL:HG11	1.60	0.82
1:1A:2121:U:H3	1:1A:2212:G:H1	1.28	0.82
1:1A:2149:G:N2	1:1A:2183:C:N3	2.27	0.82
1:1A:1104:G:H1	1:1A:1126:C:N4	1.77	0.81
19:1X:57:LEU:HD11	19:1X:78:LYS:HE2	1.63	0.80
1:2A:2136:C:H42	1:2A:2155:G:H1	1.26	0.80
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.63	0.80
1:1A:1001:G:O6	61:1A:4119:HOH:O	1.99	0.80
7:2H:159:GLU:HG3	7:2H:169:VAL:HG11	1.62	0.80
3:1D:17:THR:O	3:1D:211:ARG:NH2	2.14	0.80
17:2V:40:LEU:HB2	17:2V:46:VAL:HG22	1.63	0.79
1:2A:821:A:N1	61:2A:3845:HOH:O	2.15	0.79
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.15	0.79
1:1A:2695:C:O2	10:1O:70:LYS:NZ	2.12	0.79
13:2R:67:LEU:HD13	13:2R:76:VAL:HG21	1.62	0.79
1:1A:641:G:OP1	5:1F:40:GLN:NE2	2.16	0.79
4:2E:119:ARG:HD2	4:2E:160:TYR:HB2	1.63	0.79
1:2A:975:C:OP1	61:2A:3830:HOH:O	2.00	0.78
1:1A:2387:G:N7	61:1A:4143:HOH:O	2.16	0.78
1:2A:2345:G:H4'	1:2A:2346:A:H5''	1.64	0.78
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.13	0.78
1:1A:1829:U:H5'	3:1D:259:THR:HG22	1.67	0.77
1:2A:2287:A:H62	1:2A:2344:U:H3	1.32	0.77
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.55	0.77
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.67	0.77
1:2A:1204:A:H2	1:2A:1241:A:H62	1.30	0.77
2:2B:20:C:N4	2:2B:63:G:O6	2.16	0.77
1:1A:1110:C:N3	1:1A:1120:G:O6	2.18	0.77
1:2A:529:A:N6	1:2A:2041:U:O2	2.18	0.77
3:2D:228:PRO:O	61:2D:401:HOH:O	2.01	0.76
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.65	0.76
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.18	0.76
1:2A:1171:G:H1	1:2A:1178:C:H42	1.31	0.76
1:1A:973:G:N7	61:1A:4152:HOH:O	2.18	0.76
1:1A:641:G:OP2	5:1F:43:LYS:NZ	2.19	0.76
1:1A:2162:C:N3	1:1A:2173:G:O6	2.17	0.76
1:1A:1056:A:OP2	61:1A:4120:HOH:O	2.02	0.76
1:1A:2562:G:OP1	61:1A:4122:HOH:O	2.04	0.76
11:1P:52:GLU:OE1	11:1P:55:ARG:NH1	2.19	0.76
6:2G:44:GLY:HA2	6:2G:88:ILE:HB	1.68	0.76
5:2F:24:LEU:HD23	5:2F:115:ALA:HA	1.68	0.75
1:1A:479:C:OP1	61:1A:4121:HOH:O	2.03	0.75
12:1Q:75:THR:HG21	12:1Q:87:LYS:HE3	1.69	0.75
1:2A:2127:G:N2	1:2A:2161:C:N3	2.34	0.75
1:1A:359:C:H4'	20:1Y:73:ARG:HD3	1.67	0.75
1:2A:1689:A:H62	1:2A:1698:A:H2	1.34	0.75
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.69	0.75
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	1.69	0.75
1:2A:1363:C:OP1	23:21:61:ARG:NH1	2.20	0.75
1:2A:1002:G:N2	1:2A:1038:C:N3	42.23	0.75
1:1A:2164:C:N3	1:1A:2171:G:O6	2.19	0.75
2:2B:87:G:N2	2:2B:90:A:OP2	2.19	0.75
1:1A:2143:G:H1	1:1A:2199:C:H42	1.31	0.75
1:2A:2138:C:N3	1:2A:2153:G:N2	2.29	0.75
2:2B:8:U:N3	2:2B:113:G:O6	2.15	0.75
1:1A:325:G:OP2	20:1Y:84:ARG:NH2	2.19	0.74
1:2A:2721:A:OP1	61:2A:3831:HOH:O	2.05	0.74
1:2A:1031:G:H5''	31:29:8:LYS:HE3	1.70	0.74
1:2A:1651:G:OP1	13:2R:40:LYS:NZ	2.20	0.74
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.22	0.74
2:2B:4:C:H42	2:2B:117:G:H1	1.36	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:54:GLY:N	26:14:55:ARG:HA	2.02	0.74
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.70	0.74
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.53	0.74
1:2A:761:A:N7	61:2A:3866:HOH:O	2.20	0.74
1:2A:692:C:O2'	3:2D:38:LYS:NZ	2.20	0.74
21:2Z:121:HIS:N	21:2Z:171:ILE:O	2.21	0.74
12:2Q:109:VAL:HG13	12:2Q:113:GLN:HB3	1.70	0.73
1:1A:1057:G:OP1	16:1U:77:SER:OG	2.05	0.73
22:10:11:ARG:O	22:10:14:ARG:NH2	2.22	0.73
1:1A:1896:G:OP1	61:1A:4124:HOH:O	2.07	0.73
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.21	0.73
1:2A:2849:U:OP2	15:2T:95:ARG:NH1	2.22	0.72
1:1A:2460:A:OP1	61:1A:4101:HOH:O	2.06	0.72
1:2A:962:G:OP1	61:2A:3812:HOH:O	2.06	0.72
18:1W:65:LEU:HD12	18:1W:68:ARG:HE	1.54	0.72
1:2A:517:C:OP1	27:25:16:ARG:NH2	2.21	0.72
1:1A:2604:G:OP1	61:1A:4123:HOH:O	2.06	0.72
1:1A:2804:C:H2'	1:1A:2805:G:H8	1.55	0.72
1:1A:625:G:O2'	1:1A:702:A:N6	2.23	0.72
3:1D:83:GLU:OE1	3:1D:104:TYR:OH	2.05	0.72
5:1F:72:ARG:O	61:1F:401:HOH:O	2.08	0.72
7:1H:25:LYS:HD3	7:1H:27:LYS:HE3	1.69	0.72
1:1A:183:G:N7	61:1A:4172:HOH:O	2.21	0.72
17:2V:72:VAL:HG13	17:2V:85:LYS:HB2	1.70	0.72
1:2A:2134:A:OP2	1:2A:2157:G:N2	2.22	0.72
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.72	0.72
12:2Q:18:LYS:O	12:2Q:98:LYS:NZ	2.18	0.72
1:1A:928:G:N2	1:1A:943:C:O2	2.23	0.71
4:2E:127:ASP:OD2	61:2E:401:HOH:O	2.07	0.71
1:1A:1829:U:OP2	3:1D:274:ARG:NH2	2.22	0.71
1:1A:931:C:H42	1:1A:938:G:H1	1.39	0.71
1:2A:2129:C:N4	1:2A:2159:G:N1	2.25	0.71
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.25	0.71
22:10:10:THR:HG22	22:10:12:ASN:H	1.54	0.71
1:1A:303:C:H42	1:1A:385:G:H1	1.39	0.71
2:2B:33:G:H5'	6:2G:2:PRO:HD3	1.72	0.71
1:2A:2127:G:N1	1:2A:2161:C:N4	2.38	0.71
4:2E:48:GLN:HE21	4:2E:78:LEU:HG	1.56	0.71
11:1P:42:SER:O	61:1P:301:HOH:O	2.09	0.71
1:2A:2513:G:N2	4:2E:143:ASN:OD1	2.24	0.71
1:2A:1530:C:H42	1:2A:1539:G:H1	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2U:66:ASN:HD21	16:2U:70:ARG:HH21	1.39	0.71
1:2A:271(H):G:H1	1:2A:271(P):C:H42	1.39	0.71
1:2A:1434:A:H61	1:2A:1558:A:H62	1.39	0.70
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.08	0.70
1:2A:2143:C:N4	1:2A:2148:G:H1	1.88	0.70
1:2A:2108:C:N4	1:2A:2181:G:H1	1.89	0.70
1:1A:1104:G:N2	1:1A:1126:C:N3	2.37	0.70
1:1A:1299:A:N7	61:1A:4140:HOH:O	2.23	0.70
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.73	0.70
1:1A:1275:G:N7	61:1A:4191:HOH:O	2.24	0.70
1:1A:1552:C:H2'	1:1A:1553:A:H8	1.57	0.70
1:1A:556:C:OP2	61:1A:4125:HOH:O	2.08	0.70
1:2A:1971:A:OP1	61:2A:3832:HOH:O	2.09	0.70
1:2A:307:G:N1	1:2A:310:A:OP2	2.25	0.70
1:1A:692:C:H42	1:1A:698:G:H1	1.39	0.70
1:1A:739:C:O2'	3:1D:38:LYS:NZ	2.25	0.70
5:1F:61:GLY:O	61:1F:402:HOH:O	2.09	0.70
1:1A:2331:G:H22	14:1S:3:ARG:HD3	1.57	0.70
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.24	0.70
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.72	0.70
1:2A:2789:C:O2	1:2A:2894:G:N2	2.25	0.69
1:2A:2292:C:OP1	14:2S:17:ARG:NH2	2.25	0.69
21:2Z:97:GLU:HB3	21:2Z:125:LEU:HD11	1.74	0.69
1:2A:1607:C:N4	1:2A:1622:G:OP2	2.24	0.69
1:2A:2171:A:N3	1:2A:2172:U:N3	2.39	0.69
20:1Y:11:ASP:N	20:1Y:11:ASP:OD1	2.21	0.69
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.73	0.69
1:2A:2114:A:N6	1:2A:2115:G:H21	1.89	0.69
1:1A:2672:A:N7	7:1H:175:LYS:NZ	2.40	0.69
1:2A:2169:A:H2'	1:2A:2170:A:C8	2.27	0.69
1:2A:993:G:N7	1:2A:1213:A:N6	49.03	0.69
1:1A:1219:A:H4'	1:1A:1220:U:OP1	1.92	0.69
1:1A:2164:C:O2	1:1A:2171:G:N1	2.25	0.69
20:1Y:20:TYR:HB3	20:1Y:23:ARG:HG3	1.73	0.69
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.26	0.69
1:1A:1990:G:OP1	61:1A:4126:HOH:O	2.09	0.69
22:20:10:THR:HG22	22:20:12:ASN:H	1.58	0.69
1:2A:2494:G:H2'	1:2A:2495:G:H8	1.57	0.69
1:1A:646:A:OP2	11:1P:108:LYS:NZ	2.26	0.69
1:2A:2518:A:OP2	61:2A:3834:HOH:O	2.10	0.69
1:1A:1069:U:OP2	61:1A:4109:HOH:O	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.25	0.69
7:2H:125:VAL:HG12	7:2H:131:VAL:HG22	1.75	0.69
8:2I:92:VAL:HG22	8:2I:120:ILE:HB	1.74	0.69
1:1A:889:G:N7	61:1A:4195:HOH:O	2.25	0.69
1:2A:1169:G:N2	1:2A:1181:C:O2	2.26	0.69
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.25	0.69
7:2H:86:GLU:OE2	7:2H:130:ARG:NH1	2.25	0.69
8:2I:43:ASN:ND2	23:21:75:GLU:OE2	2.26	0.68
1:2A:2010:G:OP1	61:2A:3833:HOH:O	2.10	0.68
1:1A:1310:G:OP1	27:15:19:ARG:NH2	2.27	0.68
1:1A:1813:C:OP1	61:1A:4128:HOH:O	2.11	0.68
1:2A:775:G:O3'	61:2A:3835:HOH:O	2.10	0.68
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.76	0.68
1:1A:880:U:O2	11:1P:55:ARG:NH2	2.25	0.68
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.12	0.68
9:2N:32:THR:HG23	9:2N:37:LYS:HB2	1.74	0.68
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.74	0.68
8:1I:3:VAL:HG12	8:1I:38:LEU:HA	1.76	0.68
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.73	0.68
2:2B:22:U:H3	2:2B:61:G:H1	1.40	0.68
1:1A:1108:G:H1	1:1A:1123:A:H61	1.40	0.68
5:1F:13:SER:OG	5:1F:127:GLU:OE1	2.10	0.68
20:1Y:54:LYS:HA	20:1Y:56:PRO:HD3	1.74	0.68
12:1Q:138:ASP:OD1	12:1Q:138:ASP:N	2.24	0.68
11:2P:52:GLU:OE1	11:2P:55:ARG:NH1	2.27	0.68
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.20	0.68
1:2A:659:C:H2'	1:2A:660:G:H8	1.59	0.68
1:1A:2849:G:H5'	13:1R:46:GLY:HA2	1.76	0.67
24:22:1:MET:N	24:22:52:ASP:OD1	2.26	0.67
1:2A:974:G:OP1	1:2A:1187:G:O2'	2.10	0.67
61:1A:4108:HOH:O	4:1E:135:HIS:NE2	2.27	0.67
1:1A:1232:G:O6	61:1A:4127:HOH:O	2.11	0.67
1:1A:988:U:OP2	61:1A:4129:HOH:O	2.12	0.67
6:1G:125:PHE:O	61:1G:3101:HOH:O	2.12	0.67
5:2F:101:LEU:O	5:2F:106:ARG:NH1	2.27	0.67
1:1A:1202:A:OP2	61:1A:4130:HOH:O	2.12	0.67
1:2A:2031:A:N3	1:2A:2455:G:O2'	2.28	0.67
1:1A:1128:U:C4	1:1A:1132:A:N1	2.63	0.67
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.29	0.67
7:2H:98:LEU:HA	7:2H:103:LEU:HA	1.75	0.67
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1132:A:O2'	1:1A:1133:G:N7	2.27	0.67
7:1H:86:GLU:OE2	7:1H:132:ARG:NH2	2.27	0.67
1:2A:731:C:OP2	61:2A:3836:HOH:O	2.12	0.67
1:1A:1310:G:N7	61:1A:4206:HOH:O	2.28	0.67
1:1A:927:G:H2'	1:1A:928:G:H8	1.60	0.67
1:2A:1345:C:OP2	61:2A:3837:HOH:O	2.12	0.67
1:1A:1700:G:H3'	13:1R:2:ARG:HD3	1.77	0.67
5:2F:132:VAL:HG21	5:2F:163:VAL:HG22	1.77	0.67
1:1A:2831:A:OP2	61:1A:4117:HOH:O	2.12	0.67
1:2A:1422:G:O3'	10:2O:49:ARG:NH1	99.45	0.67
4:2E:11:MET:HG2	4:2E:24:THR:HB	1.77	0.67
14:2S:10:ARG:NE	14:2S:91:PRO:O	2.26	0.67
1:2A:1022:G:N2	1:2A:1023:U:O4	2.28	0.66
3:2D:152:GLY:O	61:2D:402:HOH:O	2.14	0.66
1:1A:1485:A:OP1	61:1A:4135:HOH:O	2.14	0.66
1:1A:2058:C:OP1	61:1A:4125:HOH:O	2.13	0.66
3:2D:232:PRO:O	61:2D:403:HOH:O	2.14	0.66
1:2A:1019:U:H2'	1:2A:1020:A:H8	1.60	0.66
14:2S:67:ARG:HG2	14:2S:71:ARG:HD2	1.78	0.66
1:1A:1020:C:OP1	61:1A:4134:HOH:O	2.14	0.66
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.78	0.66
1:1A:1139:G:H3'	1:1A:1140:U:H5''	1.78	0.66
1:1A:2239:A:OP2	61:1A:4138:HOH:O	2.14	0.66
1:1A:2641:A:O2'	1:1A:2642:G:OP2	2.13	0.66
1:1A:925:A:N6	1:1A:945:A:O2'	2.26	0.66
2:1B:58:A:OP2	61:1B:301:HOH:O	2.12	0.66
2:2B:41:U:H5	6:2G:70:VAL:H	1.43	0.66
4:1E:122:PHE:O	61:1E:401:HOH:O	2.14	0.65
1:2A:1762:A:N1	61:2A:3903:HOH:O	2.28	0.65
1:1A:1138:C:H2'	1:1A:1139:G:H5'	1.78	0.65
1:1A:992:G:OP2	61:1A:4137:HOH:O	2.14	0.65
1:2A:1462:C:H4'	1:2A:2703:C:H5'	1.78	0.65
6:2G:18:GLU:HG2	6:2G:175:LEU:HD21	1.78	0.65
12:2Q:55:VAL:HG12	12:2Q:64:ILE:HD12	1.78	0.65
26:24:16:CYS:SG	26:24:17:GLY:N	2.70	0.65
1:2A:2141:G:O6	1:2A:2150:U:O2	2.13	0.65
14:2S:68:GLN:HA	14:2S:71:ARG:HD3	1.78	0.65
19:2X:61:GLY:N	19:2X:75:ASP:OD1	2.26	0.65
24:12:22:GLU:OE2	24:12:68:ARG:NH2	2.30	0.65
1:1A:1355:G:H4'	29:17:7:PRO:HB2	1.79	0.65
1:1A:2094:G:O6	61:1A:4131:HOH:O	2.13	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.79	0.65
1:2A:1920:4OC:HM22	1:2A:1921:G:H5'	1.79	0.65
1:1A:857:U:OP1	61:1A:4140:HOH:O	2.14	0.65
1:2A:563:G:OP2	61:2A:3842:HOH:O	2.14	0.65
1:2A:789:A:N1	61:2A:3911:HOH:O	2.29	0.65
6:2G:135:LEU:HD21	6:2G:157:ILE:HD12	1.77	0.65
8:2I:3:VAL:HG12	8:2I:38:LEU:HA	1.79	0.65
1:1A:133:G:N7	61:1A:4216:HOH:O	2.29	0.65
17:1V:40:LEU:HB2	17:1V:46:VAL:HG13	1.78	0.65
22:20:11:ARG:O	22:20:14:ARG:NH2	2.28	0.65
1:2A:1019:U:H2'	1:2A:1020:A:C8	2.32	0.65
1:2A:826:U:H4'	11:2P:55:ARG:HB3	1.79	0.65
1:1A:1285:G:OP1	61:1A:4132:HOH:O	2.13	0.65
1:1A:1684:A:OP1	61:1A:4139:HOH:O	2.14	0.65
1:1A:2717:A:N3	61:1A:4218:HOH:O	2.29	0.65
1:2A:571:A:OP2	61:2A:3838:HOH:O	2.14	0.65
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.78	0.65
1:2A:1119:C:H2'	1:2A:1120:G:C8	3.65	0.64
1:2A:2582:G:OP2	61:2A:3841:HOH:O	2.14	0.64
1:1A:2227:G:H3'	1:1A:2228:G:C8	2.33	0.64
12:2Q:17:LEU:HD21	12:2Q:41:TRP:HE1	1.62	0.64
1:1A:131:C:O2	1:1A:231:G:N2	72.21	0.64
1:1A:2182:G:O6	1:1A:2183:C:N4	2.30	0.64
1:2A:1958:C:OP2	61:2A:3844:HOH:O	2.15	0.64
1:2A:900:A:H2'	1:2A:901:A:H8	1.63	0.64
18:2W:67:ASP:N	18:2W:67:ASP:OD1	2.24	0.64
1:1A:449:A:OP2	61:1A:4133:HOH:O	2.13	0.64
16:1U:104:GLN:HE21	16:1U:105:VAL:HG23	1.62	0.64
1:1A:83:A:H5''	20:1Y:8:LYS:HG2	1.78	0.64
18:2W:12:ILE:HD13	18:2W:17:VAL:HG13	1.79	0.64
18:2W:73:ALA:HB3	18:2W:106:ILE:HD12	1.80	0.64
1:1A:1099:C:H42	1:1A:1152:G:H1	1.45	0.64
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.79	0.64
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.79	0.64
1:1A:2124:U:H3	1:1A:2209:G:H1	1.44	0.64
1:1A:865:G:OP2	61:1A:4127:HOH:O	2.15	0.64
9:2N:67:LEU:HB3	9:2N:88:GLU:HG3	1.79	0.64
1:2A:1920:4OC:O5'	1:2A:1920:4OC:H6	1.98	0.64
1:1A:1313:U:OP1	61:1A:4141:HOH:O	2.15	0.64
1:1A:238:C:O2	30:18:12:LYS:NZ	2.20	0.64
2:2B:28:C:N4	2:2B:56:G:O6	2.20	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:51:G:N7	14:1S:62:LYS:NZ	2.41	0.64
20:1Y:43:ASN:HB3	20:1Y:65:ALA:HB3	1.80	0.64
1:2A:2134:A:O2'	1:2A:2159:G:N2	2.30	0.64
1:1A:1104:G:N1	1:1A:1126:C:N4	2.41	0.64
1:2A:1937:A:OP1	61:2A:3846:HOH:O	2.15	0.64
1:2A:784:A:OP1	61:2A:3840:HOH:O	2.14	0.64
1:1A:555:G:N1	1:1A:2045:G:OP1	2.28	0.63
1:2A:907:U:H4'	12:2Q:101:ARG:HH22	1.63	0.63
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	1.79	0.63
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	1.81	0.63
21:2Z:52:SER:OG	21:2Z:54:HIS:ND1	2.29	0.63
5:1F:31:HIS:NE2	5:1F:35:GLU:OE2	2.30	0.63
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.31	0.63
1:2A:2815:C:H5'	27:25:29:THR:HG21	1.79	0.63
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.62	0.63
7:2H:20:ALA:HB2	7:2H:25:LYS:HG2	1.80	0.63
15:2T:59:THR:HG23	15:2T:78:LEU:HB3	1.79	0.63
1:1A:1221:G:H1'	1:1A:1222:A:H5'	1.80	0.63
6:1G:170:ARG:NH2	6:1G:182:LYS:O	2.30	0.63
1:1A:1040:C:OP2	16:1U:54:LYS:NZ	2.30	0.63
19:1X:11:PRO:HB3	19:1X:92:LEU:HD11	1.79	0.63
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.34	0.63
1:2A:2143:C:H2'	1:2A:2144:U:O4'	1.98	0.63
1:2A:586:A:N1	1:2A:809:G:O2'	2.31	0.63
1:2A:2121:G:H1	1:2A:2177:C:N4	1.96	0.63
3:2D:85:ASP:OD2	3:2D:88:ARG:NH1	2.31	0.63
4:2E:24:THR:HG23	4:2E:184:VAL:HG13	1.81	0.63
5:1F:75:HIS:ND1	61:1F:404:HOH:O	2.31	0.63
1:2A:2105:C:H2'	1:2A:2106:G:H8	1.64	0.63
1:2A:2781:A:H5''	1:2A:2782:G:H5'	1.81	0.63
1:1A:2013:U:H2'	1:1A:2014:G:H5''	1.80	0.62
26:24:24:THR:OG1	26:24:25:TYR:N	2.32	0.62
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.81	0.62
28:16:13:CYS:SG	28:16:47:THR:HG21	2.38	0.62
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.33	0.62
1:2A:531:C:OP1	1:2A:561:G:N1	2.32	0.62
1:1A:1140:U:H1'	1:1A:1143:U:C5	2.32	0.62
1:2A:2431:U:OP1	61:2A:3849:HOH:O	2.16	0.62
6:2G:60:LEU:HD21	6:2G:92:VAL:HG11	1.82	0.62
1:2A:1652:A:OP1	13:2R:8:ARG:NH1	2.33	0.62
1:1A:1087:C:H42	1:1A:1160:G:H1	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2227:G:H3'	1:1A:2228:G:H8	1.63	0.62
8:1I:93:THR:HG22	8:1I:119:PRO:HB3	1.81	0.62
1:2A:852:G:H2'	1:2A:853:G:H8	1.64	0.62
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.32	0.62
1:1A:976:G:OP2	1:1A:1358:U:O2'	101.79	0.62
1:1A:1827:U:H2'	1:1A:1828:C:C6	2.34	0.62
1:1A:2156:A:OP1	1:1A:2178:G:N2	2.33	0.62
11:2P:62:LEU:O	30:28:13:ARG:NH1	2.33	0.62
1:1A:1817:A:H1'	1:1A:1960:A:N6	2.15	0.62
15:1T:109:GLU:O	15:1T:113:LYS:HG2	2.00	0.62
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.81	0.62
5:2F:18:ARG:NH2	5:2F:127:GLU:OE2	2.32	0.62
1:1A:2324:U:H5'	6:1G:88:ILE:HD11	1.80	0.62
1:1A:92:C:H2'	1:1A:93:G:C8	3.51	0.62
10:1O:21:CYS:HB2	10:1O:39:ILE:HD12	1.82	0.62
1:2A:2099:U:H3	1:2A:2190:G:H1	1.46	0.62
1:1A:2172:U:N3	1:1A:2173:G:N7	2.47	0.61
1:1A:831:A:O4'	3:1D:227:ASN:ND2	2.33	0.61
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.82	0.61
11:2P:39:LYS:NZ	61:2P:3101:HOH:O	2.25	0.61
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.34	0.61
8:2I:110:ASP:N	8:2I:130:TYR:OH	2.31	0.61
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.36	0.61
1:2A:441:U:O2	5:2F:46:ARG:NH2	2.32	0.61
3:2D:51:VAL:HG11	3:2D:54:ARG:HE	1.63	0.61
1:1A:1831:C:OP2	3:1D:183:ARG:NH2	2.34	0.61
3:2D:20:ASP:N	3:2D:20:ASP:OD1	2.31	0.61
26:14:15:ILE:O	26:14:33:VAL:N	2.34	0.61
5:1F:44:ARG:NH1	61:1F:403:HOH:O	2.23	0.61
1:2A:2471:C:N4	1:2A:2476:A:O2'	2.31	0.61
1:2A:1310:G:H2'	1:2A:1311:G:H8	3.42	0.61
2:2B:21:G:H1	2:2B:62:C:H42	1.48	0.61
7:2H:23:ARG:NH1	7:2H:34:GLU:OE1	2.34	0.61
23:11:59:THR:O	23:11:91:LYS:NZ	2.24	0.61
1:1A:2825:C:H5'	27:15:29:THR:HG21	1.81	0.61
23:21:46:LEU:HD13	23:21:61:ARG:HD3	1.83	0.61
30:28:28:GLY:O	30:28:36:LYS:NZ	2.29	0.61
25:13:10:LYS:NZ	25:13:15:TYR:OH	2.34	0.61
1:1A:2401:G:H5''	1:1A:2402:U:H5'	1.83	0.61
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.13	0.61
5:2F:195:ASP:OD1	5:2F:196:LEU:N	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1633:A:H2'	1:1A:1634:C:C6	2.36	0.60
1:1A:2889:C:OP2	61:1A:4144:HOH:O	2.16	0.60
8:1I:69:LYS:HG3	8:1I:138:ILE:HG12	1.81	0.60
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.16	0.60
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.36	0.60
1:2A:938:G:OP2	30:28:52:LYS:NZ	2.24	0.60
1:1A:1405:A:H2	1:1A:1418:U:O4	1.83	0.60
8:1I:116:LEU:HD21	8:1I:119:PRO:HA	1.83	0.60
1:2A:10:G:H1'	1:2A:2801(A):A:H62	1.66	0.60
1:2A:509:C:OP1	61:2A:3850:HOH:O	2.16	0.60
14:2S:11:LYS:HE3	14:2S:15:ARG:HH12	1.66	0.60
1:1A:2178:G:H2'	1:1A:2179:G:C2	2.36	0.60
1:2A:1309:G:H4'	29:27:7:PRO:HB2	1.82	0.60
6:2G:48:GLU:O	6:2G:51:ARG:NH1	2.34	0.60
1:1A:1109:G:N2	1:1A:1122:C:O2'	2.34	0.60
2:2B:45:A:O4'	6:2G:95:ARG:NH1	2.35	0.60
1:2A:1653:G:O6	13:2R:11:ASN:ND2	2.34	0.60
2:1B:113:G:N2	14:1S:45:GLY:O	2.26	0.60
1:1A:1040:C:OP1	16:1U:53:ARG:NH2	2.34	0.60
1:1A:2163:G:C4	1:1A:2164:C:H1'	2.36	0.60
1:2A:2250:G:C8	1:2A:2496:C:H5''	2.36	0.60
1:2A:952:G:OP1	12:2Q:16:ARG:NH2	2.34	0.60
1:1A:2801:C:OP1	4:1E:61:ARG:NH2	2.35	0.60
1:1A:639:G:N2	5:1F:44:ARG:O	2.34	0.60
5:2F:20:LEU:HD13	5:2F:125:LEU:HD22	1.83	0.60
5:1F:53:THR:HG22	5:1F:55:GLY:H	1.65	0.60
1:2A:1412:A:H2'	1:2A:1413:G:H8	1.67	0.60
7:2H:121:ILE:HD11	7:2H:140:LYS:HG2	1.83	0.60
1:2A:1423:G:P	10:2O:49:ARG:HH12	97.19	0.60
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.35	0.60
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.36	0.60
1:2A:1286:A:H8	1:2A:1287:A:H4'	8.01	0.60
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.20	0.60
1:2A:2342:C:O2'	1:2A:2374:C:OP1	2.19	0.60
21:2Z:124:ILE:HD13	21:2Z:163:LEU:HD11	1.84	0.60
1:1A:2457:G:OP1	5:1F:74:ARG:NH2	2.35	0.59
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.02	0.59
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.24	0.59
1:2A:816:C:OP2	61:2A:3854:HOH:O	2.17	0.59
7:2H:84:SER:HB3	7:2H:132:ARG:HH11	1.67	0.59
20:2Y:94:LYS:NZ	61:2Y:601:HOH:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1577:C:H42	1:1A:1586:G:H1	1.49	0.59
1:2A:2432:A:OP2	61:2A:3851:HOH:O	2.17	0.59
1:2A:2052:G:H4'	4:2E:143:ASN:O	2.02	0.59
5:2F:145:GLU:OE1	5:2F:145:GLU:N	2.35	0.59
12:2Q:57:HIS:HD2	12:2Q:117:ALA:HB2	1.67	0.59
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.35	0.59
1:2A:222:A:OP1	61:2A:3848:HOH:O	2.16	0.59
1:2A:900:A:O2'	1:2A:901:A:OP1	2.17	0.59
5:2F:149:ASP:OD1	5:2F:149:ASP:N	2.30	0.59
1:1A:1714:G:O2'	1:1A:2013:U:O4	2.19	0.59
11:1P:50:ARG:HD3	30:18:7:HIS:HD2	1.64	0.59
31:29:17:ILE:HD12	31:29:26:ILE:HD11	1.84	0.59
1:2A:2659:G:N7	61:2A:3917:HOH:O	2.31	0.59
1:2A:958:U:OP2	12:2Q:14:ARG:NH1	2.31	0.59
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.83	0.59
1:2A:800:A:OP1	1:2A:800:A:H8	1.86	0.59
13:2R:44:LEU:HD22	13:2R:48:VAL:HG23	1.85	0.59
16:2U:50:ARG:HH22	17:2V:72:VAL:HB	1.68	0.59
21:2Z:130:PRO:HA	21:2Z:133:ILE:HG13	1.84	0.59
1:1A:1539:C:N4	1:1A:2227:G:O2'	2.36	0.59
1:1A:2600:G:OP1	61:1A:4146:HOH:O	2.17	0.59
1:2A:2074:U:O4	61:2A:3839:HOH:O	2.14	0.59
1:2A:2291:U:OP1	1:2A:2380:C:O2'	2.21	0.59
1:1A:2140:U:H6	1:1A:2170:G:HO2'	1.51	0.59
1:1A:929:G:H1	1:1A:940:C:H42	1.51	0.59
1:2A:2375:G:N2	1:2A:2378:A:OP2	2.33	0.59
1:2A:740:U:OP1	61:2A:3856:HOH:O	2.17	0.59
7:2H:20:ALA:HB1	7:2H:21:PRO:HD2	1.85	0.59
7:2H:20:ALA:HB3	7:2H:23:ARG:HG3	1.84	0.59
11:2P:95:VAL:HG13	11:2P:125:VAL:HA	1.83	0.59
1:1A:1288:A:N1	11:1P:2:LYS:NZ	2.51	0.59
1:1A:1997:G:OP2	61:1A:4147:HOH:O	2.17	0.59
7:1H:97:ARG:NH2	7:1H:104:GLU:OE1	2.35	0.59
1:2A:1183:G:H5''	25:23:30:ARG:HH22	1.67	0.59
11:2P:50:ARG:HD3	30:28:7:HIS:HD2	1.68	0.59
1:2A:2690:C:OP2	13:2R:17:ARG:NH2	2.35	0.59
23:11:18:ILE:HG12	23:11:37:ILE:HG12	1.85	0.58
1:1A:1218:G:O2'	1:1A:1219:A:O4'	2.21	0.58
1:1A:2143:G:H1	1:1A:2199:C:N4	2.00	0.58
6:1G:101:ILE:HG22	6:1G:105:LYS:HE2	1.85	0.58
1:2A:271(G):C:H2'	1:2A:271(H):G:H8	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:5:LEU:HB2	21:2Z:47:VAL:HG21	1.85	0.58
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.36	0.58
23:21:51:VAL:HG11	23:21:74:VAL:HG21	1.84	0.58
1:2A:455:C:N4	1:2A:476:G:O6	20.06	0.58
1:2A:908:C:OP2	12:2Q:22:LYS:NZ	2.33	0.58
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.85	0.58
1:1A:532:A:H2	1:1A:1206:G:H21	76.23	0.58
1:1A:556:C:O2	61:1A:4136:HOH:O	2.14	0.58
16:1U:46:ALA:O	16:1U:50:ARG:HG2	2.04	0.58
1:2A:796:C:H2'	1:2A:797:C:C6	2.38	0.58
25:13:7:LYS:HB2	25:13:34:GLU:HG2	1.85	0.58
1:1A:2260:C:OP2	61:1A:4149:HOH:O	2.17	0.58
23:11:51:VAL:HG11	23:11:74:VAL:HG21	1.86	0.58
1:2A:1007:C:N3	1:2A:1022:G:O6	16.40	0.58
1:1A:173:C:H2'	1:1A:174:U:C6	2.38	0.58
6:1G:34:LEU:HD23	6:1G:161:THR:HG22	1.85	0.58
5:1F:188:ARG:HA	11:1P:3:LEU:HD11	1.85	0.58
1:2A:1371:G:N7	61:2A:3931:HOH:O	2.32	0.58
1:2A:662:G:O2'	1:2A:836:G:OP1	26.21	0.58
8:2I:48:GLU:HB3	8:2I:52:ARG:HH12	1.69	0.58
16:2U:28:ARG:NH1	16:2U:38:THR:OG1	2.35	0.58
1:1A:1305:G:N2	1:1A:1331:G:H1'	39.90	0.58
1:1A:2205:C:H2'	1:1A:2206:G:H8	1.67	0.58
1:1A:223:C:H2'	1:1A:224:U:H6	1.68	0.58
14:1S:39:ILE:HB	14:1S:49:VAL:HG13	1.85	0.58
1:2A:878:A:N6	1:2A:900:A:N7	2.51	0.58
1:2A:1468:C:OP1	61:2A:3852:HOH:O	2.17	0.58
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.67	0.58
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.39	0.58
1:2A:290:G:H1	1:2A:350:U:H3	1.52	0.58
1:1A:713:G:N2	30:18:2:PRO:O	2.37	0.58
27:25:33:CYS:HB2	27:25:40:LYS:HD3	1.86	0.58
1:2A:1023:U:OP2	61:2A:3817:HOH:O	2.17	0.58
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.85	0.57
1:1A:1832:G:OP2	3:1D:154:LYS:NZ	2.35	0.57
1:2A:1697:G:OP2	1:2A:1698:A:O2'	2.19	0.57
1:2A:223:A:O2'	1:2A:420:C:O2	2.22	0.57
1:2A:922:U:O2'	22:20:29:GLN:NE2	2.36	0.57
9:2N:30:ILE:HG22	9:2N:34:LEU:HD22	1.84	0.57
1:1A:1111:U:H1'	1:1A:1120:G:C2	2.39	0.57
1:1A:1639:G:H2'	1:1A:1640:G:C8	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1532:C:H41	1:2A:1537:G:H1	1.51	0.57
1:2A:1813:G:O6	61:2A:3858:HOH:O	2.17	0.57
8:2I:140:LEU:HD22	8:2I:142:VAL:HG22	1.86	0.57
10:2O:9:GLU:OE2	10:2O:18:LYS:NZ	2.37	0.57
19:2X:60:ARG:HH22	29:27:47:ARG:HH12	1.52	0.57
1:2A:1751:C:HO2'	1:2A:2861:G:HO2'	1.50	0.57
6:2G:11:TYR:HA	6:2G:15:VAL:HB	1.86	0.57
9:2N:30:ILE:O	9:2N:34:LEU:N	2.32	0.57
22:10:27:GLU:HG3	22:10:68:GLU:HA	1.85	0.57
1:1A:1121:C:H2'	1:1A:1122:C:H5'	1.86	0.57
1:1A:223:C:H2'	1:1A:224:U:C6	2.39	0.57
1:2A:2129:C:H5'	1:2A:2130:U:OP2	2.04	0.57
9:2N:20:GLY:HA2	9:2N:61:ARG:HG3	1.85	0.57
21:2Z:138:GLU:H	21:2Z:156:LYS:HE2	1.70	0.57
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.87	0.57
24:12:14:ARG:O	24:12:67:LYS:NZ	2.37	0.57
5:1F:51:THR:HB	5:1F:88:VAL:HG11	1.87	0.57
1:2A:2625:G:O6	61:2A:3843:HOH:O	2.15	0.57
6:2G:29:TRP:O	6:2G:33:ARG:NH1	2.36	0.57
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	1.87	0.57
17:2V:46:VAL:HG23	17:2V:52:VAL:HG11	1.87	0.57
1:1A:166:G:H2'	1:1A:167:G:C8	3.93	0.57
1:2A:1469:A:OP2	61:2A:3855:HOH:O	2.17	0.57
1:2A:1658:C:OP1	61:2A:3859:HOH:O	2.17	0.57
1:2A:2140:C:H1'	1:2A:2152:G:N2	2.19	0.57
1:2A:863:A:H2'	1:2A:864:G:H8	1.69	0.57
4:2E:14:ILE:HG13	4:2E:21:VAL:HG13	1.86	0.57
1:1A:1435:G:H2'	1:1A:1436:U:C6	3.10	0.57
1:1A:742:G:OP1	1:1A:1426:G:O2'	2.18	0.57
1:2A:1237:A:OP1	61:2A:3863:HOH:O	2.18	0.57
1:2A:947:G:OP2	61:2A:3861:HOH:O	2.18	0.57
13:2R:33:ARG:NH1	13:2R:115:GLU:OE1	2.36	0.57
1:1A:1711:A:OP1	61:1A:4106:HOH:O	2.17	0.57
1:1A:2339:A:H2'	1:1A:2340:A:C8	2.40	0.57
2:1B:88:C:H2'	2:1B:89:G:O4'	2.04	0.57
1:2A:2746:U:OP1	7:2H:85:LYS:NZ	2.29	0.57
1:1A:1342:G:OP1	1:1A:2721:G:O2'	2.16	0.57
1:2A:2375:G:O2'	1:2A:2377:A:N7	2.28	0.57
1:2A:1783:A:HO2'	1:2A:2607:G:HO2'	1.52	0.57
58:2A:3746:EZG:ND1	61:2A:3933:HOH:O	2.33	0.57
22:20:63:VAL:HG21	22:20:83:PRO:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:37:LEU:HD21	12:1Q:130:LYS:HE2	1.87	0.56
23:21:53:VAL:HG22	23:21:74:VAL:HG13	1.86	0.56
1:2A:2498:C:H3'	61:2A:3829:HOH:O	2.03	0.56
1:2A:516:C:OP1	27:25:13:LYS:NZ	2.34	0.56
4:2E:76:ARG:NH1	61:2E:403:HOH:O	2.38	0.56
8:2I:38:LEU:HB2	8:2I:40:THR:HG23	1.86	0.56
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.87	0.56
1:1A:493:G:OP1	29:17:33:ARG:NH1	2.38	0.56
1:1A:1159:U:H2'	1:1A:1160:G:C8	2.40	0.56
1:1A:2104:A:H5'	61:1A:4178:HOH:O	2.05	0.56
1:1A:2157:A:H5'	1:1A:2182:G:H4'	1.87	0.56
1:1A:297:C:H2'	1:1A:298:G:H8	1.71	0.56
22:20:10:THR:HG22	22:20:12:ASN:N	2.20	0.56
30:28:6:THR:HG22	30:28:63:PRO:HD2	1.87	0.56
1:2A:1530:C:N4	1:2A:1539:G:H1	2.03	0.56
2:2B:24:G:N7	2:2B:56:G:H2'	2.20	0.56
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.41	0.56
1:1A:166:G:H2'	1:1A:167:G:H8	3.54	0.56
1:1A:174:U:H2'	1:1A:175:G:H8	1.70	0.56
1:2A:1639:U:H2'	1:2A:1640:C:H5''	1.88	0.56
2:2B:72:G:O2'	2:2B:105:A:N6	2.37	0.56
1:1A:1217:G:OP2	1:1A:1219:A:N6	2.38	0.56
1:1A:2507:G:H5''	12:1Q:82:ARG:HG2	1.87	0.56
26:24:41:PRO:HG3	26:24:49:PHE:CZ	2.40	0.56
1:2A:2461:C:H2'	1:2A:2462:U:C6	2.40	0.56
1:2A:639:U:H2'	1:2A:640:C:C6	2.40	0.56
1:2A:861:A:N3	2:2B:79:C:O2'	2.38	0.56
1:1A:1151:U:H2'	1:1A:1152:G:H8	1.71	0.56
1:1A:2642:G:H2'	1:1A:2643:G:C8	2.40	0.56
1:1A:532:A:N6	1:1A:1206:G:O2'	79.79	0.56
2:1B:8:U:OP1	14:1S:15:ARG:NH2	2.38	0.56
1:2A:1310:G:H2'	1:2A:1311:G:C8	3.86	0.56
1:2A:27:G:O2'	1:2A:28:A:OP2	2.23	0.56
7:2H:45:VAL:HG12	7:2H:50:VAL:HG22	1.86	0.56
1:1A:1716:A:OP2	61:1A:4122:HOH:O	2.18	0.56
1:1A:692:C:N4	1:1A:698:G:H1	2.04	0.56
13:1R:44:LEU:HD22	13:1R:48:VAL:HG23	1.88	0.56
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.38	0.56
1:2A:1599:C:OP1	61:2A:3857:HOH:O	2.17	0.56
1:2A:218:A:OP2	61:2A:3862:HOH:O	2.18	0.56
6:2G:170:ARG:O	6:2G:174:GLU:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2367:C:H1'	22:10:39:ARG:HH21	1.70	0.56
1:2A:2121:G:H1	1:2A:2177:C:H42	1.52	0.56
21:2Z:47:VAL:O	21:2Z:50:GLN:NE2	2.39	0.56
1:1A:2177:G:H3'	1:1A:2178:G:C8	2.41	0.56
1:1A:655:G:OP2	30:18:15:LYS:NZ	2.35	0.56
20:1Y:92:ASN:N	20:1Y:93:GLY:HA2	2.19	0.56
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.41	0.56
4:2E:143:ASN:HD22	4:2E:147:PRO:HD3	1.71	0.56
18:2W:88:ARG:NH1	18:2W:94:ASP:OD2	2.36	0.56
21:2Z:92:SER:O	21:2Z:130:PRO:HG3	2.06	0.56
1:1A:1552:C:H2'	1:1A:1553:A:C8	2.41	0.56
1:1A:559:U:H2'	1:1A:560:C:C6	2.41	0.56
1:1A:347:G:C8	5:1F:171:PRO:HG3	2.41	0.56
1:2A:1508:A:H4'	1:2A:1509(A):A:C5	2.41	0.56
1:2A:882:G:H2'	1:2A:883:G:H8	1.70	0.56
1:1A:2348:A:H61	22:10:43:THR:CG2	2.19	0.55
5:1F:12:LEU:HB3	5:1F:126:VAL:HG12	1.88	0.55
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.05	0.55
8:1I:79:ILE:HB	8:1I:144:VAL:HG12	1.87	0.55
1:1A:1051:C:O2'	9:1N:28:THR:HG21	2.06	0.55
23:21:50:ARG:HG2	23:21:59:THR:HG22	1.87	0.55
1:2A:108:U:H2'	1:2A:109:G:H8	1.71	0.55
1:2A:1270:C:H2'	1:2A:1271:G:C8	6.68	0.55
1:2A:484:C:H2'	1:2A:485:C:H6	1.71	0.55
5:2F:185:ASP:OD1	5:2F:188:ARG:NH1	2.34	0.55
1:1A:122:G:OP1	1:1A:1422:C:O2'	2.15	0.55
1:1A:2584:A:C8	4:1E:144:ARG:HD3	2.41	0.55
1:2A:265:A:C8	1:2A:266:G:H1'	2.40	0.55
1:1A:2291:G:O6	22:10:14:ARG:HG3	2.07	0.55
28:16:35:GLU:OE2	28:16:50:ARG:NH1	2.39	0.55
1:1A:2158:C:H42	1:1A:2177:G:H1	0.63	0.55
8:1I:47:LEU:HG	8:1I:51:ILE:HD11	1.88	0.55
2:2B:43:C:H5''	26:24:1:MET:HG2	1.87	0.55
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.07	0.55
2:2B:83:G:H1	2:2B:94:C:H42	1.54	0.55
1:2A:1155:A:H5''	16:2U:55:ARG:NH1	2.21	0.55
1:1A:2153:G:N2	1:1A:2180:A:N1	2.55	0.55
1:1A:2658:C:OP2	1:1A:2745:G:O2'	2.19	0.55
6:1G:45:GLU:OE2	61:1G:3102:HOH:O	2.17	0.55
8:1I:65:ALA:O	8:1I:69:LYS:N	2.39	0.55
19:1X:56:THR:O	61:1X:201:HOH:O	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.41	0.55
1:2A:1266:G:N2	1:2A:1269:A:N7	9.96	0.55
1:2A:2882:A:H5'	13:2R:96:ARG:HG3	1.87	0.55
4:2E:179:GLU:HG3	15:2T:9:LEU:HD21	1.87	0.55
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.36	0.55
1:2A:602:G:O2'	1:2A:655:A:N6	2.39	0.55
5:2F:120:GLU:HG3	5:2F:122:LYS:HG2	1.89	0.55
1:1A:2101:U:O3'	23:11:35:THR:OG1	2.25	0.55
1:1A:71:U:OP1	61:1A:4148:HOH:O	2.17	0.55
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.87	0.55
14:2S:28:VAL:HG11	14:2S:98:VAL:HG13	1.88	0.55
6:1G:145:THR:HG23	6:1G:148:MET:HG2	1.89	0.55
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.88	0.55
9:1N:108:PRO:O	9:1N:113:GLY:HA3	2.07	0.55
21:2Z:166:SER:O	21:2Z:168:GLU:N	2.39	0.55
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.89	0.55
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.21	0.55
1:1A:1068:G:OP2	1:1A:1068:G:H8	6.89	0.55
1:1A:1320:A:N3	1:1A:1343:C:H1'	2.22	0.55
1:1A:2442:A:H2'	1:1A:2442:A:N3	2.22	0.55
1:1A:2732:G:OP2	61:1A:4153:HOH:O	2.18	0.55
1:1A:879:G:H5'	11:1P:45:LEU:HD21	1.89	0.55
1:2A:2393:A:H5''	11:2P:63:PRO:HB3	1.89	0.55
1:2A:2489:G:N2	1:2A:2491:U:O4	2.32	0.55
1:2A:652(D):C:H42	1:2A:652(U):G:H1	1.54	0.55
1:1A:1100:A:N6	1:1A:1151:U:N3	2.35	0.55
1:2A:111:A:O2'	24:22:65:ASN:ND2	2.34	0.55
5:2F:25:PRO:HD2	5:2F:115:ALA:HB2	1.89	0.55
12:2Q:17:LEU:HD21	12:2Q:41:TRP:NE1	2.21	0.55
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.87	0.55
1:1A:1484:U:O2	1:1A:1602:G:N2	2.41	0.54
5:2F:53:THR:HG22	5:2F:56:GLU:HG3	1.88	0.54
14:2S:58:LEU:HD12	14:2S:65:VAL:HG13	1.89	0.54
22:10:38:VAL:HB	22:10:59:LEU:HB2	1.89	0.54
1:1A:2129:C:H42	1:1A:2204:G:H1	1.54	0.54
6:1G:83:ARG:O	6:1G:86:MET:HG3	2.07	0.54
7:1H:148:ILE:HA	7:1H:151:ILE:HD12	1.89	0.54
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.08	0.54
1:2A:2141:G:H2'	1:2A:2142:C:O4'	2.07	0.54
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.43	0.54
1:2A:632:A:H2'	1:2A:633:A:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:656:G:H2'	1:2A:657:U:O4'	2.06	0.54
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.89	0.54
15:2T:122:ASP:O	15:2T:126:ALA:N	2.36	0.54
1:1A:2545:A:H2'	1:1A:2546:A:O4'	2.06	0.54
1:1A:2602:A:O3'	3:1D:239:ARG:NH2	2.40	0.54
1:1A:2713:C:OP1	61:1A:4151:HOH:O	2.18	0.54
1:1A:650:G:O6	11:1P:107:LYS:NZ	2.40	0.54
1:2A:2089:U:H3	1:2A:2230:G:H1	1.54	0.54
1:2A:740:U:H2'	1:2A:741:G:C8	2.41	0.54
2:2B:14:U:O3'	2:2B:108:U:O2'	2.23	0.54
1:1A:1105:G:H2'	1:1A:1106:U:C5	2.43	0.54
1:1A:1829:U:H5'	3:1D:259:THR:CG2	2.36	0.54
12:1Q:51:ARG:HD3	12:1Q:66:ILE:HD11	1.89	0.54
1:2A:2357:U:P	22:20:20:ARG:HE	2.30	0.54
1:2A:2357:U:OP1	22:20:20:ARG:NE	2.34	0.54
15:2T:24:PRO:HA	15:2T:49:VAL:HG23	1.89	0.54
23:11:89:GLU:O	23:11:93:GLU:HG2	2.07	0.54
1:1A:1115:A:H2'	1:1A:1119:A:N7	2.23	0.54
1:1A:2650:G:P	4:1E:82:ARG:HH12	2.31	0.54
1:2A:1183:G:H5''	25:23:30:ARG:NH2	2.23	0.54
1:2A:2128:C:H2'	1:2A:2129:C:O4'	2.06	0.54
1:2A:863:A:H2'	1:2A:864:G:C8	2.42	0.54
1:1A:1346:U:H4'	1:1A:1347:A:H5''	1.88	0.54
1:1A:1514:C:OP2	1:1A:1593:C:O2'	2.25	0.54
1:1A:1904:C:H2'	1:1A:1905:G:O4'	2.08	0.54
1:1A:542:C:OP1	27:15:16:ARG:NH2	2.41	0.54
29:27:34:ARG:HB2	29:27:42:LEU:HD22	1.89	0.54
1:2A:108:U:H2'	1:2A:109:G:C8	2.43	0.54
1:2A:2572:A:OP1	1:2A:2574:G:O2'	2.26	0.54
1:2A:686:G:H8	29:27:6:GLN:O	1.91	0.54
1:2A:922:U:H2'	1:2A:923:C:C6	2.43	0.54
7:1H:24:VAL:HG22	7:1H:35:VAL:HB	1.90	0.54
1:2A:1187:G:OP2	1:2A:1187:G:H8	1.90	0.54
1:2A:624:C:OP1	61:2A:3860:HOH:O	2.17	0.54
1:1A:798:A:OP1	61:1A:4150:HOH:O	2.18	0.54
19:2X:60:ARG:HH22	29:27:47:ARG:NH1	2.05	0.54
10:1O:38:VAL:HG13	10:1O:87:ILE:HD11	1.90	0.54
1:1A:2307:C:OP1	14:1S:10:ARG:NH1	2.40	0.54
7:2H:25:LYS:HB3	7:2H:27:LYS:HZ1	1.72	0.54
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.40	0.54
28:16:9:LEU:HD13	28:16:51:GLU:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1347:A:O2'	1:1A:1348:A:H3'	2.06	0.54
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.08	0.54
1:2A:2649:U:H2'	1:2A:2650:U:C6	2.43	0.54
1:2A:624:C:H2'	1:2A:625:G:H8	2.94	0.54
31:19:2:LYS:HE2	31:19:31:LYS:O	2.07	0.53
1:1A:2130:C:H2'	1:1A:2131:U:H6	1.73	0.53
1:1A:586:G:H22	1:1A:601:A:H2	1.56	0.53
11:1P:124:LYS:HA	11:1P:144:GLU:HB3	1.91	0.53
24:22:24:LEU:HD23	24:22:60:LEU:HD21	1.88	0.53
1:2A:1286:A:C8	1:2A:1287:A:H4'	8.12	0.53
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.08	0.53
1:2A:2483:C:N3	12:2Q:124:LYS:NZ	2.55	0.53
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.90	0.53
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.24	0.53
1:2A:2786:U:OP1	4:2E:69:LYS:NZ	2.34	0.53
22:10:38:VAL:HG12	22:10:40:GLN:HG2	1.91	0.53
29:17:21:ARG:NH1	61:17:5001:HOH:O	2.31	0.53
1:1A:715:G:H5'	1:1A:716:G:OP2	2.09	0.53
13:1R:59:ASP:N	13:1R:59:ASP:OD1	2.42	0.53
25:23:23:LEU:HD13	25:23:50:VAL:HG11	1.90	0.53
1:2A:2495:G:H5''	12:2Q:82:ARG:HG2	1.90	0.53
21:2Z:40:ASP:OD2	21:2Z:43:GLU:N	2.21	0.53
1:1A:174:U:H2'	1:1A:175:G:C8	2.43	0.53
1:1A:346:A:OP1	5:1F:168:ARG:HD2	2.08	0.53
4:1E:111:ARG:HD2	4:1E:160:TYR:CD2	2.44	0.53
7:1H:86:GLU:HB3	7:1H:165:ALA:HB2	1.89	0.53
1:2A:784:A:C5	3:2D:229:VAL:HG11	2.44	0.53
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.07	0.53
1:1A:768:C:H2'	1:1A:769:A:C8	2.44	0.53
6:1G:11:TYR:HA	6:1G:15:VAL:HB	1.89	0.53
15:1T:29:ARG:HG3	15:1T:46:GLU:HB2	1.91	0.53
15:1T:65:LYS:HE3	15:1T:67:SER:HB2	1.90	0.53
23:21:83:GLU:N	23:21:83:GLU:OE1	2.41	0.53
1:2A:1441:G:O2'	61:2A:3864:HOH:O	2.18	0.53
1:2A:566:U:H5''	11:2P:29:LYS:HE3	1.91	0.53
1:2A:568:U:H5'	1:2A:945:A:N1	2.23	0.53
21:2Z:55:HIS:CE1	21:2Z:135:GLU:HG3	2.44	0.53
1:1A:1825:U:H2'	1:1A:1826:C:C6	2.43	0.53
26:24:46:GLN:NE2	26:24:48:ARG:HD3	2.24	0.53
29:27:34:ARG:HH21	29:27:39:ARG:HG2	1.74	0.53
1:2A:1125:G:H5'	31:29:37:GLY:HA2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.43	0.53
1:2A:2137:C:O2'	1:2A:2138:C:OP2	2.25	0.53
1:2A:266:G:H5''	1:2A:268:C:H41	11.64	0.53
14:2S:11:LYS:HG3	14:2S:91:PRO:HD3	1.90	0.53
1:1A:664:U:H2'	1:1A:665:C:C6	2.44	0.53
8:1I:101:LEU:HG	8:1I:107:VAL:HB	1.88	0.53
26:24:60:GLN:O	26:24:62:ARG:NH1	2.41	0.53
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.44	0.53
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.44	0.53
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.08	0.53
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.35	0.53
1:1A:1387:U:O2	19:1X:80:ILE:HD12	2.08	0.53
1:1A:2586:G:OP1	61:1A:4155:HOH:O	2.19	0.53
3:1D:68:LYS:HD3	3:1D:70:TRP:CH2	2.44	0.53
6:1G:126:ASP:HB3	6:1G:130:ASN:HB2	1.91	0.53
11:1P:126:VAL:HG12	11:1P:148:LEU:HD23	1.90	0.53
13:1R:28:LEU:HD23	13:1R:48:VAL:HG21	1.90	0.53
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.08	0.53
1:2A:2807:G:H22	1:2A:2893:G:H1	1.57	0.53
1:2A:848:G:H2'	1:2A:849:A:C8	2.42	0.53
24:12:28:LYS:HD2	24:12:53:LEU:HD21	1.91	0.53
26:14:53:GLU:HB2	26:14:55:ARG:HA	1.91	0.53
1:1A:2504:U:H2'	1:1A:2505:U:C6	2.44	0.53
4:1E:121:ASN:ND2	61:1E:403:HOH:O	2.34	0.53
6:2G:108:ASN:HA	26:24:37:SER:HB2	1.90	0.53
1:2A:1824:G:N3	3:2D:254:THR:OG1	2.42	0.53
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.90	0.53
5:2F:133:ASN:N	5:2F:138:GLU:OE1	2.42	0.53
1:1A:302:A:O2'	1:1A:303:C:OP1	2.25	0.53
1:2A:271(G):C:H2'	1:2A:271(H):G:C8	2.43	0.53
1:1A:1123:A:H2'	1:1A:1124:U:H4'	1.90	0.52
1:1A:1291:G:OP1	11:1P:13:ASN:ND2	2.29	0.52
2:1B:65:C:HO2'	2:1B:66:A:P	2.31	0.52
2:1B:79:C:H2'	2:1B:80:U:O4'	2.09	0.52
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.09	0.52
22:20:40:GLN:HE21	22:20:57:PHE:HB3	1.73	0.52
1:2A:261:G:HO2'	1:2A:610:G:HO2'	1.53	0.52
11:2P:38:GLN:HG2	11:2P:45:LEU:H	1.74	0.52
12:2Q:1:MET:HG3	12:2Q:44:ALA:HB1	1.91	0.52
1:1A:1006:C:H42	1:1A:1023:G:H1	21.37	0.52
1:1A:149:A:H2'	1:1A:150:C:C6	2.80	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1825:U:H2'	1:1A:1826:C:H6	1.74	0.52
1:1A:2153:G:H5''	1:1A:2154:U:H3'	1.91	0.52
1:1A:906:G:O2'	1:1A:962:G:O6	2.16	0.52
4:1E:174:ASP:OD1	4:1E:175:VAL:N	2.42	0.52
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.44	0.52
1:2A:2507:C:H5''	1:2A:2573:C:N4	2.24	0.52
7:2H:33:LEU:HD11	7:2H:136:ILE:HG22	1.92	0.52
21:2Z:28:MET:HE1	21:2Z:61:LEU:HD21	1.91	0.52
1:1A:1425:A:H4'	1:1A:1426:G:OP2	2.10	0.52
1:1A:1814:A:H5'	1:1A:2620:G:H4'	1.91	0.52
5:1F:123:LEU:HD13	5:1F:192:LEU:HB3	1.90	0.52
7:1H:24:VAL:O	7:1H:35:VAL:N	2.39	0.52
9:1N:42:TRP:CH2	9:1N:44:PRO:HB3	2.44	0.52
26:24:61:ARG:NH1	26:24:62:ARG:O	2.43	0.52
1:2A:184:C:H2'	1:2A:185:U:C6	2.45	0.52
1:2A:517:C:OP2	27:25:13:LYS:HE2	2.09	0.52
3:2D:274:ARG:O	3:2D:275:LYS:HD2	2.09	0.52
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.90	0.52
10:2O:53:LYS:N	10:2O:56:ASP:OD2	2.38	0.52
10:2O:88:ASN:ND2	10:2O:92:GLU:OE1	2.40	0.52
16:2U:113:ALA:O	16:2U:117:GLN:HG2	2.08	0.52
29:17:12:ARG:NH2	29:17:44:PRO:HB3	2.24	0.52
1:1A:1108:G:H1	1:1A:1123:A:N6	2.07	0.52
1:1A:768:C:H2'	1:1A:769:A:H8	1.75	0.52
2:2B:15:A:H5''	2:2B:16:G:H8	1.73	0.52
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.74	0.52
1:1A:1154:U:H2'	1:1A:1155:C:O4'	2.10	0.52
1:1A:2176:G:C2	1:1A:2177:G:H1'	2.45	0.52
1:1A:957:A:H2'	12:1Q:9:TYR:OH	2.08	0.52
11:2P:52:GLU:HG3	30:28:57:ARG:HH22	1.74	0.52
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.09	0.52
1:2A:2116:G:N7	1:2A:2166:G:N2	2.57	0.52
1:2A:2168:G:H8	1:2A:2170:A:N7	2.07	0.52
1:2A:2206:G:H8	1:2A:2207:G:N7	2.08	0.52
1:2A:1012:U:O2	9:2N:25:ARG:NH1	2.43	0.52
12:2Q:30:GLY:O	12:2Q:134:ARG:NH1	2.43	0.52
1:1A:2152:U:H2'	1:1A:2180:A:N1	2.25	0.52
3:1D:71:ASP:HB3	3:1D:103:ARG:HH12	1.74	0.52
8:1I:70:GLU:O	8:1I:74:ASN:HB2	2.09	0.52
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.90	0.52
2:2B:43:C:OP1	26:24:6:HIS:NE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2233:U:H2'	1:2A:2234:G:C8	2.44	0.52
1:2A:315:G:H2'	1:2A:316:C:C6	2.45	0.52
1:2A:668:G:H5'	1:2A:669:G:OP2	2.10	0.52
9:2N:116:LEU:O	9:2N:119:ARG:N	2.39	0.52
24:12:9:GLN:HE21	24:12:60:LEU:HD21	1.74	0.52
1:1A:308:U:H2'	1:1A:309:C:C6	2.45	0.52
1:1A:645:G:N3	1:1A:645:G:H5'	2.25	0.52
2:1B:33:G:H5'	6:1G:2:PRO:HD3	1.91	0.52
5:1F:133:ASN:N	5:1F:138:GLU:OE1	2.31	0.52
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.45	0.52
1:2A:2155:G:C5	1:2A:2156:G:H1'	2.44	0.52
7:2H:3:ARG:HG2	7:2H:6:ARG:HE	1.75	0.52
26:14:16:CYS:SG	26:14:17:GLY:N	2.82	0.52
1:1A:1223:C:H2'	1:1A:1224:C:H6	1.74	0.52
1:1A:2082:A:OP1	61:1A:4156:HOH:O	2.19	0.52
1:1A:2130:C:H2'	1:1A:2131:U:C6	2.45	0.52
1:1A:407:U:H2'	1:1A:408:G:H8	1.75	0.52
12:1Q:30:GLY:HA2	12:1Q:107:ALA:HB2	1.90	0.52
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.44	0.52
1:2A:920:G:H2'	1:2A:921:G:H8	1.75	0.52
14:2S:10:ARG:O	14:2S:14:VAL:HG12	2.10	0.52
7:1H:33:LEU:HD21	7:1H:136:ILE:HG13	1.92	0.52
8:1I:10:GLU:O	8:1I:12:LEU:N	2.43	0.52
10:1O:120:GLU:HG2	10:1O:122:LEU:HG	1.92	0.52
1:2A:1991:U:H2'	1:2A:1992:G:H5''	1.91	0.52
1:2A:2095:C:H2'	1:2A:2096:U:O4'	2.09	0.52
10:2O:7:TYR:CE1	10:2O:20:MET:HB2	2.45	0.52
1:2A:300:A:P	20:2Y:86:ARG:HH21	2.33	0.52
1:1A:1021:G:O2'	1:1A:1202:A:N1	2.38	0.52
1:1A:606:G:N2	1:1A:632:A:N7	49.61	0.52
9:1N:62:VAL:HG21	9:1N:66:LYS:HB2	1.92	0.52
1:2A:774:A:N3	1:2A:774:A:H2'	2.25	0.52
6:2G:41:GLN:HB3	6:2G:43:LEU:HD22	1.92	0.52
1:2A:335:C:H4'	20:2Y:73:ARG:HD3	1.92	0.52
1:1A:1451:U:H2'	1:1A:1452:U:C6	2.46	0.51
1:1A:1735:U:O2	1:1A:1747:A:H5'	2.10	0.51
1:1A:2717:A:O2'	1:1A:2862:G:OP1	2.21	0.51
9:1N:62:VAL:HG23	9:1N:66:LYS:HD2	1.91	0.51
16:2U:110:VAL:HG12	16:2U:114:LYS:HE3	1.92	0.51
1:1A:1233:U:H4'	17:1V:79:VAL:HG22	1.92	0.51
1:1A:1338:U:H2'	1:1A:1339:C:C6	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1846:A:OP2	3:1D:54:ARG:NH2	2.43	0.51
4:1E:11:MET:HG2	4:1E:24:THR:HB	1.91	0.51
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	1.92	0.51
2:2B:19:G:H2'	2:2B:20:C:O4'	2.09	0.51
7:2H:8:PRO:O	7:2H:69:ARG:NH2	2.41	0.51
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.92	0.51
1:1A:1055:A:OP2	61:1A:4120:HOH:O	2.19	0.51
1:1A:2175:G:H2'	1:1A:2176:G:C8	2.45	0.51
1:1A:2376:C:H2'	1:1A:2377:G:O4'	2.11	0.51
1:1A:2564:2MU:O5'	1:1A:2564:2MU:H6	2.10	0.51
4:1E:77:ILE:HG12	4:1E:195:LEU:HD22	1.92	0.51
6:1G:41:GLN:HG2	6:1G:154:GLY:O	2.11	0.51
1:2A:2127:G:C2	1:2A:2161:C:N3	2.78	0.51
1:2A:2238:G:N3	1:2A:2238:G:H2'	2.26	0.51
1:2A:271(Q):G:H2'	1:2A:271(R):G:H8	1.76	0.51
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.44	0.51
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.92	0.51
9:2N:99:LEU:O	9:2N:103:VAL:HG23	2.10	0.51
17:2V:50:PRO:HG2	17:2V:51:VAL:HG12	1.92	0.51
1:1A:207:A:C2	1:1A:224:U:H4'	2.45	0.51
1:1A:2340:A:H2'	1:1A:2341:G:C8	2.46	0.51
1:1A:2044:U:O2'	1:1A:2629:C:H5'	2.11	0.51
1:1A:2858:G:H1'	1:1A:2877:G:N2	2.25	0.51
10:1O:73:ASP:HB2	15:1T:82:LEU:HD13	1.93	0.51
15:1T:112:ARG:HG3	15:1T:115:ARG:NH2	2.26	0.51
1:1A:24:G:O2'	18:1W:78:GLU:O	2.25	0.51
21:1Z:53:ILE:HG22	21:1Z:71:VAL:HG12	1.92	0.51
1:2A:1882:C:H5''	23:21:26:ARG:HH21	1.76	0.51
1:2A:1467:C:C5	1:2A:1546:C:H2'	2.44	0.51
1:2A:2134:A:HO2'	1:2A:2159:G:N2	2.08	0.51
1:2A:2723:C:OP2	4:2E:109:LYS:NZ	2.44	0.51
1:2A:882:G:N2	1:2A:895:U:O2	2.42	0.51
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.43	0.51
1:1A:1518:A:OP2	1:1A:1567:G:N1	2.37	0.51
1:1A:1705:C:OP1	4:1E:135:HIS:NE2	2.44	0.51
1:2A:2019:A:N7	27:25:9:LYS:HE2	2.25	0.51
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.45	0.51
1:2A:330:A:H2	1:2A:1210:A:HO2'	1.57	0.51
7:2H:90:LYS:HE2	7:2H:159:GLU:HG2	1.91	0.51
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.92	0.51
20:2Y:9:LYS:NZ	20:2Y:28:LYS:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2162:C:H2'	1:1A:2163:G:C8	2.46	0.51
1:1A:2851:C:H2'	1:1A:2852:G:H8	1.75	0.51
1:2A:1226:A:OP1	17:2V:84:LYS:NZ	2.26	0.51
1:2A:2025:C:H2'	1:2A:2026:C:C6	2.46	0.51
1:2A:305:U:H2'	1:2A:306:U:C6	2.46	0.51
1:2A:27:G:N2	1:2A:512:G:H1'	2.25	0.51
1:2A:605:C:O2	1:2A:657:U:O2'	2.23	0.51
20:2Y:1:MET:HE3	20:2Y:2:ARG:H	1.75	0.51
1:1A:2495:C:N3	12:1Q:124:LYS:NZ	2.58	0.51
1:1A:313:A:H2'	1:1A:314:G:O4'	2.10	0.51
8:1I:25:TYR:O	8:1I:29:TYR:HB3	2.09	0.51
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.29	0.51
28:26:10:LEU:HG	28:26:54:ILE:HG13	1.92	0.51
1:2A:1011:G:H1	1:2A:1018:C:H42	17.56	0.51
1:2A:1261:C:OP2	18:2W:83:LYS:NZ	2.27	0.51
1:2A:484:C:H2'	1:2A:485:C:C6	2.46	0.51
1:2A:909:A:C6	1:2A:912:C:C2	2.99	0.51
1:2A:2203:U:H4'	3:2D:151:LYS:HG2	1.93	0.51
15:2T:28:VAL:HG13	15:2T:86:ILE:HG23	1.92	0.51
22:10:70:GLN:OE1	22:10:80:HIS:NE2	2.42	0.51
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.91	0.51
1:1A:1121:C:C2'	1:1A:1122:C:H5'	2.40	0.51
1:1A:2153:G:OP1	1:1A:2154:U:O2'	2.19	0.51
1:1A:721:G:O2'	5:1F:74:ARG:HD3	2.10	0.51
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.44	0.51
7:2H:89:ILE:HG12	7:2H:162:ILE:HG12	1.92	0.51
8:2I:65:ALA:O	8:2I:69:LYS:N	2.42	0.51
1:2A:2406:U:C2	11:2P:72:PRO:HG2	2.46	0.51
1:1A:2762:A:OP1	7:1H:3:ARG:NH1	2.44	0.51
1:1A:388:A:H3'	1:1A:389:G:H8	1.75	0.51
13:1R:24:GLN:HE22	13:1R:36:THR:HG21	1.76	0.51
2:1B:8:U:O3'	14:1S:25:ARG:NH2	2.44	0.51
1:1A:2034:G:OP1	18:1W:11:ARG:NH2	2.44	0.51
1:2A:1159:U:O2'	1:2A:1160:G:OP2	4.78	0.51
1:2A:1270:C:H2'	1:2A:1271:G:H8	6.03	0.51
1:2A:2149:G:C2	1:2A:2150:U:H1'	2.46	0.51
1:2A:566:U:OP1	17:2V:80:GLN:NE2	2.40	0.51
1:2A:1653:G:H3'	13:2R:2:ARG:HD3	1.92	0.51
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.93	0.51
20:2Y:83:THR:OG1	20:2Y:84:ARG:N	2.44	0.51
1:1A:2205:C:H2'	1:1A:2206:G:C8	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2519:C:H2'	1:1A:2520:G:O4'	2.11	0.51
1:2A:122:G:OP1	1:2A:149:A:O2'	2.22	0.51
1:2A:1301:A:H2	1:2A:1626:G:N3	2.08	0.51
1:2A:1711:C:H2'	1:2A:1712:C:H6	1.76	0.51
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.44	0.51
12:2Q:38:GLU:HG3	12:2Q:127:ILE:HG22	1.93	0.51
1:1A:149:A:H2'	1:1A:150:C:H6	2.26	0.50
1:1A:2285:A:H2'	1:1A:2286:A:C8	2.46	0.50
1:1A:2303:U:H2'	1:1A:2304:C:C6	2.45	0.50
1:1A:553:A:O2'	1:1A:554:A:H5'	2.11	0.50
1:1A:909:G:H2'	1:1A:910:A:O4'	2.11	0.50
12:1Q:31:ASP:HA	12:1Q:134:ARG:NH1	2.25	0.50
1:2A:2379:G:HO2'	14:2S:17:ARG:HH12	1.51	0.50
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.11	0.50
30:18:6:THR:HG22	30:18:63:PRO:HD2	1.93	0.50
1:1A:1388:A:O2'	1:1A:1390:G:OP2	2.21	0.50
1:1A:1740:U:H1'	3:1D:14:ARG:NH2	2.26	0.50
1:1A:936:C:H2'	1:1A:937:A:O4'	4.19	0.50
1:1A:964:A:N3	2:1B:80:U:O2'	2.40	0.50
20:1Y:6:HIS:CD2	20:1Y:6:HIS:H	2.29	0.50
1:2A:1180:C:H2'	1:2A:1181:C:H6	1.76	0.50
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.46	0.50
1:2A:1912:A:OP1	61:2A:3865:HOH:O	2.19	0.50
1:2A:2305:A:H1'	6:2G:136:ARG:HB3	1.93	0.50
21:2Z:6:LYS:HZ3	21:2Z:8:TYR:HE2	1.59	0.50
1:1A:2348:A:H61	22:10:43:THR:HG21	1.76	0.50
1:1A:1398:U:OP2	61:1A:4158:HOH:O	2.19	0.50
1:1A:2085:C:OP2	61:1A:4159:HOH:O	2.19	0.50
1:1A:2800:C:H2'	1:1A:2801:C:H6	1.76	0.50
1:1A:636:G:N2	1:1A:640:A:O2'	2.44	0.50
1:1A:989:G:N7	61:1A:4255:HOH:O	2.34	0.50
4:1E:16:ARG:NH1	4:1E:173:VAL:HG13	2.26	0.50
13:1R:38:VAL:HG12	13:1R:42:LYS:HE3	1.92	0.50
16:1U:58:ARG:HA	16:1U:61:TRP:CE3	2.46	0.50
23:21:51:VAL:HG12	23:21:53:VAL:HG23	1.93	0.50
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.10	0.50
1:2A:597:U:H2'	1:2A:598:G:C8	2.47	0.50
1:2A:824:A:H1'	1:2A:2358:G:N7	2.27	0.50
8:2I:122:GLU:O	8:2I:126:TYR:OH	2.26	0.50
18:2W:18:ARG:NH1	18:2W:76:VAL:O	2.45	0.50
1:1A:1060:U:OP2	61:1A:4157:HOH:O	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1111:U:H1'	1:1A:1120:G:N1	2.26	0.50
1:1A:1223:C:H2'	1:1A:1224:C:C6	2.46	0.50
1:1A:265:U:H2'	1:1A:266:C:C6	2.46	0.50
19:1X:24:GLY:O	19:1X:83:VAL:HG22	2.12	0.50
21:1Z:132:ASN:HD21	21:1Z:160:GLY:HA3	1.75	0.50
1:2A:287:C:H2'	1:2A:288:C:C6	2.47	0.50
2:2B:66:A:H61	2:2B:109:C:H5''	1.75	0.50
31:19:32:HIS:O	31:19:34:GLN:HG3	2.11	0.50
1:1A:1086:C:H2'	1:1A:1087:C:O4'	2.10	0.50
1:1A:209:G:O2'	1:1A:222:A:N3	2.35	0.50
1:1A:2576:A:C2	1:1A:2659:U:H4'	2.47	0.50
1:1A:2851:C:H2'	1:1A:2852:G:C8	2.47	0.50
23:21:85:LEU:HD23	23:21:89:GLU:HG2	1.92	0.50
1:2A:1029:A:N1	1:2A:2465:C:O2'	2.37	0.50
1:2A:1268:A:H2'	1:2A:1269:A:C8	3.35	0.50
1:2A:2065:C:H2'	1:2A:2066:C:C6	2.46	0.50
1:2A:2453:A:N7	61:2A:3942:HOH:O	2.34	0.50
4:2E:77:ILE:HD11	4:2E:195:LEU:HD22	1.94	0.50
8:2I:50:ARG:O	8:2I:54:GLN:HB2	2.12	0.50
1:1A:1698:G:O6	61:1A:4145:HOH:O	2.17	0.50
1:1A:2227:G:H8	1:1A:2228:G:N7	2.09	0.50
1:1A:2641:A:HO2'	1:1A:2642:G:P	2.31	0.50
3:1D:77:ALA:HA	3:1D:97:TYR:HA	1.94	0.50
4:1E:14:ILE:HG13	4:1E:21:VAL:HG13	1.94	0.50
25:23:6:VAL:HG22	25:23:56:VAL:HG22	1.92	0.50
26:24:13:ARG:HG2	26:24:23:GLU:HA	1.93	0.50
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.27	0.50
1:2A:2857:G:N2	1:2A:2860:A:OP2	2.45	0.50
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.11	0.50
1:1A:2800:C:H2'	1:1A:2801:C:C6	2.46	0.50
5:1F:152:GLU:OE1	5:1F:191:ARG:HD2	2.12	0.50
14:1S:15:ARG:O	14:1S:19:LYS:HG3	2.12	0.50
1:2A:2151:G:C2	1:2A:2152:G:C8	2.99	0.50
1:2A:1983:C:H4'	1:2A:2606:C:H4'	1.93	0.50
1:2A:793:A:OP2	1:2A:2071:A:O2'	2.28	0.50
3:2D:206:LEU:O	3:2D:211:ARG:HD3	2.11	0.50
4:2E:167:VAL:HG22	4:2E:170:LEU:HD11	1.93	0.50
1:1A:1037:C:H2'	1:1A:1038:C:H6	2.13	0.50
1:1A:1615:G:H5'	3:1D:60:ARG:HA	1.94	0.50
1:1A:2198:A:H2'	1:1A:2199:C:C6	2.46	0.50
11:1P:98:GLU:HG3	11:1P:99:LEU:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2W:23:LEU:HD11	27:25:25:LEU:HB2	1.92	0.50
1:2A:1139:G:H4'	1:2A:1140:C:H5'	4.64	0.50
1:2A:8:A:H2'	1:2A:9:U:C6	2.47	0.50
1:2A:946:G:H2'	1:2A:947:G:C8	2.47	0.50
7:2H:3:ARG:NH1	7:2H:5:GLY:H	2.09	0.50
12:2Q:66:ILE:HG12	12:2Q:104:PHE:HD1	1.77	0.50
15:2T:30:VAL:HG22	15:2T:86:ILE:HG12	1.93	0.50
1:1A:99:G:H21	24:12:7:ARG:HH22	1.59	0.50
1:1A:920:G:H1	1:1A:950:C:H42	1.60	0.50
29:27:26:GLY:O	29:27:30:VAL:HG23	2.12	0.50
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.12	0.50
1:2A:946:G:H2'	1:2A:947:G:H8	1.77	0.50
5:2F:107:LYS:HG3	5:2F:206:ILE:HA	1.94	0.50
10:2O:88:ASN:HD21	10:2O:92:GLU:HB2	1.76	0.50
1:1A:1037:C:H2'	1:1A:1038:C:C6	2.90	0.49
1:1A:1138:C:C2'	1:1A:1139:G:H5'	2.41	0.49
1:1A:18:C:O2'	1:1A:577:U:OP1	2.30	0.49
1:1A:142:G:H1'	19:1X:37:THR:HG21	1.94	0.49
1:2A:1011:G:H1	1:2A:1018:C:N4	17.78	0.49
1:2A:1341:U:OP2	1:2A:1394:U:O2'	2.26	0.49
1:2A:1899:G:N3	1:2A:1899:G:H2'	2.26	0.49
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.47	0.49
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.47	0.49
1:2A:2557:G:H2'	1:2A:2558:C:H6	1.77	0.49
1:2A:271(Q):G:H2'	1:2A:271(R):G:C8	2.47	0.49
1:2A:30:G:H2'	1:2A:31:C:C6	2.47	0.49
2:2B:24:G:H4'	2:2B:25:A:C8	2.47	0.49
13:2R:26:LYS:HD3	13:2R:70:LEU:O	2.12	0.49
1:1A:2143:G:H2'	1:1A:2144:U:C6	2.47	0.49
1:1A:2346:G:O6	22:10:74:ARG:NH2	2.42	0.49
1:1A:2372:A:H2'	1:1A:2373:A:O4'	2.12	0.49
1:1A:2707:C:H2'	1:1A:2708:U:C6	2.47	0.49
1:1A:602:G:H2'	1:1A:603:C:C6	2.47	0.49
1:1A:1834:A:O2'	3:1D:259:THR:HG21	2.12	0.49
6:1G:56:ALA:O	6:1G:59:GLU:HG2	2.11	0.49
10:1O:86:ILE:HG22	10:1O:94:ARG:HD3	1.94	0.49
21:1Z:99:TYR:HB3	21:1Z:123:ASP:OD2	2.12	0.49
1:2A:2336:A:H61	22:20:43:THR:HG22	1.77	0.49
1:2A:1543:C:H5''	61:2A:4225:HOH:O	2.11	0.49
1:2A:1837:C:O2'	1:2A:1927:A:N3	2.36	0.49
1:2A:2103:C:H2'	1:2A:2104:G:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:34:C:H2'	1:2A:35:G:H8	4.09	0.49
1:1A:302:A:H2'	1:1A:303:C:C6	2.47	0.49
28:26:35:GLU:HG2	28:26:50:ARG:HD3	1.94	0.49
1:2A:833:U:O2'	30:28:57:ARG:NH1	2.45	0.49
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.48	0.49
1:2A:443:A:C5	5:2F:45:ARG:HD2	2.47	0.49
7:2H:3:ARG:HG2	7:2H:6:ARG:NE	2.27	0.49
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.12	0.49
12:2Q:35:VAL:HG12	12:2Q:130:LYS:O	2.12	0.49
1:1A:1821:C:H2'	1:1A:1822:A:C5	2.48	0.49
1:1A:2247:G:H2'	1:1A:2248:C:C6	2.47	0.49
1:1A:2381:A:H2'	1:1A:2382:G:H8	1.77	0.49
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.47	0.49
1:2A:858:U:O2	1:2A:2268:A:H2'	2.12	0.49
1:2A:529:A:H2	61:2A:3888:HOH:O	1.96	0.49
1:2A:588:U:H2'	1:2A:589:C:C6	2.47	0.49
4:2E:50:GLY:HA2	4:2E:77:ILE:O	2.13	0.49
1:1A:463:C:H2'	1:1A:464:G:H8	1.75	0.49
1:1A:1834:A:H4'	3:1D:259:THR:HG23	1.95	0.49
11:1P:59:LEU:HD21	30:18:10:ALA:HA	1.95	0.49
1:2A:2127:G:H1	1:2A:2161:C:N4	2.08	0.49
1:2A:38:A:H2'	1:2A:39:C:C6	2.48	0.49
3:2D:127:VAL:HA	3:2D:193:VAL:HG23	1.95	0.49
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.47	0.49
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.22	0.49
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.47	0.49
1:2A:2127:G:C6	1:2A:2161:C:N4	2.80	0.49
1:2A:435:C:H2'	1:2A:436:C:H6	3.68	0.49
1:2A:819:A:OP2	1:2A:1187:G:N2	2.36	0.49
1:2A:848:G:C2	1:2A:933:A:H1'	2.47	0.49
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	1.93	0.49
9:2N:24:GLY:O	9:2N:28:THR:OG1	2.29	0.49
11:2P:100:LEU:HD12	11:2P:112:LEU:HD11	1.95	0.49
29:17:20:ALA:HA	29:17:23:ARG:HH21	1.78	0.49
1:1A:1186:U:H4'	1:1A:1188:A:O4'	2.13	0.49
1:2A:1486:A:H2'	1:2A:1487:G:H8	1.76	0.49
1:2A:581:C:H2'	1:2A:582:G:C8	2.47	0.49
2:2B:43:C:O2	6:2G:95:ARG:NE	2.42	0.49
1:1A:1074:A:N6	1:1A:1171:G:H2'	2.27	0.49
1:1A:1318:A:H5''	14:1S:3:ARG:NH1	127.09	0.49
1:1A:1495:G:O2'	1:1A:1575:A:N1	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:180:A:N1	61:1A:4262:HOH:O	2.35	0.49
1:1A:2262:G:OP1	12:1Q:85:LYS:NZ	2.30	0.49
1:1A:943:C:N3	1:1A:944:C:N4	2.60	0.49
1:1A:1445:C:OP1	19:1X:25:LYS:NZ	2.45	0.49
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.13	0.49
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.46	0.49
1:1A:1057:G:OP2	16:1U:70:ARG:NH2	2.46	0.49
1:1A:155:C:O2	1:1A:166:G:N2	23.52	0.49
1:1A:2123:G:H1	1:1A:2210:C:H42	1.61	0.49
1:1A:2402:U:P	30:18:35:GLN:HE22	2.36	0.49
1:2A:197:A:O2'	61:2A:3847:HOH:O	2.15	0.49
19:2X:41:ASN:O	19:2X:45:THR:HG23	2.13	0.49
1:1A:1136:U:C2	1:1A:1148:C:H1'	2.47	0.49
1:1A:1431:G:O2'	1:1A:1442:U:O2	2.22	0.49
1:1A:1572:G:C6	1:1A:1573:G:C2	3.01	0.49
1:1A:1717:C:O2	4:1E:129:HIS:NE2	2.44	0.49
1:1A:629:U:H4'	1:1A:705:C:H4'	1.95	0.49
1:1A:2417:G:H5''	11:1P:75:ILE:HG21	1.93	0.49
1:2A:75:G:H4'	24:22:55:ARG:HH11	1.77	0.49
5:2F:126:VAL:HG21	5:2F:129:PHE:CZ	2.48	0.49
9:2N:34:LEU:HD21	9:2N:120:LEU:HB2	1.95	0.49
1:1A:225:C:H2'	1:1A:226:C:C6	2.48	0.48
1:1A:2328:C:H1'	6:1G:128:ARG:HH21	1.77	0.48
7:1H:3:ARG:CZ	7:1H:5:GLY:H	2.26	0.48
25:23:10:LYS:HB3	25:23:53:LEU:HA	1.94	0.48
1:2A:1442:G:N3	1:2A:1442:G:H2'	2.83	0.48
1:2A:994:C:O2'	1:2A:996:A:OP1	2.27	0.48
8:2I:48:GLU:HB3	8:2I:52:ARG:NH1	2.28	0.48
21:2Z:150:LEU:HB2	21:2Z:171:ILE:HD11	1.94	0.48
1:1A:449:A:H2'	1:1A:450:A:C8	2.48	0.48
1:1A:515:G:N7	18:1W:49:LYS:NZ	2.60	0.48
1:2A:1568:G:H5''	3:2D:61:LEU:HD13	1.96	0.48
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.47	0.48
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.48	0.48
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.30	0.48
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.95	0.48
15:2T:109:GLU:HG2	15:2T:112:ARG:NH2	2.28	0.48
25:13:37:LEU:HB3	25:13:43:ILE:HD13	1.96	0.48
1:1A:242:C:OP2	30:18:5:LYS:NZ	2.34	0.48
1:1A:2589:A:OP1	61:1A:4163:HOH:O	2.20	0.48
1:1A:589:U:H5''	11:1P:29:LYS:HE3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1R:87:TYR:OH	13:1R:117:VAL:O	2.26	0.48
1:2A:2317:C:N4	1:2A:2318:G:O6	2.47	0.48
1:2A:336:C:H2'	1:2A:337:C:C6	2.48	0.48
1:2A:578:A:OP2	61:2A:3868:HOH:O	2.20	0.48
2:2B:91:C:H5'	12:2Q:18:LYS:HA	1.94	0.48
1:2A:908:C:P	12:2Q:22:LYS:HZ2	2.34	0.48
1:1A:2391:G:O2'	14:1S:17:ARG:NH2	2.33	0.48
1:1A:715:G:N7	61:1A:4264:HOH:O	2.35	0.48
8:1I:46:ALA:HB1	8:1I:50:ARG:HH22	1.79	0.48
24:22:32:LEU:HD13	24:22:53:LEU:HB3	1.94	0.48
1:2A:1901:A:OP2	3:2D:255:LYS:NZ	2.31	0.48
1:2A:204:A:O3'	1:2A:205:G:H4'	2.14	0.48
1:2A:2557:G:H2'	1:2A:2558:C:C6	2.48	0.48
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.13	0.48
1:2A:514:A:N3	1:2A:581:C:O2'	2.44	0.48
6:1G:101:ILE:HD13	26:14:25:TYR:HB2	1.95	0.48
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.26	0.48
7:1H:3:ARG:HH22	7:1H:66:GLY:N	2.12	0.48
15:1T:107:ASP:OD2	15:1T:111:ARG:NH1	2.46	0.48
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.49	0.48
1:2A:2037:G:H2'	1:2A:2038:G:C8	2.48	0.48
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.13	0.48
11:2P:38:GLN:O	11:2P:39:LYS:HB3	2.14	0.48
20:2Y:31:LEU:HD23	20:2Y:31:LEU:HA	1.70	0.48
21:2Z:31:ARG:HH11	21:2Z:94:GLU:HG2	1.78	0.48
1:1A:2504:U:H2'	1:1A:2505:U:H6	1.77	0.48
1:1A:2053:A:C6	1:1A:2510:C:H1'	2.48	0.48
1:1A:993:G:OP1	61:1A:4162:HOH:O	2.20	0.48
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.47	0.48
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.94	0.48
6:2G:109:VAL:HG21	26:24:14:ILE:HD13	1.95	0.48
1:2A:1509(B):A:H2'	1:2A:1510:G:H8	1.78	0.48
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.37	0.48
1:2A:903:C:H2'	1:2A:904:C:C6	2.49	0.48
6:2G:106:LEU:O	6:2G:110:ALA:HB3	2.14	0.48
6:2G:173:LEU:HB3	6:2G:178:PHE:CD2	2.48	0.48
19:2X:88:LYS:HG2	19:2X:93:GLU:HG3	1.96	0.48
1:1A:369:A:N3	1:1A:371:A:N6	2.62	0.48
4:1E:29:GLY:HA3	61:1E:408:HOH:O	2.14	0.48
1:2A:2430:A:OP2	61:2A:3867:HOH:O	2.20	0.48
1:2A:893:C:H2'	1:2A:894:C:C5	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:880:G:H22	1:2A:898:C:H1'	1.77	0.48
1:2A:2227:A:OP1	3:2D:263:ARG:HD2	2.13	0.48
21:2Z:166:SER:C	21:2Z:168:GLU:H	2.16	0.48
1:1A:469:A:H1'	1:1A:1246:C:O4'	2.13	0.48
20:1Y:14:LEU:HB2	20:1Y:75:ILE:HD11	1.95	0.48
21:1Z:4:ARG:HH21	21:1Z:60:GLU:HG2	1.78	0.48
1:2A:1481:U:H3	1:2A:1510:G:H1	1.61	0.48
1:2A:2144:U:H1'	1:2A:2148:G:N2	2.29	0.48
1:2A:2600:A:H2'	1:2A:2601:C:C6	2.49	0.48
1:2A:666:G:OP2	1:2A:725:G:N2	99.34	0.48
1:2A:801:G:O6	5:2F:53:THR:OG1	2.32	0.48
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.13	0.48
20:2Y:91:GLU:OE1	20:2Y:91:GLU:N	2.45	0.48
28:16:12:GLU:OE1	28:16:19:ARG:NH1	2.47	0.48
1:1A:103:C:H2'	1:1A:104:C:H6	1.79	0.48
1:1A:1473:A:H4'	1:1A:1474:C:O4'	2.13	0.48
1:1A:1674:G:H2'	1:1A:1675:U:C6	2.47	0.48
28:26:25:LYS:NZ	28:26:51:GLU:OE2	2.35	0.48
1:2A:1113:U:H2'	1:2A:1114:G:C8	2.48	0.48
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.49	0.48
1:2A:2698:U:H2'	1:2A:2699:C:C6	2.49	0.48
14:2S:87:PHE:CE1	14:2S:102:ALA:HB2	2.48	0.48
1:1A:1634:C:H2'	1:1A:1635:C:H6	1.79	0.48
1:1A:1827:U:H2'	1:1A:1828:C:H6	1.79	0.48
1:1A:2564:2MU:H2'	1:1A:2566:U:OP2	2.14	0.48
1:1A:2745:G:H3'	1:1A:2746:A:O4'	2.14	0.48
1:1A:2784:C:H2'	1:1A:2785:C:C6	2.49	0.48
5:1F:116:ASP:OD2	5:1F:117:ARG:NH1	2.47	0.48
21:1Z:31:ARG:HD3	21:1Z:94:GLU:OE1	2.14	0.48
29:27:30:VAL:O	29:27:34:ARG:HG2	2.13	0.48
1:2A:1973:G:OP1	61:2A:3869:HOH:O	2.20	0.48
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.12	0.48
1:2A:2441:C:OP2	1:2A:2586:C:O2'	2.31	0.48
1:2A:560:C:H4'	16:2U:52:ARG:CZ	2.44	0.48
1:2A:957:A:H5'	12:2Q:76:LYS:HG3	1.96	0.48
2:2B:66:A:N6	2:2B:108:U:H3'	2.29	0.48
3:2D:37:LEU:HD13	3:2D:62:TYR:HB2	1.96	0.48
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.29	0.48
27:15:16:ARG:NH1	27:15:17:ASP:OD1	2.46	0.47
1:1A:116:A:C8	1:1A:117:A:C8	3.02	0.47
1:1A:1232:G:H5''	17:1V:81:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:386:U:O2'	1:1A:387:G:H5''	2.13	0.47
18:1W:78:GLU:OE2	18:1W:99:ARG:NH1	2.43	0.47
22:20:51:VAL:N	22:20:62:LEU:HD12	2.29	0.47
1:2A:1264:G:H2'	1:2A:2014:A:N6	2.28	0.47
1:2A:2127:G:N2	1:2A:2161:C:C2	2.82	0.47
5:2F:32:LEU:O	5:2F:36:VAL:HG23	2.14	0.47
14:2S:34:HIS:ND1	14:2S:53:SER:OG	2.46	0.47
22:10:43:THR:OG1	22:10:46:LYS:HG2	2.13	0.47
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.96	0.47
1:1A:1633:A:H2'	1:1A:1634:C:H6	1.77	0.47
1:1A:2122:G:H1	1:1A:2211:U:H3	1.62	0.47
1:2A:266:G:H2'	1:2A:266:G:N3	3.18	0.47
1:2A:918:A:N3	2:2B:80:U:H4'	2.29	0.47
12:2Q:66:ILE:HG12	12:2Q:104:PHE:CD1	2.48	0.47
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	1.95	0.47
1:1A:1078:A:H2	1:1A:1168:G:H22	1.62	0.47
1:1A:1379:C:OP2	61:1A:4167:HOH:O	2.20	0.47
1:1A:31:C:OP1	61:1A:4161:HOH:O	2.20	0.47
8:1I:38:LEU:HD13	8:1I:40:THR:HG23	1.96	0.47
8:1I:48:GLU:HB3	8:1I:52:ARG:HH22	1.78	0.47
15:1T:15:VAL:HG13	15:1T:79:HIS:CE1	2.49	0.47
27:25:16:ARG:HG3	27:25:17:ASP:N	2.29	0.47
1:2A:1213:A:N3	1:2A:1238:G:O2'	2.43	0.47
1:2A:2645:G:N2	1:2A:2767:C:OP2	2.48	0.47
1:2A:511:U:O4	1:2A:512:G:N1	2.47	0.47
1:2A:928:G:H8	1:2A:928:G:O5'	1.96	0.47
2:2B:42:C:O2'	6:2G:67:LYS:O	2.23	0.47
8:2I:40:THR:O	8:2I:44:LEU:HB2	2.14	0.47
13:2R:72:ASP:O	13:2R:76:VAL:HG23	2.14	0.47
14:2S:67:ARG:HH12	14:2S:103:GLU:HB2	1.77	0.47
1:1A:1405:A:H5'	1:1A:1405:A:N3	2.29	0.47
1:1A:2108:U:H2'	1:1A:2109:G:C8	2.50	0.47
1:1A:327:U:H2'	1:1A:328:G:C8	2.50	0.47
8:1I:78:THR:HA	8:1I:143:SER:HG	1.80	0.47
26:24:15:ILE:HB	26:24:32:TYR:HD1	1.79	0.47
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.33	0.47
1:2A:2224:G:H4'	1:2A:2226:C:C2	2.48	0.47
1:2A:68:G:H2'	1:2A:69:C:O4'	2.14	0.47
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.49	0.47
6:2G:101:ILE:HG22	6:2G:105:LYS:HE2	1.96	0.47
14:2S:99:LYS:HE2	14:2S:103:GLU:OE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1110:C:H2'	1:1A:1111:U:O4'	2.14	0.47
1:1A:310:C:H2'	1:1A:311:C:C6	2.49	0.47
1:1A:78:G:O6	1:1A:92:C:N4	28.96	0.47
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.96	0.47
9:1N:62:VAL:CG2	9:1N:66:LYS:HB2	2.44	0.47
12:1Q:16:ARG:O	12:1Q:18:LYS:N	2.48	0.47
25:23:16:PRO:HB2	25:23:18:ASP:OD1	2.14	0.47
26:24:12:ALA:HB3	26:24:26:SER:HB3	1.96	0.47
1:2A:2419:U:H5''	30:28:33:ASN:HB2	1.95	0.47
1:2A:1119:C:H2'	1:2A:1120:G:H8	2.93	0.47
1:2A:1270:C:N4	1:2A:1271:G:O6	13.73	0.47
1:2A:2059:A:O2'	5:2F:69:HIS:HD2	1.96	0.47
1:2A:2102:U:H2'	1:2A:2103:C:C6	2.49	0.47
1:2A:2117:A:O2'	1:2A:2118:U:H5''	2.14	0.47
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.78	0.47
1:2A:526:A:N3	1:2A:2044:C:H1'	2.30	0.47
1:2A:573:G:O2'	1:2A:574:C:H3'	2.13	0.47
1:2A:614(C):A:C4	5:2F:180:GLY:HA3	2.49	0.47
7:2H:154:PRO:HB3	7:2H:163:TYR:CZ	2.49	0.47
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.33	0.47
1:2A:446:G:OP1	16:2U:3:ARG:NH1	2.48	0.47
22:10:46:LYS:HD2	22:10:78:TYR:CZ	2.49	0.47
1:1A:1101:G:H2'	1:1A:1102:G:O4'	2.14	0.47
1:1A:1199:C:H2'	1:1A:1200:G:O4'	2.14	0.47
1:1A:1245:C:H5'	61:1A:4421:HOH:O	2.14	0.47
1:1A:2162:C:O2	1:1A:2173:G:N1	2.25	0.47
1:1A:268:G:H4'	23:11:81:LYS:HG2	1.97	0.47
28:26:34:LEU:HB2	28:26:51:GLU:HB3	1.96	0.47
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.50	0.47
1:2A:1434:A:H61	1:2A:1558:A:N6	2.09	0.47
1:2A:2141:G:C5	1:2A:2151:G:C2	3.03	0.47
1:2A:262:A:H2'	1:2A:263:C:O4'	2.14	0.47
1:2A:286:C:H2'	1:2A:287:C:C6	2.50	0.47
3:2D:3:VAL:HG13	3:2D:17:THR:HB	1.96	0.47
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.28	0.47
7:2H:97:ARG:O	7:2H:104:GLU:N	2.44	0.47
29:17:5:TRP:NE1	29:17:7:PRO:HG3	2.29	0.47
1:1A:698:G:H2'	1:1A:699:C:C6	2.49	0.47
8:1I:123:LEU:HD12	8:1I:144:VAL:HG23	1.97	0.47
1:1A:2857:U:OP1	15:1T:98:LYS:NZ	2.46	0.47
1:2A:2881:C:H2'	1:2A:2882:A:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:615:G:OP2	5:2F:43:LYS:NZ	2.22	0.47
1:2A:708:C:H42	1:2A:723:G:H1	1.63	0.47
2:2B:75:G:H22	21:2Z:73:GLN:HE21	1.63	0.47
6:2G:3:LEU:O	6:2G:8:LYS:NZ	2.41	0.47
7:2H:87:LEU:O	7:2H:131:VAL:N	2.47	0.47
10:2O:119:PRO:HB2	15:2T:68:TYR:CZ	2.50	0.47
1:1A:1441:A:OP1	61:1A:4166:HOH:O	2.20	0.47
1:1A:1775:C:H5'	1:1A:1776:G:OP2	2.14	0.47
1:1A:2162:C:N3	1:1A:2173:G:C6	2.83	0.47
1:1A:2724:U:OP1	1:1A:2727:G:H4'	2.15	0.47
3:1D:95:LEU:HD11	3:1D:105:ILE:HD13	1.95	0.47
15:1T:118:ARG:HD3	15:1T:118:ARG:HA	1.59	0.47
1:2A:2022:U:OP2	27:25:15:ARG:NH2	2.48	0.47
1:2A:2507:C:H5''	1:2A:2573:C:C4	2.49	0.47
1:2A:2674:G:H2'	1:2A:2675:A:C8	2.50	0.47
1:2A:2689:U:P	1:2A:2719:G:H22	2.38	0.47
1:2A:902:C:H2'	1:2A:903:C:H6	1.80	0.47
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.48	0.47
1:1A:1115:A:H1'	1:1A:1142:A:H4'	1.97	0.47
1:1A:1554:A:O2'	1:1A:1555:C:H5''	2.15	0.47
1:1A:273:G:N2	8:1I:50:ARG:HH11	2.12	0.47
1:1A:2856:G:H2'	1:1A:2857:U:O4'	2.15	0.47
1:1A:905:U:O2	1:1A:2280:A:H2'	2.15	0.47
1:1A:936:C:OP2	1:1A:936:C:H2'	2.14	0.47
1:2A:459:U:H5''	29:27:40:TRP:CD2	2.50	0.47
1:2A:1010:A:N3	1:2A:1153:C:H1'	2.29	0.47
1:2A:2148:G:H2'	1:2A:2149:G:C8	2.49	0.47
1:2A:2638:G:OP1	4:2E:82:ARG:NH2	2.31	0.47
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.48	0.47
1:2A:334:C:OP1	1:2A:336:C:N4	2.48	0.47
1:2A:392:C:H5''	1:2A:409:C:H5''	1.97	0.47
15:2T:26:ASP:O	15:2T:49:VAL:HG22	2.15	0.47
1:1A:2365:G:H5''	22:10:32:ARG:NH1	2.30	0.47
1:1A:1617:A:H2'	1:1A:1618:A:C8	2.50	0.47
1:1A:2205:C:O2'	1:1A:2206:G:OP1	2.30	0.47
1:1A:2658:C:H2'	1:1A:2659:U:O4'	2.15	0.47
1:1A:313:A:N6	1:1A:375:G:O2'	2.48	0.47
23:21:21:ARG:HD3	23:21:35:THR:HG21	1.95	0.47
19:2X:9:LEU:HA	24:22:36:ARG:HH21	1.80	0.47
25:23:18:ASP:OD1	25:23:18:ASP:N	2.48	0.47
1:2A:2815:C:C5'	27:25:29:THR:HG21	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2218:U:N3	23:21:55:GLY:O	2.48	0.47
1:2A:2507:C:H2'	1:2A:2508:G:O4'	2.13	0.47
1:2A:2638:G:P	4:2E:82:ARG:HH12	2.37	0.47
1:2A:34:C:H2'	1:2A:35:G:C8	4.89	0.47
1:1A:1108:G:N2	1:1A:1134:A:C6	2.83	0.47
1:1A:2732:G:O6	61:1A:4169:HOH:O	2.20	0.47
1:1A:843:C:H2'	1:1A:844:C:C6	2.49	0.47
26:24:64:GLY:C	26:24:66:SER:H	2.18	0.47
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.51	0.47
1:2A:1913:A:H4'	1:2A:1914:C:H5''	1.96	0.47
1:2A:2126:A:N3	1:2A:2127:G:H1'	2.30	0.47
1:2A:557:U:H2'	1:2A:558:G:H8	1.80	0.47
1:2A:807:U:OP2	11:2P:41:ARG:NH2	2.48	0.47
1:2A:993:G:H1'	17:2V:89:GLN:OE1	2.15	0.47
2:2B:43:C:O4'	6:2G:66:GLN:NE2	2.47	0.47
18:2W:12:ILE:O	18:2W:101:SER:OG	2.30	0.47
21:2Z:45:ASP:OD1	21:2Z:49:ARG:NE	2.35	0.47
1:1A:1109:G:C5	1:1A:1110:C:N4	2.84	0.46
1:1A:1137:G:C6	1:1A:1138:C:C4	3.03	0.46
1:1A:1546:G:H2'	1:1A:1547:C:C6	2.50	0.46
1:1A:1660:A:P	1:1A:1660:A:H8	2.38	0.46
1:1A:2671:G:OP1	7:1H:158:HIS:NE2	2.47	0.46
1:1A:580:U:H2'	1:1A:581:G:O4'	2.79	0.46
17:1V:29:PRO:HA	17:1V:61:VAL:HG22	1.97	0.46
22:20:53:MET:HG3	22:20:59:LEU:HD23	1.97	0.46
1:2A:1161:C:H2'	1:2A:1162:G:H8	1.79	0.46
1:2A:117:G:OP2	1:2A:119:A:O2'	2.29	0.46
1:2A:2114:A:H2'	1:2A:2114:A:N3	2.30	0.46
1:2A:2376:A:N3	14:2S:106:ARG:NH2	2.62	0.46
1:1A:1299:A:H2'	1:1A:1299:A:N3	4.79	0.46
1:1A:275:C:H2'	1:1A:276:C:C6	2.50	0.46
1:1A:463:C:H2'	1:1A:464:G:C8	2.50	0.46
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.16	0.46
26:24:40:HIS:CD2	26:24:41:PRO:HD2	2.50	0.46
1:2A:2096:U:H3	1:2A:2193:G:H1	1.63	0.46
23:11:91:LYS:HA	23:11:94:LEU:HD12	1.98	0.46
1:1A:1102:G:H21	1:1A:1149:A:H62	1.64	0.46
5:1F:148:LEU:HD13	5:1F:154:VAL:HG21	1.97	0.46
1:2A:1523:U:H2'	1:2A:1524:G:O4'	2.15	0.46
1:2A:443:A:H5''	1:2A:444:C:OP1	2.15	0.46
1:2A:582:G:H2'	1:2A:583:G:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2210:C:H2'	1:1A:2211:U:O4'	2.15	0.46
1:1A:1757:C:O2'	1:1A:2868:C:N3	2.43	0.46
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.45	0.46
1:1A:1836:U:O2	3:1D:50:THR:HB	2.14	0.46
12:1Q:34:LEU:HD11	12:1Q:129:THR:HB	1.96	0.46
28:26:23:THR:OG1	28:26:24:GLU:N	2.47	0.46
1:2A:1179:C:H2'	1:2A:1180:C:C6	2.51	0.46
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.50	0.46
1:2A:2065:C:H2'	1:2A:2066:C:H6	1.80	0.46
1:2A:2554:U:H2'	1:2A:2555:U:C6	2.50	0.46
1:2A:320:A:H4'	1:2A:322:A:N7	2.30	0.46
1:2A:1799:G:O3'	3:2D:183:ARG:NH1	2.48	0.46
4:2E:54:GLN:OE1	4:2E:55:ASN:N	2.48	0.46
18:2W:17:VAL:HG11	18:2W:103:ILE:HD11	1.97	0.46
19:2X:40:LYS:HG3	19:2X:51:VAL:HB	1.96	0.46
1:1A:1688:A:H2'	1:1A:1689:G:O4'	2.16	0.46
1:1A:1698:G:OP1	13:1R:40:LYS:NZ	2.49	0.46
1:1A:831:A:N6	3:1D:229:VAL:HG11	2.31	0.46
7:1H:124:GLU:HG3	7:1H:132:ARG:HB3	1.97	0.46
1:2A:1913:A:H4'	1:2A:1914:C:C5'	2.46	0.46
1:2A:2180:U:H2'	1:2A:2181:G:O4'	2.15	0.46
1:2A:2752:C:H2'	1:2A:2753:A:O4'	2.15	0.46
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.50	0.46
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.16	0.46
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.59	0.46
1:1A:1052:C:C2	1:1A:1183:G:N2	2.84	0.46
1:1A:1071:G:C4	1:1A:1180:C:H1'	2.51	0.46
1:1A:1400:A:H2'	1:1A:1401:G:O4'	2.15	0.46
1:1A:1653:C:N4	1:1A:1668:G:OP2	2.44	0.46
1:2A:1027:A:C6	1:2A:1126:A:C4	3.03	0.46
1:2A:1426:G:O2'	1:2A:1572:A:N6	2.45	0.46
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.51	0.46
1:2A:1533:G:N2	1:2A:1536:C:O2'	2.49	0.46
1:2A:200:U:O2	1:2A:386:G:N2	2.48	0.46
1:2A:538:G:H5'	9:2N:5:VAL:HG11	1.98	0.46
1:1A:231:G:C8	30:18:5:LYS:HG2	2.50	0.46
31:19:17:ILE:HD11	31:19:24:TYR:HB2	1.97	0.46
1:1A:2128:G:H2'	1:1A:2129:C:C6	2.51	0.46
1:1A:2298:A:H4'	1:1A:2299:A:O4'	2.16	0.46
1:1A:2370:G:N1	61:1A:4194:HOH:O	2.24	0.46
1:1A:738:C:H2'	1:1A:739:C:C6	3.00	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:831:A:OP2	61:1A:4165:HOH:O	2.20	0.46
12:1Q:85:LYS:HD2	12:1Q:85:LYS:N	2.31	0.46
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.98	0.46
1:1A:2694:U:O2'	15:1T:58:ASN:ND2	2.49	0.46
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.16	0.46
1:2A:1475:G:C2	1:2A:1517:G:C2	3.04	0.46
1:2A:2119:A:C5	1:2A:2170:A:C6	3.04	0.46
1:2A:276:A:H5''	1:2A:277:C:H5'	1.98	0.46
1:2A:340:A:H2'	1:2A:341:G:O4'	2.16	0.46
5:2F:56:GLU:OE1	5:2F:93:LYS:NZ	2.49	0.46
8:2I:53:ALA:O	8:2I:57:ARG:HG2	2.15	0.46
19:2X:35:THR:HG22	19:2X:37:THR:N	2.31	0.46
12:1Q:85:LYS:HD3	22:10:7:LEU:HD12	1.97	0.46
30:18:52:LYS:HE2	30:18:52:LYS:HB3	1.71	0.46
1:1A:1108:G:P	1:1A:1116:A:H1'	2.56	0.46
1:2A:1297:C:H1'	1:2A:1298:C:H5	5.01	0.46
1:2A:1530:C:O2'	1:2A:1531:C:O5'	2.30	0.46
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.51	0.46
1:2A:2320:A:H2'	1:2A:2320:A:N3	2.31	0.46
1:2A:243:U:OP1	30:28:6:THR:OG1	2.29	0.46
1:2A:1637:A:H4'	1:2A:2711:A:O2'	2.16	0.46
1:2A:2815:C:H2'	1:2A:2816:C:C6	2.51	0.46
1:2A:952:G:C6	1:2A:966:G:C6	3.04	0.46
1:1A:236:G:H4'	1:1A:413:G:C5	2.50	0.46
1:1A:329:U:H2'	1:1A:330:U:C6	2.50	0.46
1:1A:39:C:O2	5:1F:46:ARG:NH2	2.33	0.46
1:1A:704:U:H2'	1:1A:705:C:C6	2.51	0.46
9:1N:77:GLY:O	61:1N:301:HOH:O	2.20	0.46
10:1O:64:ARG:HB2	10:1O:79:PHE:CG	2.51	0.46
10:1O:86:ILE:HG21	10:1O:94:ARG:HH11	1.81	0.46
1:2A:1818:U:OP2	3:2D:157:ARG:HD3	2.15	0.46
1:2A:362:U:O2'	1:2A:363:G:H5''	2.16	0.46
1:2A:990:A:H1'	1:2A:1156:A:N3	2.30	0.46
30:18:42:ARG:NH1	61:18:5001:HOH:O	2.13	0.46
1:1A:1110:C:N3	1:1A:1120:G:C6	2.84	0.46
1:1A:2549:U:H2'	1:1A:2550:C:C6	2.51	0.46
1:1A:310:C:H2'	1:1A:311:C:H6	1.81	0.46
3:1D:275:LYS:HG3	3:1D:276:LYS:HB2	1.98	0.46
4:1E:12:THR:HG22	4:1E:13:ARG:H	1.81	0.46
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.51	0.46
7:2H:59:ARG:HD2	7:2H:59:ARG:HA	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2T:73:GLU:OE2	15:2T:103:ARG:NE	2.48	0.46
16:2U:16:LYS:HB3	16:2U:16:LYS:HE2	1.73	0.46
1:1A:2255:U:H2'	1:1A:2256:U:C6	2.51	0.45
1:1A:801:C:H2'	1:1A:802:C:H6	1.81	0.45
2:1B:14:U:O3'	2:1B:108:U:O2'	2.34	0.45
13:1R:44:LEU:HA	13:1R:44:LEU:HD23	1.85	0.45
15:1T:24:PRO:HA	15:1T:49:VAL:HG22	1.97	0.45
15:1T:91:ARG:HH11	15:1T:120:ARG:NH1	2.13	0.45
22:20:32:ARG:H	22:20:35:ASN:ND2	2.13	0.45
1:2A:2126:A:H61	1:2A:2162:G:C2'	2.28	0.45
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.31	0.45
1:2A:855:G:H2'	1:2A:856:C:C6	2.51	0.45
5:2F:120:GLU:HG3	5:2F:122:LYS:CG	2.46	0.45
11:2P:126:VAL:HG12	11:2P:148:LEU:HD23	1.97	0.45
25:13:18:ASP:OD1	25:13:18:ASP:N	2.49	0.45
26:14:41:PRO:HG3	26:14:49:PHE:CE1	2.52	0.45
1:1A:1000:C:OP1	12:1Q:87:LYS:NZ	2.32	0.45
1:1A:1221:G:H1'	1:1A:1222:A:C5'	2.46	0.45
1:1A:1343:C:OP2	61:1A:4171:HOH:O	2.21	0.45
1:1A:2120:U:H3	1:1A:2213:G:H1	1.62	0.45
1:1A:662:A:OP1	11:1P:133:SER:OG	2.31	0.45
3:1D:35:LYS:HE2	3:1D:64:ILE:HG12	1.98	0.45
6:1G:15:VAL:HG13	6:1G:175:LEU:HB3	1.98	0.45
22:20:48:GLY:H	22:20:51:VAL:HB	1.81	0.45
1:2A:851:U:O2'	25:23:42:ALA:O	2.30	0.45
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.51	0.45
1:2A:1547:C:H2'	1:2A:1548:C:C6	2.51	0.45
1:2A:2119:A:N6	1:2A:2171:A:C6	2.84	0.45
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.51	0.45
1:2A:531:C:OP1	1:2A:561:G:N2	2.49	0.45
1:2A:1814:G:H4'	3:2D:51:VAL:HG21	1.98	0.45
4:2E:9:VAL:HG23	15:2T:7:ILE:HD11	1.97	0.45
9:2N:103:VAL:O	9:2N:107:LEU:HG	2.16	0.45
10:2O:73:ASP:OD2	15:2T:32:TYR:OH	2.30	0.45
1:2A:811:U:H2'	11:2P:21:ARG:HA	1.98	0.45
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.99	0.45
1:1A:1218:G:N2	1:1A:1222:A:OP2	2.43	0.45
1:1A:1831:C:OP1	3:1D:260:ARG:NH2	2.49	0.45
1:1A:2163:G:C6	1:1A:2164:C:C2	3.04	0.45
1:1A:733:G:N2	1:1A:835:A:H61	2.15	0.45
4:1E:191:PRO:HD2	61:1E:410:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1O:66:LYS:HA	10:1O:79:PHE:O	2.15	0.45
14:1S:61:ASN:O	14:1S:65:VAL:HG23	2.16	0.45
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.69	0.45
1:2A:2473:U:H2'	1:2A:2473:U:O2	2.15	0.45
1:2A:26:G:C6	1:2A:27:G:N1	2.84	0.45
1:2A:532:A:N6	1:2A:1206:G:O2'	62.55	0.45
5:2F:155:LEU:HB2	5:2F:189:THR:HG21	1.97	0.45
7:2H:25:LYS:HE3	7:2H:27:LYS:HZ1	1.82	0.45
26:14:20:ASN:OD1	26:14:21:VAL:N	2.50	0.45
1:1A:1047:A:H2'	1:1A:1048:G:O4'	2.17	0.45
1:1A:1405:A:C2	1:1A:1418:U:O4	2.67	0.45
1:1A:2096:U:H2'	1:1A:2097:U:C6	2.52	0.45
1:1A:2786:C:H2'	1:1A:2787:C:H6	1.81	0.45
1:1A:320:C:H2'	1:1A:321:C:H6	1.81	0.45
1:1A:671:A:H2'	1:1A:672:G:O4'	2.16	0.45
14:1S:87:PHE:HB2	14:1S:112:PHE:CE1	2.51	0.45
1:1A:1057:G:P	16:1U:77:SER:HG	2.38	0.45
1:2A:1219:G:N2	1:2A:1221:C:N3	2.64	0.45
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.26	0.45
1:2A:1784:A:H5''	61:2A:3978:HOH:O	2.15	0.45
1:2A:2051:A:H5'	1:2A:2578:G:O4'	2.17	0.45
1:2A:2734:A:H2'	1:2A:2735:G:O4'	2.17	0.45
1:2A:752:A:P	29:27:3:ARG:HH22	2.39	0.45
1:2A:795:C:H2'	1:2A:796:C:C6	2.52	0.45
3:2D:222:ARG:NH1	3:2D:224:ALA:HB3	2.31	0.45
10:2O:63:VAL:HG11	10:2O:85:VAL:HG23	1.98	0.45
11:2P:121:LYS:HG2	11:2P:123:LEU:HG	1.99	0.45
13:2R:28:LEU:HD22	13:2R:48:VAL:HG21	1.99	0.45
14:2S:94:TYR:CZ	14:2S:99:LYS:HG3	2.51	0.45
1:2A:445:C:OP1	16:2U:2:PRO:HA	2.16	0.45
25:13:6:VAL:HG12	25:13:28:LEU:HD11	1.99	0.45
1:1A:2143:G:OP2	1:1A:2143:G:H8	1.98	0.45
12:1Q:38:GLU:HA	12:1Q:99:PRO:HG3	1.98	0.45
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.16	0.45
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.99	0.45
26:24:40:HIS:HD1	26:24:43:TYR:HD2	1.64	0.45
29:27:5:TRP:NE1	29:27:7:PRO:HG3	2.32	0.45
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.16	0.45
1:2A:2190:G:H2'	1:2A:2191:G:O4'	2.16	0.45
1:2A:500:G:N1	1:2A:503:A:OP2	2.50	0.45
1:2A:868:U:C4	1:2A:869:G:N7	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:848:G:C4	1:2A:933:A:H8	2.34	0.45
2:2B:80:U:H2'	2:2B:81:G:C8	2.51	0.45
6:2G:39:ILE:HG12	6:2G:157:ILE:HG12	1.99	0.45
25:13:6:VAL:HG13	25:13:54:VAL:CG1	2.39	0.45
26:14:63:TYR:CD1	26:14:63:TYR:N	2.84	0.45
30:18:32:LEU:O	30:18:36:LYS:HE3	2.17	0.45
1:1A:1110:C:O2	1:1A:1120:G:N1	2.29	0.45
1:1A:1704:C:H2'	1:1A:1705:C:C6	2.51	0.45
1:1A:441:C:H2'	1:1A:442:A:C8	2.51	0.45
1:1A:1615:G:H5''	3:1D:61:LEU:HD13	1.98	0.45
4:1E:54:GLN:HB2	4:1E:76:ARG:HG2	1.99	0.45
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.17	0.45
1:2A:1183:G:H2'	1:2A:1184:G:H8	1.82	0.45
1:2A:118:A:OP2	1:2A:119:A:H5''	2.17	0.45
1:2A:459:U:H4'	29:27:40:TRP:CZ3	2.52	0.45
6:2G:123:ASN:O	6:2G:125:PHE:N	2.49	0.45
9:2N:33:LEU:HD12	9:2N:38:HIS:CD2	2.52	0.45
1:2A:906:G:O4'	12:2Q:29:PHE:HE2	2.00	0.45
12:2Q:42:ILE:HD13	12:2Q:97:VAL:HB	1.97	0.45
13:2R:98:LEU:HB2	13:2R:113:LEU:HD11	1.99	0.45
21:2Z:159:PRO:HA	21:2Z:160:GLY:HA2	1.54	0.45
21:2Z:23:LYS:HD2	21:2Z:40:ASP:HA	1.99	0.45
1:1A:1099:C:N4	1:1A:1152:G:H1	2.11	0.45
1:1A:2171:G:C6	1:1A:2172:U:C2	3.04	0.45
1:1A:613:A:H2'	1:1A:614:C:O4'	2.16	0.45
3:1D:61:LEU:O	3:1D:63:ARG:NH1	2.50	0.45
11:1P:116:GLY:O	11:1P:137:LYS:NZ	2.37	0.45
14:1S:110:LEU:HA	14:1S:110:LEU:HD12	1.78	0.45
13:2R:33:ARG:NH2	27:25:57:VAL:O	2.49	0.45
28:26:18:ARG:HD2	28:26:42:TRP:CD1	2.51	0.45
1:2A:2186:G:H2'	1:2A:2187:G:H8	1.81	0.45
1:2A:2252:G:H2'	1:2A:2253:G:O4'	2.17	0.45
1:2A:2562:U:H4'	10:2O:25:LEU:HD21	1.98	0.45
1:2A:13:A:N6	1:2A:526:A:OP2	2.45	0.45
2:2B:38:C:O2	2:2B:48:A:H1'	2.17	0.45
7:2H:38:SER:HB2	7:2H:64:LEU:HD22	1.99	0.45
24:12:25:VAL:HG13	24:12:29:LYS:HD2	1.98	0.45
25:13:4:LEU:O	25:13:36:VAL:HA	2.17	0.45
26:14:40:HIS:HB3	26:14:43:TYR:CD2	2.52	0.45
1:1A:1099:C:C2	1:1A:1100:A:H1'	2.52	0.45
1:1A:185:A:N3	1:1A:185:A:H2'	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1921:G:H2'	1:1A:1921:G:N3	2.32	0.45
1:1A:2021:C:H4'	1:1A:2736:C:O2	2.17	0.45
1:1A:2134:G:C2	1:1A:2135:U:H1'	2.51	0.45
1:1A:2164:C:N3	1:1A:2171:G:C6	2.85	0.45
12:1Q:1:MET:HB3	12:1Q:44:ALA:HB1	1.99	0.45
1:2A:2390:U:P	30:28:35:GLN:HE22	2.40	0.45
1:2A:2663:G:H3'	1:2A:2664:G:H8	1.81	0.45
1:2A:2747:G:O6	1:2A:2755:C:H5''	2.17	0.45
1:2A:274:G:H2'	1:2A:275:G:C8	2.52	0.45
1:2A:601:C:O2	1:2A:605:C:H4'	2.17	0.45
4:2E:49:LEU:HD21	4:2E:91:VAL:HG21	1.98	0.45
11:2P:39:LYS:CB	11:2P:45:LEU:HG	2.35	0.45
14:2S:105:ALA:O	14:2S:110:LEU:HB2	2.17	0.45
1:1A:1312:G:O5'	18:1W:15:ARG:NH2	2.50	0.45
1:1A:2754:A:OP1	31:19:22:ARG:NH2	2.32	0.45
2:1B:78:A:C2	2:1B:100:A:C4	3.04	0.45
10:1O:63:VAL:HG23	10:1O:64:ARG:HG2	1.99	0.45
13:1R:54:LEU:HA	13:1R:54:LEU:HD12	1.84	0.45
15:1T:22:PHE:HB3	15:1T:88:ILE:HD11	1.98	0.45
1:2A:2792:G:N3	1:2A:2792:G:H2'	2.31	0.45
6:2G:150:ASP:OD1	6:2G:153:ARG:NH2	2.48	0.45
30:18:26:LYS:HG2	30:18:46:ARG:O	2.16	0.45
1:1A:1273:G:C2	1:1A:1274:G:H1'	3.50	0.45
1:1A:2290:A:OP2	22:10:12:ASN:ND2	2.50	0.45
1:1A:2527:C:O2'	1:1A:2528:G:H5'	2.17	0.45
2:1B:91:C:H5'	12:1Q:18:LYS:HG2	1.99	0.45
5:1F:74:ARG:H	5:1F:74:ARG:HG3	1.49	0.45
9:1N:67:LEU:HB3	9:1N:88:GLU:HG3	1.98	0.45
1:2A:1628:G:H2'	1:2A:1629:U:C6	2.52	0.45
3:2D:145:VAL:HG13	3:2D:191:ALA:HB2	1.98	0.45
12:2Q:137:TYR:CE1	21:2Z:83:PRO:HG3	2.51	0.45
16:2U:52:ARG:HG3	16:2U:55:ARG:NH2	2.31	0.45
21:2Z:45:ASP:O	21:2Z:49:ARG:HG2	2.17	0.45
2:2B:103:G:H21	21:2Z:73:GLN:NE2	2.14	0.45
31:19:10:ILE:HD11	31:19:34:GLN:HE21	1.82	0.44
1:1A:2659:U:H2'	1:1A:2660:C:C6	2.53	0.44
1:1A:2699:U:H2'	1:1A:2700:U:O4'	2.18	0.44
6:1G:11:TYR:OH	6:1G:32:PRO:O	2.30	0.44
11:1P:77:ARG:HB2	11:1P:78:PRO:HD2	1.98	0.44
1:1A:543:G:H4'	18:1W:18:ARG:NE	2.32	0.44
1:1A:794:U:H4'	18:1W:92:ARG:HH22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1X:55:ASN:O	19:1X:80:ILE:N	2.42	0.44
23:21:83:GLU:HA	23:21:84:GLY:HA2	1.75	0.44
24:22:35:LEU:HD12	24:22:53:LEU:HD12	1.99	0.44
1:2A:70:G:H5''	1:2A:112:U:O2	2.16	0.44
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.25	0.44
1:2A:2152:G:C2	1:2A:2153:G:H1'	2.52	0.44
1:2A:253:C:OP2	30:28:5:LYS:NZ	2.36	0.44
19:2X:50:LYS:HB3	19:2X:87:GLN:HE22	1.82	0.44
1:1A:2734:A:H8	1:1A:2734:A:O5'	2.00	0.44
1:1A:2830:A:OP2	13:1R:2:ARG:NH2	2.51	0.44
16:1U:102:GLU:HB3	16:1U:104:GLN:NE2	2.32	0.44
19:1X:64:LYS:HD3	19:1X:64:LYS:HA	1.82	0.44
26:24:57:GLU:HA	26:24:58:ARG:HA	1.65	0.44
1:2A:1161:C:H2'	1:2A:1162:G:C8	2.51	0.44
1:2A:1489:U:HO2'	1:2A:1490:A:H8	1.62	0.44
1:2A:2444:G:OP2	5:2F:68:LYS:NZ	2.35	0.44
1:2A:2529:G:O6	31:29:31:LYS:NZ	2.51	0.44
1:2A:479:A:HO2'	1:2A:481:G:H8	1.64	0.44
1:2A:784:A:N6	3:2D:229:VAL:HG11	2.31	0.44
11:2P:97:PRO:HG3	11:2P:112:LEU:HD12	1.99	0.44
21:2Z:163:LEU:HG	21:2Z:165:VAL:HG22	1.99	0.44
1:1A:1859:G:OP2	1:1A:1859:G:H8	2.00	0.44
3:1D:127:VAL:HA	3:1D:193:VAL:HG22	2.00	0.44
6:1G:15:VAL:HG21	6:1G:176:LEU:HD23	1.99	0.44
8:1I:6:LEU:HG	8:1I:36:ALA:HA	1.99	0.44
13:1R:56:LYS:NZ	13:1R:90:ARG:O	2.50	0.44
1:2A:1639:U:C2'	1:2A:1640:C:H5''	2.47	0.44
1:2A:211:A:H2'	1:2A:212:G:O4'	2.17	0.44
1:2A:2149:G:C6	1:2A:2150:U:C2	3.05	0.44
1:2A:2427:C:H5''	1:2A:2428:G:OP1	2.17	0.44
1:2A:455:C:N3	1:2A:472:A:H2'	2.32	0.44
1:2A:652(B):A:N6	1:2A:655:A:H1'	2.32	0.44
2:2B:55:U:H2'	2:2B:56:G:O4'	2.17	0.44
18:2W:45:TYR:CZ	18:2W:49:LYS:HE3	2.53	0.44
61:1A:5058:HOH:O	22:10:14:ARG:HB2	2.17	0.44
1:1A:1222:A:H2'	1:1A:1222:A:N3	2.33	0.44
1:1A:757:G:H2'	1:1A:758:G:C8	2.52	0.44
6:1G:61:ALA:HB1	26:14:7:PRO:HG3	1.99	0.44
15:1T:33:LYS:HA	15:1T:42:ILE:HD13	1.99	0.44
18:1W:6:ILE:HA	18:1W:103:ILE:O	2.18	0.44
1:2A:1020:A:N1	1:2A:1141:U:H1'	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2872:G:C2	1:2A:2873:A:N6	2.84	0.44
1:2A:307:G:H21	1:2A:330:A:H62	1.66	0.44
1:2A:910:A:H62	12:2Q:12:GLN:HA	1.83	0.44
6:2G:5:VAL:HG23	6:2G:8:LYS:HB2	2.00	0.44
1:2A:747:U:O2'	18:2W:92:ARG:NH1	2.50	0.44
21:2Z:53:ILE:HG22	21:2Z:71:VAL:HG12	2.00	0.44
1:1A:1653:C:H5''	1:1A:1654:A:H5'	1.98	0.44
1:1A:2346:G:H4'	1:1A:2347:A:OP2	2.17	0.44
3:1D:70:TRP:HB3	3:1D:190:TYR:CE2	2.51	0.44
13:1R:118:GLU:H	13:1R:118:GLU:CD	2.20	0.44
16:1U:17:ILE:HG13	16:1U:32:PHE:HE1	1.81	0.44
1:2A:2754:U:O2'	31:29:17:ILE:HD13	2.17	0.44
1:2A:2403:C:N3	1:2A:2415:G:C2	2.86	0.44
1:2A:2494:G:C4	1:2A:2495:G:C8	3.06	0.44
1:2A:27:G:HO2'	1:2A:28:A:P	2.39	0.44
1:2A:324:A:N6	1:2A:338:G:O2'	2.50	0.44
1:2A:942:G:OP1	11:2P:39:LYS:NZ	2.45	0.44
10:2O:80:ASP:OD2	15:2T:64:ARG:NH2	2.44	0.44
20:2Y:73:ARG:HH21	20:2Y:83:THR:C	2.21	0.44
1:1A:1088:G:H2'	1:1A:1089:C:C6	2.52	0.44
1:1A:180:A:H2'	1:1A:181:C:C6	2.52	0.44
1:1A:1830:G:N2	3:1D:155:LEU:HD12	2.32	0.44
3:1D:223:GLY:HA3	3:1D:231:HIS:CE1	2.52	0.44
8:1I:61:ARG:HA	8:1I:61:ARG:HD3	1.61	0.44
1:2A:1557:C:H5''	1:2A:1558:A:OP2	2.17	0.44
1:2A:184:C:H2'	1:2A:185:U:H6	1.83	0.44
1:2A:2360:A:H2'	1:2A:2361:A:O4'	2.18	0.44
1:2A:2593:U:H2'	1:2A:2594:C:C6	2.52	0.44
1:2A:492:A:H2'	1:2A:493:G:O4'	2.17	0.44
1:2A:597:U:H2'	1:2A:598:G:H8	1.82	0.44
9:2N:58:ASP:N	9:2N:58:ASP:OD1	2.50	0.44
11:2P:44:GLY:HA2	11:2P:45:LEU:HB2	2.00	0.44
12:2Q:2:LEU:HG	12:2Q:69:PHE:CE1	2.52	0.44
12:2Q:51:ARG:O	12:2Q:55:VAL:HG13	2.18	0.44
1:1A:1560:U:H2'	1:1A:1561:C:C6	2.53	0.44
1:1A:308:U:H2'	1:1A:309:C:H6	1.80	0.44
1:1A:510:C:H2'	1:1A:511:C:C6	2.53	0.44
1:1A:605:G:H2'	1:1A:606:G:C8	2.52	0.44
27:25:51:TYR:CE2	27:25:56:LYS:HD3	2.52	0.44
1:2A:1218:C:OP2	16:2U:15:LYS:NZ	2.49	0.44
1:2A:1252:G:N3	16:2U:33:ARG:HG2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2833:G:H4'	1:2A:2834:G:OP2	2.17	0.44
1:2A:323:G:O2'	1:2A:1205:U:N3	2.48	0.44
1:2A:330:A:HO2'	1:2A:331:A:H8	1.66	0.44
1:2A:624:C:H2'	1:2A:625:G:C8	3.66	0.44
1:2A:705:A:C2	1:2A:727:A:H1'	2.52	0.44
3:2D:166:GLN:HB2	3:2D:174:ILE:HG22	1.99	0.44
5:2F:116:ASP:OD1	5:2F:119:ARG:NH2	2.47	0.44
9:2N:34:LEU:O	9:2N:49:GLY:HA3	2.17	0.44
13:2R:44:LEU:HD23	13:2R:44:LEU:HA	1.78	0.44
14:2S:4:LEU:HA	14:2S:4:LEU:HD23	1.84	0.44
15:2T:109:GLU:HG2	15:2T:112:ARG:HH22	1.83	0.44
1:1A:1841:A:H2'	1:1A:1842:G:O4'	2.18	0.44
1:1A:2787:C:H2'	1:1A:2788:A:O4'	2.17	0.44
1:1A:2879:G:H2'	1:1A:2880:C:O4'	2.17	0.44
1:1A:942:A:H4'	1:1A:943:C:OP1	2.18	0.44
2:1B:29:A:H2'	2:1B:30:C:O4'	2.18	0.44
2:1B:31:C:H4'	6:1G:29:TRP:CH2	2.53	0.44
11:1P:100:LEU:HD12	11:1P:112:LEU:HD11	1.99	0.44
24:22:8:LYS:HA	24:22:8:LYS:HD2	1.79	0.44
1:2A:1022:G:H1	1:2A:1142(A):A:H2	1.64	0.44
1:2A:1028:A:H2'	1:2A:1029:A:C8	2.53	0.44
1:2A:1027:A:N6	1:2A:1126:A:C4	2.86	0.44
1:2A:816:C:N4	1:2A:1192:G:O6	2.51	0.44
1:2A:1217:C:H2'	1:2A:1218:C:O4'	2.61	0.44
1:2A:1263:U:C4	1:2A:1264:G:C6	3.05	0.44
1:2A:2386:C:H2'	1:2A:2387:U:C6	2.53	0.44
1:2A:2773:C:OP1	4:2E:166:THR:OG1	2.34	0.44
1:2A:2872:G:O2'	1:2A:2873:A:H5'	2.18	0.44
1:2A:699:A:H2'	1:2A:700:G:O4'	2.17	0.44
1:2A:900:A:C2'	1:2A:901:A:H8	2.27	0.44
9:2N:62:VAL:HG11	9:2N:66:LYS:HB2	1.99	0.44
19:2X:9:LEU:HB2	19:2X:29:TRP:O	2.18	0.44
1:1A:2148:A:H4'	1:1A:2149:G:OP1	2.18	0.44
1:1A:2236:G:H4'	1:1A:2238:C:C2	2.53	0.44
1:1A:2826:C:O2	1:1A:2893:A:O2'	2.35	0.44
1:1A:807:G:OP1	61:1A:4170:HOH:O	2.21	0.44
3:1D:145:VAL:HB	3:1D:155:LEU:HB2	2.00	0.44
7:1H:104:GLU:HG3	7:1H:114:VAL:HG22	2.00	0.44
8:1I:117:GLU:HG3	8:1I:118:LYS:H	1.82	0.44
21:1Z:128:VAL:HG23	21:1Z:160:GLY:O	2.17	0.44
1:2A:1016:G:H2'	1:2A:1017:G:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1242:A:N1	11:2P:4:SER:OG	2.41	0.44
1:2A:2335:A:C8	1:2A:2337:G:C5	3.06	0.44
1:2A:249:C:H4'	1:2A:250:G:O5'	2.17	0.44
1:2A:1693:U:O3'	3:2D:14:ARG:NH2	2.51	0.44
12:2Q:17:LEU:HD22	12:2Q:96:VAL:HG13	1.99	0.44
1:2A:2851:A:O2'	13:2R:64:ARG:NH2	2.48	0.44
19:2X:60:ARG:NH2	29:27:47:ARG:HH12	2.14	0.44
23:11:10:LYS:NZ	23:11:65:SER:OG	2.44	0.43
1:1A:2137:G:H8	1:1A:2137:G:O5'	2.00	0.43
1:1A:2518:U:N3	58:1A:4030:EZG:CG	2.80	0.43
1:1A:624:C:O2'	1:1A:628:C:H5''	2.18	0.43
1:1A:722:A:C8	1:1A:851:A:C6	3.05	0.43
14:1S:3:ARG:HD3	14:1S:3:ARG:HA	1.88	0.43
21:1Z:132:ASN:ND2	21:1Z:160:GLY:HA3	2.33	0.43
25:23:6:VAL:HG12	25:23:28:LEU:HD11	2.00	0.43
30:28:52:LYS:HG2	30:28:56:GLU:OE2	2.17	0.43
1:2A:2161:C:H3'	1:2A:2162:G:C8	2.53	0.43
1:2A:839:U:H2'	1:2A:840:C:C6	2.53	0.43
4:2E:9:VAL:HG22	4:2E:25:VAL:HB	2.00	0.43
7:2H:148:ILE:HG13	7:2H:148:ILE:H	1.50	0.43
14:2S:64:GLU:CD	14:2S:64:GLU:H	3.53	0.43
16:2U:49:HIS:HA	16:2U:52:ARG:HB3	1.98	0.43
19:2X:57:LEU:HD22	19:2X:78:LYS:HE2	2.00	0.43
21:2Z:144:LEU:HD23	21:2Z:145:GLU:H	1.82	0.43
1:1A:1087:C:N4	1:1A:1160:G:H1	2.15	0.43
5:1F:184:TYR:O	5:1F:188:ARG:HG3	2.18	0.43
1:1A:2885:C:O2'	15:1T:2:ASN:OD1	2.36	0.43
19:1X:41:ASN:O	19:1X:45:THR:HG23	2.18	0.43
1:2A:1315:C:H42	1:2A:1337:G:H1	1.66	0.43
1:2A:1651:G:H2'	1:2A:1652:A:O4'	2.18	0.43
1:2A:320:A:O2'	1:2A:322:A:OP2	2.36	0.43
1:2A:434:U:H2'	1:2A:435:C:C6	6.51	0.43
1:2A:657:U:H2'	1:2A:658:C:C6	2.53	0.43
1:2A:992:C:OP1	16:2U:47:TYR:OH	2.25	0.43
3:2D:253:GLN:HG3	61:2D:412:HOH:O	2.17	0.43
1:2A:535:C:O3'	16:2U:53:ARG:NH1	2.50	0.43
1:1A:1683:C:H2'	1:1A:1684:A:C8	2.53	0.43
1:1A:1973:U:O2	1:1A:1975:A:H8	2.01	0.43
1:1A:2123:G:H2'	1:1A:2124:U:C6	2.53	0.43
2:1B:5:C:O2'	2:1B:27:C:O2	2.35	0.43
10:1O:70:LYS:HE2	10:1O:70:LYS:HB3	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:24:PRO:HD3	15:1T:52:ILE:HD12	2.00	0.43
18:1W:18:ARG:HG3	18:1W:76:VAL:HB	1.99	0.43
26:24:15:ILE:HB	26:24:32:TYR:CD1	2.54	0.43
26:24:47:GLN:C	26:24:49:PHE:H	2.21	0.43
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.19	0.43
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.54	0.43
1:2A:478:A:C6	1:2A:480:A:C6	3.07	0.43
1:2A:1155:A:H5''	16:2U:55:ARG:HH11	1.83	0.43
1:1A:414:U:P	23:11:20:ARG:HH12	2.40	0.43
26:14:44:THR:O	26:14:46:GLN:N	2.51	0.43
1:1A:1654:A:H1'	1:1A:1656:A:OP2	2.18	0.43
1:1A:2343:G:O2'	1:1A:2348:A:N1	2.45	0.43
1:1A:426:G:OP2	61:1A:4164:HOH:O	2.20	0.43
2:1B:2:C:H2'	2:1B:3:C:H6	1.82	0.43
5:1F:106:ARG:H	5:1F:106:ARG:HG2	1.50	0.43
1:1A:609:A:H5'	5:1F:89:VAL:HG21	2.00	0.43
1:2A:125:G:C6	29:27:10:ARG:HG3	2.53	0.43
1:2A:1528:A:H2'	1:2A:1528(A):A:C8	2.54	0.43
1:2A:1529:G:O6	1:2A:1530:C:N4	2.51	0.43
1:2A:2274:A:C5	1:2A:2276:G:C8	3.05	0.43
1:2A:296:C:O3'	20:2Y:95:LYS:NZ	2.51	0.43
1:2A:93:G:H2'	1:2A:94:C:C6	2.53	0.43
4:2E:101:ARG:NH1	4:2E:171:GLU:HB2	2.34	0.43
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.18	0.43
1:1A:1756:U:H2'	1:1A:1757:C:C6	2.53	0.43
1:1A:1935:A:H4'	1:1A:1936:C:H5''	2.00	0.43
1:1A:2372:A:O5'	1:1A:2372:A:H8	2.02	0.43
1:1A:2819:A:H2'	1:1A:2820:A:C8	2.54	0.43
1:1A:332:G:H2'	1:1A:333:G:H8	2.94	0.43
1:1A:703:G:H2'	1:1A:704:U:O4'	2.18	0.43
1:1A:733:G:H8	29:17:6:GLN:O	2.02	0.43
2:1B:23:G:O6	61:1B:302:HOH:O	2.21	0.43
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.19	0.43
12:1Q:18:LYS:O	12:1Q:98:LYS:NZ	2.29	0.43
1:1A:1387:U:O4'	19:1X:57:LEU:HD23	2.18	0.43
1:2A:1422:G:H5''	10:2O:48:PRO:CB	100.11	0.43
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.53	0.43
1:2A:212:G:H2'	1:2A:213:A:O4'	2.19	0.43
1:2A:2133:G:O2'	1:2A:2134:A:OP1	2.30	0.43
1:2A:2334:G:H5'	14:2S:9:ARG:HG2	2.00	0.43
1:2A:2366:A:H2'	1:2A:2367:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2429:G:OP2	61:2A:3867:HOH:O	2.21	0.43
3:2D:242:ARG:HG2	3:2D:246:PRO:HG3	1.99	0.43
1:2A:2637:U:H5''	4:2E:82:ARG:NH1	2.34	0.43
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.51	0.43
14:2S:15:ARG:O	14:2S:19:LYS:HG2	2.18	0.43
15:2T:18:ASP:OD1	15:2T:18:ASP:N	2.45	0.43
30:18:23:VAL:CG1	30:18:47:LYS:HB3	2.49	0.43
1:1A:1004:A:H5'	1:1A:1024:G:O6	28.32	0.43
1:1A:1115:A:H4'	1:1A:1116:A:H8	1.83	0.43
1:1A:1410:G:N7	23:11:3:LYS:HD2	2.33	0.43
1:1A:2769:U:H1'	1:1A:2770:A:H5''	1.99	0.43
1:1A:659:C:H2'	1:1A:660:C:C6	2.54	0.43
2:1B:24:G:N7	2:1B:56:G:H2'	2.33	0.43
2:1B:65:C:O2'	2:1B:66:A:OP1	2.28	0.43
6:1G:46:ALA:HB1	6:1G:50:ALA:O	2.19	0.43
7:1H:3:ARG:HG3	7:1H:4:ILE:N	2.34	0.43
1:2A:75:G:H4'	24:22:55:ARG:NH1	2.34	0.43
25:23:6:VAL:O	25:23:34:GLU:HA	2.17	0.43
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.18	0.43
1:2A:2061:G:H5''	1:2A:2503:2MA:C2	2.48	0.43
1:2A:265:A:H8	1:2A:266:G:H1'	1.81	0.43
1:2A:557:U:H2'	1:2A:558:G:C8	2.54	0.43
1:2A:859:G:N2	1:2A:917:A:OP2	2.38	0.43
1:2A:956:G:N2	1:2A:959:A:H3'	2.33	0.43
6:2G:111:LEU:HD23	6:2G:117:PHE:CZ	2.53	0.43
6:2G:127:GLY:H	6:2G:166:ASP:CG	2.21	0.43
1:2A:2642:G:H5''	9:2N:78:TYR:CD1	2.53	0.43
14:2S:105:ALA:HB1	14:2S:110:LEU:HD22	2.01	0.43
28:16:2:ALA:HA	28:16:6:ARG:HB2	2.01	0.43
1:1A:1001:G:H5''	12:1Q:77:LYS:HD2	2.01	0.43
1:1A:1221:G:H21	1:1A:1222:A:H4'	1.84	0.43
1:1A:1851:U:C2	3:1D:202:LYS:HD3	2.53	0.43
10:1O:9:GLU:O	10:1O:83:ALA:HA	2.18	0.43
22:20:14:ARG:H	22:20:14:ARG:HG2	1.66	0.43
1:2A:2025:C:H2'	1:2A:2026:C:H6	1.83	0.43
1:2A:2143:C:N3	1:2A:2148:G:N2	2.55	0.43
1:2A:263:C:H2'	1:2A:264:C:O4'	2.19	0.43
1:2A:359:A:H2'	1:2A:360:G:O4'	2.19	0.43
1:2A:864:G:C6	1:2A:865:C:N4	2.87	0.43
2:2B:7:G:H2'	2:2B:8:U:O4'	2.19	0.43
1:1A:1627:A:H8	1:1A:1627:A:OP2	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1766:G:H1'	1:1A:1770:A:H61	1.84	0.43
1:1A:596:G:O2'	1:1A:597:C:H3'	2.19	0.43
8:1I:116:LEU:HD11	8:1I:120:ILE:HG13	2.00	0.43
8:1I:124:GLY:H	8:1I:144:VAL:HG23	1.82	0.43
10:1O:107:ARG:HD3	15:1T:37:GLY:H	1.84	0.43
18:1W:68:ARG:HH11	18:1W:111:HIS:HA	1.84	0.43
1:2A:1221(A):C:H42	1:2A:1228:G:H1	1.66	0.43
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.18	0.43
1:2A:1669:A:H5''	1:2A:2550:G:OP1	2.17	0.43
1:2A:473:G:H2'	1:2A:474:G:H8	2.78	0.43
1:2A:918:A:C2	2:2B:80:U:H4'	2.53	0.43
20:2Y:28:LYS:HD2	20:2Y:40:GLU:OE1	2.19	0.43
1:1A:1120:G:N1	1:1A:1121:C:H1'	2.34	0.43
1:1A:1514:C:OP2	1:1A:1594:C:H5	2.02	0.43
1:1A:2389:A:H2'	1:1A:2390:A:C8	2.54	0.43
1:1A:442:A:H2'	1:1A:443:C:C6	2.54	0.43
1:1A:863:C:H2'	1:1A:864:C:H6	1.83	0.43
1:1A:776:G:C6	3:1D:208:LYS:HB2	2.54	0.43
3:1D:79:VAL:O	3:1D:114:GLY:N	2.52	0.43
16:1U:97:ASP:OD1	16:1U:101:ARG:NH1	2.51	0.43
1:2A:372:G:H8	23:21:65:SER:O	2.01	0.43
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.34	0.43
1:2A:2831:G:OP1	1:2A:2834:G:H4'	2.18	0.43
1:2A:332:A:O2'	1:2A:334:C:OP2	2.28	0.43
6:2G:16:ARG:HB2	6:2G:17:PRO:HD3	2.00	0.43
6:2G:11:TYR:HB2	6:2G:176:LEU:HD21	1.99	0.43
7:2H:113:VAL:HG11	7:2H:151:ILE:HG21	2.00	0.43
14:2S:77:ALA:O	14:2S:81:GLY:N	2.52	0.43
15:2T:119:LYS:HG2	15:2T:123:GLN:HE21	1.84	0.43
1:2A:64:A:O3'	19:2X:71:GLY:HA3	2.19	0.43
21:2Z:146:ILE:HG12	21:2Z:174:VAL:HG13	2.00	0.43
25:13:35:ARG:HE	25:13:37:LEU:HD21	1.84	0.43
28:16:38:LYS:HE3	28:16:38:LYS:HB3	1.79	0.43
1:1A:1001:G:H2'	1:1A:1002:A:H2'	2.00	0.43
1:1A:2605:U:H2'	1:1A:2606:C:C6	2.54	0.43
30:28:50:LEU:HA	30:28:50:LEU:HD23	1.77	0.43
1:2A:140:G:N2	1:2A:1596:A:H4'	2.33	0.43
1:2A:2175:C:H2'	1:2A:2176:A:O4'	2.18	0.43
1:2A:2100:G:H1	1:2A:2189:U:H3	1.65	0.43
1:2A:271(H):G:H1	1:2A:271(P):C:N4	2.13	0.43
3:2D:132:PRO:HD3	3:2D:190:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:275:LYS:HA	3:2D:276:LYS:C	2.40	0.43
3:2D:275:LYS:HE3	3:2D:276:LYS:O	2.19	0.43
1:2A:674:G:O2'	5:2F:74:ARG:HD3	2.19	0.43
6:2G:170:ARG:NH2	6:2G:182:LYS:O	2.52	0.43
7:2H:127:GLU:OE1	7:2H:130:ARG:NE	2.38	0.43
11:2P:59:LEU:HD11	30:28:10:ALA:CB	2.46	0.43
14:2S:66:ALA:O	14:2S:69:VAL:HG12	2.19	0.43
14:2S:14:VAL:HG11	14:2S:90:GLY:O	2.18	0.43
1:1A:1128:U:N3	1:1A:1132:A:N6	2.30	0.42
1:1A:1139:G:H3'	1:1A:1140:U:C5'	2.47	0.42
1:1A:2296:C:OP2	28:16:6:ARG:HG3	2.19	0.42
1:1A:741:U:OP1	3:1D:59:LYS:NZ	2.50	0.42
16:1U:102:GLU:HB3	16:1U:104:GLN:HE22	1.84	0.42
1:1A:1198:C:H1'	16:1U:77:SER:HB3	2.00	0.42
21:1Z:72:ARG:HD3	21:1Z:72:ARG:HA	1.65	0.42
1:2A:1007:C:O2	1:2A:1022:G:N1	18.25	0.42
1:2A:143(A):C:H2'	1:2A:144:C:H6	1.84	0.42
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.19	0.42
1:2A:1965:C:H3'	1:2A:1966:A:H2'	2.01	0.42
1:2A:244:A:C2	1:2A:255:A:C4	3.07	0.42
1:2A:2023:G:H5'	1:2A:2617:C:H4'	2.01	0.42
1:2A:479:A:H4'	1:2A:480:A:OP1	2.18	0.42
9:2N:62:VAL:CG1	9:2N:66:LYS:HB2	2.49	0.42
1:2A:826:U:C4'	11:2P:55:ARG:HB3	2.45	0.42
20:2Y:43:ASN:O	20:2Y:64:GLU:HA	2.19	0.42
1:1A:1102:G:O6	1:1A:1147:U:H5''	2.19	0.42
1:1A:1341:C:H2'	1:1A:1342:G:H8	1.83	0.42
1:1A:2284:U:H5''	1:1A:2285:A:OP1	2.18	0.42
1:1A:27:G:N2	1:1A:537:G:H1'	2.34	0.42
1:1A:262:C:H42	1:1A:282:G:H1	1.66	0.42
5:1F:183:VAL:O	5:1F:187:VAL:HG23	2.18	0.42
9:1N:58:ASP:OD1	9:1N:58:ASP:N	2.51	0.42
10:1O:104:ARG:CZ	15:1T:34:VAL:HG11	2.50	0.42
23:21:80:LEU:HB3	23:21:82:LEU:HD21	2.01	0.42
1:2A:1219:G:H1	1:2A:1230:C:H42	1.66	0.42
1:2A:2299:G:H2'	1:2A:2300:G:H8	1.84	0.42
1:2A:2611:U:OP2	1:2A:2611:U:H3'	2.20	0.42
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.83	0.42
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	2.00	0.42
1:1A:1016:C:O2'	1:1A:1029:A:N3	2.45	0.42
1:1A:1212:C:H2'	1:1A:1213:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:125:A:H5''	1:1A:126:C:C6	2.53	0.42
1:1A:1513:G:H2'	1:1A:1594:C:H41	1.83	0.42
1:1A:2158:C:N4	1:1A:2177:G:N1	2.19	0.42
1:1A:2705:A:H2'	1:1A:2706:G:C8	2.54	0.42
1:1A:360:C:H2'	1:1A:361:C:C6	2.55	0.42
4:1E:165:VAL:O	4:1E:189:PRO:HG2	2.19	0.42
5:1F:24:LEU:HD23	5:1F:115:ALA:HA	2.02	0.42
6:1G:159:VAL:HG21	6:1G:173:LEU:HD21	2.02	0.42
8:1I:38:LEU:H	8:1I:38:LEU:HG	1.62	0.42
28:26:10:LEU:HD12	28:26:54:ILE:HA	2.01	0.42
1:2A:1354:A:O3'	3:2D:38:LYS:HE2	2.20	0.42
1:2A:1682:G:H1'	1:2A:1762:A:C6	2.54	0.42
1:2A:2108:C:N3	1:2A:2181:G:N2	2.55	0.42
1:2A:2505:G:H2'	1:2A:2576:G:O6	2.18	0.42
1:2A:2600:A:H2'	1:2A:2601:C:H6	1.84	0.42
1:2A:2747:G:OP1	7:2H:74:ASN:ND2	2.51	0.42
1:2A:2821:A:H2'	1:2A:2822:G:C8	2.54	0.42
1:2A:478:A:N1	1:2A:500:G:H4'	2.34	0.42
1:2A:915:C:H3'	1:2A:916:G:H8	1.83	0.42
3:2D:159:ALA:HB1	3:2D:198:ASN:O	2.19	0.42
7:2H:54:ARG:HB3	7:2H:65:HIS:CD2	2.54	0.42
14:2S:71:ARG:H	14:2S:71:ARG:HG3	1.65	0.42
1:1A:1613:A:OP1	3:1D:211:ARG:NH1	2.50	0.42
1:1A:1474:C:O2'	1:1A:1616:A:OP2	2.27	0.42
1:1A:2182:G:C6	1:1A:2183:C:C4	3.06	0.42
1:1A:2224:C:H2'	1:1A:2225:U:O4'	2.20	0.42
1:1A:2603:C:H2'	1:1A:2604:G:C8	2.54	0.42
1:1A:821:A:H2'	1:1A:821:A:N3	2.34	0.42
4:1E:47:VAL:HG22	4:1E:84:PHE:O	2.19	0.42
11:1P:133:SER:O	11:1P:137:LYS:HB2	2.20	0.42
18:1W:11:ARG:C	18:1W:11:ARG:HH11	2.23	0.42
29:27:34:ARG:NH2	29:27:39:ARG:HG2	2.34	0.42
1:2A:1486:A:H2'	1:2A:1487:G:C8	2.54	0.42
1:2A:1613:G:N1	1:2A:1617:C:O2'	2.46	0.42
3:2D:228:PRO:HD3	3:2D:235:GLY:CA	2.50	0.42
4:2E:170:LEU:HB3	4:2E:184:VAL:HG23	2.02	0.42
11:2P:44:GLY:CA	11:2P:45:LEU:HB2	2.49	0.42
14:2S:87:PHE:HB2	14:2S:112:PHE:CE1	2.55	0.42
1:1A:1121:C:O2	1:1A:1122:C:H2'	2.19	0.42
1:1A:1685:C:O3'	1:1A:2721:G:N2	2.53	0.42
1:1A:2314:G:H2'	1:1A:2315:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2429:C:OP1	11:1P:65:ARG:NH2	2.52	0.42
2:1B:16:G:C6	2:1B:69:G:C2	3.08	0.42
3:1D:2:ALA:O	3:1D:20:ASP:HB3	2.20	0.42
21:1Z:130:PRO:HA	21:1Z:133:ILE:HG13	2.01	0.42
1:2A:98:G:P	24:22:2:LYS:HG2	2.60	0.42
29:27:37:LYS:HD3	29:27:39:ARG:HD3	2.01	0.42
1:2A:1532:C:N4	1:2A:1537:G:N1	2.68	0.42
1:2A:18:C:H2'	1:2A:19:C:C6	2.55	0.42
1:2A:2270:G:H2'	1:2A:2271:G:O4'	2.20	0.42
1:2A:2432:A:C6	1:2A:2433:A:C6	3.07	0.42
1:2A:2823:A:OP1	4:2E:113:PHE:HB2	2.20	0.42
1:2A:473:G:H2'	1:2A:474:G:C8	3.34	0.42
5:2F:184:TYR:HE1	11:2P:3:LEU:HD21	1.84	0.42
6:2G:15:VAL:HA	6:2G:175:LEU:HD23	2.02	0.42
7:2H:145:ALA:HA	7:2H:148:ILE:HD12	2.01	0.42
15:2T:114:LEU:HD23	15:2T:114:LEU:HA	1.87	0.42
28:16:6:ARG:HH11	28:16:26:ASN:HB2	1.85	0.42
1:1A:1660:A:C6	18:1W:87:PRO:HB3	2.54	0.42
1:1A:2128:G:H1	1:1A:2205:C:H42	1.66	0.42
1:1A:2180:A:O2'	1:1A:2181:G:OP2	2.32	0.42
1:1A:2418:U:H2'	1:1A:2418:U:H6	1.60	0.42
1:1A:2807:C:N4	1:1A:2813:G:H22	2.17	0.42
1:1A:2819:A:C6	1:1A:2820:A:C6	3.07	0.42
6:1G:174:GLU:HG3	6:1G:180:PHE:CD2	2.55	0.42
22:20:69:PHE:CE1	22:20:79:VAL:HG22	2.55	0.42
29:27:24:THR:O	29:27:28:ARG:HG3	2.20	0.42
11:2P:59:LEU:HD12	30:28:58:ILE:HG12	2.01	0.42
1:2A:247:G:H4'	1:2A:386:G:C5	2.55	0.42
1:2A:271(S):G:H2'	1:2A:271(T):C:C6	2.55	0.42
15:2T:105:LEU:HB2	15:2T:110:ILE:HG13	2.01	0.42
18:1W:19:LEU:HB3	27:15:25:LEU:HD11	2.02	0.42
1:1A:1055:A:OP2	9:1N:37:LYS:NZ	2.49	0.42
1:1A:1056:A:N3	1:1A:1199:C:H1'	2.35	0.42
1:1A:1993:A:C4	3:1D:241:PRO:HD3	2.55	0.42
1:1A:2188:G:N7	1:1A:2190:G:N2	2.68	0.42
1:1A:2193:A:O2'	1:1A:2194:U:H5''	2.20	0.42
1:1A:320:C:H2'	1:1A:321:C:C6	2.55	0.42
1:1A:863:C:H2'	1:1A:864:C:C6	2.54	0.42
3:1D:183:ARG:NH2	3:1D:266:SER:HB2	2.34	0.42
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.55	0.42
1:2A:77:C:OP1	24:22:59:ARG:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.55	0.42
1:2A:2359:C:H2'	1:2A:2360:A:O4'	2.18	0.42
18:2W:43:GLY:O	18:2W:47:VAL:HG23	2.20	0.42
1:1A:2225:U:O2'	1:1A:2226:C:H5'	2.20	0.42
1:1A:2517:G:O6	1:1A:2588:G:H2'	2.20	0.42
1:1A:2821:G:N2	1:1A:2900:G:H1'	2.34	0.42
1:1A:342:C:N4	1:1A:347:G:O6	5.70	0.42
1:1A:599:U:H2'	1:1A:600:G:C8	2.55	0.42
5:1F:164:ARG:HD2	5:1F:175:THR:HG23	2.01	0.42
6:1G:138:GLN:N	6:1G:138:GLN:OE1	2.39	0.42
7:1H:88:LEU:HD23	7:1H:130:ARG:HG2	2.01	0.42
1:2A:1270:C:H4'	1:2A:1325:G:N7	2.35	0.42
1:2A:1805:U:O2	3:2D:50:THR:HB	2.20	0.42
1:2A:1493:C:N4	1:2A:2206:G:O2'	2.44	0.42
1:2A:2846:G:H2'	1:2A:2847:U:O4'	2.19	0.42
1:2A:2859:G:H2'	1:2A:2860:A:C8	2.55	0.42
1:2A:272(G):C:H42	1:2A:363(C):G:H1	1.68	0.42
1:2A:530:G:O4'	1:2A:530:G:N3	2.52	0.42
1:2A:531:C:H4'	1:2A:532:A:H5''	2.01	0.42
1:2A:848:G:N9	1:2A:933:A:H8	2.18	0.42
2:2B:55:U:O2'	6:2G:27:ASN:ND2	2.42	0.42
4:2E:52:LEU:O	4:2E:76:ARG:HG3	2.20	0.42
6:2G:111:LEU:HA	6:2G:114:ILE:HD12	2.01	0.42
10:2O:40:VAL:HG22	10:2O:59:LYS:HG2	2.00	0.42
1:2A:2296:U:OP2	14:2S:6:ALA:HB2	2.20	0.42
1:1A:2490:A:H5'	31:19:31:LYS:HE2	2.01	0.42
1:1A:2227:G:H5''	1:1A:2228:G:C8	2.55	0.42
1:1A:2418:U:H2'	1:1A:2418:U:OP2	2.20	0.42
1:1A:2803:A:H5''	1:1A:2804:C:H5''	2.01	0.42
1:1A:692:C:H2'	1:1A:693:G:O4'	2.19	0.42
1:1A:2523:U:O2'	4:1E:138:PRO:O	2.31	0.42
7:1H:152:ARG:HD3	7:1H:152:ARG:HA	1.84	0.42
9:1N:61:ARG:HD3	9:1N:61:ARG:HA	1.54	0.42
10:1O:17:ARG:HA	10:1O:17:ARG:HD3	1.90	0.42
16:1U:83:LEU:HD13	16:1U:113:ALA:HB2	2.02	0.42
1:2A:1425:G:C6	1:2A:1426:G:C6	3.07	0.42
1:2A:171:G:H2'	1:2A:172:C:H6	1.85	0.42
1:2A:2182:G:H2'	1:2A:2183:C:C6	2.55	0.42
1:2A:2769:C:H2'	1:2A:2770:G:O4'	2.19	0.42
1:2A:300:A:H8	1:2A:300:A:O5'	3.03	0.42
8:2I:93:THR:O	8:2I:97:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2O:120:GLU:HG2	10:2O:122:LEU:HG	2.01	0.42
15:2T:127:ALA:C	15:2T:129:ARG:H	2.22	0.42
1:1A:2283:G:OP1	22:10:18:ALA:HB1	2.20	0.42
27:15:16:ARG:HD2	27:15:20:ARG:NH1	2.35	0.42
27:15:5:PRO:O	61:15:201:HOH:O	2.22	0.42
1:1A:1106:U:N3	1:1A:1108:G:O2'	2.48	0.42
1:1A:2466:G:H1'	61:1A:4665:HOH:O	2.20	0.42
1:1A:2631:C:O2'	4:1E:154:LYS:HB3	2.20	0.42
1:1A:469:A:C5	5:1F:45:ARG:HD2	2.55	0.42
12:1Q:135:ASP:O	12:1Q:139:GLU:HG3	2.20	0.42
23:21:67:ILE:N	23:21:68:PRO:HD2	2.34	0.42
24:22:51:ARG:HG2	24:22:55:ARG:NH2	2.35	0.42
1:2A:1027:A:N6	1:2A:1126:A:N3	2.68	0.42
1:2A:2123:G:H2'	1:2A:2124:G:C8	2.55	0.42
1:2A:2104:G:C2	1:2A:2186:G:C2	3.08	0.42
1:2A:2207:G:H3'	1:2A:2208:A:H5''	2.02	0.42
1:2A:2689:U:H4'	1:2A:2690:C:H5'	2.02	0.42
1:2A:2809:A:N6	1:2A:2891:G:H2'	2.35	0.42
1:2A:581:C:H2'	1:2A:582:G:H8	1.84	0.42
2:2B:28:C:H2'	2:2B:29:A:O4'	2.20	0.42
2:2B:37:C:N4	2:2B:38:C:N3	2.68	0.42
13:2R:100:LEU:HA	13:2R:100:LEU:HD12	1.82	0.42
1:1A:1222:A:O2'	1:1A:1223:C:O4'	2.27	0.41
1:1A:1245:C:H1'	16:1U:2:PRO:HG3	2.01	0.41
1:1A:2142:G:C2'	1:1A:2143:G:H5'	2.50	0.41
1:1A:611:U:H2'	1:1A:612:C:C6	2.55	0.41
12:1Q:79:LEU:HD23	12:1Q:79:LEU:HA	1.88	0.41
14:1S:10:ARG:HG2	14:1S:91:PRO:HA	2.01	0.41
14:1S:93:LYS:HG2	14:1S:95:HIS:HB2	2.02	0.41
26:24:44:THR:O	26:24:46:GLN:N	2.53	0.41
1:2A:118:A:N3	1:2A:178:G:H1'	2.35	0.41
1:2A:196:A:N3	1:2A:196:A:H2'	2.36	0.41
1:2A:2483:C:H2'	1:2A:2484:G:O4'	2.20	0.41
1:2A:571:A:N6	1:2A:2499:C:O3'	2.53	0.41
5:2F:33:LEU:HA	5:2F:33:LEU:HD12	1.74	0.41
11:2P:28:GLY:O	11:2P:30:THR:N	2.53	0.41
12:2Q:12:GLN:NE2	12:2Q:72:LYS:HG3	2.35	0.41
21:2Z:54:HIS:CG	21:2Z:101:PRO:HG3	2.55	0.41
1:1A:1095:C:H1'	1:1A:1159:U:O2'	2.19	0.41
1:1A:1198:C:H4'	16:1U:77:SER:HA	2.01	0.41
1:1A:1211:U:H2'	1:1A:1212:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:18:C:H2'	1:1A:19:C:C6	2.55	0.41
1:1A:2189:U:H2'	1:1A:2190:G:O4'	2.20	0.41
1:1A:478:G:C2	1:1A:484:G:C5	3.08	0.41
1:1A:831:A:C5	3:1D:229:VAL:HG21	2.56	0.41
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	2.01	0.41
13:1R:28:LEU:HD22	13:1R:44:LEU:HD13	2.02	0.41
16:1U:85:LYS:HE3	16:1U:116:ALA:O	2.19	0.41
20:1Y:1:MET:HB3	20:1Y:2:ARG:H	1.69	0.41
1:2A:1364:G:O5'	23:21:3:LYS:HG3	2.20	0.41
25:23:39:ASP:OD1	25:23:44:ARG:NH1	2.50	0.41
1:2A:2130:U:H4'	1:2A:2133:G:H4'	2.02	0.41
1:2A:720:C:H2'	1:2A:721:C:C6	2.56	0.41
1:2A:875:G:N1	1:2A:903:C:C2	2.88	0.41
2:2B:2:C:H5''	2:2B:3:C:OP2	2.20	0.41
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	2.01	0.41
8:2I:68:LEU:O	8:2I:72:LEU:HG	2.20	0.41
14:2S:10:ARG:HH21	14:2S:91:PRO:HB2	1.85	0.41
1:1A:1053:C:OP1	9:1N:37:LYS:NZ	2.49	0.41
1:1A:1432:C:H2'	1:1A:1433:C:C6	2.55	0.41
1:1A:1760:U:H2'	1:1A:1761:G:H8	1.84	0.41
1:1A:1821:C:H5''	1:1A:1822:A:OP1	2.20	0.41
1:1A:2050:U:H2'	1:1A:2051:G:O4'	2.19	0.41
1:1A:26:G:C6	1:1A:27:G:N1	2.89	0.41
2:1B:2:C:H2'	2:1B:3:C:C6	2.55	0.41
9:1N:33:LEU:HD12	9:1N:33:LEU:HA	1.82	0.41
21:1Z:100:VAL:O	21:1Z:123:ASP:HB2	2.19	0.41
1:2A:643:A:C8	28:26:44:ARG:NH1	2.88	0.41
1:2A:1450(A):C:N3	1:2A:1451:C:N4	2.68	0.41
1:2A:16:G:H2'	1:2A:17:G:H8	1.85	0.41
1:2A:2659:G:N2	1:2A:2662:A:OP2	2.52	0.41
1:2A:2891:G:H5''	1:2A:2892:A:OP2	2.20	0.41
1:2A:39:C:H2'	1:2A:40:C:C6	2.55	0.41
1:2A:857:C:H2'	1:2A:858:U:C6	2.55	0.41
1:2A:892:G:H3'	1:2A:893:C:C5'	2.50	0.41
14:2S:19:LYS:HG2	14:2S:19:LYS:H	1.65	0.41
1:1A:898:U:O2'	25:13:42:ALA:O	2.38	0.41
1:1A:1942:4OC:O5'	1:1A:1942:4OC:H6	2.20	0.41
1:1A:1973:U:O2'	1:1A:1975:A:N7	2.42	0.41
1:1A:1314:A:C2	1:1A:2035:A:C4	3.08	0.41
1:1A:2182:G:C6	1:1A:2183:C:N4	2.88	0.41
1:1A:443:C:H2'	1:1A:444:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.55	0.41
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.59	0.41
7:1H:18:GLU:HG2	7:1H:19:VAL:N	2.35	0.41
25:23:12:PRO:HB2	25:23:20:LYS:HE3	2.03	0.41
30:28:33:ASN:HA	30:28:36:LYS:HD2	2.02	0.41
1:2A:2134:A:P	1:2A:2157:G:H22	2.44	0.41
1:2A:2815:C:H2'	1:2A:2816:C:H6	1.84	0.41
1:2A:387:U:OP2	23:21:20:ARG:NH1	2.41	0.41
6:2G:117:PHE:CZ	6:2G:179:PRO:HG2	2.55	0.41
7:2H:118:PRO:HD2	7:2H:121:ILE:HG21	2.01	0.41
8:2I:79:ILE:HB	8:2I:144:VAL:HG12	2.02	0.41
10:2O:88:ASN:ND2	10:2O:92:GLU:HB2	2.35	0.41
24:12:55:ARG:O	24:12:59:ARG:HG3	2.20	0.41
1:1A:794:U:O2	1:1A:2036:A:H1'	2.21	0.41
1:1A:2163:G:N3	1:1A:2164:C:H1'	2.36	0.41
1:1A:2541:G:H5''	1:1A:2542:A:H5''	2.02	0.41
1:1A:785:G:H3'	1:1A:786:G:C8	2.56	0.41
1:1A:928:G:H3'	1:1A:929:G:C8	2.55	0.41
12:1Q:14:ARG:HG2	12:1Q:41:TRP:HH2	1.86	0.41
22:20:53:MET:HG3	22:20:59:LEU:CD2	2.51	0.41
30:28:14:VAL:HG22	30:28:24:ALA:HB2	2.02	0.41
1:2A:1359:A:H2	1:2A:1372:U:O4	2.04	0.41
1:2A:2161:C:H3'	1:2A:2162:G:H8	1.85	0.41
1:2A:2336:A:H61	22:20:43:THR:CG2	2.33	0.41
1:2A:2404:C:O3'	11:2P:77:ARG:NH2	2.52	0.41
1:2A:2533:A:O2'	1:2A:2664:G:H5''	2.19	0.41
1:2A:300:A:N3	1:2A:319:C:H1'	2.36	0.41
4:2E:181:LEU:HA	4:2E:181:LEU:HD12	1.72	0.41
5:2F:40:GLN:NE2	5:2F:182:ASN:HB2	2.36	0.41
7:2H:3:ARG:CZ	7:2H:5:GLY:H	2.34	0.41
12:2Q:31:ASP:HA	12:2Q:134:ARG:NH1	2.34	0.41
15:2T:33:LYS:HB3	15:2T:82:LEU:HD23	2.02	0.41
16:2U:61:TRP:CZ2	16:2U:93:LYS:HG3	2.55	0.41
21:2Z:153:SER:HB3	21:2Z:167:PRO:HA	2.02	0.41
1:1A:1011:G:O4'	1:1A:2279:A:N6	2.53	0.41
1:1A:1108:G:H5''	1:1A:1116:A:O2'	2.21	0.41
1:1A:1452:U:H2'	1:1A:1453:C:C6	2.55	0.41
1:1A:2169:G:H3'	1:1A:2169:G:N3	2.36	0.41
1:1A:895:G:H2'	1:1A:896:A:C8	2.56	0.41
4:1E:21:VAL:O	4:1E:23:VAL:HG13	2.20	0.41
4:1E:52:LEU:HA	4:1E:53:PRO:HD3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:57:HIS:CD2	12:1Q:117:ALA:HB2	2.56	0.41
19:1X:25:LYS:HA	19:1X:81:VAL:O	2.21	0.41
1:2A:1364:G:P	23:21:3:LYS:HG3	2.61	0.41
1:2A:1430:C:H2'	1:2A:1431:U:H6	1.86	0.41
1:2A:1434:A:H2'	1:2A:1435:G:O4'	2.44	0.41
1:2A:1937:A:H1'	1:2A:1939:5MU:H73	2.03	0.41
1:2A:197:A:N6	1:2A:2430:A:H2'	2.35	0.41
1:2A:1998:G:H4'	1:2A:2724:C:O2'	2.19	0.41
1:2A:2516:G:C6	1:2A:2517:C:C4	3.09	0.41
1:2A:319:C:O2'	1:2A:320:A:H5'	2.20	0.41
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.20	0.41
4:2E:70:ALA:O	4:2E:72:VAL:N	2.52	0.41
5:2F:24:LEU:HD21	5:2F:114:VAL:HG12	2.01	0.41
1:2A:2565:A:H62	10:2O:28:SER:CB	2.34	0.41
10:2O:98:VAL:HG23	10:2O:118:ALA:HA	2.02	0.41
14:2S:64:GLU:HG3	14:2S:64:GLU:H	1.62	0.41
1:2A:1754:C:OP1	15:2T:96:ARG:NH1	2.53	0.41
1:1A:1073:A:C2	1:1A:2500:A:H5'	2.56	0.41
1:1A:1115:A:H2	1:1A:1141:A:HO2'	1.65	0.41
1:1A:1501:U:OP1	13:1R:77:ARG:NH1	2.40	0.41
1:1A:1698:G:N2	1:1A:2029:C:C2	2.89	0.41
1:1A:2455:C:OP1	5:1F:68:LYS:HD3	2.20	0.41
1:1A:2864:G:H2'	1:1A:2865:C:C6	2.56	0.41
1:1A:360:C:H2'	1:1A:361:C:H6	1.86	0.41
1:1A:27:G:C2	1:1A:537:G:N3	2.88	0.41
1:1A:925:A:H3'	1:1A:926:G:C8	2.55	0.41
1:1A:99:G:H21	24:12:7:ARG:NH2	2.17	0.41
7:1H:126:PRO:HB2	7:1H:127:GLU:H	1.64	0.41
8:1I:76:THR:HG22	8:1I:141:LYS:HE2	2.02	0.41
11:1P:46:LYS:HB3	11:1P:46:LYS:HE3	1.91	0.41
13:1R:37:THR:OG1	13:1R:39:PRO:HD2	2.21	0.41
14:1S:36:TYR:CD2	14:1S:36:TYR:N	2.87	0.41
19:1X:57:LEU:HD12	19:1X:57:LEU:O	2.21	0.41
28:26:26:ASN:O	28:26:29:ASN:N	2.54	0.41
1:2A:1418:G:H8	1:2A:1418:G:O5'	2.04	0.41
1:2A:1589:C:H2'	1:2A:1590:U:C6	2.55	0.41
1:2A:1830:C:H2'	1:2A:1831:G:C8	2.56	0.41
1:2A:2305:A:H2'	1:2A:2306:C:O4'	2.21	0.41
1:2A:2633:G:H2'	1:2A:2634:G:O4'	2.21	0.41
1:2A:927:G:H2'	1:2A:928:G:O4'	2.20	0.41
2:2B:38:C:H2'	2:2B:39:A:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:9:ILE:HB	7:2H:50:VAL:HB	2.03	0.41
16:2U:106:PHE:O	16:2U:110:VAL:HG23	2.20	0.41
1:1A:1535:U:HO2'	1:1A:1536:A:H8	1.64	0.41
1:1A:704:U:H2'	1:1A:705:C:H6	1.86	0.41
1:1A:782:A:N7	1:1A:808:A:H2	2.18	0.41
7:1H:4:ILE:O	7:1H:69:ARG:HD2	2.21	0.41
10:1O:63:VAL:HG11	10:1O:85:VAL:HG23	2.02	0.41
10:1O:9:GLU:H	10:1O:9:GLU:HG2	1.60	0.41
4:1E:12:THR:HG21	15:1T:11:GLU:HG2	2.03	0.41
15:1T:27:THR:O	15:1T:89:VAL:HG13	2.21	0.41
1:2A:11:G:O5'	1:2A:11:G:H8	2.04	0.41
1:2A:2150:U:H2'	1:2A:2151:G:C8	2.56	0.41
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.41	0.41
8:2I:27:ARG:HD3	23:21:71:TYR:CE2	2.55	0.41
21:2Z:158:PRO:HA	21:2Z:159:PRO:HD3	1.96	0.41
25:13:5:LYS:HG3	25:13:36:VAL:HG22	2.02	0.41
1:1A:1305:G:H22	1:1A:1331:G:H1'	40.17	0.41
1:1A:2144:U:H2'	1:1A:2145:G:O4'	2.21	0.41
1:1A:2518:U:H3	58:1A:4030:EZG:CG	2.33	0.41
1:1A:646:A:H5'	1:1A:647:G:OP2	2.21	0.41
12:1Q:37:LEU:HD21	12:1Q:130:LYS:CE	2.51	0.41
1:1A:509:A:O2'	20:1Y:49:VAL:O	2.30	0.41
26:24:48:ARG:HA	26:24:48:ARG:HD2	1.81	0.41
1:2A:1002:G:C2	1:2A:1003:G:C8	4.05	0.41
1:2A:1683:C:H2'	1:2A:1684:C:C6	2.56	0.41
1:2A:2070:G:H2'	1:2A:2071:A:C8	2.55	0.41
1:2A:2784:C:H2'	1:2A:2785:C:H6	1.85	0.41
1:2A:2787:C:H2'	1:2A:2788:C:C6	2.56	0.41
1:2A:659:C:H2'	1:2A:660:G:C8	2.47	0.41
1:2A:80:G:H1	1:2A:106:C:H42	1.67	0.41
7:2H:105:LEU:O	7:2H:113:VAL:N	2.44	0.41
1:2A:2847:U:OP2	15:2T:98:LYS:NZ	2.54	0.41
21:2Z:7:ALA:HB3	21:2Z:61:LEU:HD12	2.03	0.41
1:1A:1094:A:N1	1:1A:1158:G:O2'	2.38	0.41
1:1A:1096:A:H2'	1:1A:1097:G:O4'	2.21	0.41
1:1A:1228:G:O2'	25:13:29:ARG:NH1	2.54	0.41
1:1A:1400:A:H4'	3:1D:38:LYS:HZ3	1.86	0.41
1:1A:1468:G:H1'	1:1A:1542:A:N1	2.36	0.41
1:1A:1820:A:H2'	1:1A:1821:C:O4'	2.21	0.41
1:1A:1849:U:O4	3:1D:154:LYS:HD2	2.20	0.41
1:1A:2179:G:H4'	1:1A:2180:A:OP1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:225:C:H2'	1:1A:226:C:H6	1.84	0.41
1:1A:2756:C:OP1	31:19:33:LYS:NZ	2.43	0.41
1:1A:407:U:H2'	1:1A:408:G:C8	2.54	0.41
1:1A:764:G:H2'	1:1A:765:A:O4'	2.21	0.41
8:1I:86:THR:HG22	8:1I:123:LEU:H	1.86	0.41
8:1I:5:LEU:H	8:1I:5:LEU:HD12	1.86	0.41
19:1X:39:ILE:O	19:1X:43:VAL:HG23	2.21	0.41
26:24:26:SER:OG	26:24:27:THR:N	2.54	0.41
1:2A:116:C:H2'	1:2A:117:G:O4'	2.20	0.41
1:2A:1198:U:H2'	1:2A:1199:U:C6	2.56	0.41
1:2A:1260:G:C6	1:2A:1261:C:C4	3.09	0.41
1:2A:1818:U:H2'	3:2D:157:ARG:HD2	2.03	0.41
1:2A:2526:G:O3'	31:29:33:LYS:NZ	2.54	0.41
1:2A:1638:C:H5''	1:2A:2710:C:O2'	2.20	0.41
1:2A:521:G:H2'	1:2A:522:G:H8	1.85	0.41
1:2A:2728:U:O2'	4:2E:22:PRO:HG2	2.21	0.41
17:2V:15:GLU:O	17:2V:18:LEU:HB3	2.21	0.41
25:13:54:VAL:HG12	25:13:55:ARG:N	2.36	0.41
26:14:16:CYS:HA	26:14:33:VAL:O	2.20	0.41
1:1A:101:A:C6	1:1A:102:U:C4	3.09	0.41
1:1A:1686:U:H4'	1:1A:2711:C:H4'	2.03	0.41
1:1A:2297:C:OP2	28:16:6:ARG:HD3	2.21	0.41
1:1A:239:G:C6	1:1A:240:A:C6	3.09	0.41
1:1A:2524:C:H2'	1:1A:2525:G:O4'	2.21	0.41
1:1A:2859:U:H4'	1:1A:2878:A:C2	2.56	0.41
1:1A:34:C:H5''	1:1A:35:G:OP2	2.20	0.41
1:1A:866:A:C4	1:1A:1234:A:C2	3.09	0.41
3:1D:145:VAL:HG11	3:1D:175:LEU:HD11	2.02	0.41
1:1A:826:U:OP1	3:1D:49:ILE:HG13	2.21	0.41
3:1D:68:LYS:HB2	3:1D:70:TRP:CE2	2.55	0.41
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	2.02	0.41
13:1R:12:ARG:O	13:1R:17:ARG:NH1	2.54	0.41
14:1S:76:LYS:H	14:1S:76:LYS:HG3	1.70	0.41
15:1T:94:ALA:HB1	15:1T:99:LEU:HD21	2.03	0.41
1:2A:98:G:H5''	24:22:3:LEU:HG	2.02	0.41
27:25:49:CYS:SG	27:25:51:TYR:HB2	2.61	0.41
31:29:2:LYS:HD3	31:29:4:ARG:NH2	2.35	0.41
1:2A:1759:A:H1'	1:2A:2711:A:C2	2.56	0.41
1:2A:1826:G:H4'	3:2D:242:ARG:CZ	2.51	0.41
1:2A:2019:A:O3'	16:2U:27:LEU:HD12	2.20	0.41
1:2A:2788:C:H5''	4:2E:61:ARG:HH21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:401:A:H2'	1:2A:402:A:O4'	2.20	0.41
1:2A:56:A:H2'	1:2A:57:C:O4'	2.21	0.41
1:2A:949:C:H2'	1:2A:950:G:C8	2.56	0.41
2:2B:68:C:H2'	2:2B:69:G:H8	1.84	0.41
3:2D:66:ASP:HB2	3:2D:103:ARG:HD3	2.03	0.41
21:2Z:28:MET:HA	21:2Z:88:PHE:O	2.22	0.41
1:1A:1068:G:C5	1:1A:1185:C:C4	3.08	0.40
1:1A:1118:C:H5''	1:1A:1119:A:OP1	2.21	0.40
1:1A:1197:G:O3'	16:1U:81:HIS:HB2	2.21	0.40
1:1A:1660:A:N1	18:1W:87:PRO:HB3	2.36	0.40
1:1A:1680:G:C6	1:1A:1682:G:C4	3.09	0.40
1:1A:1810:U:H2'	61:1A:4292:HOH:O	2.20	0.40
1:1A:2039:U:O2	27:15:10:LYS:HB2	2.21	0.40
1:1A:2274:U:H5	22:10:16:SER:HB3	1.86	0.40
1:1A:965:G:N2	1:1A:2281:A:OP2	2.52	0.40
1:1A:2803:A:H5'	1:1A:2902:G:H21	1.86	0.40
1:1A:752:A:C2	1:1A:774:A:H1'	2.56	0.40
23:21:46:LEU:HD23	23:21:46:LEU:HA	1.91	0.40
23:21:89:GLU:O	23:21:93:GLU:HG2	2.21	0.40
1:2A:1007:C:N3	1:2A:1022:G:C6	16.79	0.40
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.21	0.40
1:2A:2516:G:C6	1:2A:2517:C:N4	2.90	0.40
1:2A:2647:U:H2'	1:2A:2648:C:C6	2.56	0.40
1:2A:422:A:H2'	1:2A:423:A:C8	2.56	0.40
1:2A:600:G:N2	1:2A:605:C:O3'	2.54	0.40
7:2H:17:VAL:O	7:2H:45:VAL:HG11	2.20	0.40
7:2H:20:ALA:CB	7:2H:25:LYS:HG2	2.49	0.40
8:2I:9:LEU:HD22	8:2I:12:LEU:HD12	2.03	0.40
9:2N:110:GLY:O	9:2N:114:ARG:HG3	2.20	0.40
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.56	0.40
12:2Q:2:LEU:HD12	12:2Q:2:LEU:HA	1.82	0.40
1:1A:2390:A:H4'	14:1S:23:ARG:NH1	2.35	0.40
1:1A:273:G:O2'	1:1A:274:U:H5''	2.21	0.40
1:1A:2780:C:H2'	1:1A:2781:C:H6	1.85	0.40
1:1A:954:C:OP1	12:1Q:22:LYS:HB3	2.21	0.40
2:1B:68:C:H2'	2:1B:69:G:O4'	2.20	0.40
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	2.03	0.40
10:1O:43:VAL:HG12	10:1O:54:GLU:HA	2.03	0.40
14:1S:11:LYS:HE2	14:1S:15:ARG:HH12	1.86	0.40
21:1Z:153:SER:HB3	21:1Z:167:PRO:HB3	2.03	0.40
1:2A:987:G:O2'	1:2A:1000:A:N3	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:117:G:C6	1:2A:119:A:C6	3.09	0.40
1:2A:1525:G:H2'	1:2A:1526:G:O4'	2.69	0.40
1:2A:1780:A:N6	61:2A:4058:HOH:O	2.54	0.40
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.84	0.40
1:2A:201:C:H2'	1:2A:202:U:H2'	5.71	0.40
1:2A:2019:A:H2	1:2A:2035:G:H22	1.68	0.40
1:2A:218:A:C2	1:2A:235:U:H4'	2.56	0.40
1:2A:2207:G:H2'	1:2A:2208:A:C2	2.57	0.40
1:2A:2749:A:OP1	7:2H:3:ARG:NH1	2.54	0.40
1:2A:663:G:C6	1:2A:664:C:C4	3.09	0.40
1:2A:79:G:H2'	1:2A:80:G:C8	2.60	0.40
1:2A:828:U:H2'	1:2A:829:A:C8	2.56	0.40
2:2B:59:A:H2'	2:2B:60:C:O4'	2.22	0.40
6:2G:107:LEU:HD23	6:2G:111:LEU:HD13	2.04	0.40
1:2A:1139:G:O3'	9:2N:24:GLY:HA3	2.21	0.40
11:2P:128:HIS:CD2	11:2P:148:LEU:HD11	2.56	0.40
15:2T:64:ARG:NH1	15:2T:103:ARG:HG2	2.36	0.40
21:2Z:102:LEU:HD23	21:2Z:139:VAL:HG21	2.03	0.40
27:15:16:ARG:HG2	27:15:16:ARG:HH11	1.85	0.40
1:1A:1067:A:H3'	1:1A:1067:A:N3	2.36	0.40
1:1A:1091:A:OP1	1:1A:1092:A:H3'	2.21	0.40
1:1A:791:G:N2	1:1A:1497:G:O3'	58.34	0.40
1:1A:2143:G:O6	1:1A:2198:A:N6	2.54	0.40
1:1A:2899:C:H2'	1:1A:2900:G:O4'	2.21	0.40
1:1A:434:G:H2'	1:1A:435:G:H8	1.86	0.40
1:1A:927:G:H2'	1:1A:928:G:C8	2.47	0.40
1:1A:2116:G:OP1	8:1I:22:LYS:HD2	2.21	0.40
1:2A:468:G:N7	29:27:39:ARG:NH2	2.69	0.40
1:2A:1404:C:H2'	1:2A:1405:U:H6	1.87	0.40
1:2A:1547:C:H2'	1:2A:1548:C:H6	1.87	0.40
1:2A:2173:A:H5''	1:2A:2174:C:OP2	2.22	0.40
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.56	0.40
1:2A:882:G:H1	1:2A:894:C:H42	1.69	0.40
1:2A:947:G:H2'	1:2A:948:G:C8	2.56	0.40
11:2P:38:GLN:HG2	11:2P:45:LEU:N	2.36	0.40
16:2U:66:ASN:ND2	16:2U:70:ARG:HH21	2.12	0.40
21:2Z:126:VAL:HG13	21:2Z:161:VAL:HG23	2.03	0.40
1:1A:2661:U:H2'	1:1A:2662:U:C6	2.56	0.40
1:1A:504:A:N1	1:1A:525:G:H4'	2.36	0.40
2:1B:44:G:C2	2:1B:48:A:C2	3.09	0.40
22:20:70:GLN:HG2	22:20:72:ARG:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2249:U:N3	1:2A:2253:G:OP2	2.48	0.40
1:2A:2439:A:H5'	1:2A:2439:A:C8	2.56	0.40
1:2A:250:G:C6	1:2A:251:A:C6	3.09	0.40
1:2A:2525:G:N2	1:2A:2539:C:C2	2.89	0.40
1:2A:2648:C:H2'	1:2A:2649:U:H6	1.87	0.40
1:2A:271:A:N6	1:2A:271(X):G:H1'	2.36	0.40
1:2A:395:U:O2'	1:2A:396:G:N7	2.43	0.40
1:2A:700:G:H2'	1:2A:701:G:O4'	2.21	0.40
1:2A:870:A:H5'	1:2A:871:U:OP2	2.21	0.40
5:2F:23:ASP:O	5:2F:24:LEU:HD12	2.21	0.40
6:2G:23:PHE:HB2	6:2G:25:TYR:CE2	2.56	0.40
11:2P:100:LEU:HA	11:2P:103:ALA:HB3	2.03	0.40
16:2U:68:ALA:O	16:2U:71:GLN:HB2	2.21	0.40
19:2X:64:LYS:HD3	19:2X:64:LYS:HA	1.80	0.40
21:2Z:23:LYS:HB3	21:2Z:38:TYR:CD1	2.56	0.40
30:18:23:VAL:HG13	30:18:47:LYS:HB3	2.03	0.40
1:1A:1116:A:N6	1:1A:1142:A:N3	2.70	0.40
1:1A:2230:U:O4'	23:11:52:ARG:NH2	2.43	0.40
1:1A:228:U:H2'	1:1A:229:G:O4'	2.21	0.40
1:1A:2408:G:OP1	23:11:25:LYS:NZ	2.33	0.40
1:1A:593:G:H2'	1:1A:2052:A:C5	2.57	0.40
1:1A:734:C:OP1	29:17:2:LYS:NZ	2.55	0.40
1:1A:757:G:H2'	1:1A:758:G:H8	1.85	0.40
1:1A:830:A:H2'	1:1A:830:A:N3	2.36	0.40
5:1F:53:THR:HG22	5:1F:55:GLY:N	2.34	0.40
6:1G:43:LEU:HB3	6:1G:44:GLY:H	1.50	0.40
7:1H:83:TYR:CE2	7:1H:138:LYS:HB2	2.57	0.40
8:1I:47:LEU:O	8:1I:51:ILE:HG13	2.21	0.40
21:1Z:15:PRO:O	21:1Z:19:ARG:HG3	2.21	0.40
1:2A:1878:G:C5	1:2A:1879:C:C4	3.09	0.40
1:2A:2298:A:N6	1:2A:2318:G:C8	2.89	0.40
1:2A:2262:U:H4'	1:2A:2328:A:C2	2.57	0.40
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.86	0.40
1:2A:561:G:HO2'	16:2U:45:TYR:HE1	1.69	0.40
1:2A:637:A:C6	1:2A:652:C:H4'	2.56	0.40
2:2B:33:G:N3	2:2B:50:G:N2	2.70	0.40
3:2D:155:LEU:HA	3:2D:155:LEU:HD23	4.50	0.40
6:2G:55:LYS:O	6:2G:59:GLU:N	2.28	0.40
6:2G:96:ARG:O	6:2G:99:MET:HB3	2.22	0.40
7:2H:123:PHE:CE1	7:2H:133:VAL:HG22	2.57	0.40
10:2O:4:PRO:O	10:2O:5:GLN:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	257 (94%)	16 (6%)	0	100	100
3	2D	273/276 (99%)	254 (93%)	18 (7%)	1 (0%)	34	66
4	1E	202/206 (98%)	189 (94%)	12 (6%)	1 (0%)	29	61
4	2E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	29	61
5	1F	201/210 (96%)	196 (98%)	4 (2%)	1 (0%)	29	61
5	2F	201/210 (96%)	184 (92%)	13 (6%)	4 (2%)	7	24
6	1G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	25	56
6	2G	179/182 (98%)	156 (87%)	18 (10%)	5 (3%)	5	17
7	1H	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	25	56
7	2H	172/180 (96%)	149 (87%)	20 (12%)	3 (2%)	9	29
8	1I	144/148 (97%)	133 (92%)	10 (7%)	1 (1%)	22	53
8	2I	144/148 (97%)	126 (88%)	17 (12%)	1 (1%)	22	53
9	1N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
9	2N	138/140 (99%)	126 (91%)	9 (6%)	3 (2%)	6	22
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	111 (92%)	7 (6%)	2 (2%)	9	29
11	1P	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
11	2P	147/150 (98%)	134 (91%)	11 (8%)	2 (1%)	11	34
12	1Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	22	53
12	2Q	139/141 (99%)	128 (92%)	10 (7%)	1 (1%)	22	53
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	109 (94%)	5 (4%)	2 (2%)	9	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	1S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	17	46
14	2S	108/112 (96%)	100 (93%)	6 (6%)	2 (2%)	8	26
15	1T	129/146 (88%)	120 (93%)	8 (6%)	1 (1%)	19	49
15	2T	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	19	49
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	97 (98%)	1 (1%)	1 (1%)	15	44
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	44
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/96 (97%)	84 (90%)	9 (10%)	0	100	100
20	1Y	105/110 (96%)	96 (91%)	8 (8%)	1 (1%)	15	44
20	2Y	105/110 (96%)	96 (91%)	7 (7%)	2 (2%)	8	26
21	1Z	148/206 (72%)	133 (90%)	14 (10%)	1 (1%)	22	53
21	2Z	156/206 (76%)	132 (85%)	19 (12%)	5 (3%)	4	13
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	13	39
23	11	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	63 (93%)	4 (6%)	1 (2%)	10	33
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	8	28
26	14	67/71 (94%)	55 (82%)	8 (12%)	4 (6%)	1	4
26	24	67/71 (94%)	50 (75%)	13 (19%)	4 (6%)	1	4
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	44 (86%)	7 (14%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	27	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	6	22
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
33	1b	229/256 (90%)	192 (84%)	27 (12%)	10 (4%)	2	8
33	2b	229/256 (90%)	200 (87%)	20 (9%)	9 (4%)	3	10
34	1c	204/239 (85%)	190 (93%)	11 (5%)	3 (2%)	10	33
34	2c	204/239 (85%)	173 (85%)	25 (12%)	6 (3%)	4	15
35	1d	206/209 (99%)	190 (92%)	13 (6%)	3 (2%)	10	33
35	2d	206/209 (99%)	187 (91%)	15 (7%)	4 (2%)	8	26
36	1e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	11	34
36	2e	146/162 (90%)	131 (90%)	14 (10%)	1 (1%)	22	53
37	1f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
37	2f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
38	1g	153/156 (98%)	138 (90%)	12 (8%)	3 (2%)	7	24
38	2g	153/156 (98%)	135 (88%)	15 (10%)	3 (2%)	7	24
39	1h	135/138 (98%)	129 (96%)	4 (3%)	2 (2%)	10	33
39	2h	135/138 (98%)	125 (93%)	8 (6%)	2 (2%)	10	33
40	1i	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
40	2i	125/128 (98%)	113 (90%)	12 (10%)	0	100	100
41	1j	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	3	9
41	2j	94/105 (90%)	79 (84%)	11 (12%)	4 (4%)	2	8
42	1k	112/129 (87%)	105 (94%)	6 (5%)	1 (1%)	17	46
42	2k	112/129 (87%)	103 (92%)	6 (5%)	3 (3%)	5	17
43	1l	119/132 (90%)	110 (92%)	8 (7%)	1 (1%)	19	49
43	2l	119/132 (90%)	103 (87%)	15 (13%)	1 (1%)	19	49
44	1m	121/126 (96%)	112 (93%)	9 (7%)	0	100	100
44	2m	120/126 (95%)	102 (85%)	15 (12%)	3 (2%)	5	19
45	1n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	1o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	13	39
46	2o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	13	39
47	1p	80/88 (91%)	69 (86%)	10 (12%)	1 (1%)	12	36
47	2p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
48	1q	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	15	44
48	2q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
49	1r	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	68 (84%)	12 (15%)	1 (1%)	13	39
50	2s	81/93 (87%)	66 (82%)	13 (16%)	2 (2%)	5	19
51	1t	94/106 (89%)	84 (89%)	5 (5%)	5 (5%)	2	6
51	2t	94/106 (89%)	83 (88%)	5 (5%)	6 (6%)	1	3
52	1u	21/27 (78%)	18 (86%)	2 (10%)	1 (5%)	2	7
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
All	All	11370/12128 (94%)	10425 (92%)	802 (7%)	143 (1%)	12	36

All (143) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	43	LEU
7	1H	126	PRO
26	14	53	GLU
33	1b	22	LYS
34	1c	107	GLN
38	1g	4	ARG
50	1s	81	ARG
3	2D	3	VAL
6	2G	47	LYS
12	2Q	27	VAL
26	24	45	GLY
29	27	46	VAL
33	2b	16	HIS
33	2b	17	PHE
33	2b	21	ARG
33	2b	125	PRO
36	2e	77	PRO

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Mol	Chain	Res	Type
41	2j	79	ARG
8	1I	11	ASN
20	1Y	54	LYS
26	14	45	GLY
33	1b	126	GLU
36	1e	21	ALA
38	1g	6	ARG
41	1j	79	ARG
43	1l	91	LYS
5	2F	130	ALA
7	2H	47	GLU
7	2H	126	PRO
9	2N	48	MET
10	2O	5	GLN
11	2P	29	LYS
13	2R	14	SER
17	2V	79	VAL
21	2Z	171	ILE
33	2b	95	GLN
33	2b	231	GLU
34	2c	91	LEU
34	2c	156	ARG
35	2d	179	GLU
38	2g	4	ARG
41	2j	75	ILE
42	2k	49	GLY
46	2o	88	ARG
51	2t	9	ASN
51	2t	10	LEU
51	2t	47	GLY
15	1T	37	GLY
17	1V	79	VAL
26	14	61	ARG
33	1b	20	GLU
33	1b	231	GLU
35	1d	173	TRP
35	1d	178	VAL
36	1e	86	ALA
41	1j	29	ARG
41	1j	77	PRO
46	1o	19	PRO
51	1t	47	GLY

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Mol	Chain	Res	Type
51	1t	95	ALA
4	2E	52	LEU
5	2F	21	ALA
6	2G	124	SER
7	2H	29	PRO
8	2I	116	LEU
9	2N	2	LYS
14	2S	84	GLN
20	2Y	102	CYS
20	2Y	103	GLY
21	2Z	167	PRO
26	24	61	ARG
33	2b	20	GLU
33	2b	123	ALA
34	2c	181	ASN
35	2d	181	MET
38	2g	55	GLY
51	2t	95	ALA
4	1E	52	LEU
12	1Q	17	LEU
26	14	57	GLU
33	1b	9	GLU
33	1b	17	PHE
33	1b	21	ARG
33	1b	207	ALA
38	1g	80	VAL
51	1t	100	ILE
52	1u	3	LYS
9	2N	59	LYS
11	2P	45	LEU
13	2R	2	ARG
21	2Z	142	SER
24	22	46	GLN
33	2b	158	LEU
34	2c	64	VAL
34	2c	92	ALA
34	2c	95	THR
35	2d	5	ILE
35	2d	10	ARG
38	2g	80	VAL
41	2j	31	GLY
42	2k	106	LYS

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Mol	Chain	Res	Type
44	2m	106	ASN
50	2s	76	PRO
51	2t	102	GLY
14	1S	94	TYR
33	1b	16	HIS
34	1c	66	VAL
35	1d	179	GLU
39	1h	133	LEU
48	1q	33	GLY
51	1t	10	LEU
5	2F	168	ARG
6	2G	51	ARG
6	2G	179	PRO
15	2T	117	ASP
22	20	12	ASN
26	24	29	PRO
26	24	55	ARG
39	2h	3	THR
43	2l	51	ALA
50	2s	81	ARG
51	2t	99	LEU
21	1Z	156	LYS
47	1p	53	VAL
51	1t	102	GLY
5	2F	133	ASN
10	2O	88	ASN
14	2S	96	GLY
39	1h	83	ILE
42	1k	105	VAL
21	2Z	147	GLY
42	2k	105	VAL
44	2m	4	ILE
33	1b	230	VAL
41	1j	39	PRO
6	2G	177	GLY
41	2j	39	PRO
39	2h	73	ASP
44	2m	6	GLY
34	1c	174	PRO
21	2Z	165	VAL
25	23	50	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	200 (93%)	15 (7%)	15	40
3	2D	215/218 (99%)	206 (96%)	9 (4%)	30	63
4	1E	164/166 (99%)	152 (93%)	12 (7%)	14	38
4	2E	164/166 (99%)	148 (90%)	16 (10%)	8	24
5	1F	160/166 (96%)	144 (90%)	16 (10%)	7	22
5	2F	159/166 (96%)	144 (91%)	15 (9%)	8	26
6	1G	143/156 (92%)	133 (93%)	10 (7%)	15	40
6	2G	143/156 (92%)	134 (94%)	9 (6%)	18	46
7	1H	144/148 (97%)	138 (96%)	6 (4%)	30	63
7	2H	144/148 (97%)	138 (96%)	6 (4%)	30	63
8	1I	113/124 (91%)	104 (92%)	9 (8%)	12	34
8	2I	105/124 (85%)	99 (94%)	6 (6%)	20	50
9	1N	118/119 (99%)	110 (93%)	8 (7%)	16	42
9	2N	118/119 (99%)	108 (92%)	10 (8%)	10	31
10	1O	100/100 (100%)	97 (97%)	3 (3%)	41	75
10	2O	100/100 (100%)	100 (100%)	0	100	100
11	1P	115/116 (99%)	109 (95%)	6 (5%)	23	55
11	2P	115/116 (99%)	111 (96%)	4 (4%)	36	70
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	22	53
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	11	33
13	1R	101/101 (100%)	90 (89%)	11 (11%)	6	19
13	2R	101/101 (100%)	92 (91%)	9 (9%)	9	28
14	1S	86/88 (98%)	78 (91%)	8 (9%)	9	26
14	2S	85/88 (97%)	78 (92%)	7 (8%)	11	33
15	1T	115/127 (91%)	112 (97%)	3 (3%)	46	79
15	2T	113/127 (89%)	105 (93%)	8 (7%)	14	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	85 (91%)	8 (9%)	10	30
16	2U	93/94 (99%)	91 (98%)	2 (2%)	52	83
17	1V	80/82 (98%)	73 (91%)	7 (9%)	10	29
17	2V	80/82 (98%)	71 (89%)	9 (11%)	6	18
18	1W	90/92 (98%)	87 (97%)	3 (3%)	38	72
18	2W	90/92 (98%)	83 (92%)	7 (8%)	12	35
19	1X	77/78 (99%)	73 (95%)	4 (5%)	23	55
19	2X	77/78 (99%)	74 (96%)	3 (4%)	32	66
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	19	49
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	14	39
21	1Z	135/179 (75%)	123 (91%)	12 (9%)	9	28
21	2Z	137/179 (76%)	128 (93%)	9 (7%)	16	44
22	10	65/67 (97%)	62 (95%)	3 (5%)	27	60
22	20	65/67 (97%)	63 (97%)	2 (3%)	40	74
23	11	80/83 (96%)	77 (96%)	3 (4%)	33	67
23	21	80/83 (96%)	80 (100%)	0	100	100
24	12	65/67 (97%)	62 (95%)	3 (5%)	27	60
24	22	65/67 (97%)	64 (98%)	1 (2%)	65	89
25	13	51/52 (98%)	50 (98%)	1 (2%)	55	84
25	23	50/52 (96%)	45 (90%)	5 (10%)	7	22
26	14	59/63 (94%)	55 (93%)	4 (7%)	16	42
26	24	53/63 (84%)	49 (92%)	4 (8%)	13	37
27	15	50/52 (96%)	44 (88%)	6 (12%)	5	15
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	48
28	16	51/52 (98%)	47 (92%)	4 (8%)	12	35
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	22
29	17	41/42 (98%)	37 (90%)	4 (10%)	8	24
29	27	41/42 (98%)	39 (95%)	2 (5%)	25	57
30	18	54/55 (98%)	49 (91%)	5 (9%)	9	26
30	28	54/55 (98%)	49 (91%)	5 (9%)	9	26
31	19	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	76
33	1b	192/220 (87%)	184 (96%)	8 (4%)	30	63
33	2b	187/220 (85%)	174 (93%)	13 (7%)	15	40
34	1c	142/188 (76%)	136 (96%)	6 (4%)	30	63
34	2c	140/188 (74%)	133 (95%)	7 (5%)	24	56
35	1d	169/181 (93%)	159 (94%)	10 (6%)	19	49
35	2d	173/181 (96%)	162 (94%)	11 (6%)	17	45
36	1e	113/123 (92%)	105 (93%)	8 (7%)	14	39
36	2e	114/123 (93%)	108 (95%)	6 (5%)	22	54
37	1f	84/90 (93%)	81 (96%)	3 (4%)	35	69
37	2f	85/90 (94%)	82 (96%)	3 (4%)	36	70
38	1g	119/127 (94%)	114 (96%)	5 (4%)	30	63
38	2g	120/127 (94%)	111 (92%)	9 (8%)	13	37
39	1h	114/119 (96%)	108 (95%)	6 (5%)	22	54
39	2h	114/119 (96%)	107 (94%)	7 (6%)	18	48
40	1i	90/99 (91%)	86 (96%)	4 (4%)	28	61
40	2i	89/99 (90%)	85 (96%)	4 (4%)	27	60
41	1j	66/92 (72%)	64 (97%)	2 (3%)	41	75
41	2j	69/92 (75%)	64 (93%)	5 (7%)	14	38
42	1k	82/99 (83%)	78 (95%)	4 (5%)	25	57
42	2k	83/99 (84%)	78 (94%)	5 (6%)	19	48
43	1l	96/108 (89%)	86 (90%)	10 (10%)	7	21
43	2l	96/108 (89%)	93 (97%)	3 (3%)	40	74
44	1m	93/101 (92%)	87 (94%)	6 (6%)	17	44
44	2m	92/101 (91%)	90 (98%)	2 (2%)	52	83
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	15
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	22
46	1o	78/80 (98%)	76 (97%)	2 (3%)	46	79
46	2o	78/80 (98%)	75 (96%)	3 (4%)	33	67
47	1p	69/74 (93%)	66 (96%)	3 (4%)	29	62
47	2p	68/74 (92%)	65 (96%)	3 (4%)	28	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	91 (97%)	3 (3%)	39	73
48	2q	94/97 (97%)	89 (95%)	5 (5%)	22	54
49	1r	59/77 (77%)	55 (93%)	4 (7%)	16	42
49	2r	59/77 (77%)	57 (97%)	2 (3%)	37	71
50	1s	69/80 (86%)	67 (97%)	2 (3%)	42	76
50	2s	67/80 (84%)	64 (96%)	3 (4%)	27	60
51	1t	70/82 (85%)	67 (96%)	3 (4%)	29	62
51	2t	70/82 (85%)	65 (93%)	5 (7%)	14	39
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	21	51
All	All	9303/10064 (92%)	8749 (94%)	554 (6%)	19	48

All (554) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	61	LEU
3	1D	71	ASP
3	1D	88	ARG
3	1D	113	VAL
3	1D	147	LEU
3	1D	155	LEU
3	1D	162	SER
3	1D	176	ARG
3	1D	193	VAL
3	1D	211	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	257	LEU
3	1D	273	ARG
4	1E	1	MET
4	1E	12	THR
4	1E	21	VAL
4	1E	33	VAL
4	1E	47	VAL
4	1E	73	GLU
4	1E	78	LEU
4	1E	92	THR

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Mol	Chain	Res	Type
4	1E	113	PHE
4	1E	116	VAL
4	1E	175	VAL
4	1E	181	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	70	THR
5	1F	74	ARG
5	1F	88	VAL
5	1F	95	ARG
5	1F	106	ARG
5	1F	110	LEU
5	1F	125	LEU
5	1F	161	GLU
5	1F	170	LEU
5	1F	175	THR
5	1F	183	VAL
5	1F	189	THR
5	1F	192	LEU
6	1G	3	LEU
6	1G	31	VAL
6	1G	43	LEU
6	1G	60	LEU
6	1G	109	VAL
6	1G	126	ASP
6	1G	133	LEU
6	1G	145	THR
6	1G	159	VAL
6	1G	175	LEU
7	1H	56	SER
7	1H	69	ARG
7	1H	71	LEU
7	1H	88	LEU
7	1H	134	SER
7	1H	155	SER
8	1I	1	MET
8	1I	2	LYS
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	92	VAL
8	1I	129	THR
8	1I	142	VAL
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	35	ARG
9	1N	48	MET
9	1N	62	VAL
9	1N	87	LEU
9	1N	99	LEU
10	1O	9	GLU
10	1O	97	ARG
10	1O	108	GLU
11	1P	55	ARG
11	1P	59	LEU
11	1P	83	VAL
11	1P	98	GLU
11	1P	112	LEU
11	1P	125	VAL
12	1Q	7	MET
12	1Q	89	ASN
12	1Q	109	VAL
12	1Q	110	THR
12	1Q	135	ASP
12	1Q	138	ASP
13	1R	6	SER
13	1R	24	GLN
13	1R	29	LEU
13	1R	36	THR
13	1R	37	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	67	LEU
13	1R	79	LEU
13	1R	111	LEU
13	1R	114	VAL
14	1S	3	ARG
14	1S	11	LYS
14	1S	14	VAL
14	1S	36	TYR
14	1S	42	ASP

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Mol	Chain	Res	Type
14	1S	49	VAL
14	1S	69	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	89	VAL
15	1T	118	ARG
16	1U	5	LYS
16	1U	8	VAL
16	1U	50	ARG
16	1U	59	ARG
16	1U	74	LEU
16	1U	77	SER
16	1U	83	LEU
16	1U	95	LEU
17	1V	46	VAL
17	1V	52	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	79	VAL
17	1V	82	ARG
18	1W	17	VAL
18	1W	97	LYS
18	1W	107	LEU
19	1X	45	THR
19	1X	75	ASP
19	1X	81	VAL
19	1X	92	LEU
20	1Y	1	MET
20	1Y	11	ASP
20	1Y	55	TYR
20	1Y	72	VAL
20	1Y	99	CYS
21	1Z	18	LEU
21	1Z	33	LEU
21	1Z	41	LEU
21	1Z	61	LEU
21	1Z	72	ARG
21	1Z	76	LEU
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	129	SER

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Mol	Chain	Res	Type
21	1Z	150	LEU
21	1Z	170	THR
21	1Z	171	ILE
22	10	14	ARG
22	10	32	ARG
22	10	43	THR
23	11	30	VAL
23	11	56	GLN
23	11	95	LEU
24	12	30	ARG
24	12	40	SER
24	12	70	GLN
25	13	30	ARG
26	14	27	THR
26	14	49	PHE
26	14	52	THR
26	14	53	GLU
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
27	15	33	CYS
27	15	57	VAL
27	15	58	LEU
28	16	5	VAL
28	16	19	ARG
28	16	48	VAL
28	16	51	GLU
29	17	1	MET
29	17	24	THR
29	17	41	ARG
29	17	43	THR
30	18	14	VAL
30	18	30	ARG
30	18	31	HIS
30	18	32	LEU
30	18	34	TRP
33	1b	24	TRP
33	1b	37	ASN
33	1b	73	THR
33	1b	94	ASN
33	1b	127	ILE
33	1b	160	ASP

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Mol	Chain	Res	Type
33	1b	172	ILE
33	1b	195	ASP
34	1c	3	ASN
34	1c	21	ARG
34	1c	49	SER
34	1c	112	SER
34	1c	192	THR
34	1c	196	LEU
35	1d	3	ARG
35	1d	5	ILE
35	1d	10	ARG
35	1d	31	CYS
35	1d	53	ASP
35	1d	59	ARG
35	1d	70	ILE
35	1d	73	ARG
35	1d	112	VAL
35	1d	135	LEU
36	1e	16	THR
36	1e	31	LEU
36	1e	34	VAL
36	1e	41	VAL
36	1e	45	PHE
36	1e	51	VAL
36	1e	56	GLN
36	1e	91	LEU
37	1f	72	VAL
37	1f	73	ASN
37	1f	93	SER
38	1g	12	LEU
38	1g	16	LEU
38	1g	24	THR
38	1g	90	GLU
38	1g	94	ARG
39	1h	25	ASP
39	1h	29	SER
39	1h	49	GLU
39	1h	85	ARG
39	1h	112	LEU
39	1h	133	LEU
40	1i	17	VAL
40	1i	64	THR

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Mol	Chain	Res	Type
40	1i	65	VAL
40	1i	87	GLN
41	1j	34	VAL
41	1j	84	GLN
42	1k	31	THR
42	1k	48	ILE
42	1k	109	VAL
42	1k	114	VAL
43	1l	27	LEU
43	1l	37	CYS
43	1l	52	LEU
43	1l	55	VAL
43	1l	58	VAL
43	1l	59	ARG
43	1l	83	VAL
43	1l	89	ARG
43	1l	113	ARG
43	1l	117	ARG
44	1m	4	ILE
44	1m	8	GLU
44	1m	11	ARG
44	1m	19	LEU
44	1m	109	THR
44	1m	121	LYS
45	1n	6	LEU
45	1n	13	THR
45	1n	18	VAL
45	1n	23	ARG
45	1n	32	SER
45	1n	35	ARG
46	1o	39	LEU
46	1o	87	ILE
47	1p	2	VAL
47	1p	20	VAL
47	1p	67	THR
48	1q	15	MET
48	1q	35	VAL
48	1q	68	ARG
49	1r	26	LEU
49	1r	31	LEU
49	1r	46	GLU
49	1r	47	THR

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Mol	Chain	Res	Type
50	1s	12	ASP
50	1s	28	LYS
51	1t	13	LEU
51	1t	24	LEU
51	1t	56	MET
3	2D	20	ASP
3	2D	94	LEU
3	2D	106	ILE
3	2D	113	VAL
3	2D	116	GLN
3	2D	142	VAL
3	2D	183	ARG
3	2D	204	ILE
3	2D	242	ARG
4	2E	9	VAL
4	2E	21	VAL
4	2E	23	VAL
4	2E	24	THR
4	2E	27	LEU
4	2E	52	LEU
4	2E	75	VAL
4	2E	78	LEU
4	2E	101	ARG
4	2E	113	PHE
4	2E	116	VAL
4	2E	119	ARG
4	2E	134	ILE
4	2E	181	LEU
4	2E	184	VAL
4	2E	195	LEU
5	2F	12	LEU
5	2F	20	LEU
5	2F	33	LEU
5	2F	53	THR
5	2F	57	VAL
5	2F	74	ARG
5	2F	82	ILE
5	2F	88	VAL
5	2F	132	VAL
5	2F	149	ASP
5	2F	168	ARG
5	2F	170	LEU

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Mol	Chain	Res	Type
5	2F	183	VAL
5	2F	192	LEU
5	2F	201	VAL
6	2G	5	VAL
6	2G	7	LEU
6	2G	31	VAL
6	2G	43	LEU
6	2G	133	LEU
6	2G	135	LEU
6	2G	140	ILE
6	2G	145	THR
6	2G	159	VAL
7	2H	49	VAL
7	2H	59	ARG
7	2H	103	LEU
7	2H	134	SER
7	2H	148	ILE
7	2H	152	ARG
8	2I	38	LEU
8	2I	47	LEU
8	2I	96	ASP
8	2I	108	THR
8	2I	116	LEU
8	2I	123	LEU
9	2N	23	LEU
9	2N	28	THR
9	2N	34	LEU
9	2N	43	THR
9	2N	46	VAL
9	2N	60	ILE
9	2N	73	THR
9	2N	87	LEU
9	2N	120	LEU
9	2N	140	VAL
11	2P	45	LEU
11	2P	95	VAL
11	2P	99	LEU
11	2P	112	LEU
12	2Q	1	MET
12	2Q	2	LEU
12	2Q	16	ARG
12	2Q	21	THR

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Mol	Chain	Res	Type
12	2Q	29	PHE
12	2Q	60	ARG
12	2Q	75	THR
12	2Q	101	ARG
12	2Q	110	THR
13	2R	15	SER
13	2R	18	LEU
13	2R	24	GLN
13	2R	29	LEU
13	2R	33	ARG
13	2R	44	LEU
13	2R	65	LEU
13	2R	100	LEU
13	2R	102	GLU
14	2S	21	THR
14	2S	36	TYR
14	2S	46	VAL
14	2S	58	LEU
14	2S	64	GLU
14	2S	83	LYS
14	2S	110	LEU
15	2T	6	LEU
15	2T	31	SER
15	2T	46	GLU
15	2T	64	ARG
15	2T	67	SER
15	2T	74	ARG
15	2T	96	ARG
15	2T	104	ASN
16	2U	74	LEU
16	2U	95	LEU
17	2V	14	VAL
17	2V	18	LEU
17	2V	38	LEU
17	2V	51	VAL
17	2V	52	VAL
17	2V	61	VAL
17	2V	72	VAL
17	2V	79	VAL
17	2V	82	ARG
18	2W	11	ARG
18	2W	17	VAL

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Mol	Chain	Res	Type
18	2W	19	LEU
18	2W	23	LEU
18	2W	67	ASP
18	2W	92	ARG
18	2W	96	ILE
19	2X	14	SER
19	2X	45	THR
19	2X	81	VAL
20	2Y	14	LEU
20	2Y	38	ILE
20	2Y	72	VAL
20	2Y	83	THR
20	2Y	84	ARG
20	2Y	99	CYS
21	2Z	27	VAL
21	2Z	33	LEU
21	2Z	38	TYR
21	2Z	40	ASP
21	2Z	86	VAL
21	2Z	129	SER
21	2Z	144	LEU
21	2Z	154	ASP
21	2Z	171	ILE
22	20	14	ARG
22	20	27	GLU
24	22	53	LEU
25	23	23	LEU
25	23	30	ARG
25	23	31	LEU
25	23	40	THR
25	23	53	LEU
26	24	24	THR
26	24	34	GLU
26	24	50	VAL
26	24	63	TYR
27	25	6	VAL
27	25	16	ARG
27	25	21	SER
28	26	9	LEU
28	26	13	CYS
28	26	30	THR
28	26	32	ASN

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Mol	Chain	Res	Type
28	26	51	GLU
29	27	39	ARG
29	27	41	ARG
30	28	14	VAL
30	28	23	VAL
30	28	31	HIS
30	28	32	LEU
30	28	34	TRP
31	29	7	VAL
33	2b	11	LEU
33	2b	24	TRP
33	2b	41	ILE
33	2b	48	MET
33	2b	93	VAL
33	2b	94	ASN
33	2b	102	LEU
33	2b	135	GLN
33	2b	144	ARG
33	2b	165	VAL
33	2b	178	ARG
33	2b	185	ILE
33	2b	189	ASP
34	2c	49	SER
34	2c	57	ILE
34	2c	77	ILE
34	2c	89	GLU
34	2c	128	PHE
34	2c	166	GLU
34	2c	175	LEU
35	2d	31	CYS
35	2d	76	ARG
35	2d	107	ARG
35	2d	108	LEU
35	2d	135	LEU
35	2d	141	ARG
35	2d	150	GLU
35	2d	170	VAL
35	2d	175	SER
35	2d	178	VAL
35	2d	181	MET
36	2e	25	ARG
36	2e	34	VAL

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Mol	Chain	Res	Type
36	2e	41	VAL
36	2e	73	ASN
36	2e	81	GLU
36	2e	83	GLU
37	2f	10	LEU
37	2f	28	ARG
37	2f	75	LEU
38	2g	9	VAL
38	2g	15	ASP
38	2g	16	LEU
38	2g	78	ARG
38	2g	79	ARG
38	2g	95	ARG
38	2g	98	SER
38	2g	104	LEU
38	2g	154	TYR
39	2h	2	LEU
39	2h	3	THR
39	2h	12	ARG
39	2h	25	ASP
39	2h	68	ARG
39	2h	87	SER
39	2h	112	LEU
40	2i	89	ASN
40	2i	102	LEU
40	2i	108	VAL
40	2i	111	ARG
41	2j	8	LEU
41	2j	17	ASP
41	2j	59	SER
41	2j	67	THR
41	2j	100	THR
42	2k	14	VAL
42	2k	24	SER
42	2k	81	ASP
42	2k	84	VAL
42	2k	114	VAL
43	2l	12	ARG
43	2l	113	ARG
43	2l	117	ARG
44	2m	15	VAL
44	2m	103	THR

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Mol	Chain	Res	Type
45	2n	6	LEU
45	2n	11	LYS
45	2n	25	VAL
45	2n	33	VAL
45	2n	44	LEU
46	2o	37	ASN
46	2o	51	HIS
46	2o	88	ARG
47	2p	2	VAL
47	2p	21	VAL
47	2p	60	LEU
48	2q	6	LEU
48	2q	35	VAL
48	2q	57	VAL
48	2q	79	SER
48	2q	97	SER
49	2r	37	VAL
49	2r	59	SER
50	2s	65	ASN
50	2s	71	LEU
50	2s	79	THR
51	2t	24	LEU
51	2t	70	SER
51	2t	72	LEU
51	2t	84	LEU
51	2t	89	ARG
52	2u	6	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	48	GLN
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	79	ASN
8	1I	105	HIS
12	1Q	57	HIS
13	1R	24	GLN
13	1R	71	GLN
14	1S	68	GLN
15	1T	58	ASN

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Mol	Chain	Res	Type
16	1U	104	GLN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
20	1Y	43	ASN
21	1Z	54	HIS
23	11	56	GLN
30	18	35	GLN
33	1b	37	ASN
33	1b	40	HIS
34	1c	6	HIS
34	1c	104	GLN
34	1c	162	GLN
35	1d	77	ASN
35	1d	116	GLN
35	1d	119	GLN
35	1d	123	HIS
35	1d	161	ASN
36	1e	78	HIS
37	1f	73	ASN
37	1f	100	ASN
38	1g	28	ASN
40	1i	3	GLN
40	1i	23	ASN
40	1i	34	ASN
40	1i	58	HIS
40	1i	124	GLN
41	1j	56	HIS
43	1l	99	HIS
44	1m	62	ASN
45	1n	49	HIS
47	1p	13	HIS
50	1s	83	HIS
3	2D	87	ASN
3	2D	112	GLN
3	2D	220	HIS
4	2E	48	GLN
4	2E	66	HIS
5	2F	69	HIS
5	2F	203	GLN
6	2G	66	GLN
7	2H	158	HIS

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Mol	Chain	Res	Type
9	2N	38	HIS
10	2O	5	GLN
12	2Q	12	GLN
12	2Q	57	HIS
12	2Q	123	HIS
14	2S	38	GLN
15	2T	104	ASN
15	2T	123	GLN
19	2X	31	HIS
21	2Z	55	HIS
21	2Z	73	GLN
24	22	65	ASN
26	24	46	GLN
28	26	32	ASN
31	29	20	HIS
33	2b	94	ASN
33	2b	95	GLN
34	2c	6	HIS
34	2c	162	GLN
35	2d	42	GLN
35	2d	116	GLN
35	2d	125	HIS
37	2f	73	ASN
37	2f	100	ASN
38	2g	28	ASN
38	2g	68	ASN
38	2g	86	GLN
38	2g	97	GLN
39	2h	82	HIS
40	2i	3	GLN
40	2i	31	GLN
40	2i	58	HIS
46	2o	28	GLN
47	2p	16	HIS
49	2r	63	GLN
51	2t	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2860/2915 (98%)	472 (16%)	28 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2A	2788/2915 (95%)	502 (18%)	22 (0%)
2	1B	120/121 (99%)	12 (10%)	2 (1%)
2	2B	118/121 (97%)	32 (27%)	0
32	1a	1494/1521 (98%)	243 (16%)	0
32	2a	1498/1521 (98%)	270 (18%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	12/24 (50%)	2 (16%)	0
54	1w	71/76 (93%)	22 (30%)	0
54	1y	71/76 (93%)	21 (29%)	0
54	2w	68/76 (89%)	24 (35%)	0
54	2y	69/76 (90%)	26 (37%)	0
55	1x	75/77 (97%)	12 (16%)	0
55	2x	75/77 (97%)	9 (12%)	0
All	All	9331/9620 (96%)	1650 (17%)	52 (0%)

All (1650) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	45	C
1	1A	57	G
1	1A	60	G
1	1A	62	U
1	1A	63	A
1	1A	70	A
1	1A	73	A
1	1A	74	G
1	1A	83	A
1	1A	91	G
1	1A	94	G
1	1A	112	U
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	123	G
1	1A	129	G
1	1A	162	G
1	1A	164	G
1	1A	185	A
1	1A	188	A

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Mol	Chain	Res	Type
1	1A	194	G
1	1A	203	G
1	1A	204	G
1	1A	205	A
1	1A	211	A
1	1A	212	A
1	1A	215	G
1	1A	217	A
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	262	C
1	1A	263	C
1	1A	272	U
1	1A	273	G
1	1A	275	C
1	1A	288	U
1	1A	289	G
1	1A	299	G
1	1A	303	C
1	1A	335	A
1	1A	353	G
1	1A	354	A
1	1A	376	G
1	1A	381	A
1	1A	384	G
1	1A	387	G
1	1A	388	A
1	1A	389	G
1	1A	393	A
1	1A	413	G
1	1A	432	U
1	1A	438	G
1	1A	439	A
1	1A	448	U
1	1A	455	A
1	1A	470	C
1	1A	474	U
1	1A	483	A
1	1A	507	G
1	1A	529	U
1	1A	530	A

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Mol	Chain	Res	Type
1	1A	534	C
1	1A	537	G
1	1A	555	G
1	1A	556	C
1	1A	557	A
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	586	G
1	1A	596	G
1	1A	598	A
1	1A	615	G
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	639	G
1	1A	641	G
1	1A	652	A
1	1A	662	A
1	1A	670	C
1	1A	671	A
1	1A	678	A
1	1A	693	G
1	1A	697	C
1	1A	703	G
1	1A	716	G
1	1A	724	A
1	1A	733	G
1	1A	777	C
1	1A	787	U
1	1A	804	U
1	1A	811	A
1	1A	812	G
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	831	A
1	1A	832	G
1	1A	837	C
1	1A	839	G
1	1A	852	G
1	1A	859	C

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Mol	Chain	Res	Type
1	1A	866	A
1	1A	874	U
1	1A	875	U
1	1A	879	G
1	1A	906	G
1	1A	913	A
1	1A	924	U
1	1A	926	G
1	1A	927	G
1	1A	928	G
1	1A	929	G
1	1A	931	C
1	1A	932	C
1	1A	933	C
1	1A	934	A
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	940	C
1	1A	941	U
1	1A	942	A
1	1A	943	C
1	1A	944	C
1	1A	945	A
1	1A	953	U
1	1A	956	A
1	1A	957	A
1	1A	965	G
1	1A	976	G
1	1A	977	G
1	1A	990	A
1	1A	991	G
1	1A	1003	U
1	1A	1004	A
1	1A	1006	C
1	1A	1019	G
1	1A	1020	C
1	1A	1021	G
1	1A	1029	A
1	1A	1042	A
1	1A	1051	C
1	1A	1058	U

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Mol	Chain	Res	Type
1	1A	1059	C
1	1A	1068	G
1	1A	1071	G
1	1A	1072	U
1	1A	1073	A
1	1A	1076	G
1	1A	1079	U
1	1A	1083	G
1	1A	1084	C
1	1A	1087	C
1	1A	1090	G
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1100	A
1	1A	1101	G
1	1A	1104	G
1	1A	1105	G
1	1A	1112	U
1	1A	1114	G
1	1A	1117	G
1	1A	1119	A
1	1A	1120	G
1	1A	1121	C
1	1A	1122	C
1	1A	1124	U
1	1A	1125	C
1	1A	1126	C
1	1A	1133	G
1	1A	1134	A
1	1A	1137	G
1	1A	1138	C
1	1A	1139	G
1	1A	1140	U
1	1A	1142	A
1	1A	1146	C
1	1A	1149	A
1	1A	1156	G
1	1A	1157	A
1	1A	1158	G
1	1A	1162	C
1	1A	1164	C

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Mol	Chain	Res	Type
1	1A	1175	A
1	1A	1176	U
1	1A	1180	C
1	1A	1181	G
1	1A	1187	U
1	1A	1216	G
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1222	A
1	1A	1256	U
1	1A	1263	C
1	1A	1287	A
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1319	U
1	1A	1335	C
1	1A	1346	U
1	1A	1347	A
1	1A	1349	G
1	1A	1375	U
1	1A	1388	A
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1426	G
1	1A	1430	A
1	1A	1431	G
1	1A	1441	A
1	1A	1442	U
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1474	C
1	1A	1475	G
1	1A	1485	A
1	1A	1491	A

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Mol	Chain	Res	Type
1	1A	1497	G
1	1A	1502	G
1	1A	1514	C
1	1A	1529	G
1	1A	1530	G
1	1A	1536	A
1	1A	1539	C
1	1A	1540	A
1	1A	1545	C
1	1A	1554	A
1	1A	1555	C
1	1A	1556	A
1	1A	1569	U
1	1A	1571	G
1	1A	1601	A
1	1A	1605	A
1	1A	1606	G
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1627	A
1	1A	1628	G
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1658	C
1	1A	1694	G
1	1A	1695	C
1	1A	1701	A
1	1A	1721	G
1	1A	1743	G
1	1A	1747	A
1	1A	1748	A
1	1A	1750	G
1	1A	1767	A
1	1A	1776	G
1	1A	1787	G
1	1A	1793	A
1	1A	1794	G
1	1A	1795	G
1	1A	1800	G
1	1A	1804	A

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Mol	Chain	Res	Type
1	1A	1811	A
1	1A	1813	C
1	1A	1822	A
1	1A	1831	C
1	1A	1843	A
1	1A	1847	G
1	1A	1859	G
1	1A	1860	A
1	1A	1871	G
1	1A	1878	A
1	1A	1879	A
1	1A	1892	G
1	1A	1899	A
1	1A	1911	A
1	1A	1915	C
1	1A	1922	A
1	1A	1928	G
1	1A	1941	A
1	1A	1949	A
1	1A	1951	G
1	1A	1952	G
1	1A	1953	U
1	1A	1956	C
1	1A	1959	A
1	1A	1960	A
1	1A	1977	U
1	1A	1985	U
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2006	G
1	1A	2014	G
1	1A	2015	U
1	1A	2019	G
1	1A	2042	A
1	1A	2045	G
1	1A	2053	A
1	1A	2054	G
1	1A	2055	A
1	1A	2061	C
1	1A	2065	C

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Mol	Chain	Res	Type
1	1A	2074	G
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2084	A
1	1A	2091	G
1	1A	2118	U
1	1A	2120	U
1	1A	2124	U
1	1A	2132	G
1	1A	2135	U
1	1A	2136	A
1	1A	2141	A
1	1A	2143	G
1	1A	2144	U
1	1A	2148	A
1	1A	2149	G
1	1A	2151	C
1	1A	2152	U
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2157	A
1	1A	2158	C
1	1A	2164	C
1	1A	2166	U
1	1A	2168	C
1	1A	2169	G
1	1A	2170	G
1	1A	2172	U
1	1A	2177	G
1	1A	2179	G
1	1A	2180	A
1	1A	2181	G
1	1A	2188	G
1	1A	2189	U
1	1A	2190	G
1	1A	2192	A
1	1A	2194	U
1	1A	2195	A

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Mol	Chain	Res	Type
1	1A	2196	C
1	1A	2200	C
1	1A	2203	G
1	1A	2206	G
1	1A	2207	C
1	1A	2211	U
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A
1	1A	2230	U
1	1A	2237	A
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2285	A
1	1A	2292	G
1	1A	2295	C
1	1A	2299	A
1	1A	2306	C
1	1A	2317	A
1	1A	2320	G
1	1A	2332	A
1	1A	2337	G
1	1A	2346	G
1	1A	2348	A
1	1A	2359	C
1	1A	2362	C
1	1A	2366	G
1	1A	2373	A
1	1A	2384	G
1	1A	2395	G
1	1A	2397	C
1	1A	2408	G
1	1A	2418	U
1	1A	2422	G
1	1A	2430	A
1	1A	2434	A
1	1A	2437	A
1	1A	2441	G

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Mol	Chain	Res	Type
1	1A	2442	A
1	1A	2443	U
1	1A	2447	A
1	1A	2451	A
1	1A	2453	C
1	1A	2460	A
1	1A	2483	C
1	1A	2488	A
1	1A	2489	C
1	1A	2490	A
1	1A	2502	G
1	1A	2506	G
1	1A	2514	G
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2532	C
1	1A	2537	G
1	1A	2541	G
1	1A	2561	G
1	1A	2566	U
1	1A	2576	A
1	1A	2578	A
1	1A	2579	G
1	1A	2585	C
1	1A	2594	G
1	1A	2614	A
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2641	A
1	1A	2642	G
1	1A	2646	G
1	1A	2666	A
1	1A	2681	G
1	1A	2682	A
1	1A	2701	U
1	1A	2702	C
1	1A	2703	C
1	1A	2714	U
1	1A	2715	C
1	1A	2725	A

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Mol	Chain	Res	Type
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2745	G
1	1A	2746	A
1	1A	2757	G
1	1A	2763	A
1	1A	2765	C
1	1A	2770	A
1	1A	2771	A
1	1A	2774	G
1	1A	2777	A
1	1A	2778	A
1	1A	2779	G
1	1A	2782	C
1	1A	2791	A
1	1A	2793	G
1	1A	2803	A
1	1A	2804	C
1	1A	2807	C
1	1A	2813	G
1	1A	2830	A
1	1A	2831	A
1	1A	2845	A
1	1A	2882	G
1	1A	2890	C
1	1A	2901	A
1	1A	2903	G
2	1B	2	C
2	1B	9	G
2	1B	12	C
2	1B	15	A
2	1B	25	A
2	1B	35	U
2	1B	56	G
2	1B	66	A
2	1B	67	G
2	1B	73	A
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G

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Mol	Chain	Res	Type
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	52	G
32	1a	54	C
32	1a	61	G
32	1a	79	G
32	1a	91	C
32	1a	96	U
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	145	G
32	1a	162	A
32	1a	163	C
32	1a	174	C
32	1a	183	G
32	1a	189(F)	U
32	1a	189(H)	G
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	318	G
32	1a	321	A
32	1a	328	C

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Mol	Chain	Res	Type
32	1a	332	G
32	1a	342	C
32	1a	348	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	382	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	421	U
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	439	A
32	1a	441	A
32	1a	442	C
32	1a	452	A
32	1a	453	A
32	1a	457	C
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	482	A
32	1a	483	C
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	524	G
32	1a	531	U

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Mol	Chain	Res	Type
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	562	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	596	C
32	1a	607	A
32	1a	619	U
32	1a	630	G
32	1a	631	G
32	1a	653	A
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	717	C
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	747	C
32	1a	749	C
32	1a	752	G
32	1a	755	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	859	A
32	1a	870	U
32	1a	885	G

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Mol	Chain	Res	Type
32	1a	891	U
32	1a	902	G
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	931	C
32	1a	934	C
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	997	U
32	1a	1000	U
32	1a	1001(A)	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1026	G
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1030(D)	A
32	1a	1031	G
32	1a	1033	G
32	1a	1039	C
32	1a	1040	U

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Mol	Chain	Res	Type
32	1a	1043	C
32	1a	1053	G
32	1a	1054	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1096	C
32	1a	1101	A
32	1a	1108	G
32	1a	1123	A
32	1a	1125	U
32	1a	1129	C
32	1a	1132	C
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
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	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1270	C
32	1a	1275	A
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1300	G
32	1a	1302	U

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Mol	Chain	Res	Type
32	1a	1319	A
32	1a	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1340	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1378	C
32	1a	1397	C
32	1a	1400	5MC
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
53	1v	14	A
53	1v	24	A
54	1w	2	C
54	1w	3	C
54	1w	4	C
54	1w	6	G
54	1w	7	A
54	1w	8	4SU
54	1w	14	A
54	1w	19	G

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Mol	Chain	Res	Type
54	1w	20	U
54	1w	21	A
54	1w	24	G
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	62	C
54	1w	68	C
54	1w	70	G
54	1w	71	G
54	1w	72	C
54	1w	73	A
54	1w	74	C
55	1x	9	G
55	1x	13	C
55	1x	19	G
55	1x	21	A
55	1x	47	U
55	1x	48	C
55	1x	59	A
55	1x	61	C
55	1x	68	C
55	1x	69	C
55	1x	70	G
55	1x	76	A
54	1y	6	G
54	1y	8	4SU
54	1y	9	A
54	1y	11	C
54	1y	13	C
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	35	A
54	1y	45	U
54	1y	46	7MG
54	1y	47	U
54	1y	48	C
54	1y	49	C
54	1y	54	5MU
54	1y	57	G

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Mol	Chain	Res	Type
54	1y	59	U
54	1y	65	G
54	1y	69	G
54	1y	70	G
54	1y	73	A
1	2A	11	G
1	2A	12	U
1	2A	15	G
1	2A	29	U
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U
1	2A	96	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	125	G
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	198	C
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	232	G
1	2A	243	U
1	2A	248	G
1	2A	249	C

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Mol	Chain	Res	Type
1	2A	250	G
1	2A	266	G
1	2A	271(E)	U
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	G
1	2A	272(B)	G
1	2A	272(I)	U
1	2A	272(J)	C
1	2A	277	C
1	2A	278	A
1	2A	294	A
1	2A	311	A
1	2A	312	G
1	2A	320	A
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	352	G
1	2A	354	G
1	2A	361	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	391	G
1	2A	396	G
1	2A	399	G
1	2A	405	U
1	2A	411	G
1	2A	422	A
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	474	G

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Mol	Chain	Res	Type
1	2A	481	G
1	2A	498	G
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	528	A
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(U)	G
1	2A	669	G
1	2A	686	G
1	2A	701	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	783	A
1	2A	784	A

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Mol	Chain	Res	Type
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	870	A
1	2A	874	G
1	2A	877	U
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	890	A
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	904	C
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	933	A
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G

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Mol	Chain	Res	Type
1	2A	975	C
1	2A	980	A
1	2A	983	A
1	2A	996	A
1	2A	999	U
1	2A	1012	U
1	2A	1013	C
1	2A	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	1114	G
1	2A	1116	C
1	2A	1122	G
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1137	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1143	A
1	2A	1144	G
1	2A	1171	G
1	2A	1188	U
1	2A	1208	C
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1236	G
1	2A	1244	G
1	2A	1247	A
1	2A	1248	G
1	2A	1250	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A

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Mol	Chain	Res	Type
1	2A	1273	U
1	2A	1284	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1345	C
1	2A	1347	G
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1370	C
1	2A	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1441	G
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1478	G
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1495	A
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A

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Mol	Chain	Res	Type
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1511	C
1	2A	1531	C
1	2A	1533	G
1	2A	1542	A
1	2A	1547	C
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1588	C
1	2A	1603	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1640	C
1	2A	1647	G
1	2A	1648	C
1	2A	1654	A
1	2A	1663	C
1	2A	1664	A
1	2A	1674	G
1	2A	1676	A
1	2A	1680	U
1	2A	1691	C
1	2A	1694	C
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G

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Mol	Chain	Res	Type
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1806	C
1	2A	1811	G
1	2A	1812	A
1	2A	1816	G
1	2A	1835	G
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1857	G
1	2A	1866	C
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	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	1993	U
1	2A	1996	C
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C

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Mol	Chain	Res	Type
1	2A	2051	A
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2070	G
1	2A	2093	G
1	2A	2099	U
1	2A	2104	G
1	2A	2105	C
1	2A	2108	C
1	2A	2109	U
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2130	U
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2142	C
1	2A	2146	C
1	2A	2150	U
1	2A	2153	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A

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Mol	Chain	Res	Type
1	2A	2161	C
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2171	A
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2178	C
1	2A	2182	G
1	2A	2183	C
1	2A	2185	C
1	2A	2188	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	2243	U
1	2A	2262	U
1	2A	2275	C
1	2A	2278	A
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A
1	2A	2320	A
1	2A	2322	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2346	A
1	2A	2347	C

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Mol	Chain	Res	Type
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2377	A
1	2A	2383	G
1	2A	2385	C
1	2A	2396	G
1	2A	2403	C
1	2A	2406	U
1	2A	2410	G
1	2A	2419	U
1	2A	2425	A
1	2A	2428	G
1	2A	2429	G
1	2A	2430	A
1	2A	2434	A
1	2A	2435	A
1	2A	2439	A
1	2A	2440	C
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2469	A
1	2A	2476	A
1	2A	2487	G
1	2A	2490	G
1	2A	2497	A
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2536	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2579	C

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Mol	Chain	Res	Type
1	2A	2586	C
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2641	G
1	2A	2654	A
1	2A	2664	G
1	2A	2689	U
1	2A	2691	C
1	2A	2696	U
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	2744	G
1	2A	2748	A
1	2A	2751	G
1	2A	2757	A
1	2A	2758	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2780	G
1	2A	2789	C
1	2A	2802	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2836	U
1	2A	2872	G
1	2A	2873	A
1	2A	2880	C
1	2A	2892	A

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Mol	Chain	Res	Type
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	2B	2	C
2	2B	5	C
2	2B	8	U
2	2B	9	G
2	2B	12	C
2	2B	13	A
2	2B	15	A
2	2B	19	G
2	2B	25	A
2	2B	32	C
2	2B	42	C
2	2B	52	A
2	2B	53	A
2	2B	56	G
2	2B	57	A
2	2B	63	G
2	2B	64	C
2	2B	65	C
2	2B	66	A
2	2B	67	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	84	C
2	2B	88	C
2	2B	91	C
2	2B	108	U
2	2B	110	G
2	2B	111	G
2	2B	114	C
2	2B	116	G
2	2B	119	G
32	2a	6	G
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	30	U
32	2a	32	A
32	2a	33	A

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Mol	Chain	Res	Type
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	54	C
32	2a	66	G
32	2a	73	G
32	2a	80	G
32	2a	88	A
32	2a	92	C
32	2a	97	G
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	120	A
32	2a	121	C
32	2a	131	C
32	2a	163	C
32	2a	174	C
32	2a	180	U
32	2a	182	U
32	2a	189(B)	C
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	301	G
32	2a	316	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	345	C

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Mol	Chain	Res	Type
32	2a	346	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	355	C
32	2a	363	A
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	381	C
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	470	C
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	517	G
32	2a	518	C
32	2a	527	7MG
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	560	U
32	2a	561	U
32	2a	564	C

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Mol	Chain	Res	Type
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	576	G
32	2a	577	G
32	2a	619	U
32	2a	630	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	701	C
32	2a	702	A
32	2a	721	G
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	735	C
32	2a	738	C
32	2a	749	C
32	2a	755	G
32	2a	773	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
32	2a	828	A
32	2a	834	C
32	2a	840	C
32	2a	841	U
32	2a	848	C
32	2a	853	G
32	2a	858	G
32	2a	859	A
32	2a	870	U
32	2a	902	G
32	2a	914	A

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Mol	Chain	Res	Type
32	2a	916	G
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	942	G
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	997	U
32	2a	999	C
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1029	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1033	G
32	2a	1035	A

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Mol	Chain	Res	Type
32	2a	1036	G
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1043	C
32	2a	1045	C
32	2a	1046	A
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1079	G
32	2a	1081	G
32	2a	1087	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1109	C
32	2a	1117	G
32	2a	1121	U
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1161	C
32	2a	1174	G
32	2a	1182	G
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G

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Mol	Chain	Res	Type
32	2a	1202	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1227	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1264	C
32	2a	1270	C
32	2a	1274	G
32	2a	1275	A
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	1299	A
32	2a	1300	G
32	2a	1303	C
32	2a	1305	G
32	2a	1313	U
32	2a	1320	C
32	2a	1322	C
32	2a	1323	G
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G
32	2a	1363	C
32	2a	1368	G
32	2a	1370	G
32	2a	1397	C
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C

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Mol	Chain	Res	Type
32	2a	1456	G
32	2a	1492	A
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1532	U
53	2v	13	A
53	2v	14	A
54	2w	3	C
54	2w	4	C
54	2w	8	4SU
54	2w	9	A
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	29	G
54	2w	32	PSU
54	2w	34	G
54	2w	46	7MG
54	2w	48	C
54	2w	50	U
54	2w	61	C
54	2w	64	A
54	2w	65	G
54	2w	66	U
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	71	G
54	2w	74	C
54	2w	76	A
55	2x	9	G
55	2x	19	G
55	2x	20	U
55	2x	21	A
55	2x	47	U

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Mol	Chain	Res	Type
55	2x	48	C
55	2x	62	C
55	2x	67	C
55	2x	76	A
54	2y	2	C
54	2y	14	A
54	2y	15	G
54	2y	19	G
54	2y	30	G
54	2y	34	G
54	2y	40	C
54	2y	45	U
54	2y	46	7MG
54	2y	49	C
54	2y	52	G
54	2y	53	G
54	2y	55	PSU
54	2y	56	C
54	2y	57	G
54	2y	58	A
54	2y	59	U
54	2y	60	U
54	2y	61	C
54	2y	62	C
54	2y	63	G
54	2y	65	G
54	2y	66	U
54	2y	69	G
54	2y	70	G
54	2y	73	A

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	115	G
1	1A	185	A
1	1A	271	U
1	1A	302	A
1	1A	509	A
1	1A	716	G
1	1A	811	A
1	1A	913	A

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Mol	Chain	Res	Type
1	1A	941	U
1	1A	1067	A
1	1A	1093	G
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A
1	1A	1286	U
1	1A	1554	A
1	1A	1700	G
1	1A	2014	G
1	1A	2156	A
1	1A	2205	C
1	1A	2418	U
1	1A	2442	A
1	1A	2451	A
1	1A	2641	A
1	1A	2701	U
1	1A	2769	U
2	1B	1	U
2	1B	65	C
1	2A	34	C
1	2A	195	A
1	2A	228	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	774	A
1	2A	856	C
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G

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Mol	Chain	Res	Type
1	2A	2126	A
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
55	5MU	2x	54	55	15,22,23	1.10	1 (6%)	16,32,35	1.64	2 (12%)
1	2MU	2A	2552	1,56	14,22,24	0.91	0	14,31,36	0.94	1 (7%)
55	5MC	2x	32	55	15,22,23	1.28	1 (6%)	19,32,35	1.45	3 (15%)
1	2MA	1A	2515	1,56	17,25,26	1.31	2 (11%)	19,37,40	2.01	2 (10%)
1	5MU	2A	1915	1	15,22,23	1.07	1 (6%)	16,32,35	1.81	2 (12%)
32	5MC	1a	1407	32	15,22,23	1.24	1 (6%)	19,32,35	1.37	2 (10%)
43	0TD	2l	92	43	4,9,10	3.09	1 (25%)	3,11,13	2.37	1 (33%)
32	MA6	1a	1518	32	19,26,27	0.90	1 (5%)	18,38,41	1.72	5 (27%)
55	PSU	2x	55	55	17,21,22	1.51	2 (11%)	20,30,33	3.16	6 (30%)
32	M2G	2a	966	32	20,27,28	1.42	3 (15%)	22,40,43	2.20	7 (31%)
54	5MU	2y	54	54	15,22,23	1.11	1 (6%)	16,32,35	1.72	2 (12%)
54	4SU	2y	8	54	14,21,22	1.27	1 (7%)	15,30,33	1.29	2 (13%)
1	PSU	1A	1933	1	17,21,22	1.67	4 (23%)	20,30,33	3.08	6 (30%)
1	5MC	2A	1942	1	15,22,23	1.29	1 (6%)	19,32,35	1.34	2 (10%)
1	PSU	2A	2605	1	17,21,22	1.68	2 (11%)	20,30,33	2.93	6 (30%)
1	5MU	1A	1937	1	15,22,23	1.08	1 (6%)	16,32,35	1.70	1 (6%)
1	4OC	2A	1920	1	15,22,24	0.67	0	17,31,35	1.51	2 (11%)
32	5MC	2a	1400	32	15,22,23	1.45	1 (6%)	19,32,35	1.26	2 (10%)
1	PSU	2A	1917	1	17,21,22	1.58	2 (11%)	20,30,33	3.13	6 (30%)
1	PSU	1A	1939	1	17,21,22	1.54	2 (11%)	20,30,33	3.23	6 (30%)
32	MA6	2a	1519	32	19,26,27	1.01	1 (5%)	18,38,41	1.67	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PSU	2y	39	54	17,21,22	1.69	2 (11%)	20,30,33	3.81	7 (35%)
54	5MU	1y	54	54	15,22,23	1.11	2 (13%)	16,32,35	1.91	2 (12%)
55	PSU	1x	55	55	17,21,22	1.63	2 (11%)	20,30,33	3.17	6 (30%)
1	PSU	1A	2617	1,56	17,21,22	1.67	4 (23%)	20,30,33	3.15	6 (30%)
1	2MA	2A	2503	1,56	17,25,26	1.25	2 (11%)	19,37,40	1.94	3 (15%)
54	PSU	1w	39	54	17,21,22	1.60	3 (17%)	20,30,33	3.01	5 (25%)
54	7MG	1w	46	54	22,26,27	1.74	4 (18%)	28,39,42	2.90	8 (28%)
1	5MC	1A	1984	1,56	15,22,23	1.34	1 (6%)	19,32,35	1.24	3 (15%)
54	PSU	1y	32	54	17,21,22	1.50	2 (11%)	20,30,33	3.35	6 (30%)
55	5MC	1x	32	55	15,22,23	1.27	1 (6%)	19,32,35	1.48	4 (21%)
54	7MG	2w	46	54	22,26,27	1.79	4 (18%)	28,39,42	2.64	9 (32%)
55	5MU	1x	54	55,56	15,22,23	1.07	1 (6%)	16,32,35	1.90	2 (12%)
54	7MG	2y	46	54	22,26,27	1.82	3 (13%)	28,39,42	2.92	9 (32%)
32	PSU	2a	516	32	17,21,22	1.44	2 (11%)	20,30,33	3.08	6 (30%)
54	PSU	2w	39	54	17,21,22	1.45	2 (11%)	20,30,33	3.32	6 (30%)
32	UR3	1a	1498	32	14,22,23	0.83	1 (7%)	15,32,35	0.61	0
1	OMG	2A	2251	1,55,56	18,26,27	1.32	2 (11%)	20,38,41	2.09	6 (30%)
54	PSU	1w	55	54	17,21,22	1.45	2 (11%)	20,30,33	3.43	6 (30%)
32	7MG	2a	527	32,56	22,26,27	1.74	4 (18%)	28,39,42	2.76	9 (32%)
32	5MC	1a	1404	32	15,22,23	1.32	1 (6%)	19,32,35	1.38	2 (10%)
54	4SU	1y	8	54	14,21,22	1.21	1 (7%)	15,30,33	1.67	2 (13%)
32	4OC	2a	1402	32,56	16,23,24	0.63	0	17,32,35	1.31	1 (5%)
54	MIA	2w	37	54	20,27,32	1.71	3 (15%)	22,39,47	1.84	6 (27%)
32	5MC	2a	1404	32	15,22,23	1.31	1 (6%)	19,32,35	1.37	3 (15%)
32	UR3	2a	1498	32	14,22,23	0.84	1 (7%)	15,32,35	0.80	1 (6%)
32	4OC	1a	1402	32	16,23,24	0.68	0	17,32,35	1.14	1 (5%)
54	PSU	2w	55	54	17,21,22	1.46	2 (11%)	20,30,33	3.21	6 (30%)
1	5MC	1A	1964	1	15,22,23	1.29	1 (6%)	19,32,35	1.46	3 (15%)
32	7MG	1a	527	32	22,26,27	1.88	4 (18%)	28,39,42	2.68	8 (28%)
32	5MC	2a	967	32	15,22,23	1.38	1 (6%)	19,32,35	1.29	3 (15%)
32	5MC	1a	1400	32	15,22,23	1.28	1 (6%)	19,32,35	1.52	4 (21%)
1	5MU	1A	1961	1,56	15,22,23	0.97	1 (6%)	16,32,35	1.77	2 (12%)
32	MA6	1a	1519	32	19,26,27	0.99	1 (5%)	18,38,41	1.52	4 (22%)
32	MA6	2a	1518	32	19,26,27	0.99	1 (5%)	18,38,41	1.62	3 (16%)
54	MIA	2y	37	54	18,24,32	1.11	2 (11%)	18,35,47	1.36	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	M2G	1a	966	32	20,27,28	1.46	3 (15%)	22,40,43	2.36	7 (31%)
54	MIA	1y	37	54	18,24,32	1.15	2 (11%)	18,35,47	1.27	2 (11%)
54	4SU	2w	8	54	14,21,22	1.27	1 (7%)	15,30,33	1.33	2 (13%)
32	5MC	2a	1407	32	15,22,23	1.26	1 (6%)	19,32,35	1.47	2 (10%)
55	4SU	2x	8	55,56	14,21,22	1.29	2 (14%)	15,30,33	2.37	2 (13%)
54	5MU	2w	54	54	15,22,23	1.09	1 (6%)	16,32,35	2.00	1 (6%)
1	2MU	1A	2564	1,56	14,22,24	0.89	1 (7%)	14,31,36	0.94	1 (7%)
54	PSU	2y	32	54	17,21,22	1.46	3 (17%)	20,30,33	3.16	6 (30%)
54	PSU	2w	32	54	17,21,22	1.48	2 (11%)	20,30,33	3.17	6 (30%)
54	PSU	1y	55	54	17,21,22	1.61	3 (17%)	20,30,33	3.17	7 (35%)
32	PSU	1a	516	32,56	17,21,22	1.50	3 (17%)	20,30,33	3.15	6 (30%)
1	5MU	2A	1939	1,56	15,22,23	1.09	1 (6%)	16,32,35	1.78	2 (12%)
54	PSU	2y	55	54	17,21,22	1.47	3 (17%)	20,30,33	3.32	6 (30%)
1	5MC	2A	1962	1,56	15,22,23	1.27	1 (6%)	19,32,35	1.32	3 (15%)
54	4SU	1w	8	54	14,21,22	1.37	2 (14%)	15,30,33	1.37	2 (13%)
54	PSU	1y	39	54	17,21,22	1.50	3 (17%)	20,30,33	3.23	5 (25%)
32	2MG	1a	1207	32	19,26,27	1.30	2 (10%)	21,38,41	2.27	7 (33%)
1	4OC	1A	1942	1	15,22,24	0.72	0	17,31,35	1.55	2 (11%)
1	PSU	2A	1911	1	17,21,22	1.48	2 (11%)	20,30,33	3.18	7 (35%)
55	4SU	1x	8	55	14,21,22	1.49	2 (14%)	15,30,33	2.53	2 (13%)
32	2MG	2a	1207	32	19,26,27	1.30	2 (10%)	21,38,41	2.46	8 (38%)
1	OMG	1A	2263	1,55,56	18,26,27	1.09	2 (11%)	20,38,41	2.06	6 (30%)
54	PSU	1w	32	54	17,21,22	1.50	2 (11%)	20,30,33	3.12	6 (30%)
54	5MU	1w	54	54	15,22,23	1.13	1 (6%)	16,32,35	1.74	2 (12%)
32	5MC	1a	967	32	15,22,23	1.23	1 (6%)	19,32,35	1.38	2 (10%)
54	MIA	1w	37	54	24,31,32	2.24	4 (16%)	26,44,47	2.48	9 (34%)
43	0TD	1l	92	43	4,9,10	3.15	1 (25%)	3,11,13	3.65	1 (33%)
54	7MG	1y	46	54	22,26,27	1.87	4 (18%)	28,39,42	3.06	10 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	2x	54	55	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MU	2A	2552	1,56	-	1/7/27/28	0/2/2/2
55	5MC	2x	32	55	-	0/5/25/26	0/2/2/2
1	2MA	1A	2515	1,56	-	2/3/25/26	0/3/3/3
1	5MU	2A	1915	1	-	2/5/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/3/12/14	-
32	MA6	1a	1518	32	-	3/7/29/30	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
54	5MU	2y	54	54	-	3/5/25/26	0/2/2/2
54	4SU	2y	8	54	-	0/5/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/5/25/26	0/2/2/2
1	4OC	2A	1920	1	-	1/7/27/30	0/2/2/2
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	2/5/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	1,56	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	1/3/25/26	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	1/7/37/38	0/3/3/3
1	5MC	1A	1984	1,56	-	2/5/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/5/25/26	0/2/2/2
54	7MG	2w	46	54	-	3/7/37/38	0/3/3/3
55	5MU	1x	54	55,56	-	0/5/25/26	0/2/2/2
54	7MG	2y	46	54	-	2/7/37/38	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
1	OMG	2A	2251	1,55,56	-	0/5/27/28	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	3/7/37/38	0/3/3/3
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	4SU	1y	8	54	-	4/5/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
54	MIA	2w	37	54	-	3/7/29/34	0/3/3/3
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1964	1	-	0/5/25/26	0/2/2/2
32	7MG	1a	527	32	-	3/7/37/38	0/3/3/3
32	5MC	2a	967	32	-	1/5/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
1	5MU	1A	1961	1,56	-	0/5/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
54	MIA	2y	37	54	-	3/3/25/34	0/3/3/3
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
54	4SU	2w	8	54	-	1/5/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
55	4SU	2x	8	55,56	-	1/5/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/5/25/26	0/2/2/2
1	2MU	1A	2564	1,56	-	0/7/27/28	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	1/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	0/5/25/26	0/2/2/2
54	PSU	2y	55	54	-	5/7/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	2/5/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/5/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
1	4OC	1A	1942	1	-	0/7/27/30	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/5/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
1	OMG	1A	2263	1,55,56	-	0/5/27/28	0/3/3/3
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	967	32	-	2/5/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/11/33/34	0/3/3/3
43	0TD	1l	92	43	-	1/3/12/14	-
54	7MG	1y	46	54	-	3/7/37/38	0/3/3/3

All (149) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C13-C14	7.37	1.53	1.32
54	1w	37	MIA	C2-S10	-6.46	1.70	1.75
54	2w	37	MIA	C2-S10	-6.14	1.70	1.75
43	1l	92	0TD	CB-SB	-6.02	1.69	1.84
43	2l	92	0TD	CB-SB	-5.95	1.69	1.84
32	1a	527	7MG	C6-C5	5.50	1.49	1.41
32	2a	1400	5MC	C5-C4	5.20	1.49	1.41
1	2A	2605	PSU	C5-C1'	-5.17	1.47	1.52
32	2a	527	7MG	C6-C5	5.09	1.48	1.41
1	1A	2617	PSU	C5-C1'	-5.08	1.47	1.52
54	2w	46	7MG	C6-C5	5.01	1.48	1.41
54	2y	39	PSU	C5-C1'	-5.00	1.48	1.52
54	1y	46	7MG	C6-C5	5.00	1.48	1.41
32	2a	967	5MC	C5-C4	4.98	1.49	1.41
54	1y	46	7MG	C5-C4	4.91	1.48	1.39
54	1y	55	PSU	C5-C1'	-4.90	1.48	1.52
54	2y	46	7MG	C6-C5	4.79	1.48	1.41
32	2a	1404	5MC	C5-C4	4.74	1.48	1.41
32	1a	527	7MG	C5-C4	4.74	1.48	1.39
1	1A	1984	5MC	C5-C4	4.74	1.48	1.41
54	2y	46	7MG	C5-C4	4.72	1.48	1.39
1	2A	1942	5MC	C5-C4	4.70	1.48	1.41
1	1A	1933	PSU	C5-C1'	-4.67	1.48	1.52
32	1a	1404	5MC	C5-C4	4.65	1.48	1.41
55	2x	32	5MC	C5-C4	4.65	1.48	1.41
55	1x	55	PSU	C5-C1'	-4.63	1.48	1.52
32	1a	1207	2MG	C6-C5	4.62	1.49	1.41
32	2a	1207	2MG	C6-C5	4.57	1.49	1.41
1	1A	1964	5MC	C5-C4	4.57	1.48	1.41
1	2A	2251	OMG	C6-C5	4.56	1.49	1.41
54	1w	39	PSU	C5-C1'	-4.56	1.48	1.52
54	1w	46	7MG	C5-C4	4.54	1.48	1.39
55	1x	32	5MC	C5-C4	4.47	1.48	1.41
54	2w	46	7MG	C5-C4	4.46	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1400	5MC	C5-C4	4.45	1.48	1.41
1	2A	1962	5MC	C5-C4	4.44	1.48	1.41
1	2A	1917	PSU	C5-C1'	-4.42	1.48	1.52
32	1a	966	M2G	C6-C5	4.40	1.48	1.41
32	2a	966	M2G	C6-C5	4.40	1.48	1.41
32	2a	1407	5MC	C5-C4	4.37	1.48	1.41
32	1a	967	5MC	C5-C4	4.37	1.48	1.41
54	1w	8	4SU	C4-S4	-4.36	1.59	1.67
54	1w	46	7MG	C6-C5	4.33	1.47	1.41
1	1A	2515	2MA	C6-C5	4.28	1.47	1.41
32	1a	1407	5MC	C5-C4	4.28	1.48	1.41
32	2a	527	7MG	C5-C4	4.26	1.47	1.39
1	1A	1939	PSU	C5-C1'	-4.20	1.48	1.52
1	2A	2503	2MA	C6-C5	4.09	1.47	1.41
55	2x	55	PSU	C5-C1'	-4.04	1.48	1.52
54	2y	8	4SU	C4-S4	-4.01	1.60	1.67
54	2w	32	PSU	C4-C5	4.00	1.50	1.41
54	2w	8	4SU	C4-S4	-4.00	1.60	1.67
55	1x	8	4SU	C4-S4	-3.85	1.60	1.67
54	1y	32	PSU	C5-C1'	-3.83	1.49	1.52
32	1a	516	PSU	C5-C1'	-3.82	1.49	1.52
54	1w	32	PSU	C5-C1'	-3.81	1.49	1.52
1	2A	1911	PSU	C5-C1'	-3.80	1.49	1.52
54	2y	55	PSU	C4-C5	3.79	1.49	1.41
54	2y	32	PSU	C5-C1'	-3.78	1.49	1.52
55	2x	8	4SU	C4-S4	-3.75	1.60	1.67
54	1y	8	4SU	C4-S4	-3.73	1.60	1.67
54	2w	39	PSU	C5-C1'	-3.72	1.49	1.52
55	1x	8	4SU	C2-N3	-3.72	1.30	1.38
54	1y	39	PSU	C5-C1'	-3.72	1.49	1.52
32	1a	966	M2G	C2-N2	3.65	1.40	1.34
54	2y	54	5MU	C4-C5	3.65	1.49	1.41
54	2w	55	PSU	C5-C1'	-3.64	1.49	1.52
54	2y	39	PSU	C4-C5	3.63	1.49	1.41
54	1w	54	5MU	C4-C5	3.63	1.49	1.41
54	1w	55	PSU	C5-C1'	-3.55	1.49	1.52
54	1y	32	PSU	C4-C5	3.55	1.49	1.41
54	1w	55	PSU	C4-C5	3.54	1.49	1.41
54	1w	46	7MG	C5-N7	-3.51	1.33	1.39
1	1A	2263	OMG	C6-C5	3.49	1.47	1.41
54	2w	55	PSU	C4-C5	3.49	1.48	1.41
54	2y	46	7MG	C5-N7	-3.48	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	54	5MU	C4-C5	3.48	1.48	1.41
32	2a	516	PSU	C4-C5	3.48	1.48	1.41
54	1y	54	5MU	C4-C5	3.47	1.48	1.41
32	2a	516	PSU	C5-C1'	-3.47	1.49	1.52
55	2x	55	PSU	C4-C5	3.46	1.48	1.41
54	1w	32	PSU	C4-C5	3.45	1.48	1.41
1	2A	1915	5MU	C4-C5	3.43	1.48	1.41
54	1y	39	PSU	C4-C5	3.43	1.48	1.41
1	2A	1939	5MU	C4-C5	3.42	1.48	1.41
32	1a	527	7MG	C5-N7	-3.39	1.34	1.39
54	2y	32	PSU	C4-C5	3.33	1.48	1.41
55	1x	54	5MU	C4-C5	3.32	1.48	1.41
54	2w	54	5MU	C4-C5	3.31	1.48	1.41
55	1x	55	PSU	C4-C5	3.31	1.48	1.41
1	2A	1917	PSU	C4-C5	3.30	1.48	1.41
1	1A	1937	5MU	C4-C5	3.29	1.48	1.41
1	2A	1911	PSU	C4-C5	3.27	1.48	1.41
54	2w	39	PSU	C4-C5	3.26	1.48	1.41
1	1A	1933	PSU	C4-C5	3.25	1.48	1.41
54	1y	46	7MG	C5-N7	-3.24	1.34	1.39
32	2a	527	7MG	C5-N7	-3.24	1.34	1.39
54	2w	46	7MG	C5-N7	-3.19	1.34	1.39
32	1a	516	PSU	C4-C5	3.18	1.48	1.41
54	1w	39	PSU	C4-C5	3.18	1.48	1.41
32	2a	966	M2G	C2-N2	3.17	1.40	1.34
54	1y	55	PSU	C4-C5	3.15	1.48	1.41
54	2y	55	PSU	C5-C1'	-3.12	1.49	1.52
54	2w	32	PSU	C5-C1'	-3.09	1.49	1.52
1	2A	2605	PSU	C4-C5	3.06	1.48	1.41
1	1A	1961	5MU	C4-C5	3.02	1.47	1.41
1	1A	1939	PSU	C4-C5	2.99	1.47	1.41
54	2y	37	MIA	C5-C4	2.75	1.48	1.40
54	1y	37	MIA	C5-C4	2.73	1.48	1.40
54	1y	37	MIA	C2-N3	2.70	1.36	1.32
32	2a	1518	MA6	C5-C4	2.66	1.48	1.40
54	1w	37	MIA	C5-C4	2.61	1.47	1.40
1	2A	2251	OMG	C5-C4	2.57	1.47	1.40
54	2w	37	MIA	C5-C4	2.57	1.47	1.40
54	2y	37	MIA	C2-N3	2.55	1.36	1.32
55	2x	8	4SU	C2-N3	-2.55	1.33	1.38
32	2a	1519	MA6	C5-C4	2.53	1.47	1.40
32	1a	1519	MA6	C5-C4	2.52	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	966	M2G	C5-C4	2.51	1.47	1.40
54	2w	46	7MG	C4-N9	-2.48	1.33	1.38
32	2a	1207	2MG	C5-C4	2.47	1.47	1.40
32	1a	966	M2G	C5-C4	2.46	1.47	1.40
32	1a	527	7MG	C4-N9	-2.45	1.33	1.38
1	1A	2617	PSU	C4-C5	2.45	1.46	1.41
32	1a	1207	2MG	C5-C4	2.43	1.47	1.40
54	1w	46	7MG	C4-N9	-2.42	1.33	1.38
32	1a	1518	MA6	C5-C4	2.42	1.47	1.40
1	1A	2515	2MA	C5-C4	2.40	1.47	1.40
32	1a	516	PSU	O4'-C1'	-2.38	1.41	1.44
1	1A	2263	OMG	C5-C4	2.29	1.47	1.40
1	2A	2503	2MA	C5-C4	2.27	1.46	1.40
32	2a	527	7MG	C4-N9	-2.24	1.34	1.38
1	1A	1933	PSU	O4'-C1'	-2.17	1.41	1.44
54	2y	55	PSU	C2-N1	-2.16	1.33	1.38
1	1A	2564	2MU	C2-N3	-2.16	1.33	1.38
54	1y	46	7MG	C4-N3	2.16	1.37	1.34
1	1A	2617	PSU	C2-N3	-2.14	1.33	1.38
32	2a	1498	UR3	C4-N3	2.14	1.41	1.38
32	1a	1498	UR3	C4-N3	2.12	1.41	1.38
54	2w	37	MIA	C6-N1	2.10	1.35	1.32
54	1y	39	PSU	O4'-C1'	-2.10	1.41	1.44
54	1w	37	MIA	C6-N1	2.09	1.35	1.32
54	1y	54	5MU	C2-N3	-2.05	1.34	1.38
1	1A	1933	PSU	C2-N1	-2.04	1.34	1.38
54	2y	32	PSU	O4'-C1'	-2.04	1.41	1.44
54	1w	39	PSU	O4'-C1'	-2.02	1.41	1.44
54	1y	55	PSU	O4'-C1'	-2.02	1.41	1.44
1	1A	2617	PSU	C2-N1	-2.01	1.34	1.38
54	1w	8	4SU	C2-N3	-2.01	1.34	1.38

All (347) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	46	7MG	N3-C4-N9	10.09	139.87	126.91
54	1w	46	7MG	N3-C4-N9	9.51	139.12	126.91
54	2w	39	PSU	N1-C2-N3	-9.44	120.93	128.43
54	2y	46	7MG	N3-C4-N9	9.37	138.95	126.91
32	2a	527	7MG	N3-C4-N9	9.19	138.71	126.91
54	1y	32	PSU	N1-C2-N3	-9.09	121.20	128.43
54	1y	39	PSU	N1-C2-N3	-9.06	121.22	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	55	PSU	N1-C2-N3	-9.04	121.24	128.43
32	1a	516	PSU	N1-C2-N3	-9.02	121.26	128.43
1	1A	1939	PSU	N1-C2-N3	-9.01	121.27	128.43
54	2w	32	PSU	N1-C2-N3	-8.90	121.36	128.43
1	1A	2617	PSU	N1-C2-N3	-8.85	121.39	128.43
1	2A	1911	PSU	N1-C2-N3	-8.85	121.40	128.43
54	2y	32	PSU	N1-C2-N3	-8.82	121.42	128.43
32	1a	527	7MG	N3-C4-N9	8.74	138.13	126.91
54	1w	32	PSU	N1-C2-N3	-8.63	121.57	128.43
32	2a	516	PSU	N1-C2-N3	-8.62	121.57	128.43
55	1x	8	4SU	C2-N3-C4	8.59	127.61	115.15
54	1w	55	PSU	N1-C2-N3	-8.56	121.62	128.43
54	2y	39	PSU	C5-C1'-C2'	-8.53	100.11	115.32
54	2w	55	PSU	N1-C2-N3	-8.53	121.65	128.43
54	2w	46	7MG	N3-C4-N9	8.45	137.77	126.91
54	2y	39	PSU	N1-C2-N3	-8.44	121.72	128.43
55	2x	55	PSU	N1-C2-N3	-8.39	121.76	128.43
55	1x	55	PSU	N1-C2-N3	-8.22	121.90	128.43
1	2A	2605	PSU	N1-C2-N3	-8.02	122.05	128.43
54	1w	39	PSU	N1-C2-N3	-8.01	122.06	128.43
1	2A	1917	PSU	N1-C2-N3	-7.98	122.09	128.43
54	1w	37	MIA	C12-C13-C14	-7.92	111.73	127.14
55	2x	8	4SU	C2-N3-C4	7.88	126.58	115.15
54	1y	55	PSU	N1-C2-N3	-7.84	122.20	128.43
1	1A	1933	PSU	N1-C2-N3	-7.80	122.23	128.43
54	1y	32	PSU	C4-N3-C2	7.64	121.59	115.14
54	2y	55	PSU	C4-N3-C2	7.56	121.52	115.14
54	2w	54	5MU	C4-N3-C2	7.47	121.45	115.14
54	1y	39	PSU	C4-N3-C2	7.37	121.36	115.14
54	2w	39	PSU	C4-N3-C2	7.25	121.27	115.14
54	2w	32	PSU	C4-N3-C2	7.22	121.24	115.14
1	2A	1911	PSU	C4-N3-C2	7.20	121.22	115.14
54	2y	39	PSU	C4-N3-C2	7.20	121.22	115.14
1	1A	1939	PSU	C4-N3-C2	7.13	121.16	115.14
55	1x	54	5MU	C4-N3-C2	7.05	121.09	115.14
54	1w	55	PSU	C4-N3-C2	7.03	121.08	115.14
54	1y	54	5MU	C4-N3-C2	6.90	120.97	115.14
1	1A	1933	PSU	C4-N3-C2	6.87	120.95	115.14
1	2A	1917	PSU	C4-N3-C2	6.87	120.94	115.14
54	2y	32	PSU	C4-N3-C2	6.80	120.89	115.14
32	1a	516	PSU	C4-N3-C2	6.80	120.89	115.14
54	1w	32	PSU	C4-N3-C2	6.80	120.88	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	516	PSU	C4-N3-C2	6.72	120.82	115.14
55	1x	55	PSU	C4-N3-C2	6.68	120.78	115.14
55	2x	55	PSU	C4-N3-C2	6.59	120.71	115.14
1	2A	1915	5MU	C4-N3-C2	6.57	120.69	115.14
54	2w	55	PSU	C4-N3-C2	6.55	120.67	115.14
54	1w	39	PSU	C4-N3-C2	6.42	120.56	115.14
54	1y	55	PSU	C4-N3-C2	6.24	120.41	115.14
54	1w	54	5MU	C4-N3-C2	6.20	120.38	115.14
1	1A	1937	5MU	C4-N3-C2	6.16	120.34	115.14
43	1l	92	0TD	CSB-SB-CB	-6.14	89.78	101.85
54	2y	54	5MU	C4-N3-C2	6.13	120.32	115.14
1	1A	2617	PSU	C4-N3-C2	6.08	120.28	115.14
1	1A	2515	2MA	C2-N3-C4	5.95	120.36	115.52
55	1x	55	PSU	C5-C4-N3	-5.83	117.85	125.36
54	2y	39	PSU	C5-C4-N3	-5.79	117.90	125.36
1	2A	1939	5MU	C4-N3-C2	5.76	120.00	115.14
54	1w	55	PSU	C5-C1'-C2'	-5.75	105.05	115.32
1	2A	2503	2MA	C2-N3-C4	5.75	120.20	115.52
54	1y	32	PSU	C5-C4-N3	-5.72	117.99	125.36
1	1A	1933	PSU	C5-C4-N3	-5.72	117.99	125.36
32	2a	527	7MG	N7-C8-N9	-5.67	95.27	103.38
55	2x	54	5MU	C4-N3-C2	5.65	119.91	115.14
54	2y	55	PSU	C5-C4-N3	-5.63	118.10	125.36
1	2A	1917	PSU	C5-C4-N3	-5.62	118.11	125.36
54	1y	55	PSU	C5-C4-N3	-5.62	118.12	125.36
1	1A	1961	5MU	C4-N3-C2	5.60	119.87	115.14
54	1w	55	PSU	C5-C4-N3	-5.55	118.22	125.36
54	1y	46	7MG	C5-C4-N3	-5.52	117.48	126.49
1	2A	2605	PSU	C4-N3-C2	5.51	119.79	115.14
54	1y	39	PSU	C5-C4-N3	-5.47	118.31	125.36
54	1y	46	7MG	C6-N1-C2	5.46	124.60	115.93
54	2y	46	7MG	C6-N1-C2	5.39	124.49	115.93
54	1w	39	PSU	C5-C4-N3	-5.36	118.45	125.36
54	2w	32	PSU	C5-C4-N3	-5.34	118.48	125.36
54	1w	46	7MG	N7-C8-N9	-5.33	95.76	103.38
32	1a	966	M2G	C2-N3-C4	5.31	121.31	115.28
32	1a	527	7MG	C5-C4-N3	-5.31	117.82	126.49
54	2w	46	7MG	N7-C8-N9	-5.31	95.79	103.38
55	2x	55	PSU	C5-C4-N3	-5.29	118.54	125.36
54	2y	32	PSU	C5-C4-N3	-5.29	118.55	125.36
54	1w	32	PSU	C5-C4-N3	-5.26	118.58	125.36
1	2A	1911	PSU	C5-C4-N3	-5.22	118.64	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	46	7MG	C5-C4-N3	-5.20	118.00	126.49
32	2a	516	PSU	C5-C4-N3	-5.20	118.67	125.36
32	2a	966	M2G	C6-N1-C2	5.16	122.32	116.18
32	2a	527	7MG	C5-C4-N3	-5.14	118.09	126.49
1	1A	1939	PSU	C5-C4-N3	-5.14	118.74	125.36
32	1a	966	M2G	C6-N1-C2	5.10	122.25	116.18
54	2w	55	PSU	C5-C4-N3	-5.08	118.81	125.36
1	1A	2515	2MA	C5-C6-N1	-5.06	117.75	123.06
54	2w	39	PSU	C5-C4-N3	-5.02	118.89	125.36
1	2A	2503	2MA	C5-C6-N1	-5.00	117.81	123.06
54	2y	46	7MG	N7-C8-N9	-4.99	96.24	103.38
54	1w	46	7MG	C6-N1-C2	4.94	123.78	115.93
1	2A	2251	OMG	C2-N3-C4	4.94	121.00	115.36
54	1y	46	7MG	N7-C8-N9	-4.92	96.34	103.38
32	1a	516	PSU	C5-C4-N3	-4.90	119.04	125.36
54	1w	46	7MG	C5-C4-N3	-4.89	118.50	126.49
32	2a	1207	2MG	C2-N3-C4	4.86	120.80	115.28
1	1A	1942	4OC	C2-N3-C4	4.85	121.26	116.34
54	2w	46	7MG	C5-C4-N3	-4.81	118.64	126.49
32	1a	527	7MG	N7-C8-N9	-4.79	96.53	103.38
54	2w	37	MIA	C2-N3-C4	4.77	121.90	115.32
1	2A	2605	PSU	C5-C6-N1	-4.75	118.61	124.44
32	1a	1207	2MG	C2-N3-C4	4.74	120.66	115.28
32	2a	966	M2G	C2-N3-C4	4.69	120.61	115.28
1	1A	2617	PSU	C5-C4-N3	-4.68	119.33	125.36
1	1A	2617	PSU	C5-C6-N1	-4.65	118.73	124.44
54	1y	8	4SU	C2-N3-C4	4.63	121.87	115.15
54	1y	55	PSU	C5-C6-N1	-4.63	118.75	124.44
1	2A	2605	PSU	C5-C4-N3	-4.60	119.43	125.36
54	2w	46	7MG	C6-N1-C2	4.60	123.23	115.93
54	2y	46	7MG	C6-C5-C4	4.55	120.09	115.20
54	1w	46	7MG	C6-C5-C4	4.52	120.05	115.20
54	1w	39	PSU	C5-C6-N1	-4.52	118.88	124.44
1	1A	2263	OMG	C2-N3-C4	4.50	120.49	115.36
54	1y	46	7MG	C6-C5-C4	4.49	120.02	115.20
54	2y	39	PSU	C5-C6-N1	-4.48	118.93	124.44
1	2A	1920	4OC	C2-N3-C4	4.48	120.89	116.34
54	1y	55	PSU	C5-C1'-C2'	-4.48	107.33	115.32
55	2x	55	PSU	C5-C6-N1	-4.44	118.98	124.44
32	1a	527	7MG	C6-C5-C4	4.44	119.96	115.20
1	1A	2617	PSU	C6-N1-C2	4.43	122.66	115.36
54	2w	55	PSU	C5-C1'-C2'	-4.42	107.44	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1207	2MG	C5-C6-N1	-4.41	117.40	123.43
1	2A	2605	PSU	C6-N1-C2	4.30	122.46	115.36
54	2w	39	PSU	C6-N1-C2	4.29	122.44	115.36
32	1a	516	PSU	C6-N1-C2	4.28	122.42	115.36
32	1a	1404	5MC	C2-N3-C4	4.27	121.17	116.02
32	2a	966	M2G	C5-C6-N1	-4.27	117.59	123.43
32	2a	1207	2MG	C5-C6-N1	-4.27	117.59	123.43
32	2a	1207	2MG	C6-C5-C4	-4.27	116.72	120.80
55	2x	8	4SU	C5-C4-N3	-4.26	118.14	123.83
54	2w	55	PSU	C6-N1-C2	4.24	122.36	115.36
32	1a	527	7MG	C6-N1-C2	4.22	122.64	115.93
32	1a	516	PSU	C5-C6-N1	-4.22	119.25	124.44
54	2w	55	PSU	C5-C6-N1	-4.20	119.28	124.44
54	2w	39	PSU	C5-C6-N1	-4.20	119.28	124.44
54	2y	32	PSU	C5-C6-N1	-4.19	119.29	124.44
54	2y	32	PSU	C6-N1-C2	4.18	122.25	115.36
55	1x	55	PSU	C5-C6-N1	-4.18	119.31	124.44
54	2y	55	PSU	C6-N1-C2	4.17	122.24	115.36
55	2x	55	PSU	C6-N1-C2	4.15	122.21	115.36
55	1x	8	4SU	C5-C4-N3	-4.15	118.28	123.83
54	1y	39	PSU	C6-N1-C2	4.13	122.18	115.36
54	1w	8	4SU	C2-N3-C4	4.13	121.14	115.15
54	1w	32	PSU	C6-N1-C2	4.13	122.17	115.36
1	1A	1939	PSU	C6-N1-C2	4.13	122.17	115.36
1	2A	1917	PSU	C5-C6-N1	-4.12	119.37	124.44
32	2a	516	PSU	C6-N1-C2	4.12	122.16	115.36
32	1a	966	M2G	N3-C2-N2	4.12	121.36	117.18
32	2a	527	7MG	C6-N1-C2	4.11	122.46	115.93
54	1w	37	MIA	C2-N3-C4	4.10	120.98	115.32
54	2w	32	PSU	C6-N1-C2	4.08	122.09	115.36
32	1a	1207	2MG	C6-N1-C2	4.08	122.48	115.18
54	2y	39	PSU	C6-N1-C2	4.07	122.07	115.36
54	2y	46	7MG	C5-C6-N1	-4.07	114.79	123.14
1	1A	1939	PSU	C5-C6-N1	-4.06	119.45	124.44
54	1w	39	PSU	C6-N1-C2	4.05	122.05	115.36
32	2a	1207	2MG	C6-N1-C2	4.04	122.42	115.18
54	1w	46	7MG	C5-C6-N1	-4.03	114.85	123.14
1	1A	2263	OMG	C6-N1-C2	4.03	122.33	115.93
54	1w	55	PSU	C6-N1-C2	4.02	122.00	115.36
1	1A	1933	PSU	C5-C6-N1	-4.02	119.50	124.44
1	1A	2263	OMG	C5-C6-N1	-4.01	117.94	123.43
32	2a	1402	4OC	CM4-N4-C4	-4.01	119.53	122.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	516	PSU	C5-C6-N1	-4.00	119.53	124.44
54	1y	32	PSU	C6-N1-C2	3.99	121.94	115.36
54	1y	55	PSU	C6-N1-C2	3.95	121.88	115.36
55	1x	55	PSU	C6-N1-C2	3.95	121.87	115.36
1	2A	1911	PSU	C6-N1-C2	3.94	121.86	115.36
43	2l	92	0TD	CSB-SB-CB	-3.93	94.12	101.85
54	1w	37	MIA	C5-C6-N1	-3.92	117.55	120.81
32	2a	1407	5MC	C2-N3-C4	3.92	120.75	116.02
54	1w	55	PSU	C5-C6-N1	-3.91	119.63	124.44
54	1y	39	PSU	C5-C6-N1	-3.90	119.65	124.44
54	1y	46	7MG	C5-C6-N1	-3.89	115.14	123.14
32	2a	527	7MG	C6-C5-C4	3.88	119.37	115.20
32	1a	966	M2G	C5-C6-N1	-3.86	118.15	123.43
32	1a	967	5MC	C2-N3-C4	3.86	120.68	116.02
32	1a	527	7MG	C5-C6-N1	-3.83	115.27	123.14
32	1a	1400	5MC	C2-N3-C4	3.83	120.64	116.02
54	1w	32	PSU	C5-C6-N1	-3.81	119.75	124.44
1	2A	1917	PSU	C6-N1-C2	3.81	121.64	115.36
1	2A	2251	OMG	C5-C6-N1	-3.80	118.23	123.43
1	1A	1933	PSU	C6-N1-C2	3.79	121.62	115.36
54	2w	8	4SU	C2-N3-C4	3.79	120.64	115.15
32	2a	967	5MC	C2-N3-C4	3.78	120.58	116.02
54	1w	37	MIA	C16-C14-C13	-3.77	111.76	122.65
32	2a	966	M2G	C6-C5-C4	-3.76	117.21	120.80
1	2A	1942	5MC	C2-N3-C4	3.75	120.54	116.02
32	2a	1518	MA6	C4-C5-N7	-3.71	105.53	109.40
54	2y	8	4SU	C2-N3-C4	3.68	120.48	115.15
54	1w	37	MIA	C15-C14-C13	-3.67	112.03	122.65
32	1a	1207	2MG	C6-C5-C4	-3.67	117.30	120.80
32	2a	1207	2MG	C4-C5-N7	-3.64	105.61	109.40
32	1a	1407	5MC	C2-N3-C4	3.64	120.41	116.02
54	2w	46	7MG	C5-C6-N1	-3.64	115.67	123.14
54	1y	32	PSU	C5-C6-N1	-3.63	119.97	124.44
1	2A	1911	PSU	C5-C6-N1	-3.62	119.98	124.44
1	2A	2251	OMG	C6-C5-C4	-3.62	117.34	120.80
1	2A	2251	OMG	C6-N1-C2	3.61	121.67	115.93
55	2x	32	5MC	C2-N3-C4	3.61	120.37	116.02
54	2w	46	7MG	C6-C5-C4	3.60	119.07	115.20
54	2y	39	PSU	O4'-C1'-C5	3.60	115.50	109.93
32	2a	1207	2MG	CM2-N2-C2	-3.59	119.25	123.59
55	1x	55	PSU	C5-C1'-C2'	-3.59	108.91	115.32
32	1a	1207	2MG	C4-C5-N7	-3.59	105.66	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1964	5MC	C2-N3-C4	3.57	120.32	116.02
32	2a	1519	MA6	C4-C5-N7	-3.52	105.73	109.40
55	1x	32	5MC	C2-N3-C4	3.52	120.27	116.02
32	1a	1518	MA6	N3-C2-N1	-3.52	123.17	128.68
1	2A	1917	PSU	C5-C1'-C2'	-3.50	109.07	115.32
54	1y	32	PSU	C5-C1'-C2'	-3.50	109.08	115.32
32	2a	1518	MA6	C9-N6-C6	-3.49	108.94	119.51
54	2y	37	MIA	N3-C2-N1	-3.49	123.23	128.68
54	1y	37	MIA	N3-C2-N1	-3.46	123.28	128.68
54	1y	8	4SU	C5-C4-N3	-3.45	119.22	123.83
32	1a	1402	4OC	CM4-N4-C4	-3.43	120.02	122.97
32	1a	1518	MA6	C4-C5-N7	-3.43	105.82	109.40
32	2a	527	7MG	C5-C6-N1	-3.42	116.12	123.14
1	2A	1939	5MU	C5-C6-N1	-3.39	118.54	122.19
32	1a	966	M2G	C6-C5-C4	-3.38	117.57	120.80
54	2w	32	PSU	C5-C6-N1	-3.34	120.33	124.44
1	2A	1962	5MC	C2-N3-C4	3.34	120.04	116.02
54	2w	37	MIA	C5-C6-N1	-3.33	118.05	120.81
32	2a	1518	MA6	N3-C2-N1	-3.32	123.49	128.68
32	2a	1207	2MG	N2-C2-N1	3.31	120.14	116.96
1	1A	2263	OMG	C6-C5-C4	-3.30	117.64	120.80
54	2y	55	PSU	C5-C6-N1	-3.30	120.38	124.44
1	1A	1984	5MC	C2-N3-C4	3.28	119.98	116.02
32	1a	1519	MA6	N3-C2-N1	-3.28	123.56	128.68
32	1a	1518	MA6	C9-N6-C6	-3.26	109.64	119.51
32	2a	1404	5MC	C2-N3-C4	3.25	119.94	116.02
1	1A	1961	5MU	C5-C6-N1	-3.24	118.70	122.19
32	1a	967	5MC	N4-C4-N3	3.21	121.57	117.03
32	1a	966	M2G	CM2-N2-C2	-3.20	118.24	121.29
32	1a	1400	5MC	N4-C4-N3	3.20	121.55	117.03
32	1a	1519	MA6	C9-N6-C6	-3.19	109.84	119.51
1	2A	2251	OMG	C4-C5-N7	-3.19	106.07	109.40
1	1A	2263	OMG	N3-C2-N1	-3.17	123.00	127.22
32	2a	1400	5MC	C2-N3-C4	3.16	119.83	116.02
1	1A	1933	PSU	C5-C1'-C2'	-3.10	109.78	115.32
32	1a	1519	MA6	C4-C5-N7	-3.10	106.16	109.40
54	2w	37	MIA	C12-N6-C6	-3.10	120.21	122.87
32	2a	1519	MA6	N1-C6-N6	3.09	120.30	117.06
32	1a	1207	2MG	CM2-N2-C2	-3.07	119.88	123.59
54	1w	37	MIA	C2-N1-C6	3.06	122.67	117.19
1	2A	1911	PSU	C5-C1'-C2'	-3.02	109.93	115.32
1	1A	1939	PSU	C5-C1'-C2'	-2.99	109.99	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	32	5MC	N4-C4-N3	2.96	121.22	117.03
32	2a	1519	MA6	C9-N6-C6	-2.95	110.57	119.51
32	2a	1400	5MC	C5-C6-N1	-2.93	119.04	122.19
54	2y	55	PSU	C5-C1'-C2'	-2.92	110.11	115.32
32	2a	966	M2G	C4-C5-N7	-2.92	106.36	109.40
54	1w	46	7MG	C5-C4-N9	-2.91	102.37	106.44
32	1a	1407	5MC	N4-C4-N3	2.90	121.14	117.03
32	2a	527	7MG	C8-N7-C5	2.89	116.46	108.94
1	2A	1942	5MC	N4-C4-N3	2.88	121.11	117.03
32	2a	1519	MA6	N3-C2-N1	-2.87	124.19	128.68
1	1A	1964	5MC	N4-C4-N3	2.87	121.08	117.03
54	2w	37	MIA	C4-C5-N7	-2.86	106.42	109.40
1	1A	2617	PSU	C5-C1'-C2'	-2.83	110.27	115.32
54	2y	37	MIA	C4-C5-N7	-2.81	106.47	109.40
32	1a	1518	MA6	C10-N6-C9	-2.79	107.14	116.12
32	2a	1407	5MC	N4-C4-N3	2.78	120.97	117.03
54	1y	37	MIA	C4-C5-N7	-2.76	106.52	109.40
54	1y	46	7MG	C5-C4-N9	-2.72	102.64	106.44
54	1w	37	MIA	C12-N6-C6	-2.72	118.52	122.55
54	2w	37	MIA	C2-N1-C6	2.71	122.04	117.19
1	2A	2251	OMG	N3-C2-N1	-2.70	123.62	127.22
54	2w	8	4SU	C5-C4-N3	-2.68	120.25	123.83
54	1y	46	7MG	C8-N7-C5	2.66	115.86	108.94
54	1w	8	4SU	C5-C4-N3	-2.63	120.31	123.83
32	1a	966	M2G	C4-C5-N7	-2.62	106.67	109.40
1	1A	1964	5MC	C5-C6-N1	-2.62	119.37	122.19
32	1a	527	7MG	C8-N7-C5	2.62	115.74	108.94
54	1w	37	MIA	C4-C5-N7	-2.61	106.68	109.40
54	2y	46	7MG	C8-N7-C5	2.61	115.72	108.94
54	2y	8	4SU	C5-C4-N3	-2.60	120.35	123.83
32	2a	1404	5MC	N4-C4-N3	2.59	120.70	117.03
54	2w	46	7MG	C8-N7-C5	2.58	115.66	108.94
1	2A	1962	5MC	C5-C6-N1	-2.58	119.41	122.19
54	2w	37	MIA	N3-C2-N1	-2.58	122.23	126.98
55	2x	55	PSU	C5-C1'-C2'	-2.54	110.79	115.32
54	1w	46	7MG	C8-N7-C5	2.54	115.55	108.94
55	1x	32	5MC	N4-C4-N3	2.54	120.62	117.03
1	2A	1962	5MC	N4-C4-N3	2.54	120.62	117.03
32	2a	1207	2MG	C1'-N9-C4	-2.53	122.19	126.64
54	1w	37	MIA	N3-C2-N1	-2.52	122.34	126.98
54	1y	54	5MU	C5-C6-N1	-2.52	119.48	122.19
54	1w	54	5MU	C5-C6-N1	-2.51	119.49	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2503	2MA	C4-C5-N7	-2.47	106.83	109.40
54	2w	39	PSU	C5-C1'-C2'	-2.46	110.93	115.32
1	1A	1942	4OC	N4-C4-N3	2.45	120.37	116.49
32	2a	1404	5MC	C5-C6-N1	-2.44	119.56	122.19
32	1a	1404	5MC	N4-C4-N3	2.44	120.48	117.03
55	1x	32	5MC	C5-C6-N1	-2.44	119.56	122.19
55	2x	54	5MU	C5-C6-N1	-2.43	119.57	122.19
54	2y	46	7MG	C5-C4-N9	-2.43	103.03	106.44
1	1A	2263	OMG	C4-C5-N7	-2.43	106.87	109.40
1	2A	1920	4OC	N4-C4-N3	2.40	120.29	116.49
55	2x	32	5MC	C5-C6-N1	-2.40	119.61	122.19
54	1y	46	7MG	C2-N3-C4	2.36	120.42	113.89
1	1A	1984	5MC	C5-C6-N1	-2.36	119.65	122.19
32	1a	516	PSU	O4'-C1'-C2'	2.33	108.44	104.66
54	2w	32	PSU	C4-C5-C1'	2.33	125.52	121.12
32	2a	1498	UR3	C3U-N3-C4	2.33	121.21	118.12
32	2a	527	7MG	C5-C4-N9	-2.32	103.19	106.44
32	1a	1400	5MC	CM5-C5-C4	-2.31	119.39	121.72
1	2A	2605	PSU	C5-C1'-C2'	-2.29	111.24	115.32
32	2a	967	5MC	N4-C4-N3	2.26	120.23	117.03
1	2A	1915	5MU	C5-C6-N1	-2.26	119.76	122.19
54	2y	54	5MU	C5-C6-N1	-2.24	119.78	122.19
1	1A	2564	2MU	C5-C4-N3	-2.23	118.39	123.31
32	1a	1207	2MG	N2-C2-N1	2.22	119.10	116.96
55	1x	32	5MC	CM5-C5-C4	-2.22	119.47	121.72
54	1w	32	PSU	C5-C1'-C2'	-2.22	111.36	115.32
32	2a	966	M2G	N1-C2-N2	2.22	119.43	117.19
55	1x	54	5MU	C5-C6-N1	-2.19	119.83	122.19
32	2a	966	M2G	CM2-N2-C2	-2.18	119.21	121.29
32	1a	1519	MA6	N1-C6-N6	2.15	119.32	117.06
32	2a	527	7MG	C2-N3-C4	2.15	119.82	113.89
54	2w	46	7MG	C2-N3-C4	2.14	119.81	113.89
54	1y	46	7MG	C4-N9-C1'	2.14	131.67	126.60
54	2y	46	7MG	C2-N3-C4	2.12	119.75	113.89
32	1a	527	7MG	C2-N3-C4	2.10	119.68	113.89
1	1A	1984	5MC	N4-C4-N3	2.09	119.99	117.03
32	1a	1518	MA6	C10-N6-C6	-2.06	113.26	119.51
32	2a	516	PSU	O4'-C1'-C2'	2.06	108.00	104.66
32	2a	967	5MC	C5-C6-N1	-2.06	119.98	122.19
54	2y	37	MIA	C2-N1-C6	2.04	122.25	118.75
54	2w	46	7MG	C5-C4-N9	-2.04	103.58	106.44
1	2A	2552	2MU	C5-C4-N3	-2.03	118.84	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1400	5MC	C5-C6-N1	-2.03	120.01	122.19
54	2y	32	PSU	O4'-C1'-C2'	2.03	107.94	104.66
54	1y	55	PSU	O4'-C1'-C2'	2.02	107.94	104.66
1	2A	1911	PSU	O4'-C1'-C2'	2.01	107.91	104.66

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	2l	92	0TD	CG-CB-SB-CSB
32	1a	1518	MA6	C5-C6-N6-C9
32	1a	1518	MA6	C5-C6-N6-C10
54	2y	54	5MU	C2'-C1'-N1-C6
32	2a	1400	5MC	O4'-C1'-N1-C6
32	2a	1400	5MC	C2'-C1'-N1-C6
54	1y	54	5MU	C3'-C4'-C5'-O5'
54	1y	54	5MU	O4'-C4'-C5'-O5'
1	1A	1984	5MC	O4'-C1'-N1-C6
1	1A	1984	5MC	C2'-C1'-N1-C6
54	2w	46	7MG	O4'-C4'-C5'-O5'
54	2w	46	7MG	C3'-C4'-C5'-O5'
54	2y	46	7MG	C2'-C1'-N9-C8
54	1y	8	4SU	C2'-C1'-N1-C6
54	2w	37	MIA	N1-C6-N6-C12
54	2w	37	MIA	N3-C2-S10-C11
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	1518	MA6	C5-C6-N6-C9
54	2y	37	MIA	O4'-C4'-C5'-O5'
54	2y	37	MIA	C3'-C4'-C5'-O5'
54	2w	8	4SU	C2'-C1'-N1-C6
55	2x	8	4SU	C2'-C1'-N1-C6
54	2y	55	PSU	C2'-C1'-C5-C4
54	2y	55	PSU	C2'-C1'-C5-C6
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
54	1w	37	MIA	C12-C13-C14-C16
43	1l	92	0TD	CG-CB-SB-CSB
54	1y	46	7MG	C4'-C5'-O5'-P
54	2y	54	5MU	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	2a	527	7MG	C3'-C4'-C5'-O5'
54	2w	37	MIA	N1-C2-S10-C11
54	2y	54	5MU	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
54	1y	8	4SU	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1518	MA6	N1-C6-N6-C9
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	1518	MA6	N1-C6-N6-C9
32	2a	527	7MG	O4'-C4'-C5'-O5'
54	1y	46	7MG	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10
32	2a	1518	MA6	C5-C6-N6-C10
1	2A	2552	2MU	O4'-C4'-C5'-O5'
54	1w	46	7MG	C4'-C5'-O5'-P
54	2y	46	7MG	C2'-C1'-N9-C4
1	2A	1915	5MU	O4'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
54	2w	46	7MG	C4'-C5'-O5'-P
32	1a	967	5MC	O4'-C4'-C5'-O5'
1	2A	1920	4OC	C3'-C2'-O2'-CM2
32	2a	967	5MC	O4'-C4'-C5'-O5'
54	2y	37	MIA	C4'-C5'-O5'-P
32	2a	527	7MG	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
32	1a	1402	4OC	C3'-C4'-C5'-O5'
54	1y	8	4SU	C4'-C5'-O5'-P
1	2A	2503	2MA	O4'-C4'-C5'-O5'
54	2y	55	PSU	O4'-C1'-C5-C6
32	1a	527	7MG	C4'-C5'-O5'-P
54	2y	55	PSU	O4'-C1'-C5-C4
54	1y	46	7MG	C2'-C1'-N9-C8
54	2w	32	PSU	C2'-C1'-C5-C6
1	1A	2515	2MA	C4'-C5'-O5'-P
1	1A	2515	2MA	O4'-C4'-C5'-O5'
1	2A	1915	5MU	C3'-C4'-C5'-O5'
32	1a	967	5MC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
54	2y	55	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1915	5MU	1	0
1	2A	1920	4OC	2	0
1	2A	2503	2MA	1	0
1	1A	2564	2MU	2	0
1	2A	1939	5MU	2	0
1	1A	1942	4OC	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2625 ligands modelled in this entry, 2621 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	SF4	1d	501	35	0,12,12	0.00	-	-		
60	SF4	2d	501	35	0,12,12	0.00	-	-		
58	EZG	2A	3746	-	21,26,26	3.67	3 (14%)	26,35,35	1.14	3 (11%)
58	EZG	1A	4030	-	21,26,26	2.80	3 (14%)	26,35,35	1.55	4 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	2d	501	35	-	-	0/6/5/5
58	EZG	1A	4030	-	-	5/24/26/26	0/2/2/2
60	SF4	1d	501	35	-	-	0/6/5/5
58	EZG	2A	3746	-	-	8/24/26/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	2A	3746	EZG	OAC-NAY	13.98	1.46	1.22
58	1A	4030	EZG	CAT-CAW	-8.54	1.39	1.51
58	2A	3746	EZG	CAT-CAW	-7.81	1.40	1.51
58	1A	4030	EZG	OAC-NAY	7.73	1.35	1.22
58	1A	4030	EZG	CAU-NAY	-4.83	1.33	1.45
58	2A	3746	EZG	CAU-NAY	-4.63	1.34	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1A	4030	EZG	CAW-CAX-NAP	5.11	119.74	110.05
58	1A	4030	EZG	CAT-CAW-CAX	2.98	116.89	111.64
58	2A	3746	EZG	CAX-NAP-C	-2.97	117.83	123.07
58	1A	4030	EZG	CAI-CAG-CAT	-2.64	118.54	121.20
58	2A	3746	EZG	CAW-CAX-NAP	2.42	114.63	110.05
58	1A	4030	EZG	CAM-CAX-NAP	-2.28	105.64	109.27
58	2A	3746	EZG	CAI-CAU-NAY	2.10	120.95	119.38

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	2A	3746	EZG	O-C-CA-CB
58	2A	3746	EZG	NAP-C-CA-CB
58	2A	3746	EZG	NAP-C-CA-N
58	2A	3746	EZG	OAD-CAM-CAX-CAW
58	2A	3746	EZG	OAD-CAM-CAX-NAP
58	2A	3746	EZG	O-C-CA-N
58	2A	3746	EZG	N-CA-CB-CG
58	1A	4030	EZG	N-CA-CB-CG
58	1A	4030	EZG	CAM-CAX-NAP-C
58	1A	4030	EZG	OAD-CAM-CAX-NAP
58	2A	3746	EZG	C-CA-CB-CG
58	1A	4030	EZG	C-CA-CB-CG

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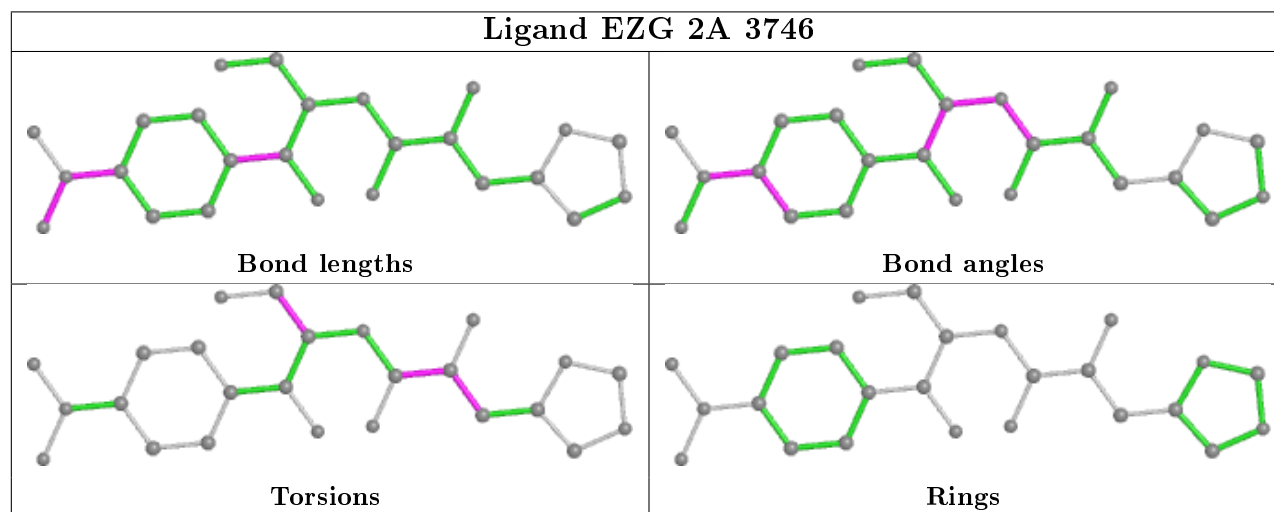
Mol	Chain	Res	Type	Atoms
58	1A	4030	EZG	OAE-CAW-CAX-CAM

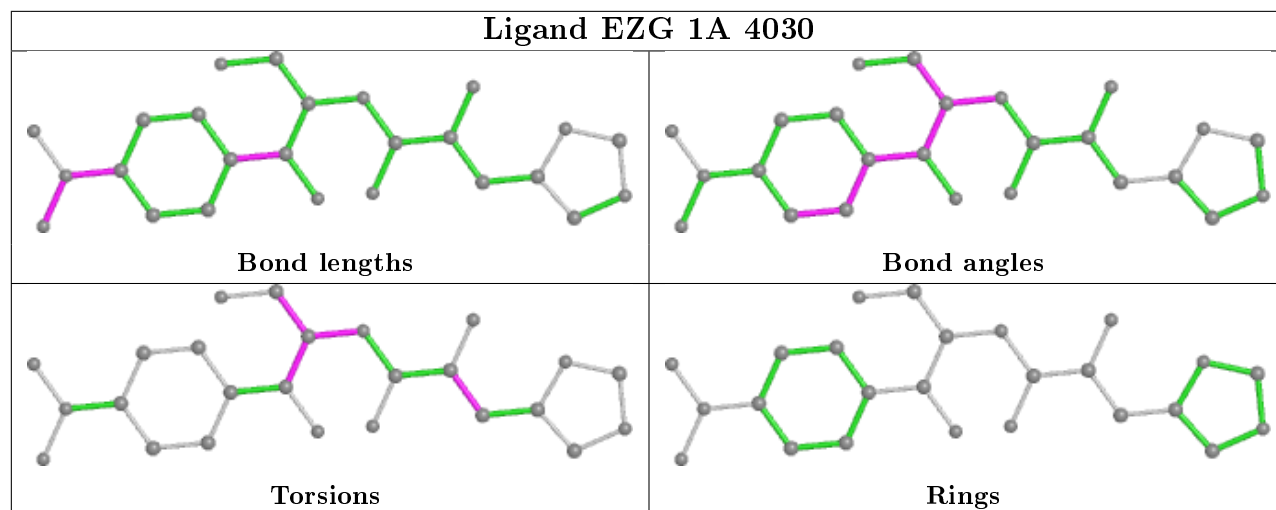
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	2A	3746	EZG	1	0
58	1A	4030	EZG	2	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	0.07	15 (0%) 91 88	13, 30, 88, 101	0
1	2A	2789/2915 (95%)	0.07	13 (0%) 91 88	25, 51, 87, 100	0
2	1B	120/121 (99%)	-0.15	0 100 100	23, 43, 57, 85	0
2	2B	120/121 (99%)	-0.15	0 100 100	53, 71, 80, 89	0
3	1D	275/276 (99%)	0.12	2 (0%) 87 84	16, 31, 46, 75	0
3	2D	275/276 (99%)	0.15	0 100 100	23, 43, 56, 66	0
4	1E	204/206 (99%)	0.02	0 100 100	13, 33, 54, 71	0
4	2E	204/206 (99%)	0.25	2 (0%) 82 77	28, 54, 67, 74	0
5	1F	203/210 (96%)	0.00	1 (0%) 91 88	15, 35, 62, 82	0
5	2F	203/210 (96%)	0.18	3 (1%) 73 68	30, 62, 74, 82	0
6	1G	181/182 (99%)	-0.15	0 100 100	35, 51, 69, 78	0
6	2G	181/182 (99%)	0.40	8 (4%) 34 24	56, 72, 78, 83	0
7	1H	174/180 (96%)	-0.13	0 100 100	34, 46, 59, 66	0
7	2H	174/180 (96%)	1.62	67 (38%) 0 0	61, 75, 81, 86	0
8	1I	146/148 (98%)	-0.06	1 (0%) 87 84	39, 67, 75, 81	0
8	2I	146/148 (98%)	0.14	2 (1%) 75 70	50, 66, 77, 81	0
9	1N	140/140 (100%)	-0.09	0 100 100	21, 35, 55, 68	0
9	2N	140/140 (100%)	0.55	4 (2%) 51 41	43, 58, 72, 75	0
10	1O	122/122 (100%)	-0.03	0 100 100	22, 35, 50, 56	0
10	2O	122/122 (100%)	0.33	0 100 100	43, 54, 67, 70	0
11	1P	149/150 (99%)	0.02	0 100 100	14, 40, 62, 66	0
11	2P	149/150 (99%)	1.25	37 (24%) 0 0	30, 61, 75, 83	0
12	1Q	141/141 (100%)	0.17	0 100 100	22, 36, 49, 72	0
12	2Q	141/141 (100%)	1.01	20 (14%) 2 1	41, 60, 70, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.19	0 100 100	18, 29, 44, 54	0
13	2R	118/118 (100%)	0.29	1 (0%) 86 81	33, 46, 55, 66	0
14	1S	110/112 (98%)	-0.12	1 (0%) 84 80	32, 44, 55, 60	0
14	2S	110/112 (98%)	1.33	24 (21%) 0 0	58, 67, 76, 79	0
15	1T	131/146 (89%)	-0.04	0 100 100	25, 39, 61, 71	0
15	2T	131/146 (89%)	0.43	5 (3%) 40 30	46, 58, 69, 75	0
16	1U	116/118 (98%)	0.03	0 100 100	14, 25, 42, 56	0
16	2U	116/118 (98%)	0.31	1 (0%) 84 80	35, 55, 67, 73	0
17	1V	101/101 (100%)	-0.17	0 100 100	19, 34, 53, 69	0
17	2V	101/101 (100%)	0.07	0 100 100	36, 63, 74, 78	0
18	1W	112/113 (99%)	-0.01	0 100 100	21, 26, 48, 71	0
18	2W	112/113 (99%)	0.23	1 (0%) 84 80	33, 44, 59, 85	0
19	1X	95/96 (98%)	-0.09	0 100 100	19, 31, 53, 75	0
19	2X	95/96 (98%)	0.00	0 100 100	40, 53, 64, 72	0
20	1Y	107/110 (97%)	-0.18	0 100 100	29, 43, 61, 72	0
20	2Y	107/110 (97%)	0.33	2 (1%) 66 59	54, 65, 74, 78	0
21	1Z	154/206 (74%)	0.07	3 (1%) 66 59	35, 57, 79, 85	0
21	2Z	160/206 (77%)	1.33	40 (25%) 0 0	61, 75, 84, 91	0
22	10	83/85 (97%)	0.25	5 (6%) 21 14	18, 31, 51, 56	0
22	20	83/85 (97%)	0.72	9 (10%) 5 3	36, 58, 69, 74	0
23	11	97/98 (98%)	0.21	1 (1%) 82 77	20, 38, 62, 70	0
23	21	97/98 (98%)	0.42	5 (5%) 27 18	35, 50, 68, 73	0
24	12	70/72 (97%)	-0.08	0 100 100	29, 41, 53, 64	0
24	22	70/72 (97%)	-0.09	0 100 100	47, 62, 70, 73	0
25	13	59/60 (98%)	-0.11	0 100 100	19, 31, 54, 72	0
25	23	59/60 (98%)	1.12	10 (16%) 1 1	48, 58, 70, 76	0
26	14	69/71 (97%)	-0.00	2 (2%) 51 41	43, 65, 83, 84	0
26	24	69/71 (97%)	-0.02	3 (4%) 35 25	67, 77, 86, 87	0
27	15	59/60 (98%)	-0.02	1 (1%) 70 63	14, 28, 41, 50	0
27	25	59/60 (98%)	0.09	1 (1%) 70 63	32, 46, 56, 64	0
28	16	53/54 (98%)	0.16	1 (1%) 66 59	27, 36, 50, 55	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.90	6 (11%) 5 3	42, 54, 67, 68	0
29	17	48/49 (97%)	0.13	1 (2%) 63 54	16, 21, 50, 60	0
29	27	48/49 (97%)	0.16	0 100 100	24, 35, 51, 60	0
30	18	64/65 (98%)	0.21	1 (1%) 72 66	21, 27, 37, 55	0
30	28	64/65 (98%)	1.63	18 (28%) 0 0	40, 49, 58, 68	0
31	19	37/37 (100%)	0.55	0 100 100	22, 33, 50, 55	0
31	29	37/37 (100%)	1.50	11 (29%) 0 0	53, 62, 71, 75	0
32	1a	1488/1521 (97%)	0.03	9 (0%) 89 86	32, 59, 86, 102	0
32	2a	1491/1521 (98%)	0.13	28 (1%) 66 59	43, 69, 89, 101	0
33	1b	231/256 (90%)	0.59	15 (6%) 18 11	59, 73, 82, 85	0
33	2b	231/256 (90%)	1.30	57 (24%) 0 0	64, 79, 85, 90	0
34	1c	206/239 (86%)	0.63	21 (10%) 6 3	51, 66, 74, 80	0
34	2c	206/239 (86%)	1.46	63 (30%) 0 0	66, 78, 82, 85	0
35	1d	208/209 (99%)	0.50	11 (5%) 26 17	50, 64, 76, 83	0
35	2d	208/209 (99%)	0.60	13 (6%) 20 12	53, 62, 72, 81	0
36	1e	148/162 (91%)	0.40	6 (4%) 37 27	48, 60, 70, 78	0
36	2e	148/162 (91%)	0.97	24 (16%) 1 1	58, 71, 79, 86	0
37	1f	100/101 (99%)	0.10	0 100 100	48, 60, 69, 70	0
37	2f	100/101 (99%)	0.08	1 (1%) 82 77	51, 63, 70, 76	0
38	1g	155/156 (99%)	0.43	16 (10%) 6 3	51, 62, 74, 88	0
38	2g	155/156 (99%)	0.79	19 (12%) 4 2	62, 71, 78, 84	0
39	1h	137/138 (99%)	0.29	4 (2%) 51 41	48, 61, 67, 72	0
39	2h	137/138 (99%)	0.68	14 (10%) 6 3	64, 71, 77, 85	0
40	1i	127/128 (99%)	1.23	29 (22%) 0 0	46, 69, 77, 83	0
40	2i	127/128 (99%)	2.35	69 (54%) 0 0	68, 77, 82, 88	0
41	1j	97/105 (92%)	1.18	25 (25%) 0 0	52, 71, 78, 83	0
41	2j	96/105 (91%)	1.82	37 (38%) 0 0	70, 78, 85, 87	0
42	1k	114/129 (88%)	0.26	1 (0%) 84 80	40, 58, 72, 79	0
42	2k	114/129 (88%)	0.45	7 (6%) 21 13	49, 66, 74, 78	0
43	1l	121/132 (91%)	0.01	0 100 100	33, 47, 59, 66	0
43	2l	121/132 (91%)	0.53	8 (6%) 18 11	53, 61, 71, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.35	9 (7%) 15 8	47, 59, 70, 74	0
44	2m	122/126 (96%)	0.61	17 (13%) 2 1	62, 75, 81, 85	0
45	1n	60/61 (98%)	1.05	10 (16%) 1 1	50, 59, 67, 71	0
45	2n	60/61 (98%)	2.95	41 (68%) 0 0	68, 77, 81, 87	0
46	1o	88/89 (98%)	0.13	2 (2%) 60 51	44, 59, 70, 75	0
46	2o	88/89 (98%)	-0.09	1 (1%) 80 75	53, 65, 74, 75	0
47	1p	82/88 (93%)	0.50	5 (6%) 21 13	51, 61, 70, 75	0
47	2p	82/88 (93%)	0.29	1 (1%) 79 73	55, 62, 71, 75	0
48	1q	99/105 (94%)	0.34	3 (3%) 50 40	47, 59, 72, 75	0
48	2q	99/105 (94%)	0.98	20 (20%) 1 0	55, 65, 73, 75	0
49	1r	68/88 (77%)	0.34	4 (5%) 22 14	48, 61, 71, 73	0
49	2r	68/88 (77%)	0.00	2 (2%) 51 41	57, 63, 73, 77	0
50	1s	83/93 (89%)	0.26	1 (1%) 79 73	49, 64, 73, 77	0
50	2s	83/93 (89%)	0.80	16 (19%) 1 0	71, 78, 84, 87	0
51	1t	96/106 (90%)	0.70	14 (14%) 2 1	50, 64, 73, 78	0
51	2t	96/106 (90%)	1.18	18 (18%) 1 1	52, 63, 76, 79	0
52	1u	23/27 (85%)	1.35	4 (17%) 1 1	52, 59, 63, 70	0
52	2u	23/27 (85%)	2.20	12 (52%) 0 0	67, 73, 80, 80	0
53	1v	13/24 (54%)	1.10	3 (23%) 0 0	42, 56, 81, 90	0
53	2v	13/24 (54%)	1.10	2 (15%) 2 1	59, 74, 91, 97	0
54	1w	67/76 (88%)	0.14	5 (7%) 14 8	32, 82, 93, 96	0
54	1y	67/76 (88%)	0.36	5 (7%) 14 8	28, 88, 96, 100	0
54	2w	65/76 (85%)	0.25	3 (4%) 32 22	54, 87, 95, 99	0
54	2y	66/76 (86%)	0.57	7 (10%) 6 3	49, 90, 94, 97	0
55	1x	72/77 (93%)	-0.08	0 100 100	32, 58, 76, 85	0
55	2x	72/77 (93%)	-0.14	0 100 100	45, 71, 81, 83	0
All	All	20875/21748 (95%)	0.29	1010 (4%) 30 21	13, 57, 83, 102	0

All (1010) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	2n	34	TYR	8.6
44	2m	123	ALA	7.6

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Mol	Chain	Res	Type	RSRZ
40	2i	14	VAL	7.4
38	2g	82	GLY	7.1
44	1m	124	PRO	7.1
45	2n	25	VAL	7.0
45	2n	39	LEU	6.9
40	2i	28	VAL	6.9
38	1g	82	GLY	6.8
41	2j	55	LYS	6.7
45	2n	38	GLY	6.6
31	29	37	GLY	6.5
45	2n	2	ALA	6.5
44	2m	124	PRO	6.2
41	1j	10	GLY	6.2
41	2j	47	PHE	6.1
21	2Z	144	LEU	6.0
21	2Z	170	THR	5.7
40	2i	114	TYR	5.7
33	2b	211	ILE	5.5
34	2c	201	TYR	5.5
41	2j	48	THR	5.4
33	2b	201	ILE	5.4
36	2e	10	MET	5.4
34	2c	188	LEU	5.3
40	2i	36	TYR	5.3
44	1m	123	ALA	5.2
11	2P	79	ARG	5.2
44	2m	102	ARG	5.2
30	28	16	ILE	5.2
21	2Z	121	HIS	5.2
40	2i	9	ARG	5.1
41	2j	63	PHE	5.1
36	2e	31	LEU	5.0
41	2j	50	ILE	5.0
33	2b	165	VAL	5.0
34	2c	171	GLY	4.9
33	2b	210	SER	4.9
7	2H	45	VAL	4.9
12	2Q	104	PHE	4.9
40	2i	27	THR	4.9
40	2i	115	GLY	4.9
45	2n	35	ARG	4.8
7	2H	133	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
40	2i	66	ARG	4.8
38	1g	84	ASN	4.8
1	2A	229	A	4.8
40	2i	7	THR	4.8
45	2n	11	LYS	4.8
32	2a	1034	G	4.7
52	2u	15	ARG	4.7
7	2H	7	LEU	4.7
40	2i	62	TYR	4.7
40	2i	19	LEU	4.7
45	2n	12	ARG	4.7
45	2n	61	TRP	4.6
33	2b	187	LEU	4.6
41	2j	54	PHE	4.6
36	2e	11	ILE	4.6
41	2j	62	HIS	4.6
40	2i	108	VAL	4.6
41	2j	65	LEU	4.5
45	2n	37	PHE	4.5
40	2i	125	TYR	4.5
40	2i	64	THR	4.5
54	2w	71	G	4.5
21	2Z	149	SER	4.5
34	2c	7	PRO	4.4
38	1g	85	TYR	4.4
11	2P	118	GLY	4.4
22	10	5	LYS	4.4
7	2H	113	VAL	4.4
32	2a	1030(B)	C	4.4
40	2i	117	HIS	4.3
33	2b	164	VAL	4.3
51	2t	9	ASN	4.3
34	2c	182	ILE	4.3
33	2b	77	ALA	4.3
48	2q	38	ARG	4.3
45	2n	13	THR	4.2
54	1w	70	G	4.2
22	10	6	GLY	4.2
34	2c	170	GLN	4.2
34	2c	157	ILE	4.2
39	2h	133	LEU	4.2
21	2Z	126	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
45	2n	7	ILE	4.2
34	2c	6	HIS	4.2
32	2a	1033	G	4.2
33	2b	163	PHE	4.2
40	2i	15	ALA	4.2
40	2i	110	GLU	4.2
41	2j	46	ARG	4.2
34	1c	196	LEU	4.1
40	2i	26	VAL	4.1
41	2j	52	GLY	4.1
33	2b	71	VAL	4.1
30	28	65	GLU	4.1
34	2c	8	ILE	4.1
53	2v	12	A	4.1
45	2n	31	ARG	4.1
40	2i	127	LYS	4.1
36	2e	20	GLN	4.0
32	2a	1257	U	4.0
12	2Q	22	LYS	4.0
21	2Z	51	ALA	4.0
40	1i	106	ALA	4.0
52	2u	16	GLY	4.0
7	2H	2	SER	4.0
44	2m	90	LEU	4.0
21	1Z	149	SER	4.0
12	2Q	103	MET	4.0
31	29	17	ILE	4.0
11	2P	78	PRO	4.0
34	2c	23	TYR	4.0
34	2c	167	TRP	3.9
41	2j	56	HIS	3.9
52	2u	6	ARG	3.9
40	2i	13	ALA	3.9
34	2c	198	VAL	3.9
3	1D	276	LYS	3.9
40	1i	65	VAL	3.9
40	2i	65	VAL	3.9
30	28	61	LEU	3.8
32	2a	1035	A	3.8
28	26	54	ILE	3.8
34	2c	124	ILE	3.8
47	1p	1	MET	3.8

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Mol	Chain	Res	Type	RSRZ
21	2Z	48	PHE	3.8
45	2n	22	THR	3.8
52	2u	11	GLY	3.8
40	2i	72	GLY	3.8
13	2R	69	ASP	3.8
11	2P	123	LEU	3.8
44	2m	122	LYS	3.7
7	2H	103	LEU	3.7
36	2e	18	ARG	3.7
44	2m	104	ARG	3.7
33	2b	200	ILE	3.7
41	2j	58	ASP	3.7
7	2H	76	VAL	3.7
45	2n	57	ARG	3.7
14	2S	26	LEU	3.7
38	2g	81	GLY	3.7
40	2i	124	GLN	3.7
52	2u	14	TRP	3.7
40	1i	76	ALA	3.7
45	2n	54	PRO	3.7
23	11	2	SER	3.7
41	2j	10	GLY	3.6
7	2H	141	VAL	3.6
11	2P	106	LEU	3.6
45	2n	58	LYS	3.6
36	2e	12	LEU	3.6
31	29	15	LYS	3.6
25	23	51	ALA	3.6
11	2P	85	LEU	3.6
28	26	11	LEU	3.6
34	1c	15	THR	3.6
38	1g	80	VAL	3.6
34	2c	187	ALA	3.6
1	1A	931	C	3.6
36	2e	8	GLU	3.6
34	2c	184	TYR	3.6
38	2g	154	TYR	3.6
41	1j	98	ILE	3.6
35	2d	47	ARG	3.6
40	2i	4	TYR	3.6
40	2i	126	SER	3.6
7	2H	115	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
40	2i	109	VAL	3.6
34	2c	12	LEU	3.5
22	20	7	LEU	3.5
41	1j	35	SER	3.5
51	1t	29	LYS	3.5
33	2b	120	ALA	3.5
34	2c	189	ALA	3.5
45	2n	6	LEU	3.5
11	2P	75	ILE	3.5
34	2c	202	ILE	3.5
33	2b	152	PHE	3.5
38	1g	79	ARG	3.5
54	2w	70	G	3.5
34	1c	179	ARG	3.5
34	2c	179	ARG	3.5
33	2b	80	ILE	3.5
34	2c	60	ALA	3.5
14	2S	32	LEU	3.5
22	20	2	ALA	3.5
40	2i	5	TYR	3.5
7	2H	70	THR	3.4
21	1Z	169	GLU	3.4
7	2H	94	TYR	3.4
36	2e	119	LEU	3.4
45	2n	53	LEU	3.4
7	2H	114	VAL	3.4
33	2b	108	ILE	3.4
34	2c	14	ILE	3.4
38	1g	83	ALA	3.4
33	2b	16	HIS	3.4
44	2m	120	LYS	3.4
45	1n	2	ALA	3.4
35	1d	167	GLY	3.4
21	2Z	125	LEU	3.4
7	2H	36	PRO	3.4
14	2S	14	VAL	3.4
34	2c	186	PHE	3.4
35	1d	166	LYS	3.4
36	2e	16	THR	3.4
53	2v	24	A	3.4
11	2P	70	GLN	3.4
43	2l	5	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
39	2h	83	ILE	3.4
21	2Z	1	MET	3.4
34	2c	163	ALA	3.4
45	2n	29	ARG	3.3
38	2g	84	ASN	3.3
45	2n	17	LYS	3.3
7	2H	105	LEU	3.3
41	2j	98	ILE	3.3
33	2b	48	MET	3.3
52	2u	17	THR	3.3
7	2H	96	ALA	3.3
33	2b	70	PHE	3.3
40	2i	17	VAL	3.3
40	2i	12	GLU	3.3
51	2t	73	HIS	3.3
22	10	4	LYS	3.3
11	2P	125	VAL	3.3
38	2g	156	TRP	3.3
34	2c	154	SER	3.3
1	1A	1140	U	3.3
38	1g	81	GLY	3.3
38	2g	4	ARG	3.3
54	1w	71	G	3.3
40	2i	121	ARG	3.3
7	2H	6	ARG	3.3
41	1j	65	LEU	3.3
40	1i	113	LYS	3.3
48	1q	28	PRO	3.3
7	2H	3	ARG	3.3
28	26	10	LEU	3.3
33	2b	31	TYR	3.2
45	2n	33	VAL	3.2
41	2j	85	LEU	3.2
41	1j	62	HIS	3.2
40	2i	81	ILE	3.2
21	2Z	139	VAL	3.2
44	2m	88	ARG	3.2
45	2n	56	VAL	3.2
38	1g	156	TRP	3.2
45	2n	36	PHE	3.2
34	2c	200	ALA	3.2
45	2n	30	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
7	2H	159	GLU	3.2
39	2h	2	LEU	3.2
33	2b	197	VAL	3.2
45	2n	60	SER	3.2
54	1w	3	C	3.2
41	2j	44	VAL	3.2
43	2l	18	VAL	3.2
45	2n	15	LYS	3.2
21	2Z	83	PRO	3.2
41	2j	71	LEU	3.2
33	2b	19	HIS	3.2
52	1u	6	ARG	3.2
30	28	64	TYR	3.2
45	2n	14	PRO	3.2
32	2a	1149	C	3.2
34	2c	5	ILE	3.1
43	2l	7	ILE	3.1
41	2j	49	VAL	3.1
33	2b	135	GLN	3.1
35	1d	168	ARG	3.1
45	2n	23	ARG	3.1
54	1w	72	C	3.1
40	1i	117	HIS	3.1
40	2i	116	LYS	3.1
7	2H	52	VAL	3.1
21	2Z	150	LEU	3.1
35	2d	176	LEU	3.1
36	2e	9	LYS	3.1
16	2U	90	VAL	3.1
21	2Z	47	VAL	3.1
21	2Z	141	VAL	3.1
48	2q	23	VAL	3.1
33	2b	121	LEU	3.1
38	1g	16	LEU	3.1
34	1c	193	TYR	3.1
33	1b	186	ALA	3.1
34	2c	37	GLN	3.1
40	1i	70	LYS	3.1
51	2t	24	LEU	3.1
44	2m	97	PRO	3.1
34	1c	14	ILE	3.1
36	2e	22	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	2A	2155	G	3.1
48	2q	22	LEU	3.1
36	2e	84	PHE	3.1
7	2H	162	ILE	3.1
52	2u	13	ILE	3.1
1	2A	2125	G	3.1
21	2Z	140	ASP	3.1
12	2Q	19	GLY	3.1
21	2Z	122	ARG	3.1
34	2c	159	GLY	3.1
40	2i	90	PRO	3.1
7	2H	35	VAL	3.1
11	2P	65	ARG	3.1
36	2e	25	ARG	3.1
1	1A	1114	G	3.1
33	2b	66	GLY	3.1
40	2i	63	ILE	3.1
44	2m	105	THR	3.1
11	2P	83	VAL	3.0
50	2s	45	VAL	3.0
41	1j	97	GLU	3.0
31	29	23	VAL	3.0
11	2P	80	TYR	3.0
32	2a	1001(A)	G	3.0
32	2a	1002	G	3.0
40	2i	18	PHE	3.0
51	2t	63	ILE	3.0
1	2A	888	C	3.0
40	2i	42	ARG	3.0
33	2b	146	GLN	3.0
41	2j	74	ILE	3.0
14	2S	46	VAL	3.0
48	2q	30	PRO	3.0
32	2a	1116	C	3.0
34	2c	33	LEU	3.0
45	1n	57	ARG	3.0
40	1i	47	LEU	3.0
41	1j	71	LEU	3.0
34	1c	13	GLY	3.0
7	2H	131	VAL	3.0
50	2s	70	LYS	3.0
32	1a	1002	G	3.0

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Mol	Chain	Res	Type	RSRZ
34	2c	206	GLU	3.0
43	2l	64	TYR	3.0
11	2P	115	LEU	3.0
33	2b	102	LEU	3.0
40	2i	37	PHE	3.0
40	1i	112	LYS	3.0
35	2d	198	VAL	3.0
34	2c	149	ALA	3.0
33	1b	187	LEU	3.0
33	2b	94	ASN	3.0
21	2Z	79	ARG	3.0
12	2Q	40	ALA	2.9
33	2b	92	TYR	2.9
41	1j	8	LEU	2.9
44	2m	78	ILE	2.9
33	2b	186	ALA	2.9
34	2c	160	ALA	2.9
14	2S	33	LYS	2.9
14	2S	93	LYS	2.9
33	2b	136	VAL	2.9
41	2j	51	ARG	2.9
7	2H	168	PRO	2.9
33	2b	142	LEU	2.9
51	2t	72	LEU	2.9
40	1i	4	TYR	2.9
40	2i	16	ARG	2.9
33	2b	215	LEU	2.9
50	2s	80	TYR	2.9
34	2c	39	ILE	2.9
12	2Q	102	VAL	2.9
36	1e	10	MET	2.9
6	2G	3	LEU	2.9
54	2y	36	A	2.9
21	2Z	137	ILE	2.9
48	2q	21	VAL	2.9
52	1u	17	THR	2.9
12	2Q	28	ALA	2.9
34	2c	196	LEU	2.9
22	10	3	HIS	2.9
22	20	3	HIS	2.9
1	2A	652(B)	A	2.9
7	2H	164	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
41	1j	5	ARG	2.9
54	2y	64	A	2.9
51	2t	55	ILE	2.9
40	2i	35	GLU	2.9
1	1A	932	C	2.9
7	2H	71	LEU	2.9
40	2i	123	PRO	2.9
28	26	20	ASN	2.9
12	2Q	97	VAL	2.9
51	2t	29	LYS	2.9
50	2s	79	THR	2.9
25	23	29	ARG	2.9
35	1d	170	VAL	2.9
43	2l	55	VAL	2.9
48	2q	9	VAL	2.9
42	2k	50	TYR	2.8
26	24	49	PHE	2.8
48	2q	33	GLY	2.8
7	2H	145	ALA	2.8
35	2d	160	GLN	2.8
7	2H	10	PRO	2.8
7	2H	102	ALA	2.8
41	1j	59	SER	2.8
51	2t	64	ASP	2.8
34	2c	4	LYS	2.8
32	1a	1257	U	2.8
34	2c	174	PRO	2.8
33	2b	122	PHE	2.8
7	2H	169	VAL	2.8
34	1c	18	TRP	2.8
21	2Z	138	GLU	2.8
38	2g	86	GLN	2.8
38	2g	79	ARG	2.8
41	2j	57	LYS	2.8
51	1t	74	LYS	2.8
7	2H	89	ILE	2.8
12	2Q	33	GLY	2.8
33	1b	200	ILE	2.8
40	2i	32	ASP	2.8
21	2Z	91	LEU	2.8
32	2a	1003	G	2.8
33	2b	69	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
41	2j	66	ARG	2.8
41	2j	95	GLU	2.8
54	2y	65	G	2.8
28	26	50	ARG	2.8
33	1b	226	ARG	2.8
51	2t	80	ARG	2.8
51	1t	14	LYS	2.8
11	2P	51	PHE	2.8
25	23	54	VAL	2.8
21	2Z	80	ARG	2.8
38	2g	115	ARG	2.8
52	2u	9	ARG	2.8
34	1c	8	ILE	2.8
44	2m	100	GLY	2.8
11	2P	58	THR	2.8
38	2g	16	LEU	2.8
40	2i	79	LEU	2.8
41	1j	60	ARG	2.8
1	1A	942	A	2.8
1	1A	1110	C	2.8
40	1i	8	GLY	2.8
40	2i	67	GLY	2.8
12	2Q	66	ILE	2.8
7	2H	49	VAL	2.8
11	2P	126	VAL	2.8
21	2Z	128	VAL	2.8
26	14	46	GLN	2.8
33	2b	123	ALA	2.8
33	2b	161	ALA	2.8
26	14	54	GLY	2.7
33	2b	214	ILE	2.7
41	1j	45	ARG	2.7
43	2l	32	PHE	2.7
44	2m	121	LYS	2.7
11	2P	109	GLY	2.7
40	2i	111	ARG	2.7
40	1i	18	PHE	2.7
33	2b	184	VAL	2.7
11	2P	81	GLN	2.7
51	1t	18	GLN	2.7
40	2i	61	ALA	2.7
51	1t	12	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
34	2c	185	GLY	2.7
14	2S	58	LEU	2.7
33	2b	81	VAL	2.7
34	2c	32	LEU	2.7
40	1i	75	ASP	2.7
51	2t	59	ALA	2.7
18	2W	112	GLY	2.7
35	2d	167	GLY	2.7
21	2Z	57	ILE	2.7
40	1i	81	ILE	2.7
7	2H	77	LYS	2.7
14	2S	13	ARG	2.7
42	2k	126	ARG	2.7
36	2e	17	ALA	2.7
40	2i	106	ALA	2.7
22	20	52	GLY	2.7
1	2A	2127	G	2.7
40	2i	33	PHE	2.7
32	1a	1030	C	2.7
6	2G	2	PRO	2.7
34	2c	172	ARG	2.7
51	2t	83	ARG	2.7
50	2s	83	HIS	2.7
20	2Y	5	MET	2.7
33	1b	163	PHE	2.7
6	2G	39	ILE	2.7
40	2i	10	ARG	2.7
22	10	7	LEU	2.7
33	1b	165	VAL	2.7
21	2Z	106	GLY	2.7
34	1c	10	PHE	2.7
35	1d	165	MET	2.7
27	25	29	THR	2.7
38	1g	4	ARG	2.7
51	2t	26	ASN	2.7
30	28	49	VAL	2.7
41	2j	40	LEU	2.7
36	2e	98	THR	2.7
7	2H	128	PRO	2.7
51	2t	66	ALA	2.7
35	2d	49	ARG	2.7
1	2A	2173	A	2.6

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Mol	Chain	Res	Type	RSRZ
28	16	54	ILE	2.6
40	1i	114	TYR	2.6
34	1c	178	LEU	2.6
40	2i	56	LEU	2.6
41	2j	72	VAL	2.6
33	2b	203	GLY	2.6
34	2c	13	GLY	2.6
45	2n	55	GLY	2.6
33	1b	207	ALA	2.6
50	2s	36	ARG	2.6
51	2t	25	ARG	2.6
41	2j	64	GLU	2.6
11	2P	68	GLN	2.6
40	1i	64	THR	2.6
40	2i	82	ALA	2.6
30	28	29	LYS	2.6
38	1g	153	HIS	2.6
39	2h	111	ILE	2.6
9	2N	45	ASN	2.6
34	2c	158	GLY	2.6
46	2o	60	VAL	2.6
34	1c	177	THR	2.6
45	2n	42	ILE	2.6
11	2P	59	LEU	2.6
40	1i	19	LEU	2.6
40	2i	120	ARG	2.6
4	2E	10	GLY	2.6
8	2I	19	VAL	2.6
40	2i	105	ASP	2.6
1	1A	1142	A	2.6
40	2i	52	ALA	2.6
31	29	26	ILE	2.6
25	23	53	LEU	2.6
44	1m	90	LEU	2.6
7	2H	13	LYS	2.6
34	1c	206	GLU	2.6
11	2P	91	PHE	2.6
41	2j	42	THR	2.6
54	2y	53	G	2.6
34	2c	21	ARG	2.6
38	1g	78	ARG	2.6
30	28	25	MET	2.6

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Mol	Chain	Res	Type	RSRZ
22	20	75	LEU	2.6
33	1b	27	LYS	2.6
38	2g	32	ARG	2.6
40	2i	83	ARG	2.6
45	2n	41	ARG	2.6
30	28	15	LYS	2.6
31	29	16	VAL	2.6
38	2g	85	TYR	2.6
41	1j	64	GLU	2.6
33	2b	188	ALA	2.6
41	2j	43	ARG	2.6
46	1o	87	ILE	2.6
7	2H	144	VAL	2.6
40	1i	36	TYR	2.6
42	2k	25	TYR	2.6
11	2P	76	LYS	2.6
11	2P	114	ILE	2.5
33	2b	83	MET	2.5
49	2r	85	LEU	2.5
7	2H	17	VAL	2.5
40	1i	111	ARG	2.5
45	1n	58	LYS	2.5
43	2l	68	ALA	2.5
7	2H	34	GLU	2.5
7	2H	108	GLY	2.5
7	2H	116	GLU	2.5
41	1j	95	GLU	2.5
45	2n	4	LYS	2.5
7	2H	100	GLY	2.5
15	2T	52	ILE	2.5
30	28	20	GLY	2.5
51	2t	62	LEU	2.5
7	2H	84	SER	2.5
32	2a	1250	A	2.5
40	2i	92	TYR	2.5
9	2N	44	PRO	2.5
38	2g	113	GLU	2.5
33	2b	101	MET	2.5
39	2h	9	MET	2.5
41	2j	34	VAL	2.5
45	1n	56	VAL	2.5
33	1b	195	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
14	2S	37	ALA	2.5
36	1e	132	ALA	2.5
7	2H	151	ILE	2.5
25	23	26	LEU	2.5
35	2d	94	LEU	2.5
44	1m	56	LEU	2.5
35	2d	56	VAL	2.5
14	2S	111	GLU	2.5
21	2Z	72	ARG	2.5
21	2Z	50	GLN	2.5
42	2k	59	TYR	2.5
38	2g	27	ILE	2.5
7	2H	74	ASN	2.5
33	1b	179	LYS	2.5
41	1j	36	GLY	2.5
48	2q	32	TYR	2.5
12	2Q	37	LEU	2.5
23	21	2	SER	2.5
30	28	2	PRO	2.5
1	2A	896	A	2.5
53	1v	13	A	2.5
28	26	42	TRP	2.5
30	28	34	TRP	2.5
7	2H	106	THR	2.5
38	2g	83	ALA	2.5
11	2P	88	LEU	2.5
14	2S	82	ILE	2.5
33	2b	127	ILE	2.5
41	2j	8	LEU	2.5
44	2m	66	LEU	2.5
7	2H	95	ARG	2.5
1	1A	934	A	2.5
21	2Z	156	LYS	2.5
34	2c	65	ALA	2.5
41	2j	32	ALA	2.5
34	2c	177	THR	2.5
34	1c	12	LEU	2.5
7	2H	123	PHE	2.4
1	1A	1141	A	2.4
39	2h	21	LYS	2.4
34	2c	41	GLY	2.4
53	1v	23	A	2.4

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Mol	Chain	Res	Type	RSRZ
7	2H	97	ARG	2.4
30	28	46	ARG	2.4
40	1i	50	LEU	2.4
5	2F	183	VAL	2.4
34	2c	10	PHE	2.4
33	2b	195	ASP	2.4
7	2H	167	GLU	2.4
41	1j	9	ARG	2.4
25	23	23	LEU	2.4
31	29	25	VAL	2.4
39	2h	15	ASN	2.4
22	20	8	GLY	2.4
31	29	13	LYS	2.4
39	1h	83	ILE	2.4
21	2Z	96	VAL	2.4
36	2e	45	PHE	2.4
39	1h	93	VAL	2.4
48	2q	35	VAL	2.4
32	2a	1030(C)	G	2.4
32	2a	1224	G	2.4
51	2t	68	LYS	2.4
44	1m	4	ILE	2.4
50	1s	71	LEU	2.4
51	2t	13	LEU	2.4
22	20	69	PHE	2.4
34	2c	55	VAL	2.4
26	24	54	GLY	2.4
3	1D	275	LYS	2.4
11	2P	119	GLU	2.4
12	2Q	38	GLU	2.4
51	1t	9	ASN	2.4
21	2Z	124	ILE	2.4
32	2a	1030(A)	G	2.4
33	2b	185	ILE	2.4
45	2n	49	HIS	2.4
35	2d	20	TYR	2.4
41	1j	66	ARG	2.4
48	2q	11	VAL	2.4
40	2i	38	GLN	2.4
36	1e	89	ILE	2.4
36	2e	13	ILE	2.4
48	2q	84	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	2A	883	G	2.4
36	2e	27	ARG	2.4
33	2b	72	GLY	2.4
38	1g	154	TYR	2.4
50	2s	52	TYR	2.4
32	1a	1447	A	2.4
14	2S	20	ARG	2.4
33	2b	40	HIS	2.4
38	2g	78	ARG	2.4
14	2S	87	PHE	2.4
7	2H	82	GLY	2.4
11	2P	110	TYR	2.4
33	1b	167	PRO	2.4
33	2b	131	PRO	2.4
21	2Z	87	ASP	2.4
32	2a	973	G	2.4
32	2a	1202	G	2.4
40	1i	119	ALA	2.4
23	21	98	LEU	2.4
49	1r	76	LEU	2.4
47	1p	2	VAL	2.3
48	2q	42	TYR	2.3
29	17	48	LYS	2.3
48	2q	7	THR	2.3
33	2b	207	ALA	2.3
34	2c	164	ARG	2.3
50	2s	38	SER	2.3
36	1e	81	GLU	2.3
40	2i	80	GLY	2.3
45	2n	51	GLY	2.3
54	1y	56	C	2.3
21	2Z	86	VAL	2.3
44	1m	105	THR	2.3
33	1b	215	LEU	2.3
7	2H	119	GLU	2.3
7	2H	124	GLU	2.3
50	2s	35	SER	2.3
21	2Z	88	PHE	2.3
52	1u	16	GLY	2.3
1	2A	2146	C	2.3
23	21	62	VAL	2.3
27	15	60	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
41	1j	72	VAL	2.3
40	1i	15	ALA	2.3
40	2i	45	ALA	2.3
6	2G	140	ILE	2.3
21	2Z	59	LEU	2.3
34	2c	178	LEU	2.3
39	2h	17	THR	2.3
48	2q	31	LEU	2.3
49	1r	78	LEU	2.3
14	2S	12	PHE	2.3
41	1j	7	LYS	2.3
41	1j	11	PHE	2.3
1	1A	933	C	2.3
32	2a	1249	C	2.3
45	1n	41	ARG	2.3
32	1a	204	U	2.3
32	2a	1150	U	2.3
7	2H	41	MET	2.3
26	24	57	GLU	2.3
33	2b	118	LEU	2.3
34	2c	175	LEU	2.3
41	1j	63	PHE	2.3
7	2H	43	VAL	2.3
32	2a	1251	A	2.3
54	1y	35	A	2.3
11	2P	97	PRO	2.3
50	2s	42	PRO	2.3
34	2c	145	GLY	2.3
34	2c	3	ASN	2.3
51	2t	70	SER	2.3
23	21	30	VAL	2.3
49	2r	46	GLU	2.3
32	2a	1112	C	2.3
14	2S	4	LEU	2.3
34	1c	201	TYR	2.3
45	2n	10	ALA	2.3
54	1y	1	G	2.3
35	1d	101	LEU	2.3
5	2F	131	GLY	2.3
22	20	76	GLY	2.3
36	2e	64	ARG	2.3
33	2b	76	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
7	2H	138	LYS	2.3
45	2n	8	GLU	2.3
45	2n	50	LYS	2.3
40	2i	49	PRO	2.3
1	1A	935	C	2.3
7	2H	132	ARG	2.3
9	2N	74	ARG	2.3
14	2S	3	ARG	2.3
34	2c	43	LEU	2.3
44	2m	99	ARG	2.3
48	2q	88	TYR	2.3
51	1t	24	LEU	2.3
54	2w	72	C	2.3
21	1Z	147	GLY	2.3
14	2S	112	PHE	2.3
40	1i	118	LYS	2.3
1	1A	1139	G	2.3
11	2P	74	GLU	2.3
12	2Q	12	GLN	2.3
51	1t	70	SER	2.2
12	2Q	17	LEU	2.2
12	2Q	39	PRO	2.2
14	2S	110	LEU	2.2
33	1b	61	LEU	2.2
35	1d	135	LEU	2.2
36	2e	43	LEU	2.2
52	1u	14	TRP	2.2
1	2A	2128	C	2.2
7	2H	24	VAL	2.2
33	2b	67	THR	2.2
48	2q	39	SER	2.2
32	1a	1532	U	2.2
45	1n	50	LYS	2.2
36	1e	86	ALA	2.2
34	1c	57	ILE	2.2
34	2c	173	VAL	2.2
36	2e	90	VAL	2.2
48	2q	10	VAL	2.2
30	28	19	SER	2.2
1	1A	1112	U	2.2
21	2Z	148	ASP	2.2
34	2c	183	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
45	2n	32	SER	2.2
4	2E	52	LEU	2.2
32	2a	1117	G	2.2
50	2s	84	GLY	2.2
54	1y	20	U	2.2
33	2b	17	PHE	2.2
33	2b	32	ILE	2.2
34	1c	124	ILE	2.2
38	2g	42	ILE	2.2
48	2q	44	ALA	2.2
49	1r	38	GLU	2.2
44	1m	87	TYR	2.2
51	1t	68	LYS	2.2
11	2P	112	LEU	2.2
41	2j	59	SER	2.2
30	18	65	GLU	2.2
44	2m	96	LEU	2.2
7	2H	148	ILE	2.2
44	1m	97	PRO	2.2
34	2c	30	ARG	2.2
9	2N	103	VAL	2.2
5	2F	196	LEU	2.2
35	1d	179	GLU	2.2
52	2u	5	ASP	2.2
34	2c	15	THR	2.2
38	1g	77	SER	2.2
40	1i	46	ALA	2.2
46	1o	65	ARG	2.2
51	1t	8	ARG	2.2
48	2q	87	LYS	2.2
51	1t	63	ILE	2.2
7	2H	83	TYR	2.2
40	1i	109	VAL	2.2
11	2P	92	GLU	2.2
11	2P	93	GLY	2.2
12	2Q	15	GLY	2.2
6	2G	97	ASP	2.2
7	2H	51	ARG	2.2
21	2Z	155	LEU	2.2
30	28	21	LYS	2.2
39	2h	84	ARG	2.2
40	2i	85	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
39	2h	16	ALA	2.2
21	2Z	98	MET	2.2
38	1g	86	GLN	2.2
52	2u	23	PRO	2.2
7	2H	85	LYS	2.2
33	2b	97	TRP	2.2
40	1i	110	GLU	2.2
34	1c	11	ARG	2.2
35	1d	3	ARG	2.2
38	1g	3	ARG	2.2
39	2h	91	ARG	2.2
35	1d	78	LEU	2.2
7	2H	122	THR	2.2
36	2e	19	MET	2.2
45	1n	49	HIS	2.2
14	2S	9	ARG	2.2
22	20	5	LYS	2.2
38	2g	80	VAL	2.2
34	2c	132	ARG	2.2
14	2S	41	ASP	2.2
39	1h	133	LEU	2.2
41	1j	90	LEU	2.2
45	2n	16	PHE	2.2
33	1b	71	VAL	2.2
41	2j	96	ILE	2.1
50	2s	53	ASN	2.1
30	28	3	LYS	2.1
32	1a	1003	G	2.1
42	2k	121	PRO	2.1
34	2c	176	HIS	2.1
41	2j	60	ARG	2.1
41	2j	87	THR	2.1
5	1F	89	VAL	2.1
15	2T	100	TYR	2.1
34	2c	193	TYR	2.1
36	2e	114	GLY	2.1
32	2a	1004	A	2.1
12	2Q	25	ASP	2.1
40	2i	11	LYS	2.1
45	1n	61	TRP	2.1
11	2P	101	VAL	2.1
42	2k	49	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
48	1q	7	THR	2.1
20	2Y	67	LEU	2.1
30	28	26	LYS	2.1
40	2i	47	LEU	2.1
7	2H	9	ILE	2.1
1	1A	1105	G	2.1
41	1j	48	THR	2.1
40	1i	125	TYR	2.1
7	2H	101	ARG	2.1
14	1S	20	ARG	2.1
31	29	12	ASP	2.1
11	2P	140	ALA	2.1
12	2Q	121	ALA	2.1
47	1p	7	ALA	2.1
1	2A	652(T)	C	2.1
11	2P	1	MET	2.1
50	2s	76	PRO	2.1
25	23	52	HIS	2.1
34	1c	64	VAL	2.1
40	2i	95	LYS	2.1
33	2b	190	THR	2.1
39	2h	10	LEU	2.1
41	1j	47	PHE	2.1
47	1p	25	ARG	2.1
47	2p	25	ARG	2.1
51	1t	62	LEU	2.1
32	1a	1001(A)	G	2.1
34	2c	162	GLN	2.1
40	2i	91	ASP	2.1
25	23	21	ALA	2.1
45	2n	59	ALA	2.1
6	2G	75	LYS	2.1
30	28	12	LYS	2.1
43	2l	31	PRO	2.1
44	2m	119	GLY	2.1
14	2S	28	VAL	2.1
40	1i	86	VAL	2.1
48	2q	43	LEU	2.1
41	1j	58	ASP	2.1
30	28	58	ILE	2.1
41	2j	38	ILE	2.1
7	2H	44	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
14	2S	85	VAL	2.1
32	2a	1039	C	2.1
32	2a	1114	C	2.1
39	1h	119	LEU	2.1
14	2S	92	TYR	2.1
21	2Z	9	TYR	2.1
31	29	2	LYS	2.1
31	29	24	TYR	2.1
40	2i	88	TYR	2.1
21	2Z	162	GLU	2.1
25	23	47	VAL	2.1
32	2a	1032	G	2.1
49	1r	39	VAL	2.1
32	2a	1252	A	2.1
50	2s	10	PHE	2.1
51	1t	72	LEU	2.1
53	1v	24	A	2.1
7	2H	72	ILE	2.1
15	2T	14	TYR	2.1
33	2b	68	ILE	2.1
34	1c	39	ILE	2.1
34	2c	57	ILE	2.1
37	2f	59	TYR	2.1
39	2h	80	ILE	2.1
41	2j	6	ILE	2.1
42	2k	89	ALA	2.1
50	2s	68	GLY	2.1
6	2G	70	VAL	2.1
7	2H	125	VAL	2.1
35	1d	133	VAL	2.1
35	2d	98	GLU	2.1
8	2l	137	PRO	2.1
40	1i	28	VAL	2.1
47	1p	21	VAL	2.1
21	2Z	70	LEU	2.0
40	2i	40	LEU	2.0
48	1q	98	LEU	2.0
54	1y	13	C	2.0
35	2d	209	ARG	2.0
38	2g	24	THR	2.0
40	2i	55	ALA	2.0
51	1t	80	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
33	1b	72	GLY	2.0
34	2c	26	LYS	2.0
6	2G	159	VAL	2.0
50	2s	30	LEU	2.0
11	2P	77	ARG	2.0
12	2Q	107	ALA	2.0
32	2a	1191	A	2.0
34	1c	189	ALA	2.0
11	2P	108	LYS	2.0
35	2d	207	TYR	2.0
44	1m	122	LYS	2.0
45	1n	17	LYS	2.0
54	2y	60	U	2.0
15	2T	1	MET	2.0
39	2h	19	VAL	2.0
15	2T	76	PHE	2.0
23	2l	68	PRO	2.0
25	23	2	PRO	2.0
40	1i	37	PHE	2.0
42	1k	98	LEU	2.0
35	2d	168	ARG	2.0
34	1c	182	ILE	2.0
1	1A	2196	C	2.0
32	1a	1029	C	2.0
40	2i	30	GLY	2.0
54	1w	1	G	2.0
11	2P	60	MET	2.0
52	2u	24	ARG	2.0
7	2H	140	LYS	2.0
40	2i	43	ALA	2.0
1	2A	1026	U	2.0
32	2a	1036	G	2.0
36	1e	82	VAL	2.0
36	2e	120	THR	2.0
54	2y	1	G	2.0
54	2y	34	G	2.0
8	1I	1	MET	2.0
45	1n	16	PHE	2.0
52	2u	10	ARG	2.0
12	2Q	18	LYS	2.0
14	2S	83	LYS	2.0
21	2Z	5	LEU	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(Å ²)	Q<0.9
54	PSU	1y	55	20/21	0.76	0.28	85,93,105,123	0
54	5MU	1y	54	21/22	0.78	0.32	79,87,99,114	0
54	4SU	1y	8	20/21	0.80	0.20	91,96,103,105	0
54	PSU	2y	55	20/21	0.80	0.27	85,92,104,109	0
54	7MG	1w	46	24/25	0.82	0.15	76,87,106,118	0
54	5MU	2y	54	21/22	0.82	0.33	84,91,97,115	0
54	7MG	2y	46	24/25	0.83	0.23	83,92,97,112	0
54	7MG	2w	46	24/25	0.83	0.14	78,92,98,107	0
54	7MG	1y	46	24/25	0.84	0.22	86,94,99,108	0
54	4SU	2w	8	20/21	0.85	0.15	85,89,104,109	0
54	4SU	2y	8	20/21	0.85	0.14	83,95,104,112	0
54	MIA	2y	37	22/30	0.86	0.21	69,81,100,111	0
54	PSU	1y	32	20/21	0.88	0.19	71,81,88,90	0
54	PSU	2y	39	20/21	0.88	0.24	77,84,98,102	0
54	PSU	2y	32	20/21	0.88	0.17	69,84,92,94	0
54	MIA	1y	37	22/30	0.90	0.17	70,78,88,93	0
55	PSU	2x	55	20/21	0.91	0.13	67,78,81,81	0
43	0TD	2l	92	10/11	0.91	0.30	58,64,65,80	0
54	4SU	1w	8	20/21	0.91	0.12	74,81,92,95	0
54	PSU	2w	55	20/21	0.91	0.12	75,81,89,94	0
54	5MU	2w	54	21/22	0.92	0.12	68,75,81,83	0
54	PSU	1w	55	20/21	0.92	0.14	61,70,79,80	0
54	PSU	1y	39	20/21	0.92	0.17	70,77,87,90	0
55	5MU	2x	54	21/22	0.92	0.16	77,81,86,94	0
54	PSU	2w	32	20/21	0.93	0.27	67,78,88,89	0
54	PSU	2w	39	20/21	0.93	0.19	60,73,79,81	0
1	5MU	2A	1915	21/22	0.93	0.16	59,64,71,73	0
55	4SU	2x	8	20/21	0.93	0.13	69,73,78,81	0
32	5MC	2a	967	21/22	0.93	0.30	62,67,71,73	0
32	PSU	2a	516	20/21	0.93	0.14	50,70,74,75	0
32	7MG	2a	527	24/25	0.94	0.17	46,56,67,71	0
32	M2G	2a	966	25/26	0.94	0.26	60,65,72,79	0
32	5MC	2a	1400	21/22	0.94	0.23	60,67,71,73	0
43	0TD	1l	92	10/11	0.94	0.21	43,48,51,69	0
55	5MC	2x	32	21/22	0.94	0.18	65,68,73,74	0
1	5MU	1A	1937	21/22	0.95	0.17	43,49,54,56	0
32	7MG	1a	527	24/25	0.95	0.18	34,42,51,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MIA	2w	37	25/30	0.95	0.17	60,68,74,78	0
32	5MC	2a	1404	21/22	0.95	0.17	47,51,56,61	0
55	PSU	1x	55	20/21	0.95	0.13	53,58,67,72	0
1	PSU	2A	1911	20/21	0.95	0.15	50,60,65,67	0
32	2MG	2a	1207	24/25	0.95	0.15	74,77,86,91	0
54	PSU	1w	32	20/21	0.95	0.19	57,62,68,69	0
54	MIA	1w	37	29/30	0.95	0.23	41,51,60,64	0
1	PSU	2A	1917	20/21	0.95	0.14	55,60,65,69	0
1	4OC	2A	1920	21/23	0.95	0.18	53,58,64,66	0
32	5MC	2a	1407	21/22	0.96	0.19	44,48,55,60	0
32	4OC	2a	1402	22/23	0.96	0.16	52,58,64,67	0
32	2MG	1a	1207	24/25	0.96	0.17	57,62,67,68	0
32	MA6	2a	1518	24/25	0.96	0.19	47,59,63,66	0
55	4SU	1x	8	20/21	0.96	0.15	50,57,65,67	0
1	PSU	1A	1939	20/21	0.96	0.16	38,46,53,54	0
55	5MU	1x	54	21/22	0.96	0.14	55,62,70,76	0
32	MA6	2a	1519	24/25	0.96	0.21	47,56,64,66	0
32	PSU	1a	516	20/21	0.96	0.15	32,49,53,54	0
1	5MC	2A	1942	21/22	0.96	0.17	49,56,62,66	0
1	PSU	1A	1933	20/21	0.97	0.19	30,37,44,45	0
32	5MC	1a	1400	21/22	0.97	0.21	37,47,50,55	0
32	MA6	1a	1519	24/25	0.97	0.20	33,39,43,44	0
32	5MC	1a	1407	21/22	0.97	0.20	28,34,39,40	0
32	5MC	1a	1404	21/22	0.97	0.19	31,38,42,44	0
32	UR3	2a	1498	21/22	0.97	0.18	44,50,54,63	0
54	PSU	1w	39	20/21	0.97	0.17	44,60,69,70	0
54	5MU	1w	54	21/22	0.97	0.17	44,60,67,72	0
32	M2G	1a	966	25/26	0.97	0.22	41,48,56,63	0
1	5MU	2A	1939	21/22	0.97	0.17	34,38,43,44	0
1	2MU	2A	2552	21/23	0.97	0.18	31,41,45,52	0
1	5MC	2A	1962	21/22	0.97	0.17	32,45,48,61	0
32	MA6	1a	1518	24/25	0.98	0.20	31,38,40,40	0
1	OMG	2A	2251	24/25	0.98	0.20	32,37,42,45	0
32	4OC	1a	1402	22/23	0.98	0.18	38,42,47,53	0
1	5MC	1A	1984	21/22	0.98	0.17	24,31,36,41	0
1	4OC	1A	1942	21/23	0.98	0.17	32,39,45,47	0
1	5MC	1A	1964	21/22	0.98	0.18	30,39,46,50	0
55	5MC	1x	32	21/22	0.98	0.20	44,50,57,66	0
1	2MU	1A	2564	21/23	0.98	0.19	18,23,28,31	0
1	PSU	2A	2605	20/21	0.98	0.17	27,31,37,38	0
1	PSU	1A	2617	20/21	0.98	0.18	16,20,25,28	0
1	5MU	1A	1961	21/22	0.98	0.18	19,23,26,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	2MA	2A	2503	23/24	0.98	0.21	24,33,37,46	0
32	5MC	1a	967	21/22	0.98	0.20	45,50,58,64	0
1	2MA	1A	2515	23/24	0.98	0.20	11,16,19,22	0
32	UR3	1a	1498	21/22	0.99	0.19	27,39,42,46	0
1	OMG	1A	2263	24/25	0.99	0.17	14,18,24,25	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
56	MG	2y	3006	1/1	0.34	0.13	88,88,88,88	0
56	MG	2a	1640	1/1	0.36	0.22	62,62,62,62	0
56	MG	2A	3720	1/1	0.47	0.17	97,97,97,97	0
56	MG	1A	3209	1/1	0.52	0.29	61,61,61,61	0
56	MG	1A	3898	1/1	0.56	0.15	71,71,71,71	0
56	MG	1A	3986	1/1	0.60	0.24	67,67,67,67	0
56	MG	1A	3242	1/1	0.63	0.26	59,59,59,59	0
56	MG	2a	1769	1/1	0.63	0.13	75,75,75,75	0
59	ZN	24	501	1/1	0.64	0.09	103,103,103,103	0
56	MG	2A	3258	1/1	0.64	0.17	58,58,58,58	0
56	MG	1A	3414	1/1	0.66	0.28	55,55,55,55	0
56	MG	1A	3201	1/1	0.67	0.51	42,42,42,42	0
56	MG	2a	1750	1/1	0.68	0.09	60,60,60,60	0
56	MG	2A	3383	1/1	0.68	0.22	56,56,56,56	0
56	MG	1a	3129	1/1	0.69	0.15	65,65,65,65	0
56	MG	2A	3615	1/1	0.69	0.34	66,66,66,66	0
56	MG	2A	3457	1/1	0.69	0.20	58,58,58,58	0
56	MG	1A	3366	1/1	0.69	0.29	50,50,50,50	0
56	MG	2A	3374	1/1	0.70	0.15	41,41,41,41	0
56	MG	2B	3013	1/1	0.70	0.16	74,74,74,74	0
56	MG	2a	1637	1/1	0.70	0.13	52,52,52,52	0
56	MG	2A	3420	1/1	0.71	0.23	67,67,67,67	0
56	MG	1B	211	1/1	0.71	0.74	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3630	1/1	0.71	0.18	55,55,55,55	0
56	MG	1A	3971	1/1	0.71	0.15	65,65,65,65	0
56	MG	1w	110	1/1	0.72	0.19	75,75,75,75	0
56	MG	28	102	1/1	0.72	0.15	64,64,64,64	0
56	MG	2A	3332	1/1	0.72	0.25	56,56,56,56	0
56	MG	1A	3977	1/1	0.72	0.13	44,44,44,44	0
56	MG	2A	3570	1/1	0.73	0.20	56,56,56,56	0
56	MG	1A	3436	1/1	0.73	0.16	62,62,62,62	0
56	MG	1A	3458	1/1	0.73	0.15	68,68,68,68	0
56	MG	2w	106	1/1	0.73	0.33	59,59,59,59	0
56	MG	1Z	3003	1/1	0.73	0.17	52,52,52,52	0
56	MG	2A	3247	1/1	0.73	0.13	63,63,63,63	0
56	MG	2a	1740	1/1	0.73	0.16	60,60,60,60	0
56	MG	2A	3702	1/1	0.74	0.13	59,59,59,59	0
56	MG	2v	3002	1/1	0.74	0.55	67,67,67,67	0
56	MG	2A	3031	1/1	0.74	0.28	57,57,57,57	0
56	MG	2A	3587	1/1	0.74	0.16	55,55,55,55	0
56	MG	1A	3802	1/1	0.74	0.22	54,54,54,54	0
56	MG	2w	109	1/1	0.74	0.13	63,63,63,63	0
56	MG	1A	3907	1/1	0.74	0.21	39,39,39,39	0
56	MG	2A	3353	1/1	0.74	0.16	35,35,35,35	0
56	MG	1X	101	1/1	0.75	0.09	73,73,73,73	0
56	MG	2A	3636	1/1	0.75	0.18	55,55,55,55	0
56	MG	1A	3920	1/1	0.75	0.21	39,39,39,39	0
56	MG	1A	3766	1/1	0.75	0.23	36,36,36,36	0
56	MG	1r	3001	1/1	0.75	0.16	61,61,61,61	0
56	MG	2B	3002	1/1	0.75	0.38	62,62,62,62	0
56	MG	2A	3163	1/1	0.75	0.26	44,44,44,44	0
56	MG	1A	3305	1/1	0.75	0.20	51,51,51,51	0
56	MG	1B	236	1/1	0.75	0.31	65,65,65,65	0
56	MG	2y	3003	1/1	0.76	0.13	59,59,59,59	0
56	MG	2A	3215	1/1	0.76	0.15	58,58,58,58	0
56	MG	1A	3226	1/1	0.76	0.82	49,49,49,49	0
56	MG	1A	3834	1/1	0.76	0.16	51,51,51,51	0
56	MG	2y	3001	1/1	0.76	0.23	64,64,64,64	0
56	MG	2A	3259	1/1	0.76	0.20	53,53,53,53	0
56	MG	2r	3002	1/1	0.76	0.14	64,64,64,64	0
56	MG	2A	3201	1/1	0.76	0.20	55,55,55,55	0
56	MG	2A	3710	1/1	0.76	0.07	76,76,76,76	0
56	MG	1A	3319	1/1	0.76	0.23	53,53,53,53	0
56	MG	1E	310	1/1	0.77	0.16	60,60,60,60	0
56	MG	2A	3491	1/1	0.77	0.13	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3550	1/1	0.77	0.15	58,58,58,58	0
56	MG	2A	3198	1/1	0.77	0.17	43,43,43,43	0
56	MG	2W	202	1/1	0.77	0.54	46,46,46,46	0
56	MG	2a	1656	1/1	0.77	0.14	68,68,68,68	0
56	MG	1D	313	1/1	0.77	0.21	52,52,52,52	0
56	MG	1a	3141	1/1	0.78	0.17	64,64,64,64	0
56	MG	2A	3586	1/1	0.78	0.12	44,44,44,44	0
56	MG	2A	3266	1/1	0.78	0.11	54,54,54,54	0
56	MG	1B	208	1/1	0.78	0.23	59,59,59,59	0
56	MG	1A	3883	1/1	0.78	0.21	59,59,59,59	0
56	MG	2a	1644	1/1	0.78	0.20	62,62,62,62	0
56	MG	2a	1806	1/1	0.78	0.11	76,76,76,76	0
56	MG	1A	3293	1/1	0.78	0.23	51,51,51,51	0
56	MG	1A	3361	1/1	0.78	0.37	57,57,57,57	0
56	MG	2A	3394	1/1	0.78	0.20	29,29,29,29	0
56	MG	1A	3044	1/1	0.78	0.16	37,37,37,37	0
56	MG	2A	3140	1/1	0.78	0.22	60,60,60,60	0
56	MG	2A	3175	1/1	0.78	0.36	43,43,43,43	0
56	MG	1A	3959	1/1	0.79	0.12	76,76,76,76	0
56	MG	2A	3088	1/1	0.79	0.15	40,40,40,40	0
56	MG	2A	3285	1/1	0.79	0.13	58,58,58,58	0
56	MG	1A	3794	1/1	0.79	0.18	18,18,18,18	0
56	MG	2a	1773	1/1	0.79	0.20	70,70,70,70	0
56	MG	1A	3882	1/1	0.79	0.14	62,62,62,62	0
56	MG	2B	3012	1/1	0.79	0.16	75,75,75,75	0
56	MG	2A	3244	1/1	0.79	0.18	47,47,47,47	0
56	MG	1A	3679	1/1	0.79	0.23	14,14,14,14	0
56	MG	2a	1714	1/1	0.79	0.28	68,68,68,68	0
56	MG	1D	301	1/1	0.79	0.28	44,44,44,44	0
56	MG	2v	3003	1/1	0.79	0.20	66,66,66,66	0
56	MG	1A	3459	1/1	0.79	0.20	53,53,53,53	0
56	MG	2y	3005	1/1	0.79	0.09	88,88,88,88	0
56	MG	2a	1799	1/1	0.80	0.12	59,59,59,59	0
56	MG	2G	3001	1/1	0.80	0.10	60,60,60,60	0
56	MG	2A	3093	1/1	0.80	0.13	58,58,58,58	0
56	MG	2a	1705	1/1	0.80	0.13	54,54,54,54	0
56	MG	2A	3033	1/1	0.80	0.18	52,52,52,52	0
56	MG	1B	213	1/1	0.80	0.84	55,55,55,55	0
56	MG	2A	3160	1/1	0.80	0.17	47,47,47,47	0
56	MG	1a	3024	1/1	0.80	0.16	52,52,52,52	0
56	MG	2a	1617	1/1	0.80	0.15	73,73,73,73	0
56	MG	2B	3016	1/1	0.80	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3593	1/1	0.80	0.12	30,30,30,30	0
56	MG	1e	201	1/1	0.80	0.38	59,59,59,59	0
56	MG	2x	103	1/1	0.80	0.22	63,63,63,63	0
56	MG	2A	3256	1/1	0.80	0.18	46,46,46,46	0
56	MG	2A	3560	1/1	0.80	0.08	50,50,50,50	0
56	MG	1a	3170	1/1	0.80	0.09	66,66,66,66	0
56	MG	1l	202	1/1	0.81	0.16	85,85,85,85	0
56	MG	2t	3001	1/1	0.81	0.09	53,53,53,53	0
56	MG	2a	1607	1/1	0.81	0.18	73,73,73,73	0
56	MG	27	101	1/1	0.81	0.34	44,44,44,44	0
56	MG	1A	3804	1/1	0.81	0.16	45,45,45,45	0
56	MG	1a	3162	1/1	0.81	0.22	62,62,62,62	0
56	MG	1B	212	1/1	0.81	0.29	46,46,46,46	0
56	MG	2E	305	1/1	0.81	0.14	51,51,51,51	0
56	MG	2A	3128	1/1	0.81	0.26	35,35,35,35	0
56	MG	2a	1662	1/1	0.81	0.11	59,59,59,59	0
56	MG	2a	1772	1/1	0.81	0.17	54,54,54,54	0
56	MG	1A	3408	1/1	0.81	0.30	40,40,40,40	0
56	MG	2A	3723	1/1	0.81	0.31	67,67,67,67	0
56	MG	2a	1603	1/1	0.81	0.17	73,73,73,73	0
56	MG	1a	3175	1/1	0.81	0.09	58,58,58,58	0
56	MG	2A	3046	1/1	0.81	0.15	58,58,58,58	0
56	MG	1a	3049	1/1	0.81	0.16	60,60,60,60	0
56	MG	2A	3536	1/1	0.81	0.14	54,54,54,54	0
56	MG	1Z	3002	1/1	0.81	0.15	46,46,46,46	0
56	MG	1A	3086	1/1	0.81	0.15	55,55,55,55	0
56	MG	1A	3844	1/1	0.81	0.08	23,23,23,23	0
56	MG	2A	3389	1/1	0.81	0.20	35,35,35,35	0
56	MG	28	101	1/1	0.81	0.20	49,49,49,49	0
56	MG	2a	1616	1/1	0.81	0.11	67,67,67,67	0
56	MG	2A	3261	1/1	0.81	0.20	50,50,50,50	0
56	MG	2A	3439	1/1	0.81	0.11	49,49,49,49	0
56	MG	2A	3701	1/1	0.81	0.11	50,50,50,50	0
56	MG	1A	3341	1/1	0.81	0.37	38,38,38,38	0
56	MG	1A	3760	1/1	0.81	0.13	44,44,44,44	0
56	MG	1a	3149	1/1	0.81	0.54	76,76,76,76	0
56	MG	2A	3058	1/1	0.81	0.20	65,65,65,65	0
56	MG	1A	3523	1/1	0.82	0.12	46,46,46,46	0
56	MG	1A	3230	1/1	0.82	0.19	44,44,44,44	0
56	MG	2A	3229	1/1	0.82	0.24	34,34,34,34	0
56	MG	1A	3367	1/1	0.82	0.22	46,46,46,46	0
56	MG	1B	232	1/1	0.82	0.14	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3357	1/1	0.82	0.23	43,43,43,43	0
56	MG	2a	1667	1/1	0.82	0.17	61,61,61,61	0
56	MG	1A	3227	1/1	0.82	0.13	49,49,49,49	0
56	MG	16	103	1/1	0.82	0.53	56,56,56,56	0
56	MG	2A	3524	1/1	0.82	0.12	61,61,61,61	0
56	MG	2A	3196	1/1	0.82	0.19	53,53,53,53	0
56	MG	1A	3795	1/1	0.82	0.17	50,50,50,50	0
56	MG	2a	1651	1/1	0.82	0.08	60,60,60,60	0
56	MG	1A	3166	1/1	0.82	0.37	31,31,31,31	0
56	MG	1A	3914	1/1	0.82	0.21	54,54,54,54	0
56	MG	2A	3747	1/1	0.82	0.17	35,35,35,35	0
56	MG	1A	3363	1/1	0.82	0.17	32,32,32,32	0
56	MG	2a	1738	1/1	0.82	0.12	71,71,71,71	0
56	MG	1a	3069	1/1	0.82	0.15	59,59,59,59	0
56	MG	1A	3248	1/1	0.82	0.14	49,49,49,49	0
56	MG	2a	1829	1/1	0.82	0.30	68,68,68,68	0
56	MG	2A	3558	1/1	0.82	0.28	50,50,50,50	0
56	MG	1V	202	1/1	0.82	0.42	44,44,44,44	0
56	MG	1A	3789	1/1	0.82	0.21	44,44,44,44	0
56	MG	1A	4048	1/1	0.82	0.64	31,31,31,31	0
56	MG	2A	3687	1/1	0.82	0.29	65,65,65,65	0
56	MG	2A	3447	1/1	0.82	0.22	27,27,27,27	0
56	MG	1a	3154	1/1	0.82	0.10	59,59,59,59	0
56	MG	1a	3006	1/1	0.82	0.20	59,59,59,59	0
56	MG	1A	3423	1/1	0.83	0.17	38,38,38,38	0
56	MG	2a	1681	1/1	0.83	0.22	69,69,69,69	0
56	MG	2A	3257	1/1	0.83	0.18	57,57,57,57	0
56	MG	2a	1648	1/1	0.83	0.23	63,63,63,63	0
56	MG	2a	1609	1/1	0.83	0.12	57,57,57,57	0
56	MG	1v	3001	1/1	0.83	0.11	72,72,72,72	0
56	MG	2a	1694	1/1	0.83	0.27	66,66,66,66	0
56	MG	1a	3026	1/1	0.83	0.11	72,72,72,72	0
56	MG	1A	3299	1/1	0.83	0.35	28,28,28,28	0
56	MG	2A	3065	1/1	0.83	0.16	52,52,52,52	0
56	MG	2a	1613	1/1	0.83	0.15	60,60,60,60	0
56	MG	1A	3308	1/1	0.83	0.16	49,49,49,49	0
56	MG	2A	3158	1/1	0.83	0.32	49,49,49,49	0
56	MG	1A	3935	1/1	0.83	0.15	43,43,43,43	0
56	MG	1A	3315	1/1	0.83	0.25	37,37,37,37	0
56	MG	1A	3801	1/1	0.83	0.25	71,71,71,71	0
56	MG	1A	4041	1/1	0.83	0.54	35,35,35,35	0
56	MG	2B	3014	1/1	0.83	0.31	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3638	1/1	0.83	0.16	66,66,66,66	0
56	MG	1a	3018	1/1	0.83	0.29	55,55,55,55	0
56	MG	2a	1636	1/1	0.83	0.09	66,66,66,66	0
56	MG	2j	8001	1/1	0.83	0.11	66,66,66,66	0
56	MG	1A	3904	1/1	0.83	0.15	71,71,71,71	0
56	MG	2A	3653	1/1	0.83	0.22	37,37,37,37	0
56	MG	2A	3436	1/1	0.83	0.14	62,62,62,62	0
56	MG	2A	3225	1/1	0.83	0.18	53,53,53,53	0
56	MG	2a	1647	1/1	0.84	0.13	80,80,80,80	0
56	MG	1A	3781	1/1	0.84	0.19	51,51,51,51	0
56	MG	2A	3205	1/1	0.84	0.15	55,55,55,55	0
56	MG	2A	3425	1/1	0.84	0.11	59,59,59,59	0
56	MG	1B	210	1/1	0.84	0.15	50,50,50,50	0
56	MG	1A	3672	1/1	0.84	0.22	68,68,68,68	0
56	MG	2T	3001	1/1	0.84	0.26	52,52,52,52	0
56	MG	2A	3087	1/1	0.84	0.08	59,59,59,59	0
56	MG	2a	1722	1/1	0.84	0.18	79,79,79,79	0
56	MG	1w	111	1/1	0.84	0.13	69,69,69,69	0
56	MG	1a	3046	1/1	0.84	0.09	54,54,54,54	0
56	MG	2A	3672	1/1	0.84	0.26	46,46,46,46	0
56	MG	1A	3350	1/1	0.84	0.31	44,44,44,44	0
56	MG	1A	3246	1/1	0.84	0.13	37,37,37,37	0
56	MG	2A	3263	1/1	0.84	0.19	54,54,54,54	0
56	MG	2a	1697	1/1	0.84	0.10	64,64,64,64	0
56	MG	2A	3133	1/1	0.84	0.27	44,44,44,44	0
56	MG	2A	3443	1/1	0.84	0.14	34,34,34,34	0
56	MG	1N	204	1/1	0.84	0.60	46,46,46,46	0
56	MG	2a	1736	1/1	0.84	0.11	82,82,82,82	0
56	MG	2a	1663	1/1	0.84	0.13	48,48,48,48	0
56	MG	1A	3931	1/1	0.84	0.22	47,47,47,47	0
56	MG	2A	3621	1/1	0.84	0.09	49,49,49,49	0
56	MG	1y	103	1/1	0.84	0.26	82,82,82,82	0
56	MG	2a	1788	1/1	0.84	0.12	55,55,55,55	0
56	MG	2a	1802	1/1	0.84	0.23	69,69,69,69	0
56	MG	2a	1604	1/1	0.84	0.16	48,48,48,48	0
56	MG	2A	3296	1/1	0.84	0.40	54,54,54,54	0
56	MG	2A	3329	1/1	0.84	0.22	46,46,46,46	0
56	MG	1A	3065	1/1	0.84	0.39	62,62,62,62	0
56	MG	2x	104	1/1	0.84	0.13	64,64,64,64	0
56	MG	2a	1751	1/1	0.84	0.12	87,87,87,87	0
56	MG	2q	203	1/1	0.84	0.20	75,75,75,75	0
56	MG	2A	3312	1/1	0.84	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2F	302	1/1	0.84	0.13	50,50,50,50	0
56	MG	1a	3083	1/1	0.85	0.19	54,54,54,54	0
56	MG	1a	3168	1/1	0.85	0.15	63,63,63,63	0
56	MG	1A	3143	1/1	0.85	0.47	37,37,37,37	0
56	MG	1A	3083	1/1	0.85	0.26	55,55,55,55	0
56	MG	1a	3084	1/1	0.85	0.28	54,54,54,54	0
56	MG	1a	3205	1/1	0.85	0.11	69,69,69,69	0
56	MG	2F	304	1/1	0.85	0.10	64,64,64,64	0
56	MG	1A	3960	1/1	0.85	0.23	51,51,51,51	0
56	MG	1a	3014	1/1	0.85	0.39	55,55,55,55	0
56	MG	2a	1605	1/1	0.85	0.13	61,61,61,61	0
56	MG	2a	1615	1/1	0.85	0.22	54,54,54,54	0
56	MG	1A	3137	1/1	0.85	0.42	40,40,40,40	0
56	MG	2U	203	1/1	0.85	0.41	55,55,55,55	0
56	MG	2a	1792	1/1	0.85	0.09	61,61,61,61	0
56	MG	1A	3207	1/1	0.85	0.28	52,52,52,52	0
56	MG	2B	3003	1/1	0.85	0.21	60,60,60,60	0
56	MG	1A	3984	1/1	0.85	0.11	52,52,52,52	0
56	MG	1A	3895	1/1	0.85	0.15	71,71,71,71	0
56	MG	2A	3293	1/1	0.85	0.28	46,46,46,46	0
56	MG	2A	3497	1/1	0.85	0.18	63,63,63,63	0
56	MG	1a	3177	1/1	0.85	0.15	57,57,57,57	0
56	MG	2a	1815	1/1	0.85	0.16	61,61,61,61	0
56	MG	2A	3094	1/1	0.85	0.16	47,47,47,47	0
56	MG	1w	103	1/1	0.85	0.37	68,68,68,68	0
56	MG	2A	3501	1/1	0.85	0.19	53,53,53,53	0
56	MG	1A	3316	1/1	0.85	0.41	34,34,34,34	0
56	MG	2O	8001	1/1	0.85	0.20	56,56,56,56	0
56	MG	2A	3311	1/1	0.85	0.23	50,50,50,50	0
56	MG	1a	3206	1/1	0.85	0.18	51,51,51,51	0
56	MG	2A	3076	1/1	0.85	0.13	45,45,45,45	0
56	MG	2A	3714	1/1	0.85	0.14	50,50,50,50	0
56	MG	2a	1822	1/1	0.85	0.22	52,52,52,52	0
56	MG	2A	3356	1/1	0.85	0.08	42,42,42,42	0
56	MG	2a	1631	1/1	0.85	0.09	66,66,66,66	0
56	MG	2a	1791	1/1	0.85	0.12	69,69,69,69	0
56	MG	1x	109	1/1	0.85	0.11	57,57,57,57	0
56	MG	2A	3185	1/1	0.85	0.19	46,46,46,46	0
56	MG	1x	103	1/1	0.85	0.27	54,54,54,54	0
56	MG	2a	1784	1/1	0.85	0.11	66,66,66,66	0
56	MG	2A	3472	1/1	0.85	0.23	42,42,42,42	0
56	MG	1w	108	1/1	0.85	0.16	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3640	1/1	0.85	0.16	36,36,36,36	0
56	MG	2D	304	1/1	0.85	0.14	53,53,53,53	0
56	MG	2A	3267	1/1	0.85	0.20	52,52,52,52	0
56	MG	1a	3061	1/1	0.85	0.14	56,56,56,56	0
56	MG	1A	3680	1/1	0.85	0.30	36,36,36,36	0
56	MG	1a	3089	1/1	0.85	0.15	40,40,40,40	0
56	MG	2B	3019	1/1	0.85	0.30	82,82,82,82	0
56	MG	2A	3571	1/1	0.85	0.10	57,57,57,57	0
56	MG	1A	3644	1/1	0.85	0.14	12,12,12,12	0
56	MG	1A	3903	1/1	0.86	0.11	23,23,23,23	0
56	MG	1A	3621	1/1	0.86	0.17	44,44,44,44	0
56	MG	2a	1755	1/1	0.86	0.06	70,70,70,70	0
56	MG	1A	3592	1/1	0.86	0.13	30,30,30,30	0
56	MG	1A	4016	1/1	0.86	0.11	55,55,55,55	0
56	MG	1A	3718	1/1	0.86	0.20	39,39,39,39	0
56	MG	2a	1602	1/1	0.86	0.21	54,54,54,54	0
56	MG	1A	3057	1/1	0.86	0.26	45,45,45,45	0
56	MG	2a	1724	1/1	0.86	0.11	73,73,73,73	0
56	MG	1A	3939	1/1	0.86	0.15	44,44,44,44	0
56	MG	15	107	1/1	0.86	0.21	45,45,45,45	0
56	MG	2A	3002	1/1	0.86	0.13	61,61,61,61	0
56	MG	1A	3590	1/1	0.86	0.22	36,36,36,36	0
56	MG	1A	3480	1/1	0.86	0.64	35,35,35,35	0
56	MG	2a	1732	1/1	0.86	0.11	56,56,56,56	0
56	MG	1Q	204	1/1	0.86	0.17	41,41,41,41	0
56	MG	2A	3468	1/1	0.86	0.11	40,40,40,40	0
56	MG	1A	3416	1/1	0.86	0.15	17,17,17,17	0
56	MG	2a	1612	1/1	0.86	0.11	58,58,58,58	0
56	MG	1a	3161	1/1	0.86	0.08	53,53,53,53	0
56	MG	2A	3650	1/1	0.86	0.09	52,52,52,52	0
56	MG	1A	3951	1/1	0.86	0.12	62,62,62,62	0
56	MG	1A	3691	1/1	0.86	0.30	55,55,55,55	0
56	MG	2A	3220	1/1	0.86	0.13	49,49,49,49	0
56	MG	2A	3083	1/1	0.86	0.10	53,53,53,53	0
56	MG	1A	3455	1/1	0.86	0.51	28,28,28,28	0
56	MG	2A	3514	1/1	0.86	0.22	56,56,56,56	0
56	MG	2A	3618	1/1	0.86	0.18	71,71,71,71	0
56	MG	1a	3064	1/1	0.86	0.21	54,54,54,54	0
56	MG	1A	3047	1/1	0.86	0.14	50,50,50,50	0
56	MG	2a	1752	1/1	0.86	0.16	62,62,62,62	0
56	MG	1p	101	1/1	0.86	0.24	55,55,55,55	0
56	MG	2w	102	1/1	0.86	0.14	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	1666	1/1	0.86	0.10	51,51,51,51	0
56	MG	2A	3208	1/1	0.86	0.23	49,49,49,49	0
56	MG	2g	8001	1/1	0.86	0.15	59,59,59,59	0
56	MG	2A	3616	1/1	0.86	0.12	51,51,51,51	0
56	MG	2x	101	1/1	0.86	0.12	52,52,52,52	0
56	MG	2A	3738	1/1	0.86	0.17	63,63,63,63	0
56	MG	1S	3003	1/1	0.86	0.21	61,61,61,61	0
56	MG	2A	3539	1/1	0.86	0.10	59,59,59,59	0
56	MG	2A	3281	1/1	0.86	0.09	60,60,60,60	0
56	MG	2A	3277	1/1	0.86	0.37	54,54,54,54	0
56	MG	2a	1661	1/1	0.86	0.11	63,63,63,63	0
56	MG	2A	3231	1/1	0.86	0.31	49,49,49,49	0
56	MG	1A	3465	1/1	0.86	0.20	55,55,55,55	0
56	MG	2A	3544	1/1	0.86	0.24	30,30,30,30	0
56	MG	2B	3008	1/1	0.86	0.30	59,59,59,59	0
56	MG	1S	3001	1/1	0.86	0.18	47,47,47,47	0
56	MG	2A	3604	1/1	0.86	0.10	58,58,58,58	0
56	MG	2A	3676	1/1	0.86	0.13	79,79,79,79	0
56	MG	2A	3542	1/1	0.86	0.13	36,36,36,36	0
56	MG	2Z	8001	1/1	0.86	0.26	73,73,73,73	0
56	MG	2A	3546	1/1	0.87	0.15	45,45,45,45	0
56	MG	1a	3038	1/1	0.87	0.20	55,55,55,55	0
56	MG	1A	3513	1/1	0.87	0.16	29,29,29,29	0
56	MG	2B	3009	1/1	0.87	0.14	63,63,63,63	0
56	MG	1A	3832	1/1	0.87	0.13	69,69,69,69	0
56	MG	2A	3307	1/1	0.87	0.14	35,35,35,35	0
56	MG	1A	4012	1/1	0.87	0.26	47,47,47,47	0
56	MG	2A	3156	1/1	0.87	0.18	42,42,42,42	0
56	MG	2A	3730	1/1	0.87	0.35	32,32,32,32	0
56	MG	1A	3277	1/1	0.87	0.13	37,37,37,37	0
56	MG	1A	4053	1/1	0.87	0.45	42,42,42,42	0
56	MG	2A	3082	1/1	0.87	0.18	69,69,69,69	0
56	MG	1A	3169	1/1	0.87	0.13	53,53,53,53	0
56	MG	2A	3612	1/1	0.87	0.20	65,65,65,65	0
56	MG	1w	101	1/1	0.87	0.30	74,74,74,74	0
56	MG	2A	3053	1/1	0.87	0.14	30,30,30,30	0
56	MG	2A	3131	1/1	0.87	0.13	40,40,40,40	0
56	MG	2A	3568	1/1	0.87	0.16	47,47,47,47	0
56	MG	1A	3052	1/1	0.87	0.14	31,31,31,31	0
56	MG	2B	3010	1/1	0.87	0.11	64,64,64,64	0
56	MG	1A	3792	1/1	0.87	0.18	19,19,19,19	0
56	MG	1A	3780	1/1	0.87	0.23	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3516	1/1	0.87	0.13	30,30,30,30	0
56	MG	2A	3102	1/1	0.87	0.37	44,44,44,44	0
56	MG	1A	3198	1/1	0.87	0.12	43,43,43,43	0
56	MG	1A	3965	1/1	0.87	0.16	63,63,63,63	0
56	MG	1A	3346	1/1	0.87	0.18	43,43,43,43	0
56	MG	2A	3286	1/1	0.87	0.17	46,46,46,46	0
56	MG	2A	3426	1/1	0.87	0.18	48,48,48,48	0
56	MG	1a	3207	1/1	0.87	0.09	41,41,41,41	0
56	MG	1A	3002	1/1	0.87	0.18	46,46,46,46	0
56	MG	1A	3741	1/1	0.87	0.11	40,40,40,40	0
56	MG	2a	1645	1/1	0.87	0.61	74,74,74,74	0
56	MG	1a	3165	1/1	0.87	0.09	60,60,60,60	0
56	MG	2A	3188	1/1	0.87	0.12	57,57,57,57	0
56	MG	1A	3106	1/1	0.87	0.54	24,24,24,24	0
56	MG	1A	3980	1/1	0.87	0.21	62,62,62,62	0
56	MG	2A	3021	1/1	0.87	0.32	58,58,58,58	0
56	MG	2A	3322	1/1	0.87	0.37	55,55,55,55	0
56	MG	1a	3130	1/1	0.87	0.14	46,46,46,46	0
56	MG	1a	3186	1/1	0.87	0.19	48,48,48,48	0
56	MG	1B	220	1/1	0.87	0.14	57,57,57,57	0
56	MG	2A	3349	1/1	0.87	0.17	30,30,30,30	0
56	MG	1D	307	1/1	0.87	0.17	39,39,39,39	0
56	MG	2A	3715	1/1	0.87	0.09	56,56,56,56	0
56	MG	1A	3989	1/1	0.87	0.10	49,49,49,49	0
56	MG	2Q	3003	1/1	0.87	0.64	52,52,52,52	0
56	MG	2A	3186	1/1	0.87	0.15	51,51,51,51	0
56	MG	2a	1808	1/1	0.87	0.19	58,58,58,58	0
56	MG	2a	1620	1/1	0.87	0.21	64,64,64,64	0
56	MG	1A	3313	1/1	0.87	0.39	35,35,35,35	0
56	MG	1a	3180	1/1	0.87	0.10	62,62,62,62	0
56	MG	2a	1745	1/1	0.87	0.13	64,64,64,64	0
56	MG	2A	3689	1/1	0.87	0.13	56,56,56,56	0
56	MG	1E	308	1/1	0.87	0.17	28,28,28,28	0
56	MG	2A	3193	1/1	0.88	0.12	51,51,51,51	0
56	MG	1A	3373	1/1	0.88	0.12	41,41,41,41	0
56	MG	2a	1797	1/1	0.88	0.13	70,70,70,70	0
56	MG	2A	3744	1/1	0.88	0.10	40,40,40,40	0
56	MG	2a	1671	1/1	0.88	0.16	58,58,58,58	0
56	MG	1A	3398	1/1	0.88	0.12	37,37,37,37	0
56	MG	2A	3115	1/1	0.88	0.18	39,39,39,39	0
56	MG	1a	3050	1/1	0.88	0.12	50,50,50,50	0
56	MG	1A	3085	1/1	0.88	0.14	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3133	1/1	0.88	0.22	43,43,43,43	0
56	MG	1a	3020	1/1	0.88	0.09	47,47,47,47	0
56	MG	1A	3527	1/1	0.88	0.24	66,66,66,66	0
56	MG	1A	3461	1/1	0.88	0.18	55,55,55,55	0
56	MG	1a	3073	1/1	0.88	0.12	59,59,59,59	0
56	MG	20	3001	1/1	0.88	0.15	52,52,52,52	0
56	MG	21	3001	1/1	0.88	0.54	36,36,36,36	0
56	MG	1A	3309	1/1	0.88	0.14	32,32,32,32	0
56	MG	1A	3843	1/1	0.88	0.10	66,66,66,66	0
56	MG	2A	3045	1/1	0.88	0.14	55,55,55,55	0
56	MG	1A	4065	1/1	0.88	0.12	36,36,36,36	0
56	MG	2A	3606	1/1	0.88	0.12	49,49,49,49	0
56	MG	2A	3202	1/1	0.88	0.14	56,56,56,56	0
56	MG	1A	3368	1/1	0.88	0.39	39,39,39,39	0
56	MG	2A	3213	1/1	0.88	0.11	50,50,50,50	0
56	MG	2A	3117	1/1	0.88	0.21	61,61,61,61	0
56	MG	1A	3297	1/1	0.88	0.13	35,35,35,35	0
56	MG	1A	3425	1/1	0.88	0.14	34,34,34,34	0
56	MG	1A	3549	1/1	0.88	0.11	30,30,30,30	0
56	MG	2A	3433	1/1	0.88	0.19	60,60,60,60	0
56	MG	2w	105	1/1	0.88	0.14	72,72,72,72	0
56	MG	2A	3166	1/1	0.88	0.13	47,47,47,47	0
56	MG	1A	3730	1/1	0.88	0.35	42,42,42,42	0
56	MG	2A	3690	1/1	0.88	0.14	58,58,58,58	0
56	MG	1A	3881	1/1	0.88	0.11	44,44,44,44	0
56	MG	2A	3280	1/1	0.88	0.47	50,50,50,50	0
56	MG	2A	3249	1/1	0.88	0.14	54,54,54,54	0
56	MG	1A	3779	1/1	0.88	0.10	50,50,50,50	0
56	MG	2A	3520	1/1	0.88	0.10	52,52,52,52	0
56	MG	2A	3052	1/1	0.88	0.14	36,36,36,36	0
56	MG	2A	3360	1/1	0.88	0.13	25,25,25,25	0
56	MG	1a	3096	1/1	0.88	0.18	47,47,47,47	0
56	MG	1A	4027	1/1	0.88	0.30	61,61,61,61	0
56	MG	2A	3241	1/1	0.88	0.18	55,55,55,55	0
56	MG	2D	307	1/1	0.88	0.27	35,35,35,35	0
56	MG	1A	3506	1/1	0.88	0.09	24,24,24,24	0
56	MG	1A	3283	1/1	0.88	0.33	28,28,28,28	0
56	MG	2y	3007	1/1	0.88	0.14	81,81,81,81	0
56	MG	1t	3001	1/1	0.88	0.20	57,57,57,57	0
56	MG	2A	3737	1/1	0.88	0.26	42,42,42,42	0
56	MG	2A	3071	1/1	0.88	0.08	60,60,60,60	0
56	MG	2A	3321	1/1	0.88	0.21	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3967	1/1	0.88	0.27	53,53,53,53	0
56	MG	1A	3282	1/1	0.88	0.21	56,56,56,56	0
56	MG	1E	306	1/1	0.88	0.12	38,38,38,38	0
56	MG	1A	3294	1/1	0.88	0.21	40,40,40,40	0
56	MG	2v	3004	1/1	0.88	0.19	73,73,73,73	0
56	MG	1a	3017	1/1	0.88	0.20	57,57,57,57	0
56	MG	2a	1713	1/1	0.88	0.13	48,48,48,48	0
56	MG	1A	3916	1/1	0.88	0.13	54,54,54,54	0
56	MG	2A	3492	1/1	0.88	0.22	49,49,49,49	0
56	MG	16	101	1/1	0.88	0.17	35,35,35,35	0
56	MG	1x	101	1/1	0.88	0.19	54,54,54,54	0
56	MG	1a	3059	1/1	0.88	0.09	61,61,61,61	0
56	MG	1l	102	1/1	0.88	0.21	72,72,72,72	0
56	MG	2A	3515	1/1	0.88	0.19	44,44,44,44	0
56	MG	1A	3761	1/1	0.88	0.14	48,48,48,48	0
56	MG	2E	307	1/1	0.88	0.20	60,60,60,60	0
56	MG	2A	3376	1/1	0.88	0.17	45,45,45,45	0
56	MG	1A	3944	1/1	0.88	0.13	39,39,39,39	0
56	MG	1A	3321	1/1	0.88	0.41	45,45,45,45	0
56	MG	2A	3441	1/1	0.88	0.14	62,62,62,62	0
56	MG	2a	1610	1/1	0.88	0.81	63,63,63,63	0
56	MG	1A	3135	1/1	0.88	0.27	23,23,23,23	0
56	MG	2a	1639	1/1	0.88	0.21	60,60,60,60	0
56	MG	2A	3174	1/1	0.88	0.24	47,47,47,47	0
56	MG	2a	1770	1/1	0.89	0.17	59,59,59,59	0
56	MG	20	3002	1/1	0.89	0.07	52,52,52,52	0
56	MG	2A	3659	1/1	0.89	0.18	41,41,41,41	0
56	MG	2A	3753	1/1	0.89	0.55	52,52,52,52	0
56	MG	1F	306	1/1	0.89	0.18	36,36,36,36	0
56	MG	1A	3094	1/1	0.89	0.13	56,56,56,56	0
56	MG	2A	3207	1/1	0.89	0.28	40,40,40,40	0
56	MG	1A	3306	1/1	0.89	0.15	43,43,43,43	0
56	MG	2a	1719	1/1	0.89	0.14	55,55,55,55	0
56	MG	2A	3048	1/1	0.89	0.12	57,57,57,57	0
56	MG	1A	3473	1/1	0.89	0.18	42,42,42,42	0
56	MG	2a	1701	1/1	0.89	0.10	72,72,72,72	0
56	MG	2A	3223	1/1	0.89	0.13	45,45,45,45	0
56	MG	1A	3759	1/1	0.89	0.13	32,32,32,32	0
56	MG	2a	1800	1/1	0.89	0.23	61,61,61,61	0
56	MG	2q	202	1/1	0.89	0.24	59,59,59,59	0
56	MG	1A	3333	1/1	0.89	0.51	43,43,43,43	0
56	MG	1A	3584	1/1	0.89	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3194	1/1	0.89	0.21	51,51,51,51	0
56	MG	2a	1641	1/1	0.89	0.13	53,53,53,53	0
56	MG	13	102	1/1	0.89	0.13	46,46,46,46	0
56	MG	2A	3682	1/1	0.89	0.13	61,61,61,61	0
56	MG	2B	3001	1/1	0.89	0.55	75,75,75,75	0
56	MG	2A	3547	1/1	0.89	0.25	47,47,47,47	0
56	MG	1a	3027	1/1	0.89	0.24	58,58,58,58	0
56	MG	1w	106	1/1	0.89	0.10	70,70,70,70	0
56	MG	1A	3566	1/1	0.89	0.17	62,62,62,62	0
56	MG	1A	3713	1/1	0.89	0.11	48,48,48,48	0
56	MG	2A	3396	1/1	0.89	0.14	29,29,29,29	0
56	MG	2A	3086	1/1	0.89	0.14	62,62,62,62	0
56	MG	2A	3049	1/1	0.89	0.12	53,53,53,53	0
56	MG	1A	3104	1/1	0.89	0.22	45,45,45,45	0
56	MG	1A	3263	1/1	0.89	0.09	48,48,48,48	0
56	MG	1A	3427	1/1	0.89	0.67	29,29,29,29	0
56	MG	2A	3545	1/1	0.89	0.18	45,45,45,45	0
56	MG	1A	3197	1/1	0.89	0.13	32,32,32,32	0
56	MG	1A	3997	1/1	0.89	0.20	45,45,45,45	0
56	MG	1A	3548	1/1	0.89	0.14	52,52,52,52	0
56	MG	1A	3796	1/1	0.89	0.17	33,33,33,33	0
56	MG	2l	202	1/1	0.89	0.43	66,66,66,66	0
56	MG	1N	202	1/1	0.89	0.13	36,36,36,36	0
56	MG	10	105	1/1	0.89	0.10	50,50,50,50	0
56	MG	1P	203	1/1	0.89	0.42	33,33,33,33	0
56	MG	1A	3947	1/1	0.89	0.14	49,49,49,49	0
56	MG	2A	3044	1/1	0.89	0.08	61,61,61,61	0
56	MG	2a	1626	1/1	0.89	0.08	50,50,50,50	0
56	MG	1A	3711	1/1	0.89	0.15	44,44,44,44	0
56	MG	2A	3507	1/1	0.89	0.10	67,67,67,67	0
56	MG	1B	226	1/1	0.89	0.14	67,67,67,67	0
56	MG	1A	3355	1/1	0.89	0.49	30,30,30,30	0
56	MG	2A	3666	1/1	0.89	0.14	46,46,46,46	0
56	MG	2A	3228	1/1	0.89	0.38	38,38,38,38	0
56	MG	1a	3003	1/1	0.89	0.20	56,56,56,56	0
56	MG	2A	3592	1/1	0.89	0.12	43,43,43,43	0
56	MG	2a	1826	1/1	0.89	0.12	55,55,55,55	0
56	MG	2a	1824	1/1	0.89	0.18	63,63,63,63	0
56	MG	2A	3338	1/1	0.89	0.26	42,42,42,42	0
56	MG	1B	229	1/1	0.89	0.09	57,57,57,57	0
56	MG	1a	3044	1/1	0.89	0.15	46,46,46,46	0
56	MG	2A	3530	1/1	0.89	0.16	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3018	1/1	0.89	0.14	43,43,43,43	0
56	MG	25	504	1/1	0.89	0.36	67,67,67,67	0
56	MG	1A	4047	1/1	0.89	0.39	29,29,29,29	0
56	MG	2a	1708	1/1	0.89	0.14	61,61,61,61	0
56	MG	1A	3697	1/1	0.89	0.20	27,27,27,27	0
56	MG	1A	3339	1/1	0.89	0.26	48,48,48,48	0
56	MG	1a	3192	1/1	0.89	0.09	62,62,62,62	0
56	MG	2A	3015	1/1	0.89	0.15	37,37,37,37	0
56	MG	1A	3317	1/1	0.89	0.47	45,45,45,45	0
56	MG	1A	3586	1/1	0.89	0.19	17,17,17,17	0
56	MG	1A	3735	1/1	0.89	0.14	22,22,22,22	0
56	MG	2A	3067	1/1	0.89	0.22	46,46,46,46	0
56	MG	2A	3731	1/1	0.89	0.11	37,37,37,37	0
56	MG	1A	3609	1/1	0.89	0.08	61,61,61,61	0
56	MG	1O	205	1/1	0.89	0.38	57,57,57,57	0
56	MG	2a	1642	1/1	0.89	0.21	55,55,55,55	0
56	MG	2a	1748	1/1	0.89	0.14	60,60,60,60	0
56	MG	2A	3518	1/1	0.89	0.13	45,45,45,45	0
56	MG	2a	1621	1/1	0.89	0.55	65,65,65,65	0
56	MG	1A	4009	1/1	0.89	0.22	41,41,41,41	0
56	MG	1A	3823	1/1	0.89	0.13	50,50,50,50	0
56	MG	2a	1650	1/1	0.89	0.16	68,68,68,68	0
56	MG	1A	3430	1/1	0.89	0.66	40,40,40,40	0
56	MG	1A	3439	1/1	0.89	0.31	37,37,37,37	0
56	MG	2A	3024	1/1	0.89	0.20	50,50,50,50	0
56	MG	1A	3054	1/1	0.89	0.12	26,26,26,26	0
56	MG	1A	3456	1/1	0.89	0.41	33,33,33,33	0
56	MG	1A	3828	1/1	0.89	0.19	62,62,62,62	0
56	MG	1A	3432	1/1	0.89	0.15	31,31,31,31	0
56	MG	1A	3415	1/1	0.89	0.45	38,38,38,38	0
56	MG	2B	3018	1/1	0.89	0.86	80,80,80,80	0
56	MG	1x	114	1/1	0.89	0.14	67,67,67,67	0
56	MG	1O	207	1/1	0.89	0.10	54,54,54,54	0
56	MG	2A	3695	1/1	0.89	0.25	58,58,58,58	0
56	MG	2a	1633	1/1	0.89	0.11	63,63,63,63	0
56	MG	2A	3001	1/1	0.89	0.09	44,44,44,44	0
56	MG	1A	3356	1/1	0.89	0.19	48,48,48,48	0
56	MG	1A	3568	1/1	0.89	0.10	30,30,30,30	0
56	MG	2A	3434	1/1	0.90	0.16	46,46,46,46	0
56	MG	1a	3143	1/1	0.90	0.08	74,74,74,74	0
56	MG	2A	3529	1/1	0.90	0.24	59,59,59,59	0
56	MG	1A	4015	1/1	0.90	0.19	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3092	1/1	0.90	0.17	38,38,38,38	0
56	MG	1a	3047	1/1	0.90	0.28	46,46,46,46	0
56	MG	1B	209	1/1	0.90	0.09	53,53,53,53	0
56	MG	25	503	1/1	0.90	0.41	40,40,40,40	0
56	MG	1A	3990	1/1	0.90	0.08	38,38,38,38	0
56	MG	1A	3027	1/1	0.90	0.35	27,27,27,27	0
56	MG	2A	3480	1/1	0.90	0.21	47,47,47,47	0
56	MG	2a	1674	1/1	0.90	0.20	55,55,55,55	0
56	MG	1A	4060	1/1	0.90	0.62	19,19,19,19	0
56	MG	2A	3656	1/1	0.90	0.08	68,68,68,68	0
56	MG	1A	3108	1/1	0.90	0.15	25,25,25,25	0
56	MG	1A	3746	1/1	0.90	0.31	49,49,49,49	0
56	MG	10	104	1/1	0.90	0.12	49,49,49,49	0
56	MG	1A	3171	1/1	0.90	0.24	29,29,29,29	0
56	MG	2a	1820	1/1	0.90	0.21	60,60,60,60	0
56	MG	1E	313	1/1	0.90	0.10	25,25,25,25	0
56	MG	2A	3735	1/1	0.90	0.35	45,45,45,45	0
56	MG	1A	3203	1/1	0.90	0.16	27,27,27,27	0
56	MG	2U	202	1/1	0.90	0.82	55,55,55,55	0
56	MG	1a	3043	1/1	0.90	0.12	50,50,50,50	0
56	MG	2A	3366	1/1	0.90	0.14	67,67,67,67	0
56	MG	1A	3671	1/1	0.90	0.09	14,14,14,14	0
56	MG	1a	3101	1/1	0.90	0.15	42,42,42,42	0
56	MG	2A	3532	1/1	0.90	0.18	62,62,62,62	0
56	MG	2A	3073	1/1	0.90	0.16	38,38,38,38	0
56	MG	1A	3797	1/1	0.90	0.18	33,33,33,33	0
56	MG	2A	3167	1/1	0.90	0.14	42,42,42,42	0
56	MG	1A	3296	1/1	0.90	0.12	37,37,37,37	0
56	MG	2F	303	1/1	0.90	0.88	55,55,55,55	0
56	MG	2A	3354	1/1	0.90	0.14	53,53,53,53	0
56	MG	1A	3815	1/1	0.90	0.08	35,35,35,35	0
56	MG	1A	3998	1/1	0.90	0.13	55,55,55,55	0
56	MG	2w	101	1/1	0.90	0.18	65,65,65,65	0
56	MG	1A	3117	1/1	0.90	0.16	48,48,48,48	0
56	MG	2a	1742	1/1	0.90	0.08	70,70,70,70	0
56	MG	1A	3271	1/1	0.90	0.14	53,53,53,53	0
56	MG	2a	1762	1/1	0.90	0.13	52,52,52,52	0
56	MG	1A	3839	1/1	0.90	0.14	34,34,34,34	0
56	MG	2A	3183	1/1	0.90	0.20	38,38,38,38	0
56	MG	1A	3314	1/1	0.90	0.34	42,42,42,42	0
56	MG	2B	3017	1/1	0.90	0.20	61,61,61,61	0
56	MG	1A	3803	1/1	0.90	0.34	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3252	1/1	0.90	0.16	38,38,38,38	0
56	MG	1x	115	1/1	0.90	0.12	50,50,50,50	0
56	MG	2a	1704	1/1	0.90	0.18	52,52,52,52	0
56	MG	2A	3302	1/1	0.90	0.24	43,43,43,43	0
56	MG	1F	308	1/1	0.90	0.11	42,42,42,42	0
56	MG	2A	3484	1/1	0.90	0.11	70,70,70,70	0
56	MG	2A	3688	1/1	0.90	0.14	57,57,57,57	0
56	MG	2A	3692	1/1	0.90	0.07	52,52,52,52	0
56	MG	1a	3048	1/1	0.90	0.47	43,43,43,43	0
56	MG	2A	3400	1/1	0.90	0.25	72,72,72,72	0
56	MG	1w	102	1/1	0.90	0.10	76,76,76,76	0
56	MG	1A	3170	1/1	0.90	0.08	63,63,63,63	0
56	MG	1A	3453	1/1	0.90	0.38	41,41,41,41	0
56	MG	1A	3534	1/1	0.90	0.13	39,39,39,39	0
56	MG	1a	3030	1/1	0.90	0.18	43,43,43,43	0
56	MG	1a	3109	1/1	0.90	0.17	30,30,30,30	0
56	MG	2A	3035	1/1	0.90	0.15	52,52,52,52	0
56	MG	1A	3531	1/1	0.90	0.13	19,19,19,19	0
56	MG	2A	3582	1/1	0.90	0.15	44,44,44,44	0
56	MG	1a	3076	1/1	0.90	0.17	48,48,48,48	0
56	MG	1A	3411	1/1	0.90	0.12	45,45,45,45	0
56	MG	1A	4006	1/1	0.90	0.20	41,41,41,41	0
56	MG	1A	3721	1/1	0.90	0.26	53,53,53,53	0
56	MG	2A	3177	1/1	0.90	0.31	36,36,36,36	0
56	MG	2E	303	1/1	0.90	0.18	50,50,50,50	0
56	MG	2A	3218	1/1	0.90	0.14	39,39,39,39	0
56	MG	2A	3232	1/1	0.90	0.12	54,54,54,54	0
56	MG	1x	110	1/1	0.90	0.12	59,59,59,59	0
56	MG	1B	231	1/1	0.90	0.24	59,59,59,59	0
56	MG	2T	3002	1/1	0.90	0.25	59,59,59,59	0
56	MG	2A	3375	1/1	0.90	0.11	36,36,36,36	0
56	MG	2A	3318	1/1	0.90	0.34	42,42,42,42	0
56	MG	2A	3429	1/1	0.90	0.22	59,59,59,59	0
56	MG	1N	203	1/1	0.90	0.13	51,51,51,51	0
56	MG	2A	3097	1/1	0.90	0.14	42,42,42,42	0
56	MG	1A	3014	1/1	0.90	0.32	27,27,27,27	0
56	MG	2A	3136	1/1	0.90	0.15	36,36,36,36	0
56	MG	2a	1686	1/1	0.90	0.22	67,67,67,67	0
56	MG	1y	102	1/1	0.90	0.09	83,83,83,83	0
56	MG	1A	3495	1/1	0.90	0.10	31,31,31,31	0
56	MG	1A	3332	1/1	0.90	0.11	34,34,34,34	0
56	MG	2A	3613	1/1	0.90	0.11	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1G	3001	1/1	0.90	0.14	29,29,29,29	0
56	MG	2A	3170	1/1	0.90	0.21	44,44,44,44	0
56	MG	1A	3941	1/1	0.90	0.09	34,34,34,34	0
56	MG	1A	3859	1/1	0.90	0.12	61,61,61,61	0
56	MG	1A	3565	1/1	0.90	0.19	26,26,26,26	0
56	MG	1O	201	1/1	0.90	0.15	45,45,45,45	0
56	MG	2A	3639	1/1	0.90	0.22	56,56,56,56	0
56	MG	2A	3098	1/1	0.90	0.36	68,68,68,68	0
56	MG	2A	3381	1/1	0.90	0.18	33,33,33,33	0
56	MG	2A	3752	1/1	0.90	0.29	61,61,61,61	0
56	MG	1A	3658	1/1	0.90	0.10	46,46,46,46	0
56	MG	2E	306	1/1	0.90	0.12	43,43,43,43	0
56	MG	2A	3705	1/1	0.90	0.19	64,64,64,64	0
56	MG	1A	3127	1/1	0.90	0.15	37,37,37,37	0
56	MG	1A	3479	1/1	0.90	0.13	30,30,30,30	0
56	MG	1A	3707	1/1	0.90	0.12	45,45,45,45	0
56	MG	2A	3103	1/1	0.90	0.48	46,46,46,46	0
56	MG	2A	3111	1/1	0.90	0.21	36,36,36,36	0
56	MG	1A	3861	1/1	0.90	0.13	58,58,58,58	0
56	MG	1A	3900	1/1	0.90	0.13	44,44,44,44	0
56	MG	1w	107	1/1	0.90	0.30	64,64,64,64	0
56	MG	1A	3775	1/1	0.90	0.13	41,41,41,41	0
56	MG	1a	3092	1/1	0.90	0.11	55,55,55,55	0
56	MG	1A	3121	1/1	0.90	0.39	33,33,33,33	0
56	MG	2A	3646	1/1	0.90	0.13	59,59,59,59	0
56	MG	2a	1700	1/1	0.90	0.28	62,62,62,62	0
56	MG	1A	3937	1/1	0.90	0.10	40,40,40,40	0
56	MG	1A	3377	1/1	0.90	0.45	40,40,40,40	0
56	MG	1A	3619	1/1	0.90	0.16	36,36,36,36	0
56	MG	1F	307	1/1	0.90	0.12	40,40,40,40	0
56	MG	2a	1693	1/1	0.90	0.31	75,75,75,75	0
56	MG	1A	3036	1/1	0.90	0.21	26,26,26,26	0
56	MG	1l	104	1/1	0.90	0.10	59,59,59,59	0
56	MG	2a	1709	1/1	0.90	0.12	49,49,49,49	0
56	MG	2A	3008	1/1	0.90	0.14	34,34,34,34	0
56	MG	1A	3670	1/1	0.90	0.11	43,43,43,43	0
56	MG	1a	3077	1/1	0.90	0.09	42,42,42,42	0
56	MG	1E	301	1/1	0.90	0.59	26,26,26,26	0
56	MG	1A	3968	1/1	0.90	0.20	55,55,55,55	0
56	MG	2l	204	1/1	0.90	0.12	43,43,43,43	0
56	MG	2A	3358	1/1	0.90	0.14	47,47,47,47	0
56	MG	1A	3653	1/1	0.90	0.17	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3622	1/1	0.90	0.08	56,56,56,56	0
56	MG	27	102	1/1	0.90	0.17	47,47,47,47	0
56	MG	2A	3245	1/1	0.90	0.11	59,59,59,59	0
56	MG	1A	3288	1/1	0.90	0.08	47,47,47,47	0
56	MG	1A	3431	1/1	0.90	0.40	34,34,34,34	0
56	MG	2A	3347	1/1	0.90	0.10	53,53,53,53	0
56	MG	2A	3191	1/1	0.91	0.14	56,56,56,56	0
56	MG	2a	1710	1/1	0.91	0.15	64,64,64,64	0
56	MG	1A	3262	1/1	0.91	0.11	33,33,33,33	0
56	MG	2a	1691	1/1	0.91	0.36	56,56,56,56	0
56	MG	2A	3195	1/1	0.91	0.28	50,50,50,50	0
56	MG	1A	3175	1/1	0.91	0.44	21,21,21,21	0
56	MG	1A	3426	1/1	0.91	0.22	44,44,44,44	0
56	MG	2a	1646	1/1	0.91	0.14	71,71,71,71	0
56	MG	2a	1759	1/1	0.91	0.17	50,50,50,50	0
56	MG	1A	3331	1/1	0.91	0.21	39,39,39,39	0
56	MG	1A	3243	1/1	0.91	0.29	25,25,25,25	0
56	MG	1A	3438	1/1	0.91	0.10	29,29,29,29	0
56	MG	1A	3345	1/1	0.91	0.17	24,24,24,24	0
56	MG	2a	1796	1/1	0.91	0.15	54,54,54,54	0
56	MG	2a	1657	1/1	0.91	0.16	36,36,36,36	0
56	MG	2A	3392	1/1	0.91	0.13	33,33,33,33	0
56	MG	2A	3313	1/1	0.91	0.19	41,41,41,41	0
56	MG	1A	3349	1/1	0.91	0.13	39,39,39,39	0
56	MG	1A	3291	1/1	0.91	0.21	38,38,38,38	0
56	MG	1A	3397	1/1	0.91	0.15	51,51,51,51	0
56	MG	2A	3238	1/1	0.91	0.14	60,60,60,60	0
56	MG	2A	3489	1/1	0.91	0.14	48,48,48,48	0
56	MG	2d	502	1/1	0.91	0.12	58,58,58,58	0
56	MG	1a	3036	1/1	0.91	0.10	49,49,49,49	0
56	MG	1A	3500	1/1	0.91	0.16	20,20,20,20	0
56	MG	1a	3156	1/1	0.91	0.16	50,50,50,50	0
56	MG	2a	1804	1/1	0.91	0.10	48,48,48,48	0
56	MG	1A	3469	1/1	0.91	0.19	43,43,43,43	0
56	MG	2A	3552	1/1	0.91	0.20	35,35,35,35	0
56	MG	1A	3769	1/1	0.91	0.16	15,15,15,15	0
56	MG	2A	3384	1/1	0.91	0.11	27,27,27,27	0
56	MG	2a	1715	1/1	0.91	0.15	50,50,50,50	0
56	MG	2A	3551	1/1	0.91	0.22	48,48,48,48	0
56	MG	2A	3386	1/1	0.91	0.24	43,43,43,43	0
56	MG	1A	3955	1/1	0.91	0.12	32,32,32,32	0
56	MG	2a	1723	1/1	0.91	0.14	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	3100	1/1	0.91	0.11	61,61,61,61	0
56	MG	2a	1696	1/1	0.91	0.15	48,48,48,48	0
56	MG	2a	1678	1/1	0.91	0.11	65,65,65,65	0
56	MG	2A	3217	1/1	0.91	0.28	51,51,51,51	0
56	MG	1A	3188	1/1	0.91	0.10	12,12,12,12	0
56	MG	2A	3226	1/1	0.91	0.33	42,42,42,42	0
56	MG	1A	3450	1/1	0.91	0.11	40,40,40,40	0
56	MG	2a	1765	1/1	0.91	0.14	64,64,64,64	0
56	MG	2a	1711	1/1	0.91	0.24	67,67,67,67	0
56	MG	1a	3057	1/1	0.91	0.15	43,43,43,43	0
56	MG	1A	3510	1/1	0.91	0.18	50,50,50,50	0
56	MG	1A	3249	1/1	0.91	0.35	31,31,31,31	0
56	MG	1A	4025	1/1	0.91	0.22	24,24,24,24	0
56	MG	1A	3558	1/1	0.91	0.13	16,16,16,16	0
56	MG	1A	3924	1/1	0.91	0.11	34,34,34,34	0
56	MG	2A	3742	1/1	0.91	0.34	52,52,52,52	0
56	MG	2a	1684	1/1	0.91	0.18	49,49,49,49	0
56	MG	1A	3909	1/1	0.91	0.20	46,46,46,46	0
56	MG	1a	3194	1/1	0.91	0.08	59,59,59,59	0
56	MG	1A	3608	1/1	0.91	0.20	54,54,54,54	0
56	MG	2a	1833	1/1	0.91	0.06	62,62,62,62	0
56	MG	19	502	1/1	0.91	0.16	39,39,39,39	0
56	MG	1A	3222	1/1	0.91	0.23	51,51,51,51	0
56	MG	2A	3219	1/1	0.91	0.32	54,54,54,54	0
56	MG	1A	3692	1/1	0.91	0.12	29,29,29,29	0
56	MG	1A	3370	1/1	0.91	0.21	37,37,37,37	0
56	MG	2a	1821	1/1	0.91	0.18	66,66,66,66	0
56	MG	2a	1778	1/1	0.91	0.21	68,68,68,68	0
56	MG	2A	3728	1/1	0.91	0.17	56,56,56,56	0
56	MG	2A	3708	1/1	0.91	0.17	63,63,63,63	0
56	MG	2A	3248	1/1	0.91	0.18	44,44,44,44	0
56	MG	1A	3429	1/1	0.91	0.38	29,29,29,29	0
56	MG	2a	1818	1/1	0.91	0.10	48,48,48,48	0
56	MG	2A	3572	1/1	0.91	0.22	66,66,66,66	0
56	MG	1a	3123	1/1	0.91	0.13	60,60,60,60	0
56	MG	1A	3958	1/1	0.91	0.17	32,32,32,32	0
56	MG	1A	3595	1/1	0.91	0.14	40,40,40,40	0
56	MG	1A	3887	1/1	0.91	0.23	16,16,16,16	0
56	MG	2A	3584	1/1	0.91	0.32	50,50,50,50	0
56	MG	17	105	1/1	0.91	0.15	34,34,34,34	0
56	MG	2A	3221	1/1	0.91	0.16	54,54,54,54	0
56	MG	2A	3042	1/1	0.91	0.15	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3237	1/1	0.91	0.15	49,49,49,49	0
56	MG	1T	201	1/1	0.91	0.18	42,42,42,42	0
56	MG	1A	4018	1/1	0.91	0.34	24,24,24,24	0
56	MG	1a	3001	1/1	0.91	0.14	52,52,52,52	0
56	MG	1a	3053	1/1	0.91	0.17	56,56,56,56	0
56	MG	1A	3618	1/1	0.91	0.16	55,55,55,55	0
56	MG	1A	3141	1/1	0.91	0.21	38,38,38,38	0
56	MG	2A	3176	1/1	0.91	0.24	41,41,41,41	0
56	MG	2A	3273	1/1	0.91	0.35	57,57,57,57	0
56	MG	1a	3174	1/1	0.91	0.08	51,51,51,51	0
56	MG	2A	3139	1/1	0.91	0.13	41,41,41,41	0
56	MG	2A	3458	1/1	0.91	0.22	40,40,40,40	0
56	MG	1a	3190	1/1	0.91	0.16	51,51,51,51	0
56	MG	2A	3538	1/1	0.91	0.28	49,49,49,49	0
56	MG	1a	3181	1/1	0.91	0.14	41,41,41,41	0
56	MG	1a	3093	1/1	0.91	0.16	49,49,49,49	0
56	MG	2A	3289	1/1	0.91	0.21	53,53,53,53	0
56	MG	2A	3234	1/1	0.91	0.33	47,47,47,47	0
56	MG	1A	3435	1/1	0.91	0.13	56,56,56,56	0
56	MG	1A	3417	1/1	0.91	0.16	42,42,42,42	0
56	MG	1A	3107	1/1	0.91	0.26	24,24,24,24	0
56	MG	1A	3681	1/1	0.91	0.12	23,23,23,23	0
56	MG	2a	1786	1/1	0.91	0.12	66,66,66,66	0
56	MG	2a	1638	1/1	0.91	0.24	49,49,49,49	0
56	MG	1A	3674	1/1	0.91	0.20	56,56,56,56	0
56	MG	1A	3491	1/1	0.91	0.19	17,17,17,17	0
58	EZG	2A	3746	25/25	0.91	0.32	35,43,49,51	0
56	MG	1D	303	1/1	0.91	0.27	26,26,26,26	0
56	MG	1A	3620	1/1	0.91	0.11	49,49,49,49	0
56	MG	1A	3923	1/1	0.91	0.24	39,39,39,39	0
56	MG	1A	3563	1/1	0.91	0.08	35,35,35,35	0
56	MG	1a	3142	1/1	0.91	0.10	64,64,64,64	0
56	MG	2a	1767	1/1	0.91	0.08	39,39,39,39	0
56	MG	2A	3658	1/1	0.91	0.17	36,36,36,36	0
56	MG	1A	3783	1/1	0.91	0.27	31,31,31,31	0
56	MG	2A	3390	1/1	0.91	0.12	58,58,58,58	0
56	MG	1A	3200	1/1	0.91	0.15	44,44,44,44	0
56	MG	2A	3036	1/1	0.91	0.19	48,48,48,48	0
56	MG	1a	3022	1/1	0.91	0.09	48,48,48,48	0
56	MG	2A	3635	1/1	0.91	0.14	57,57,57,57	0
56	MG	2A	3212	1/1	0.91	0.12	59,59,59,59	0
56	MG	2A	3581	1/1	0.91	0.12	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3537	1/1	0.91	0.18	30,30,30,30	0
56	MG	2A	3483	1/1	0.91	0.15	59,59,59,59	0
56	MG	1A	3224	1/1	0.91	0.16	42,42,42,42	0
56	MG	1A	3409	1/1	0.91	0.15	54,54,54,54	0
56	MG	1a	3068	1/1	0.91	0.14	62,62,62,62	0
56	MG	1A	4021	1/1	0.91	0.14	47,47,47,47	0
56	MG	2A	3619	1/1	0.91	0.09	60,60,60,60	0
56	MG	1A	3371	1/1	0.91	0.23	39,39,39,39	0
56	MG	1A	3264	1/1	0.91	0.09	39,39,39,39	0
56	MG	1A	3379	1/1	0.91	0.39	53,53,53,53	0
56	MG	1A	3055	1/1	0.91	0.12	54,54,54,54	0
56	MG	1A	3413	1/1	0.91	0.28	55,55,55,55	0
56	MG	2A	3018	1/1	0.91	0.36	51,51,51,51	0
56	MG	1A	3812	1/1	0.91	0.16	43,43,43,43	0
56	MG	1A	3148	1/1	0.91	0.27	26,26,26,26	0
56	MG	1A	4045	1/1	0.91	0.60	39,39,39,39	0
56	MG	1A	3192	1/1	0.91	0.17	54,54,54,54	0
56	MG	2A	3757	1/1	0.91	0.26	55,55,55,55	0
56	MG	1a	3176	1/1	0.91	0.10	59,59,59,59	0
56	MG	2a	1611	1/1	0.91	0.10	65,65,65,65	0
56	MG	2q	204	1/1	0.91	0.16	65,65,65,65	0
56	MG	2A	3607	1/1	0.91	0.13	48,48,48,48	0
56	MG	1A	3241	1/1	0.91	0.14	58,58,58,58	0
56	MG	1A	3743	1/1	0.91	0.20	42,42,42,42	0
56	MG	1A	3100	1/1	0.91	0.20	38,38,38,38	0
56	MG	2A	3652	1/1	0.92	0.16	38,38,38,38	0
56	MG	2A	3125	1/1	0.92	0.32	32,32,32,32	0
56	MG	1A	3374	1/1	0.92	0.41	40,40,40,40	0
56	MG	23	101	1/1	0.92	0.61	54,54,54,54	0
56	MG	2A	3410	1/1	0.92	0.31	61,61,61,61	0
56	MG	2Q	3002	1/1	0.92	0.21	41,41,41,41	0
56	MG	2A	3159	1/1	0.92	0.14	50,50,50,50	0
56	MG	2A	3025	1/1	0.92	0.26	54,54,54,54	0
56	MG	1G	3005	1/1	0.92	0.08	52,52,52,52	0
56	MG	2a	1764	1/1	0.92	0.17	51,51,51,51	0
56	MG	1A	3482	1/1	0.92	0.28	38,38,38,38	0
56	MG	1A	3304	1/1	0.92	0.43	41,41,41,41	0
56	MG	1A	3376	1/1	0.92	0.23	31,31,31,31	0
56	MG	1A	3991	1/1	0.92	0.14	66,66,66,66	0
56	MG	1A	3445	1/1	0.92	0.10	47,47,47,47	0
56	MG	2a	1634	1/1	0.92	0.11	59,59,59,59	0
56	MG	2A	3685	1/1	0.92	0.14	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3464	1/1	0.92	0.17	39,39,39,39	0
56	MG	2A	3022	1/1	0.92	0.18	38,38,38,38	0
56	MG	2A	3147	1/1	0.92	0.28	50,50,50,50	0
56	MG	1A	4036	1/1	0.92	0.56	29,29,29,29	0
56	MG	2a	1614	1/1	0.92	0.09	52,52,52,52	0
56	MG	2A	3206	1/1	0.92	0.34	42,42,42,42	0
56	MG	1a	3063	1/1	0.92	0.16	53,53,53,53	0
56	MG	1n	502	1/1	0.92	0.13	51,51,51,51	0
56	MG	1X	102	1/1	0.92	0.21	35,35,35,35	0
56	MG	1a	3189	1/1	0.92	0.12	53,53,53,53	0
56	MG	20	3003	1/1	0.92	0.11	56,56,56,56	0
56	MG	2a	1780	1/1	0.92	0.07	57,57,57,57	0
56	MG	1A	3217	1/1	0.92	0.29	19,19,19,19	0
56	MG	1A	3238	1/1	0.92	0.16	33,33,33,33	0
56	MG	1A	3025	1/1	0.92	0.27	42,42,42,42	0
56	MG	1A	3110	1/1	0.92	0.17	27,27,27,27	0
56	MG	1T	202	1/1	0.92	0.21	47,47,47,47	0
56	MG	2A	3210	1/1	0.92	0.35	58,58,58,58	0
56	MG	1a	3134	1/1	0.92	0.22	47,47,47,47	0
56	MG	1R	204	1/1	0.92	0.33	33,33,33,33	0
56	MG	2A	3657	1/1	0.92	0.20	41,41,41,41	0
56	MG	1x	111	1/1	0.92	0.15	64,64,64,64	0
56	MG	1q	201	1/1	0.92	0.08	50,50,50,50	0
56	MG	1a	3193	1/1	0.92	0.16	47,47,47,47	0
56	MG	2a	1624	1/1	0.92	0.11	78,78,78,78	0
56	MG	2A	3490	1/1	0.92	0.07	72,72,72,72	0
56	MG	2a	1793	1/1	0.92	0.14	53,53,53,53	0
56	MG	1A	3284	1/1	0.92	0.20	42,42,42,42	0
56	MG	1A	3985	1/1	0.92	0.17	60,60,60,60	0
56	MG	2A	3269	1/1	0.92	0.14	36,36,36,36	0
56	MG	1A	3280	1/1	0.92	0.50	26,26,26,26	0
56	MG	1A	3739	1/1	0.92	0.34	29,29,29,29	0
56	MG	2A	3609	1/1	0.92	0.22	36,36,36,36	0
56	MG	2a	1798	1/1	0.92	0.14	60,60,60,60	0
56	MG	1A	3050	1/1	0.92	0.27	45,45,45,45	0
56	MG	1A	3889	1/1	0.92	0.14	39,39,39,39	0
56	MG	2A	3478	1/1	0.92	0.60	38,38,38,38	0
56	MG	2A	3562	1/1	0.92	0.10	40,40,40,40	0
56	MG	2A	3279	1/1	0.92	0.10	64,64,64,64	0
56	MG	1A	3876	1/1	0.92	0.21	34,34,34,34	0
56	MG	2A	3644	1/1	0.92	0.14	57,57,57,57	0
56	MG	1a	3150	1/1	0.92	0.11	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3292	1/1	0.92	0.17	43,43,43,43	0
56	MG	1A	3700	1/1	0.92	0.09	27,27,27,27	0
56	MG	2A	3691	1/1	0.92	0.11	68,68,68,68	0
56	MG	1A	3071	1/1	0.92	0.14	31,31,31,31	0
56	MG	2A	3590	1/1	0.92	0.15	50,50,50,50	0
56	MG	1a	3111	1/1	0.92	0.17	45,45,45,45	0
56	MG	1A	3744	1/1	0.92	0.12	41,41,41,41	0
56	MG	2A	3300	1/1	0.92	0.20	58,58,58,58	0
56	MG	1A	3878	1/1	0.92	0.11	16,16,16,16	0
56	MG	1A	3302	1/1	0.92	0.78	32,32,32,32	0
56	MG	1A	3648	1/1	0.92	0.10	20,20,20,20	0
56	MG	2A	3402	1/1	0.92	0.15	49,49,49,49	0
56	MG	1A	3831	1/1	0.92	0.13	68,68,68,68	0
56	MG	2A	3017	1/1	0.92	0.11	59,59,59,59	0
56	MG	1a	3203	1/1	0.92	0.20	69,69,69,69	0
56	MG	2A	3733	1/1	0.92	0.17	30,30,30,30	0
56	MG	1A	3179	1/1	0.92	0.37	23,23,23,23	0
56	MG	2A	3187	1/1	0.92	0.26	54,54,54,54	0
56	MG	1A	3219	1/1	0.92	0.29	19,19,19,19	0
56	MG	2A	3588	1/1	0.92	0.09	52,52,52,52	0
56	MG	1A	3511	1/1	0.92	0.22	20,20,20,20	0
56	MG	2A	3204	1/1	0.92	0.15	43,43,43,43	0
56	MG	1A	3380	1/1	0.92	0.29	33,33,33,33	0
56	MG	1A	3420	1/1	0.92	0.13	49,49,49,49	0
56	MG	2A	3155	1/1	0.92	0.09	34,34,34,34	0
56	MG	2F	301	1/1	0.92	0.16	35,35,35,35	0
56	MG	1A	3087	1/1	0.92	0.18	47,47,47,47	0
56	MG	2A	3449	1/1	0.92	0.11	63,63,63,63	0
56	MG	2A	3684	1/1	0.92	0.08	68,68,68,68	0
56	MG	1A	3218	1/1	0.92	0.07	23,23,23,23	0
56	MG	2A	3283	1/1	0.92	0.14	42,42,42,42	0
56	MG	2A	3697	1/1	0.92	0.28	50,50,50,50	0
56	MG	1A	3265	1/1	0.92	0.18	26,26,26,26	0
56	MG	2a	1743	1/1	0.92	0.10	70,70,70,70	0
56	MG	12	3001	1/1	0.92	0.15	44,44,44,44	0
56	MG	1A	3298	1/1	0.92	0.16	40,40,40,40	0
56	MG	1a	3164	1/1	0.92	0.13	58,58,58,58	0
56	MG	1a	3112	1/1	0.92	0.09	48,48,48,48	0
56	MG	2A	3466	1/1	0.92	0.16	41,41,41,41	0
56	MG	2A	3116	1/1	0.92	0.11	55,55,55,55	0
56	MG	1A	3476	1/1	0.92	0.13	27,27,27,27	0
56	MG	2A	3276	1/1	0.92	0.21	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3666	1/1	0.92	0.05	50,50,50,50	0
56	MG	2A	3299	1/1	0.92	0.33	43,43,43,43	0
56	MG	2a	1653	1/1	0.92	0.07	67,67,67,67	0
56	MG	1A	4059	1/1	0.92	0.26	22,22,22,22	0
56	MG	2A	3502	1/1	0.92	0.16	42,42,42,42	0
56	MG	1A	3762	1/1	0.92	0.14	12,12,12,12	0
56	MG	1l	203	1/1	0.92	0.17	50,50,50,50	0
56	MG	1A	3708	1/1	0.92	0.10	42,42,42,42	0
56	MG	2A	3620	1/1	0.92	0.09	34,34,34,34	0
56	MG	2a	1819	1/1	0.92	0.08	52,52,52,52	0
56	MG	1A	3505	1/1	0.92	0.22	31,31,31,31	0
56	MG	2A	3446	1/1	0.92	0.14	32,32,32,32	0
56	MG	1A	3970	1/1	0.92	0.05	53,53,53,53	0
56	MG	1A	3460	1/1	0.92	0.10	41,41,41,41	0
56	MG	1A	3072	1/1	0.92	0.31	27,27,27,27	0
56	MG	1A	3921	1/1	0.92	0.21	43,43,43,43	0
56	MG	1A	3024	1/1	0.92	0.12	32,32,32,32	0
56	MG	2A	3477	1/1	0.92	0.13	64,64,64,64	0
56	MG	2A	3640	1/1	0.92	0.24	47,47,47,47	0
56	MG	1A	3786	1/1	0.92	0.11	34,34,34,34	0
56	MG	1A	3466	1/1	0.92	0.17	39,39,39,39	0
56	MG	1A	3261	1/1	0.92	0.10	35,35,35,35	0
56	MG	1A	3945	1/1	0.92	0.34	30,30,30,30	0
56	MG	1A	3698	1/1	0.92	0.12	41,41,41,41	0
56	MG	2A	3250	1/1	0.92	0.15	51,51,51,51	0
56	MG	1A	3922	1/1	0.92	0.09	49,49,49,49	0
56	MG	1D	311	1/1	0.92	0.14	36,36,36,36	0
56	MG	2A	3481	1/1	0.92	0.25	58,58,58,58	0
56	MG	2A	3346	1/1	0.92	0.11	48,48,48,48	0
56	MG	1a	3013	1/1	0.92	0.15	45,45,45,45	0
56	MG	2A	3382	1/1	0.92	0.24	46,46,46,46	0
56	MG	2a	1761	1/1	0.92	0.22	34,34,34,34	0
56	MG	2A	3681	1/1	0.92	0.23	49,49,49,49	0
56	MG	1B	204	1/1	0.92	0.12	29,29,29,29	0
56	MG	2D	306	1/1	0.92	0.66	43,43,43,43	0
56	MG	1A	3215	1/1	0.92	0.18	54,54,54,54	0
56	MG	2W	203	1/1	0.92	0.12	41,41,41,41	0
56	MG	2A	3211	1/1	0.92	0.11	68,68,68,68	0
56	MG	1A	3145	1/1	0.92	0.62	34,34,34,34	0
56	MG	1A	3194	1/1	0.92	0.21	35,35,35,35	0
56	MG	2A	3316	1/1	0.92	0.16	53,53,53,53	0
56	MG	1a	3055	1/1	0.92	0.14	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1Q	205	1/1	0.92	0.11	28,28,28,28	0
56	MG	2a	1664	1/1	0.92	0.17	56,56,56,56	0
56	MG	1A	3641	1/1	0.92	0.18	13,13,13,13	0
56	MG	1A	3849	1/1	0.92	0.27	35,35,35,35	0
56	MG	1A	3190	1/1	0.92	0.08	43,43,43,43	0
56	MG	1a	3011	1/1	0.92	0.14	41,41,41,41	0
56	MG	2A	3075	1/1	0.92	0.16	51,51,51,51	0
56	MG	1A	3837	1/1	0.92	0.19	54,54,54,54	0
56	MG	2A	3743	1/1	0.92	0.19	51,51,51,51	0
56	MG	2A	3591	1/1	0.92	0.12	34,34,34,34	0
56	MG	1A	3152	1/1	0.92	0.17	43,43,43,43	0
56	MG	1A	3938	1/1	0.92	0.26	40,40,40,40	0
56	MG	1A	3183	1/1	0.92	0.09	39,39,39,39	0
56	MG	1A	3512	1/1	0.92	0.08	40,40,40,40	0
56	MG	1A	3472	1/1	0.92	0.14	41,41,41,41	0
56	MG	2a	1783	1/1	0.92	0.11	62,62,62,62	0
56	MG	1A	3838	1/1	0.92	0.11	53,53,53,53	0
56	MG	2a	1747	1/1	0.92	0.12	56,56,56,56	0
56	MG	2a	1775	1/1	0.92	0.15	74,74,74,74	0
56	MG	1Y	502	1/1	0.92	0.10	67,67,67,67	0
56	MG	2a	1729	1/1	0.92	0.10	61,61,61,61	0
56	MG	1A	3825	1/1	0.92	0.47	43,43,43,43	0
56	MG	1A	3195	1/1	0.92	0.49	27,27,27,27	0
56	MG	2A	3134	1/1	0.92	0.08	51,51,51,51	0
56	MG	1A	3749	1/1	0.92	0.23	31,31,31,31	0
56	MG	1A	3231	1/1	0.92	0.27	45,45,45,45	0
56	MG	2A	3698	1/1	0.92	0.16	58,58,58,58	0
56	MG	2A	3408	1/1	0.92	0.09	53,53,53,53	0
56	MG	2R	3001	1/1	0.92	0.50	58,58,58,58	0
56	MG	2A	3006	1/1	0.93	0.08	44,44,44,44	0
56	MG	2a	1739	1/1	0.93	0.14	57,57,57,57	0
56	MG	2A	3057	1/1	0.93	0.13	47,47,47,47	0
56	MG	2A	3467	1/1	0.93	0.22	28,28,28,28	0
56	MG	2A	3703	1/1	0.93	0.14	50,50,50,50	0
56	MG	2A	3595	1/1	0.93	0.09	59,59,59,59	0
56	MG	1A	3386	1/1	0.93	0.10	33,33,33,33	0
56	MG	1A	3424	1/1	0.93	0.56	32,32,32,32	0
56	MG	1A	3444	1/1	0.93	0.14	18,18,18,18	0
56	MG	2A	3305	1/1	0.93	0.15	51,51,51,51	0
56	MG	2A	3503	1/1	0.93	0.16	54,54,54,54	0
56	MG	1a	3099	1/1	0.93	0.10	72,72,72,72	0
56	MG	2a	1807	1/1	0.93	0.11	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3013	1/1	0.93	0.13	27,27,27,27	0
56	MG	10	103	1/1	0.93	0.15	54,54,54,54	0
56	MG	2A	3628	1/1	0.93	0.20	40,40,40,40	0
56	MG	2A	3506	1/1	0.93	0.13	48,48,48,48	0
56	MG	1A	3993	1/1	0.93	0.30	44,44,44,44	0
56	MG	1A	3758	1/1	0.93	0.13	32,32,32,32	0
56	MG	1A	3559	1/1	0.93	0.20	15,15,15,15	0
56	MG	2A	3416	1/1	0.93	0.13	40,40,40,40	0
56	MG	1a	3116	1/1	0.93	0.09	35,35,35,35	0
56	MG	1a	3088	1/1	0.93	0.06	57,57,57,57	0
56	MG	2A	3625	1/1	0.93	0.08	52,52,52,52	0
56	MG	1A	3109	1/1	0.93	0.41	50,50,50,50	0
56	MG	2U	204	1/1	0.93	0.83	60,60,60,60	0
56	MG	2A	3565	1/1	0.93	0.12	45,45,45,45	0
56	MG	1B	207	1/1	0.93	0.43	40,40,40,40	0
56	MG	2A	3099	1/1	0.93	0.10	38,38,38,38	0
56	MG	1s	101	1/1	0.93	0.20	62,62,62,62	0
56	MG	1A	3867	1/1	0.93	0.14	19,19,19,19	0
56	MG	1x	102	1/1	0.93	0.26	49,49,49,49	0
56	MG	1A	3628	1/1	0.93	0.13	16,16,16,16	0
56	MG	1A	3182	1/1	0.93	0.20	33,33,33,33	0
56	MG	1a	3166	1/1	0.93	0.08	49,49,49,49	0
56	MG	2A	3486	1/1	0.93	0.12	53,53,53,53	0
56	MG	1A	3365	1/1	0.93	0.21	39,39,39,39	0
56	MG	1A	3447	1/1	0.93	0.32	47,47,47,47	0
56	MG	1A	3835	1/1	0.93	0.17	42,42,42,42	0
56	MG	2A	3262	1/1	0.93	0.14	44,44,44,44	0
56	MG	2A	3298	1/1	0.93	0.12	50,50,50,50	0
56	MG	2a	1658	1/1	0.93	0.12	59,59,59,59	0
56	MG	1A	3144	1/1	0.93	0.13	37,37,37,37	0
56	MG	2a	1737	1/1	0.93	0.04	57,57,57,57	0
56	MG	1A	3030	1/1	0.93	0.59	20,20,20,20	0
56	MG	2R	3002	1/1	0.93	0.25	56,56,56,56	0
56	MG	2A	3456	1/1	0.93	0.17	26,26,26,26	0
56	MG	1a	3128	1/1	0.93	0.09	50,50,50,50	0
56	MG	2a	1695	1/1	0.93	0.16	56,56,56,56	0
56	MG	1A	3441	1/1	0.93	0.07	49,49,49,49	0
56	MG	2A	3216	1/1	0.93	0.15	51,51,51,51	0
56	MG	1S	3002	1/1	0.93	0.20	36,36,36,36	0
56	MG	2A	3050	1/1	0.93	0.14	38,38,38,38	0
56	MG	1a	3032	1/1	0.93	0.19	54,54,54,54	0
56	MG	2A	3331	1/1	0.93	0.16	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3060	1/1	0.93	0.08	26,26,26,26	0
56	MG	2a	1702	1/1	0.93	0.14	56,56,56,56	0
56	MG	1A	3811	1/1	0.93	0.08	32,32,32,32	0
56	MG	1A	3957	1/1	0.93	0.12	55,55,55,55	0
56	MG	1A	3902	1/1	0.93	0.10	55,55,55,55	0
56	MG	2A	3593	1/1	0.93	0.16	47,47,47,47	0
56	MG	2A	3476	1/1	0.93	0.12	44,44,44,44	0
56	MG	1A	3836	1/1	0.93	0.09	56,56,56,56	0
56	MG	1A	3860	1/1	0.93	0.27	54,54,54,54	0
56	MG	1I	3001	1/1	0.93	0.31	64,64,64,64	0
56	MG	2a	1688	1/1	0.93	0.14	53,53,53,53	0
56	MG	1A	3737	1/1	0.93	0.14	29,29,29,29	0
56	MG	2I	201	1/1	0.93	0.23	51,51,51,51	0
56	MG	1A	3239	1/1	0.93	0.28	38,38,38,38	0
56	MG	1A	3560	1/1	0.93	0.23	26,26,26,26	0
56	MG	1A	3020	1/1	0.93	0.15	18,18,18,18	0
56	MG	1A	3933	1/1	0.93	0.14	54,54,54,54	0
56	MG	2A	3756	1/1	0.93	0.14	33,33,33,33	0
56	MG	1A	3387	1/1	0.93	0.20	37,37,37,37	0
56	MG	1a	3040	1/1	0.93	0.12	41,41,41,41	0
56	MG	2a	1630	1/1	0.93	0.23	57,57,57,57	0
56	MG	2a	1669	1/1	0.93	0.23	56,56,56,56	0
56	MG	2A	3523	1/1	0.93	0.14	37,37,37,37	0
56	MG	1A	3118	1/1	0.93	0.11	29,29,29,29	0
56	MG	1a	3010	1/1	0.93	0.09	45,45,45,45	0
56	MG	1N	201	1/1	0.93	0.54	45,45,45,45	0
56	MG	2A	3603	1/1	0.93	0.11	37,37,37,37	0
56	MG	2A	3361	1/1	0.93	0.11	46,46,46,46	0
56	MG	2a	1643	1/1	0.93	0.21	61,61,61,61	0
56	MG	1A	3705	1/1	0.93	0.17	39,39,39,39	0
56	MG	1A	4014	1/1	0.93	0.34	33,33,33,33	0
56	MG	1a	3105	1/1	0.93	0.11	59,59,59,59	0
56	MG	1A	3798	1/1	0.93	0.26	45,45,45,45	0
56	MG	1a	3103	1/1	0.93	0.07	46,46,46,46	0
56	MG	1A	3340	1/1	0.93	0.13	47,47,47,47	0
56	MG	1B	228	1/1	0.93	0.15	24,24,24,24	0
56	MG	1A	3101	1/1	0.93	0.44	28,28,28,28	0
56	MG	1A	3603	1/1	0.93	0.16	43,43,43,43	0
56	MG	2a	1757	1/1	0.93	0.12	48,48,48,48	0
56	MG	2A	3334	1/1	0.93	0.28	58,58,58,58	0
56	MG	1A	3391	1/1	0.93	0.16	46,46,46,46	0
56	MG	1A	3048	1/1	0.93	0.45	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	3214	1/1	0.93	0.40	58,58,58,58	0
56	MG	1a	3159	1/1	0.93	0.14	41,41,41,41	0
56	MG	1n	503	1/1	0.93	0.08	38,38,38,38	0
56	MG	1A	3336	1/1	0.93	0.25	35,35,35,35	0
56	MG	2T	3003	1/1	0.93	0.11	41,41,41,41	0
56	MG	1A	3463	1/1	0.93	0.38	38,38,38,38	0
56	MG	2A	3145	1/1	0.93	0.15	48,48,48,48	0
56	MG	15	106	1/1	0.93	0.24	19,19,19,19	0
56	MG	2A	3308	1/1	0.93	0.15	54,54,54,54	0
56	MG	2A	3663	1/1	0.93	0.17	47,47,47,47	0
56	MG	1A	3329	1/1	0.93	0.10	41,41,41,41	0
56	MG	2A	3222	1/1	0.93	0.16	44,44,44,44	0
56	MG	1A	3712	1/1	0.93	0.25	34,34,34,34	0
56	MG	1A	3819	1/1	0.93	0.11	29,29,29,29	0
56	MG	1a	3104	1/1	0.93	0.17	45,45,45,45	0
56	MG	2a	1673	1/1	0.93	0.10	57,57,57,57	0
56	MG	1A	3715	1/1	0.93	0.10	23,23,23,23	0
56	MG	2A	3471	1/1	0.93	0.20	37,37,37,37	0
56	MG	1A	3383	1/1	0.93	0.18	42,42,42,42	0
56	MG	1A	3172	1/1	0.93	0.40	44,44,44,44	0
56	MG	1A	3105	1/1	0.93	0.24	30,30,30,30	0
56	MG	1A	3287	1/1	0.93	0.13	30,30,30,30	0
56	MG	2A	3011	1/1	0.93	0.15	54,54,54,54	0
56	MG	2A	3535	1/1	0.93	0.14	27,27,27,27	0
56	MG	1a	3091	1/1	0.93	0.22	46,46,46,46	0
56	MG	2A	3460	1/1	0.93	0.15	39,39,39,39	0
56	MG	2A	3517	1/1	0.93	0.09	51,51,51,51	0
56	MG	2a	1760	1/1	0.93	0.24	60,60,60,60	0
56	MG	1a	3052	1/1	0.93	0.10	58,58,58,58	0
56	MG	2l	203	1/1	0.93	0.17	62,62,62,62	0
56	MG	1A	3631	1/1	0.93	0.16	32,32,32,32	0
56	MG	2A	3179	1/1	0.93	0.17	45,45,45,45	0
56	MG	2A	3224	1/1	0.93	0.16	54,54,54,54	0
56	MG	1V	201	1/1	0.93	0.10	40,40,40,40	0
56	MG	2A	3445	1/1	0.93	0.10	47,47,47,47	0
56	MG	2A	3037	1/1	0.93	0.11	61,61,61,61	0
56	MG	1a	3072	1/1	0.93	0.09	54,54,54,54	0
56	MG	1a	3029	1/1	0.93	0.10	49,49,49,49	0
56	MG	2D	302	1/1	0.93	0.16	39,39,39,39	0
56	MG	2a	1811	1/1	0.93	0.15	71,71,71,71	0
56	MG	1A	3772	1/1	0.93	0.20	22,22,22,22	0
56	MG	2A	3108	1/1	0.93	0.30	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	3157	1/1	0.93	0.13	58,58,58,58	0
56	MG	1A	3953	1/1	0.93	0.15	40,40,40,40	0
56	MG	1A	3434	1/1	0.93	0.17	47,47,47,47	0
56	MG	2a	1685	1/1	0.93	0.10	53,53,53,53	0
56	MG	1a	3139	1/1	0.93	0.20	56,56,56,56	0
56	MG	2A	3135	1/1	0.93	0.25	49,49,49,49	0
56	MG	1a	3115	1/1	0.93	0.13	48,48,48,48	0
56	MG	1A	3493	1/1	0.93	0.32	23,23,23,23	0
56	MG	1A	3596	1/1	0.93	0.19	44,44,44,44	0
56	MG	2a	1730	1/1	0.93	0.11	65,65,65,65	0
56	MG	1A	3817	1/1	0.93	0.13	20,20,20,20	0
56	MG	1Z	3001	1/1	0.93	0.26	42,42,42,42	0
56	MG	2A	3309	1/1	0.93	0.15	52,52,52,52	0
56	MG	1A	3251	1/1	0.93	0.42	25,25,25,25	0
56	MG	1a	3117	1/1	0.93	0.09	27,27,27,27	0
56	MG	1A	3199	1/1	0.93	0.52	32,32,32,32	0
56	MG	1A	3098	1/1	0.93	0.51	36,36,36,36	0
56	MG	1B	218	1/1	0.93	0.19	40,40,40,40	0
56	MG	1A	3093	1/1	0.93	0.09	31,31,31,31	0
56	MG	2A	3254	1/1	0.93	0.17	34,34,34,34	0
56	MG	2A	3377	1/1	0.93	0.20	37,37,37,37	0
56	MG	1A	3330	1/1	0.93	0.17	28,28,28,28	0
56	MG	1E	307	1/1	0.93	0.55	50,50,50,50	0
56	MG	2a	1707	1/1	0.93	0.22	68,68,68,68	0
56	MG	1A	3897	1/1	0.93	0.14	44,44,44,44	0
56	MG	2a	1682	1/1	0.93	0.08	48,48,48,48	0
56	MG	1O	206	1/1	0.93	0.36	60,60,60,60	0
56	MG	2A	3184	1/1	0.93	0.31	52,52,52,52	0
56	MG	2A	3118	1/1	0.93	0.19	42,42,42,42	0
56	MG	2A	3079	1/1	0.93	0.09	57,57,57,57	0
56	MG	2A	3161	1/1	0.93	0.36	46,46,46,46	0
56	MG	2A	3614	1/1	0.93	0.12	51,51,51,51	0
56	MG	2A	3153	1/1	0.93	0.16	49,49,49,49	0
56	MG	2A	3253	1/1	0.93	0.54	68,68,68,68	0
56	MG	2A	3722	1/1	0.93	0.14	47,47,47,47	0
56	MG	1A	3347	1/1	0.93	0.14	42,42,42,42	0
56	MG	2A	3683	1/1	0.93	0.28	42,42,42,42	0
56	MG	2A	3168	1/1	0.93	0.11	39,39,39,39	0
56	MG	1A	3202	1/1	0.93	0.29	27,27,27,27	0
56	MG	1A	3405	1/1	0.93	0.60	46,46,46,46	0
56	MG	1A	3244	1/1	0.93	0.24	34,34,34,34	0
56	MG	2A	3233	1/1	0.93	0.26	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3178	1/1	0.93	0.17	44,44,44,44	0
56	MG	2A	3127	1/1	0.93	0.22	56,56,56,56	0
56	MG	2A	3199	1/1	0.93	0.12	53,53,53,53	0
56	MG	2a	1795	1/1	0.93	0.37	64,64,64,64	0
56	MG	1A	3252	1/1	0.93	0.29	32,32,32,32	0
56	MG	1A	3555	1/1	0.93	0.09	29,29,29,29	0
56	MG	1a	3146	1/1	0.93	0.16	64,64,64,64	0
56	MG	1A	3851	1/1	0.93	0.18	44,44,44,44	0
56	MG	2A	3406	1/1	0.93	0.13	40,40,40,40	0
56	MG	1A	3344	1/1	0.93	0.37	31,31,31,31	0
56	MG	1A	3019	1/1	0.93	0.16	32,32,32,32	0
56	MG	1A	3869	1/1	0.93	0.19	19,19,19,19	0
56	MG	2A	3255	1/1	0.93	0.22	54,54,54,54	0
56	MG	1A	3872	1/1	0.93	0.33	27,27,27,27	0
56	MG	1A	3570	1/1	0.93	0.19	57,57,57,57	0
56	MG	2A	3126	1/1	0.93	0.17	50,50,50,50	0
56	MG	2A	3106	1/1	0.93	0.08	50,50,50,50	0
56	MG	1A	3301	1/1	0.93	0.12	39,39,39,39	0
56	MG	1A	3058	1/1	0.93	0.19	33,33,33,33	0
56	MG	17	102	1/1	0.94	0.30	31,31,31,31	0
56	MG	2j	8002	1/1	0.94	0.05	62,62,62,62	0
56	MG	2A	3197	1/1	0.94	0.14	39,39,39,39	0
56	MG	1A	3885	1/1	0.94	0.12	16,16,16,16	0
56	MG	2U	201	1/1	0.94	0.08	49,49,49,49	0
56	MG	1A	3335	1/1	0.94	0.43	33,33,33,33	0
56	MG	1A	3606	1/1	0.94	0.18	61,61,61,61	0
56	MG	1A	3638	1/1	0.94	0.15	56,56,56,56	0
56	MG	1A	3307	1/1	0.94	0.10	49,49,49,49	0
56	MG	2A	3121	1/1	0.94	0.15	31,31,31,31	0
56	MG	1A	3029	1/1	0.94	0.36	17,17,17,17	0
56	MG	1a	3209	1/1	0.94	0.20	60,60,60,60	0
56	MG	1A	4013	1/1	0.94	0.13	21,21,21,21	0
56	MG	2V	3002	1/1	0.94	0.13	56,56,56,56	0
56	MG	2A	3304	1/1	0.94	0.20	49,49,49,49	0
56	MG	2A	3678	1/1	0.94	0.21	71,71,71,71	0
56	MG	1A	3039	1/1	0.94	0.18	26,26,26,26	0
56	MG	2a	1690	1/1	0.94	0.07	57,57,57,57	0
56	MG	2A	3123	1/1	0.94	0.07	58,58,58,58	0
56	MG	2A	3242	1/1	0.94	0.13	47,47,47,47	0
56	MG	1A	3449	1/1	0.94	0.19	52,52,52,52	0
56	MG	1A	3326	1/1	0.94	0.17	25,25,25,25	0
56	MG	2A	3314	1/1	0.94	0.37	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3273	1/1	0.94	0.09	38,38,38,38	0
56	MG	1A	3687	1/1	0.94	0.11	33,33,33,33	0
56	MG	1A	3312	1/1	0.94	0.24	42,42,42,42	0
56	MG	2A	3130	1/1	0.94	0.20	51,51,51,51	0
56	MG	2A	3563	1/1	0.94	0.19	55,55,55,55	0
56	MG	2a	1622	1/1	0.94	0.40	39,39,39,39	0
56	MG	2A	3154	1/1	0.94	0.32	51,51,51,51	0
56	MG	1A	3488	1/1	0.94	0.12	23,23,23,23	0
56	MG	2A	3626	1/1	0.94	0.16	46,46,46,46	0
56	MG	2A	3528	1/1	0.94	0.08	58,58,58,58	0
56	MG	2A	3485	1/1	0.94	0.22	56,56,56,56	0
56	MG	2A	3357	1/1	0.94	0.15	21,21,21,21	0
56	MG	2A	3409	1/1	0.94	0.11	54,54,54,54	0
56	MG	2A	3531	1/1	0.94	0.11	60,60,60,60	0
56	MG	1A	3382	1/1	0.94	0.12	41,41,41,41	0
56	MG	2A	3064	1/1	0.94	0.44	44,44,44,44	0
56	MG	1A	3934	1/1	0.94	0.16	22,22,22,22	0
56	MG	1A	3352	1/1	0.94	0.18	36,36,36,36	0
56	MG	1A	3626	1/1	0.94	0.14	23,23,23,23	0
56	MG	2A	3554	1/1	0.94	0.14	24,24,24,24	0
56	MG	2A	3654	1/1	0.94	0.26	33,33,33,33	0
56	MG	1B	214	1/1	0.94	0.11	42,42,42,42	0
56	MG	1A	4007	1/1	0.94	0.66	39,39,39,39	0
56	MG	1a	3124	1/1	0.94	0.13	54,54,54,54	0
56	MG	2A	3432	1/1	0.94	0.30	56,56,56,56	0
56	MG	1A	3369	1/1	0.94	0.11	38,38,38,38	0
56	MG	2a	1608	1/1	0.94	0.14	47,47,47,47	0
56	MG	1a	3090	1/1	0.94	0.07	41,41,41,41	0
56	MG	1A	3407	1/1	0.94	0.08	45,45,45,45	0
56	MG	1A	3487	1/1	0.94	0.13	34,34,34,34	0
56	MG	2a	1727	1/1	0.94	0.12	87,87,87,87	0
56	MG	1a	3144	1/1	0.94	0.19	66,66,66,66	0
56	MG	2a	1670	1/1	0.94	0.11	55,55,55,55	0
56	MG	1A	3751	1/1	0.94	0.32	23,23,23,23	0
56	MG	1A	3536	1/1	0.94	0.08	25,25,25,25	0
56	MG	1a	3147	1/1	0.94	0.05	58,58,58,58	0
56	MG	1A	4011	1/1	0.94	0.21	37,37,37,37	0
56	MG	1A	3269	1/1	0.94	0.21	35,35,35,35	0
56	MG	1F	303	1/1	0.94	0.19	35,35,35,35	0
56	MG	2a	1628	1/1	0.94	0.30	49,49,49,49	0
56	MG	2A	3146	1/1	0.94	0.15	50,50,50,50	0
56	MG	2A	3055	1/1	0.94	0.16	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3384	1/1	0.94	0.08	38,38,38,38	0
56	MG	2A	3442	1/1	0.94	0.17	23,23,23,23	0
56	MG	2A	3435	1/1	0.94	0.11	47,47,47,47	0
56	MG	1A	3174	1/1	0.94	0.39	32,32,32,32	0
56	MG	2A	3573	1/1	0.94	0.30	37,37,37,37	0
56	MG	1A	3228	1/1	0.94	0.29	40,40,40,40	0
56	MG	2A	3706	1/1	0.94	0.14	42,42,42,42	0
56	MG	2a	1785	1/1	0.94	0.15	63,63,63,63	0
56	MG	2a	1756	1/1	0.94	0.13	43,43,43,43	0
56	MG	2a	1654	1/1	0.94	0.27	58,58,58,58	0
56	MG	2A	3675	1/1	0.94	0.09	62,62,62,62	0
56	MG	1A	3443	1/1	0.94	0.15	32,32,32,32	0
56	MG	1A	3805	1/1	0.94	0.20	60,60,60,60	0
56	MG	2A	3574	1/1	0.94	0.07	46,46,46,46	0
56	MG	2a	1672	1/1	0.94	0.17	50,50,50,50	0
56	MG	2a	1652	1/1	0.94	0.09	55,55,55,55	0
56	MG	1A	3827	1/1	0.94	0.13	47,47,47,47	0
56	MG	1A	3396	1/1	0.94	0.28	44,44,44,44	0
56	MG	2A	3061	1/1	0.94	0.17	30,30,30,30	0
56	MG	1A	3787	1/1	0.94	0.14	36,36,36,36	0
56	MG	1A	3303	1/1	0.94	0.16	44,44,44,44	0
56	MG	1a	3155	1/1	0.94	0.18	53,53,53,53	0
56	MG	2A	3287	1/1	0.94	0.25	47,47,47,47	0
56	MG	2a	1623	1/1	0.94	0.14	46,46,46,46	0
56	MG	1A	3378	1/1	0.94	0.40	27,27,27,27	0
56	MG	1A	3092	1/1	0.94	0.17	44,44,44,44	0
56	MG	1A	3076	1/1	0.94	0.25	26,26,26,26	0
56	MG	1A	3790	1/1	0.94	0.36	27,27,27,27	0
56	MG	2B	3007	1/1	0.94	0.10	56,56,56,56	0
56	MG	1A	3709	1/1	0.94	0.17	30,30,30,30	0
56	MG	18	102	1/1	0.94	0.12	29,29,29,29	0
56	MG	2A	3373	1/1	0.94	0.17	25,25,25,25	0
56	MG	2A	3707	1/1	0.94	0.15	47,47,47,47	0
56	MG	1A	3756	1/1	0.94	0.65	27,27,27,27	0
56	MG	1A	3089	1/1	0.94	0.15	21,21,21,21	0
56	MG	2R	3004	1/1	0.94	0.19	49,49,49,49	0
56	MG	1A	4049	1/1	0.94	0.77	30,30,30,30	0
56	MG	1a	3178	1/1	0.94	0.06	54,54,54,54	0
56	MG	1A	4042	1/1	0.94	0.13	40,40,40,40	0
56	MG	1A	3457	1/1	0.94	0.14	32,32,32,32	0
56	MG	1A	4054	1/1	0.94	0.47	37,37,37,37	0
56	MG	1a	3012	1/1	0.94	0.10	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3706	1/1	0.94	0.11	27,27,27,27	0
56	MG	1A	3134	1/1	0.94	0.46	30,30,30,30	0
56	MG	1A	3311	1/1	0.94	0.19	37,37,37,37	0
56	MG	2A	3182	1/1	0.94	0.64	43,43,43,43	0
56	MG	1x	108	1/1	0.94	0.13	61,61,61,61	0
56	MG	1A	4029	1/1	0.94	0.33	36,36,36,36	0
56	MG	1a	3004	1/1	0.94	0.14	50,50,50,50	0
56	MG	1A	3281	1/1	0.94	0.34	29,29,29,29	0
56	MG	1m	201	1/1	0.94	0.10	57,57,57,57	0
56	MG	2A	3294	1/1	0.94	0.28	45,45,45,45	0
56	MG	1A	3919	1/1	0.94	0.15	42,42,42,42	0
56	MG	1A	3581	1/1	0.94	0.19	19,19,19,19	0
56	MG	2A	3543	1/1	0.94	0.13	45,45,45,45	0
56	MG	1A	3026	1/1	0.94	0.13	30,30,30,30	0
56	MG	1A	3276	1/1	0.94	0.16	40,40,40,40	0
56	MG	1A	3571	1/1	0.94	0.12	17,17,17,17	0
56	MG	2A	3718	1/1	0.94	0.10	56,56,56,56	0
56	MG	2A	3559	1/1	0.94	0.16	61,61,61,61	0
56	MG	1a	3062	1/1	0.94	0.08	36,36,36,36	0
56	MG	2A	3624	1/1	0.94	0.22	62,62,62,62	0
56	MG	2A	3444	1/1	0.94	0.20	42,42,42,42	0
56	MG	2A	3623	1/1	0.94	0.27	46,46,46,46	0
56	MG	2A	3142	1/1	0.94	0.13	46,46,46,46	0
56	MG	1a	3008	1/1	0.94	0.17	51,51,51,51	0
56	MG	2A	3431	1/1	0.94	0.17	24,24,24,24	0
56	MG	1a	3212	1/1	0.94	0.13	41,41,41,41	0
56	MG	1a	3051	1/1	0.94	0.12	55,55,55,55	0
56	MG	13	101	1/1	0.94	0.53	39,39,39,39	0
56	MG	2A	3632	1/1	0.94	0.32	62,62,62,62	0
56	MG	2a	1677	1/1	0.94	0.15	55,55,55,55	0
56	MG	1a	3167	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3208	1/1	0.94	0.14	29,29,29,29	0
56	MG	1D	302	1/1	0.94	0.19	21,21,21,21	0
56	MG	1a	3197	1/1	0.94	0.10	39,39,39,39	0
56	MG	1R	205	1/1	0.94	0.10	34,34,34,34	0
56	MG	1A	3521	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3583	1/1	0.94	0.45	40,40,40,40	0
56	MG	2A	3378	1/1	0.94	0.16	25,25,25,25	0
56	MG	1B	224	1/1	0.94	0.09	54,54,54,54	0
56	MG	1A	3468	1/1	0.94	0.08	37,37,37,37	0
56	MG	1A	3646	1/1	0.94	0.16	19,19,19,19	0
56	MG	1a	3023	1/1	0.94	0.15	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4043	1/1	0.94	0.45	23,23,23,23	0
56	MG	2W	201	1/1	0.94	0.16	50,50,50,50	0
56	MG	2A	3339	1/1	0.94	0.10	58,58,58,58	0
56	MG	1A	3256	1/1	0.94	0.10	33,33,33,33	0
56	MG	1a	3060	1/1	0.94	0.07	50,50,50,50	0
56	MG	1A	4001	1/1	0.94	0.11	45,45,45,45	0
56	MG	2A	3414	1/1	0.94	0.14	49,49,49,49	0
56	MG	2A	3278	1/1	0.94	0.14	57,57,57,57	0
56	MG	2A	3251	1/1	0.94	0.20	49,49,49,49	0
56	MG	2A	3007	1/1	0.94	0.10	32,32,32,32	0
56	MG	1A	3982	1/1	0.94	0.23	46,46,46,46	0
56	MG	2A	3417	1/1	0.94	0.18	35,35,35,35	0
56	MG	2A	3282	1/1	0.94	0.10	51,51,51,51	0
56	MG	2X	3001	1/1	0.94	0.14	46,46,46,46	0
56	MG	1a	3126	1/1	0.94	0.13	46,46,46,46	0
56	MG	2A	3056	1/1	0.94	0.09	52,52,52,52	0
56	MG	2A	3014	1/1	0.94	0.21	54,54,54,54	0
56	MG	2A	3113	1/1	0.94	0.21	48,48,48,48	0
56	MG	1l	201	1/1	0.94	0.17	31,31,31,31	0
56	MG	1A	3410	1/1	0.94	0.12	45,45,45,45	0
56	MG	2A	3070	1/1	0.94	0.15	33,33,33,33	0
56	MG	2a	1728	1/1	0.94	0.09	46,46,46,46	0
56	MG	1A	3462	1/1	0.94	0.31	22,22,22,22	0
56	MG	2A	3181	1/1	0.94	0.16	35,35,35,35	0
56	MG	2a	1720	1/1	0.94	0.18	66,66,66,66	0
56	MG	1A	3799	1/1	0.94	0.23	29,29,29,29	0
56	MG	2A	3667	1/1	0.94	0.11	63,63,63,63	0
56	MG	1A	3043	1/1	0.94	0.15	19,19,19,19	0
56	MG	2A	3470	1/1	0.94	0.22	53,53,53,53	0
56	MG	1A	4062	1/1	0.94	0.13	21,21,21,21	0
56	MG	1A	3841	1/1	0.94	0.14	33,33,33,33	0
56	MG	2A	3755	1/1	0.94	0.81	48,48,48,48	0
56	MG	1A	3564	1/1	0.94	0.21	36,36,36,36	0
56	MG	1X	103	1/1	0.94	0.25	29,29,29,29	0
56	MG	2A	3054	1/1	0.94	0.41	53,53,53,53	0
56	MG	1B	215	1/1	0.94	0.06	34,34,34,34	0
56	MG	2A	3580	1/1	0.94	0.15	39,39,39,39	0
56	MG	1A	4037	1/1	0.94	0.55	28,28,28,28	0
56	MG	2A	3605	1/1	0.94	0.13	42,42,42,42	0
56	MG	1B	203	1/1	0.94	0.20	39,39,39,39	0
56	MG	1A	3274	1/1	0.94	0.22	40,40,40,40	0
56	MG	1A	3673	1/1	0.94	0.13	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	3191	1/1	0.94	0.08	53,53,53,53	0
56	MG	2A	3601	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3704	1/1	0.94	0.25	28,28,28,28	0
56	MG	2A	3101	1/1	0.94	0.17	30,30,30,30	0
58	EZG	1A	4030	25/25	0.94	0.27	19,29,40,41	0
56	MG	1A	3159	1/1	0.94	0.34	36,36,36,36	0
56	MG	1A	3272	1/1	0.94	0.12	34,34,34,34	0
56	MG	1A	3158	1/1	0.94	0.17	31,31,31,31	0
56	MG	1A	3747	1/1	0.94	0.08	31,31,31,31	0
56	MG	2a	1675	1/1	0.94	0.07	53,53,53,53	0
56	MG	2A	3655	1/1	0.94	0.15	53,53,53,53	0
56	MG	2A	3265	1/1	0.94	0.17	46,46,46,46	0
56	MG	1A	3526	1/1	0.94	0.22	42,42,42,42	0
56	MG	1A	3988	1/1	0.94	0.09	34,34,34,34	0
56	MG	1a	3067	1/1	0.94	0.16	46,46,46,46	0
56	MG	2V	3001	1/1	0.94	0.39	46,46,46,46	0
56	MG	1A	3943	1/1	0.94	0.16	38,38,38,38	0
56	MG	1A	3514	1/1	0.94	0.17	21,21,21,21	0
56	MG	1A	3857	1/1	0.94	0.16	32,32,32,32	0
56	MG	1a	3135	1/1	0.94	0.12	52,52,52,52	0
56	MG	25	502	1/1	0.94	0.59	47,47,47,47	0
56	MG	1A	4004	1/1	0.94	0.27	55,55,55,55	0
56	MG	1B	225	1/1	0.94	0.17	57,57,57,57	0
56	MG	17	101	1/1	0.94	0.19	27,27,27,27	0
56	MG	1A	3826	1/1	0.94	0.16	27,27,27,27	0
56	MG	1A	3940	1/1	0.94	0.10	29,29,29,29	0
56	MG	2A	3651	1/1	0.94	0.13	42,42,42,42	0
56	MG	2A	3157	1/1	0.94	0.11	51,51,51,51	0
56	MG	1a	3148	1/1	0.94	0.09	55,55,55,55	0
56	MG	1G	3004	1/1	0.94	0.11	38,38,38,38	0
56	MG	2A	3152	1/1	0.94	0.18	45,45,45,45	0
56	MG	1A	3004	1/1	0.94	0.16	21,21,21,21	0
56	MG	1A	3928	1/1	0.94	0.17	37,37,37,37	0
56	MG	1A	3981	1/1	0.94	0.12	30,30,30,30	0
56	MG	1A	3504	1/1	0.94	0.08	48,48,48,48	0
56	MG	1a	3196	1/1	0.94	0.07	46,46,46,46	0
56	MG	15	101	1/1	0.94	0.38	27,27,27,27	0
56	MG	2A	3110	1/1	0.94	0.18	37,37,37,37	0
56	MG	1A	3695	1/1	0.94	0.21	50,50,50,50	0
56	MG	2a	1716	1/1	0.94	0.18	43,43,43,43	0
56	MG	1A	3168	1/1	0.94	0.19	43,43,43,43	0
56	MG	1U	203	1/1	0.94	0.23	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3461	1/1	0.94	0.15	45,45,45,45	0
56	MG	1B	202	1/1	0.94	0.24	42,42,42,42	0
56	MG	2A	3112	1/1	0.94	0.12	52,52,52,52	0
56	MG	1A	3075	1/1	0.94	0.13	34,34,34,34	0
56	MG	2A	3578	1/1	0.94	0.20	27,27,27,27	0
56	MG	1A	3073	1/1	0.94	0.48	42,42,42,42	0
56	MG	1A	3624	1/1	0.94	0.13	26,26,26,26	0
56	MG	1A	3061	1/1	0.94	0.11	39,39,39,39	0
56	MG	2A	3677	1/1	0.94	0.15	48,48,48,48	0
56	MG	1A	3080	1/1	0.94	0.24	41,41,41,41	0
56	MG	2O	8002	1/1	0.94	0.12	52,52,52,52	0
56	MG	1A	3845	1/1	0.94	0.30	42,42,42,42	0
56	MG	1A	3710	1/1	0.94	0.20	28,28,28,28	0
56	MG	1A	3942	1/1	0.94	0.10	47,47,47,47	0
56	MG	1A	3992	1/1	0.94	0.18	49,49,49,49	0
56	MG	1A	3005	1/1	0.94	0.13	36,36,36,36	0
56	MG	2A	3340	1/1	0.94	0.19	30,30,30,30	0
56	MG	1A	3389	1/1	0.94	0.21	34,34,34,34	0
56	MG	2A	3104	1/1	0.94	0.12	51,51,51,51	0
56	MG	2A	3326	1/1	0.94	0.11	48,48,48,48	0
56	MG	1A	3210	1/1	0.94	0.42	25,25,25,25	0
56	MG	2A	3421	1/1	0.94	0.11	39,39,39,39	0
56	MG	1B	230	1/1	0.94	0.31	42,42,42,42	0
56	MG	2d	503	1/1	0.94	0.12	56,56,56,56	0
56	MG	2A	3004	1/1	0.94	0.14	37,37,37,37	0
56	MG	1A	3323	1/1	0.94	0.22	19,19,19,19	0
56	MG	2A	3495	1/1	0.94	0.28	60,60,60,60	0
56	MG	2A	3080	1/1	0.94	0.11	28,28,28,28	0
56	MG	2A	3351	1/1	0.94	0.13	43,43,43,43	0
56	MG	1b	3002	1/1	0.94	0.10	53,53,53,53	0
56	MG	1A	3478	1/1	0.94	0.20	47,47,47,47	0
56	MG	1A	4052	1/1	0.94	0.40	31,31,31,31	0
56	MG	1A	3205	1/1	0.94	0.59	28,28,28,28	0
56	MG	1A	3572	1/1	0.95	0.20	12,12,12,12	0
56	MG	1A	3102	1/1	0.95	0.27	31,31,31,31	0
56	MG	1A	3327	1/1	0.95	0.18	10,10,10,10	0
56	MG	2B	3006	1/1	0.95	0.17	65,65,65,65	0
56	MG	2A	3643	1/1	0.95	0.08	43,43,43,43	0
56	MG	2A	3487	1/1	0.95	0.20	62,62,62,62	0
56	MG	2A	3180	1/1	0.95	0.24	33,33,33,33	0
56	MG	1A	3532	1/1	0.95	0.16	29,29,29,29	0
56	MG	1a	3138	1/1	0.95	0.16	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2B	3004	1/1	0.95	0.16	60,60,60,60	0
56	MG	1A	3418	1/1	0.95	0.56	30,30,30,30	0
56	MG	1A	3204	1/1	0.95	0.29	39,39,39,39	0
56	MG	2A	3333	1/1	0.95	0.12	25,25,25,25	0
56	MG	1A	3185	1/1	0.95	0.15	26,26,26,26	0
56	MG	2A	3596	1/1	0.95	0.15	32,32,32,32	0
56	MG	1A	3682	1/1	0.95	0.09	55,55,55,55	0
56	MG	1A	3901	1/1	0.95	0.30	44,44,44,44	0
56	MG	2A	3719	1/1	0.95	0.14	70,70,70,70	0
56	MG	1A	3422	1/1	0.95	0.50	43,43,43,43	0
56	MG	2A	3585	1/1	0.95	0.20	34,34,34,34	0
56	MG	1A	3582	1/1	0.95	0.12	26,26,26,26	0
56	MG	2A	3413	1/1	0.95	0.16	55,55,55,55	0
56	MG	1w	105	1/1	0.95	0.12	64,64,64,64	0
56	MG	1A	3016	1/1	0.95	0.20	40,40,40,40	0
56	MG	2a	1823	1/1	0.95	0.09	53,53,53,53	0
56	MG	1A	3637	1/1	0.95	0.13	20,20,20,20	0
56	MG	1a	3039	1/1	0.95	0.10	47,47,47,47	0
56	MG	2A	3023	1/1	0.95	0.12	41,41,41,41	0
56	MG	1A	3177	1/1	0.95	0.09	34,34,34,34	0
56	MG	1A	3494	1/1	0.95	0.11	35,35,35,35	0
56	MG	2A	3430	1/1	0.95	0.11	53,53,53,53	0
56	MG	1x	104	1/1	0.95	0.22	54,54,54,54	0
56	MG	1A	3056	1/1	0.95	0.14	50,50,50,50	0
56	MG	10	102	1/1	0.95	0.23	25,25,25,25	0
56	MG	1A	3597	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	4035	1/1	0.95	0.10	38,38,38,38	0
56	MG	1A	3300	1/1	0.95	0.18	29,29,29,29	0
56	MG	1A	3576	1/1	0.95	0.15	15,15,15,15	0
56	MG	1A	3694	1/1	0.95	0.08	51,51,51,51	0
56	MG	1A	3234	1/1	0.95	0.11	43,43,43,43	0
56	MG	1a	3056	1/1	0.95	0.11	50,50,50,50	0
56	MG	1x	112	1/1	0.95	0.16	45,45,45,45	0
56	MG	1A	3125	1/1	0.95	0.28	19,19,19,19	0
56	MG	2a	1683	1/1	0.95	0.20	33,33,33,33	0
56	MG	1A	3467	1/1	0.95	0.27	49,49,49,49	0
56	MG	2a	1632	1/1	0.95	0.11	67,67,67,67	0
56	MG	1A	3412	1/1	0.95	0.37	37,37,37,37	0
56	MG	1A	3146	1/1	0.95	0.55	23,23,23,23	0
56	MG	1a	3151	1/1	0.95	0.20	62,62,62,62	0
56	MG	1A	3187	1/1	0.95	0.08	28,28,28,28	0
56	MG	2a	1692	1/1	0.95	0.32	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	3188	1/1	0.95	0.10	47,47,47,47	0
56	MG	1a	3200	1/1	0.95	0.15	41,41,41,41	0
56	MG	1U	205	1/1	0.95	0.20	23,23,23,23	0
56	MG	1A	3720	1/1	0.95	0.14	41,41,41,41	0
56	MG	2A	3372	1/1	0.95	0.23	42,42,42,42	0
56	MG	1A	3879	1/1	0.95	0.18	18,18,18,18	0
56	MG	1A	3740	1/1	0.95	0.15	46,46,46,46	0
56	MG	1A	3569	1/1	0.95	0.14	17,17,17,17	0
56	MG	1A	3079	1/1	0.95	0.16	32,32,32,32	0
56	MG	2a	1746	1/1	0.95	0.08	67,67,67,67	0
56	MG	1A	3533	1/1	0.95	0.10	47,47,47,47	0
56	MG	1a	3033	1/1	0.95	0.07	57,57,57,57	0
56	MG	1A	3324	1/1	0.95	0.13	33,33,33,33	0
56	MG	2A	3290	1/1	0.95	0.19	39,39,39,39	0
56	MG	1A	3112	1/1	0.95	0.16	40,40,40,40	0
56	MG	1A	3912	1/1	0.95	0.15	25,25,25,25	0
56	MG	1A	3428	1/1	0.95	0.21	26,26,26,26	0
56	MG	1A	3059	1/1	0.95	0.20	36,36,36,36	0
56	MG	2A	3107	1/1	0.95	0.17	27,27,27,27	0
56	MG	1A	3421	1/1	0.95	0.46	37,37,37,37	0
56	MG	1A	3129	1/1	0.95	0.36	27,27,27,27	0
56	MG	1A	3905	1/1	0.95	0.07	54,54,54,54	0
56	MG	1A	3062	1/1	0.95	0.11	12,12,12,12	0
56	MG	1A	3285	1/1	0.95	0.14	34,34,34,34	0
56	MG	1W	3003	1/1	0.95	0.10	33,33,33,33	0
56	MG	1A	3899	1/1	0.95	0.09	35,35,35,35	0
56	MG	1A	3247	1/1	0.95	0.23	27,27,27,27	0
56	MG	1A	3659	1/1	0.95	0.20	40,40,40,40	0
56	MG	1a	3037	1/1	0.95	0.14	61,61,61,61	0
56	MG	1A	3160	1/1	0.95	0.60	29,29,29,29	0
56	MG	2A	3274	1/1	0.95	0.29	45,45,45,45	0
56	MG	1A	3616	1/1	0.95	0.16	58,58,58,58	0
56	MG	1A	3322	1/1	0.95	0.36	38,38,38,38	0
56	MG	1A	4008	1/1	0.95	0.36	24,24,24,24	0
56	MG	1A	3808	1/1	0.95	0.17	34,34,34,34	0
56	MG	2A	3419	1/1	0.95	0.07	55,55,55,55	0
56	MG	2A	3040	1/1	0.95	0.34	39,39,39,39	0
56	MG	1A	3232	1/1	0.95	0.10	17,17,17,17	0
56	MG	1A	3726	1/1	0.95	0.06	35,35,35,35	0
56	MG	2A	3526	1/1	0.95	0.11	49,49,49,49	0
56	MG	2a	1789	1/1	0.95	0.09	54,54,54,54	0
56	MG	2D	305	1/1	0.95	0.10	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3714	1/1	0.95	0.19	26,26,26,26	0
56	MG	1A	3979	1/1	0.95	0.10	56,56,56,56	0
56	MG	1A	3777	1/1	0.95	0.10	36,36,36,36	0
56	MG	2A	3227	1/1	0.95	0.09	40,40,40,40	0
56	MG	1a	3042	1/1	0.95	0.18	44,44,44,44	0
56	MG	1A	3647	1/1	0.95	0.16	16,16,16,16	0
56	MG	1a	3132	1/1	0.95	0.08	34,34,34,34	0
56	MG	1A	3956	1/1	0.95	0.07	67,67,67,67	0
56	MG	1x	106	1/1	0.95	0.15	66,66,66,66	0
56	MG	1A	3767	1/1	0.95	0.10	41,41,41,41	0
56	MG	1A	3782	1/1	0.95	0.09	34,34,34,34	0
56	MG	1A	3551	1/1	0.95	0.15	17,17,17,17	0
56	MG	1A	3528	1/1	0.95	0.15	23,23,23,23	0
56	MG	1a	3021	1/1	0.95	0.14	40,40,40,40	0
56	MG	1a	3210	1/1	0.95	0.14	41,41,41,41	0
56	MG	2A	3100	1/1	0.95	0.15	59,59,59,59	0
56	MG	2A	3579	1/1	0.95	0.09	51,51,51,51	0
56	MG	2A	3237	1/1	0.95	0.15	43,43,43,43	0
56	MG	2A	3365	1/1	0.95	0.11	38,38,38,38	0
56	MG	1a	3118	1/1	0.95	0.09	65,65,65,65	0
56	MG	2a	1680	1/1	0.95	0.16	45,45,45,45	0
56	MG	2A	3301	1/1	0.95	0.14	40,40,40,40	0
56	MG	1A	3629	1/1	0.95	0.23	60,60,60,60	0
56	MG	2a	1828	1/1	0.95	0.22	64,64,64,64	0
56	MG	1a	3065	1/1	0.95	0.15	41,41,41,41	0
56	MG	1A	4040	1/1	0.95	0.47	34,34,34,34	0
56	MG	2a	1831	1/1	0.95	0.09	53,53,53,53	0
56	MG	1a	3122	1/1	0.95	0.11	40,40,40,40	0
56	MG	2A	3494	1/1	0.95	0.26	49,49,49,49	0
56	MG	1A	3613	1/1	0.95	0.10	30,30,30,30	0
56	MG	2A	3173	1/1	0.95	0.14	45,45,45,45	0
56	MG	2A	3005	1/1	0.95	0.11	42,42,42,42	0
56	MG	1B	201	1/1	0.95	0.10	49,49,49,49	0
56	MG	2A	3010	1/1	0.95	0.18	31,31,31,31	0
56	MG	1A	3703	1/1	0.95	0.22	24,24,24,24	0
56	MG	2A	3319	1/1	0.95	0.13	62,62,62,62	0
56	MG	1V	203	1/1	0.95	0.21	63,63,63,63	0
56	MG	2A	3132	1/1	0.95	0.07	58,58,58,58	0
56	MG	2A	3189	1/1	0.95	0.07	38,38,38,38	0
56	MG	1B	221	1/1	0.95	0.10	36,36,36,36	0
56	MG	1A	3926	1/1	0.95	0.16	18,18,18,18	0
56	MG	1A	3750	1/1	0.95	0.08	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3380	1/1	0.95	0.17	25,25,25,25	0
56	MG	11	103	1/1	0.95	0.08	31,31,31,31	0
56	MG	1A	3785	1/1	0.95	0.20	35,35,35,35	0
56	MG	2a	1809	1/1	0.95	0.15	58,58,58,58	0
56	MG	2A	3726	1/1	0.95	0.17	43,43,43,43	0
56	MG	2a	1718	1/1	0.95	0.14	55,55,55,55	0
56	MG	2A	3348	1/1	0.95	0.13	47,47,47,47	0
56	MG	2B	3011	1/1	0.95	0.14	69,69,69,69	0
56	MG	2A	3337	1/1	0.95	0.27	27,27,27,27	0
56	MG	2A	3599	1/1	0.95	0.09	61,61,61,61	0
56	MG	1A	3401	1/1	0.95	0.10	38,38,38,38	0
56	MG	2a	1771	1/1	0.95	0.11	62,62,62,62	0
56	MG	1B	237	1/1	0.95	0.16	46,46,46,46	0
56	MG	2A	3566	1/1	0.95	0.13	56,56,56,56	0
56	MG	1B	233	1/1	0.95	0.13	50,50,50,50	0
56	MG	2a	1779	1/1	0.95	0.11	60,60,60,60	0
56	MG	1A	3833	1/1	0.95	0.14	58,58,58,58	0
56	MG	2A	3600	1/1	0.95	0.11	56,56,56,56	0
56	MG	1A	3381	1/1	0.95	0.08	46,46,46,46	0
56	MG	1A	3471	1/1	0.95	0.23	45,45,45,45	0
56	MG	1A	4046	1/1	0.95	0.44	20,20,20,20	0
56	MG	1a	3005	1/1	0.95	0.11	41,41,41,41	0
56	MG	1A	3279	1/1	0.95	0.18	41,41,41,41	0
56	MG	1a	3163	1/1	0.95	0.17	47,47,47,47	0
56	MG	1A	3724	1/1	0.95	0.10	44,44,44,44	0
56	MG	1A	3664	1/1	0.95	0.19	43,43,43,43	0
56	MG	2A	3499	1/1	0.95	0.15	41,41,41,41	0
56	MG	1a	3183	1/1	0.95	0.10	51,51,51,51	0
56	MG	2D	301	1/1	0.95	0.24	54,54,54,54	0
56	MG	1A	4058	1/1	0.95	0.24	69,69,69,69	0
56	MG	2a	1782	1/1	0.95	0.14	58,58,58,58	0
56	MG	18	103	1/1	0.95	0.22	41,41,41,41	0
56	MG	2A	3748	1/1	0.95	0.14	27,27,27,27	0
56	MG	2a	1629	1/1	0.95	0.18	73,73,73,73	0
56	MG	2A	3498	1/1	0.95	0.06	46,46,46,46	0
56	MG	1D	314	1/1	0.95	0.30	29,29,29,29	0
56	MG	1A	3524	1/1	0.95	0.16	20,20,20,20	0
56	MG	1A	3111	1/1	0.95	0.28	30,30,30,30	0
56	MG	2a	1744	1/1	0.95	0.11	67,67,67,67	0
56	MG	2A	3214	1/1	0.95	0.08	49,49,49,49	0
56	MG	2A	3564	1/1	0.95	0.17	42,42,42,42	0
56	MG	2w	104	1/1	0.95	0.14	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3297	1/1	0.95	0.24	51,51,51,51	0
56	MG	2A	3427	1/1	0.95	0.08	46,46,46,46	0
56	MG	1a	3097	1/1	0.95	0.08	62,62,62,62	0
56	MG	1A	4039	1/1	0.95	0.45	33,33,33,33	0
56	MG	2A	3479	1/1	0.95	0.15	34,34,34,34	0
56	MG	1A	3611	1/1	0.95	0.19	45,45,45,45	0
56	MG	2A	3645	1/1	0.95	0.15	33,33,33,33	0
56	MG	2A	3385	1/1	0.95	0.21	27,27,27,27	0
56	MG	1A	3151	1/1	0.95	0.21	36,36,36,36	0
56	MG	1A	3354	1/1	0.95	0.08	39,39,39,39	0
56	MG	1A	3562	1/1	0.95	0.16	18,18,18,18	0
56	MG	2A	3350	1/1	0.95	0.13	50,50,50,50	0
56	MG	1x	105	1/1	0.95	0.13	59,59,59,59	0
56	MG	2f	3001	1/1	0.95	0.11	40,40,40,40	0
56	MG	1G	3003	1/1	0.95	0.11	51,51,51,51	0
56	MG	1A	3975	1/1	0.95	0.08	51,51,51,51	0
56	MG	2a	1777	1/1	0.95	0.10	55,55,55,55	0
56	MG	1A	3973	1/1	0.95	0.13	47,47,47,47	0
56	MG	1A	3627	1/1	0.95	0.13	26,26,26,26	0
56	MG	2A	3725	1/1	0.95	0.13	47,47,47,47	0
56	MG	1A	3763	1/1	0.95	0.15	22,22,22,22	0
56	MG	1A	3342	1/1	0.95	0.32	21,21,21,21	0
56	MG	2A	3027	1/1	0.95	0.14	32,32,32,32	0
56	MG	1A	3372	1/1	0.95	0.13	35,35,35,35	0
56	MG	1A	3575	1/1	0.95	0.12	11,11,11,11	0
56	MG	2A	3577	1/1	0.95	0.21	45,45,45,45	0
56	MG	1A	3788	1/1	0.95	0.10	25,25,25,25	0
56	MG	2A	3240	1/1	0.95	0.12	51,51,51,51	0
56	MG	1A	3600	1/1	0.95	0.26	50,50,50,50	0
56	MG	1A	3961	1/1	0.95	0.10	36,36,36,36	0
56	MG	2a	1635	1/1	0.95	0.15	39,39,39,39	0
56	MG	1A	3492	1/1	0.95	0.25	35,35,35,35	0
56	MG	2A	3454	1/1	0.95	0.14	52,52,52,52	0
56	MG	2a	1725	1/1	0.95	0.14	49,49,49,49	0
56	MG	2A	3665	1/1	0.95	0.11	36,36,36,36	0
56	MG	2A	3448	1/1	0.95	0.14	33,33,33,33	0
56	MG	2a	1794	1/1	0.95	0.15	58,58,58,58	0
56	MG	1a	3133	1/1	0.95	0.15	47,47,47,47	0
56	MG	1A	3351	1/1	0.95	0.11	34,34,34,34	0
56	MG	1A	3103	1/1	0.95	0.25	33,33,33,33	0
56	MG	1A	4003	1/1	0.95	0.10	32,32,32,32	0
56	MG	2A	3699	1/1	0.95	0.11	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3650	1/1	0.95	0.17	34,34,34,34	0
56	MG	1A	4002	1/1	0.95	0.15	32,32,32,32	0
56	MG	1a	3007	1/1	0.95	0.17	50,50,50,50	0
56	MG	2a	1721	1/1	0.95	0.04	73,73,73,73	0
56	MG	2A	3141	1/1	0.95	0.13	40,40,40,40	0
56	MG	1A	3542	1/1	0.95	0.16	44,44,44,44	0
56	MG	1a	3187	1/1	0.95	0.06	43,43,43,43	0
56	MG	1B	235	1/1	0.95	0.16	55,55,55,55	0
56	MG	1A	3722	1/1	0.95	0.14	29,29,29,29	0
56	MG	1A	3078	1/1	0.95	0.39	26,26,26,26	0
56	MG	1A	3969	1/1	0.95	0.13	41,41,41,41	0
56	MG	1y	104	1/1	0.95	0.13	44,44,44,44	0
56	MG	1A	4061	1/1	0.95	0.31	38,38,38,38	0
56	MG	1A	3768	1/1	0.95	0.06	33,33,33,33	0
56	MG	2A	3438	1/1	0.95	0.10	36,36,36,36	0
56	MG	1A	3913	1/1	0.95	0.25	39,39,39,39	0
56	MG	1a	3087	1/1	0.95	0.19	44,44,44,44	0
56	MG	1D	309	1/1	0.95	0.23	28,28,28,28	0
56	MG	1a	3108	1/1	0.95	0.21	40,40,40,40	0
56	MG	2A	3474	1/1	0.95	0.15	35,35,35,35	0
56	MG	1A	3890	1/1	0.95	0.15	36,36,36,36	0
56	MG	1A	3683	1/1	0.95	0.28	41,41,41,41	0
56	MG	2A	3610	1/1	0.95	0.12	47,47,47,47	0
56	MG	1A	3259	1/1	0.95	0.16	45,45,45,45	0
56	MG	2a	1754	1/1	0.95	0.09	61,61,61,61	0
56	MG	2A	3230	1/1	0.95	0.10	41,41,41,41	0
56	MG	2A	3124	1/1	0.95	0.18	48,48,48,48	0
56	MG	2a	1817	1/1	0.95	0.16	51,51,51,51	0
56	MG	1a	3158	1/1	0.95	0.06	47,47,47,47	0
56	MG	2A	3295	1/1	0.95	0.26	43,43,43,43	0
56	MG	2Q	3001	1/1	0.95	0.07	54,54,54,54	0
56	MG	2A	3345	1/1	0.95	0.12	63,63,63,63	0
56	MG	1A	3475	1/1	0.95	0.27	28,28,28,28	0
56	MG	1A	3731	1/1	0.95	0.21	16,16,16,16	0
56	MG	2A	3598	1/1	0.95	0.14	39,39,39,39	0
56	MG	1a	3211	1/1	0.95	0.15	35,35,35,35	0
56	MG	2B	3015	1/1	0.95	0.14	51,51,51,51	0
56	MG	2a	1803	1/1	0.95	0.08	51,51,51,51	0
56	MG	1A	3950	1/1	0.95	0.14	54,54,54,54	0
56	MG	1A	3388	1/1	0.95	0.19	30,30,30,30	0
56	MG	2A	3264	1/1	0.95	0.40	47,47,47,47	0
56	MG	1A	3193	1/1	0.95	0.18	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4055	1/1	0.95	0.66	31,31,31,31	0
56	MG	1A	3574	1/1	0.95	0.15	16,16,16,16	0
56	MG	1a	3169	1/1	0.95	0.09	38,38,38,38	0
56	MG	2A	3069	1/1	0.95	0.23	39,39,39,39	0
56	MG	1a	3019	1/1	0.95	0.10	54,54,54,54	0
56	MG	2A	3271	1/1	0.95	0.25	45,45,45,45	0
56	MG	2A	3081	1/1	0.95	0.09	53,53,53,53	0
56	MG	1A	3096	1/1	0.95	0.25	26,26,26,26	0
56	MG	1a	3066	1/1	0.95	0.10	58,58,58,58	0
56	MG	2a	1618	1/1	0.95	0.43	51,51,51,51	0
56	MG	2a	1655	1/1	0.95	0.17	67,67,67,67	0
56	MG	2A	3200	1/1	0.95	0.24	50,50,50,50	0
56	MG	1a	3074	1/1	0.95	0.16	49,49,49,49	0
56	MG	2A	3513	1/1	0.95	0.11	52,52,52,52	0
56	MG	2A	3567	1/1	0.95	0.10	44,44,44,44	0
56	MG	1A	3545	1/1	0.95	0.15	25,25,25,25	0
56	MG	1A	3976	1/1	0.95	0.09	50,50,50,50	0
56	MG	2A	3549	1/1	0.95	0.15	43,43,43,43	0
56	MG	2A	3576	1/1	0.95	0.10	52,52,52,52	0
56	MG	2A	3533	1/1	0.95	0.34	52,52,52,52	0
56	MG	1A	3818	1/1	0.95	0.05	21,21,21,21	0
56	MG	2A	3716	1/1	0.95	0.09	44,44,44,44	0
56	MG	1A	3082	1/1	0.95	0.15	40,40,40,40	0
56	MG	1A	4022	1/1	0.95	0.14	46,46,46,46	0
56	MG	2A	3095	1/1	0.95	0.12	52,52,52,52	0
56	MG	2A	3190	1/1	0.96	0.13	44,44,44,44	0
56	MG	2A	3012	1/1	0.96	0.10	44,44,44,44	0
56	MG	1A	3733	1/1	0.96	0.07	55,55,55,55	0
56	MG	2A	3342	1/1	0.96	0.18	49,49,49,49	0
56	MG	1w	104	1/1	0.96	0.07	36,36,36,36	0
56	MG	1a	3171	1/1	0.96	0.07	55,55,55,55	0
56	MG	1A	3191	1/1	0.96	0.21	24,24,24,24	0
56	MG	1U	202	1/1	0.96	0.11	30,30,30,30	0
56	MG	1A	3474	1/1	0.96	0.17	38,38,38,38	0
56	MG	1A	3253	1/1	0.96	0.72	24,24,24,24	0
56	MG	1A	3852	1/1	0.96	0.15	55,55,55,55	0
56	MG	1A	3508	1/1	0.96	0.10	26,26,26,26	0
56	MG	1R	201	1/1	0.96	0.16	36,36,36,36	0
56	MG	1A	3963	1/1	0.96	0.08	33,33,33,33	0
56	MG	1A	3216	1/1	0.96	0.14	25,25,25,25	0
56	MG	1A	3550	1/1	0.96	0.19	26,26,26,26	0
56	MG	2A	3637	1/1	0.96	0.10	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3028	1/1	0.96	0.17	42,42,42,42	0
56	MG	2A	3727	1/1	0.96	0.12	49,49,49,49	0
56	MG	1A	3081	1/1	0.96	0.17	24,24,24,24	0
56	MG	1A	3212	1/1	0.96	0.18	50,50,50,50	0
56	MG	1A	3594	1/1	0.96	0.32	46,46,46,46	0
56	MG	1A	3675	1/1	0.96	0.15	66,66,66,66	0
56	MG	2A	3066	1/1	0.96	0.57	40,40,40,40	0
56	MG	1X	105	1/1	0.96	0.16	44,44,44,44	0
56	MG	2A	3679	1/1	0.96	0.15	49,49,49,49	0
56	MG	2a	1625	1/1	0.96	0.10	67,67,67,67	0
56	MG	1A	3213	1/1	0.96	0.18	36,36,36,36	0
56	MG	2A	3749	1/1	0.96	0.36	34,34,34,34	0
56	MG	1A	3138	1/1	0.96	0.46	30,30,30,30	0
56	MG	1A	3362	1/1	0.96	0.25	33,33,33,33	0
56	MG	2A	3617	1/1	0.96	0.24	43,43,43,43	0
56	MG	2A	3317	1/1	0.96	0.25	36,36,36,36	0
56	MG	2A	3664	1/1	0.96	0.21	41,41,41,41	0
56	MG	1A	3847	1/1	0.96	0.14	18,18,18,18	0
56	MG	1A	3402	1/1	0.96	0.08	28,28,28,28	0
56	MG	1A	3400	1/1	0.96	0.17	33,33,33,33	0
56	MG	1A	3290	1/1	0.96	0.10	46,46,46,46	0
56	MG	1a	3120	1/1	0.96	0.08	43,43,43,43	0
56	MG	2A	3352	1/1	0.96	0.10	50,50,50,50	0
56	MG	1A	3278	1/1	0.96	0.18	40,40,40,40	0
56	MG	1A	3546	1/1	0.96	0.11	14,14,14,14	0
56	MG	2a	1606	1/1	0.96	0.07	43,43,43,43	0
56	MG	2e	3001	1/1	0.96	0.11	60,60,60,60	0
56	MG	1y	101	1/1	0.96	0.10	35,35,35,35	0
56	MG	1A	3765	1/1	0.96	0.20	19,19,19,19	0
56	MG	2R	3003	1/1	0.96	0.15	48,48,48,48	0
56	MG	2A	3642	1/1	0.96	0.12	43,43,43,43	0
56	MG	1A	4023	1/1	0.96	0.56	21,21,21,21	0
56	MG	1A	3813	1/1	0.96	0.16	29,29,29,29	0
56	MG	1A	3877	1/1	0.96	0.20	28,28,28,28	0
56	MG	2x	102	1/1	0.96	0.19	57,57,57,57	0
56	MG	1A	3167	1/1	0.96	0.22	47,47,47,47	0
56	MG	2A	3537	1/1	0.96	0.15	46,46,46,46	0
56	MG	1F	305	1/1	0.96	0.39	28,28,28,28	0
56	MG	1A	3503	1/1	0.96	0.18	22,22,22,22	0
56	MG	1a	3081	1/1	0.96	0.09	67,67,67,67	0
56	MG	1A	3929	1/1	0.96	0.33	35,35,35,35	0
56	MG	2A	3464	1/1	0.96	0.25	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	3145	1/1	0.96	0.22	48,48,48,48	0
56	MG	1B	227	1/1	0.96	0.12	36,36,36,36	0
56	MG	1a	3152	1/1	0.96	0.10	60,60,60,60	0
56	MG	1A	3547	1/1	0.96	0.13	22,22,22,22	0
56	MG	2A	3680	1/1	0.96	0.08	62,62,62,62	0
56	MG	1A	3359	1/1	0.96	0.12	32,32,32,32	0
56	MG	1R	202	1/1	0.96	0.08	30,30,30,30	0
56	MG	2A	3510	1/1	0.96	0.11	50,50,50,50	0
56	MG	2A	3310	1/1	0.96	0.11	58,58,58,58	0
56	MG	1A	3771	1/1	0.96	0.18	17,17,17,17	0
56	MG	2a	1774	1/1	0.96	0.15	44,44,44,44	0
56	MG	1W	3001	1/1	0.96	0.19	34,34,34,34	0
59	ZN	2n	501	1/1	0.96	0.05	93,93,93,93	0
56	MG	2a	1825	1/1	0.96	0.17	56,56,56,56	0
56	MG	2A	3105	1/1	0.96	0.22	34,34,34,34	0
56	MG	1a	3075	1/1	0.96	0.11	46,46,46,46	0
56	MG	1A	3630	1/1	0.96	0.24	38,38,38,38	0
56	MG	1a	3119	1/1	0.96	0.15	52,52,52,52	0
56	MG	1P	201	1/1	0.96	0.46	16,16,16,16	0
56	MG	1A	3360	1/1	0.96	0.18	32,32,32,32	0
56	MG	2A	3399	1/1	0.96	0.19	57,57,57,57	0
56	MG	1a	3110	1/1	0.96	0.13	50,50,50,50	0
56	MG	1A	3719	1/1	0.96	0.08	47,47,47,47	0
56	MG	2A	3670	1/1	0.96	0.18	46,46,46,46	0
56	MG	2A	3493	1/1	0.96	0.09	28,28,28,28	0
56	MG	1A	3888	1/1	0.96	0.14	15,15,15,15	0
56	MG	2A	3246	1/1	0.96	0.24	48,48,48,48	0
56	MG	1A	3113	1/1	0.96	0.48	27,27,27,27	0
56	MG	1A	3598	1/1	0.96	0.34	48,48,48,48	0
56	MG	1P	202	1/1	0.96	0.27	23,23,23,23	0
56	MG	1A	3684	1/1	0.96	0.12	44,44,44,44	0
56	MG	1A	3886	1/1	0.96	0.10	24,24,24,24	0
56	MG	2A	3391	1/1	0.96	0.14	41,41,41,41	0
56	MG	1A	3591	1/1	0.96	0.16	30,30,30,30	0
56	MG	1A	3063	1/1	0.96	0.31	23,23,23,23	0
56	MG	1A	3119	1/1	0.96	0.18	49,49,49,49	0
56	MG	1A	3440	1/1	0.96	0.33	28,28,28,28	0
56	MG	1A	3553	1/1	0.96	0.14	10,10,10,10	0
56	MG	2a	1768	1/1	0.96	0.05	55,55,55,55	0
56	MG	1A	3235	1/1	0.96	0.14	22,22,22,22	0
56	MG	1A	3853	1/1	0.96	0.07	38,38,38,38	0
56	MG	2A	3074	1/1	0.96	0.15	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3039	1/1	0.96	0.15	25,25,25,25	0
56	MG	1a	3137	1/1	0.96	0.15	51,51,51,51	0
56	MG	2B	3005	1/1	0.96	0.10	55,55,55,55	0
56	MG	1A	3123	1/1	0.96	0.16	21,21,21,21	0
56	MG	1a	3140	1/1	0.96	0.10	38,38,38,38	0
56	MG	1A	3403	1/1	0.96	0.23	33,33,33,33	0
56	MG	1A	3399	1/1	0.96	0.14	42,42,42,42	0
56	MG	2A	3724	1/1	0.96	0.15	66,66,66,66	0
56	MG	2A	3371	1/1	0.96	0.19	22,22,22,22	0
56	MG	1a	3113	1/1	0.96	0.14	40,40,40,40	0
56	MG	2A	3169	1/1	0.96	0.07	45,45,45,45	0
56	MG	1A	3649	1/1	0.96	0.19	16,16,16,16	0
56	MG	1F	304	1/1	0.96	0.34	20,20,20,20	0
56	MG	2A	3034	1/1	0.96	0.16	56,56,56,56	0
56	MG	1A	3806	1/1	0.96	0.11	45,45,45,45	0
56	MG	2U	205	1/1	0.96	0.23	49,49,49,49	0
56	MG	1A	4033	1/1	0.96	0.60	25,25,25,25	0
56	MG	2a	1627	1/1	0.96	0.22	53,53,53,53	0
56	MG	1A	3774	1/1	0.96	0.11	56,56,56,56	0
56	MG	2A	3569	1/1	0.96	0.03	63,63,63,63	0
56	MG	1A	3816	1/1	0.96	0.27	46,46,46,46	0
56	MG	1a	3094	1/1	0.96	0.26	40,40,40,40	0
56	MG	2A	3137	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	3140	1/1	0.96	0.54	23,23,23,23	0
56	MG	1D	310	1/1	0.96	0.20	33,33,33,33	0
56	MG	1a	3009	1/1	0.96	0.10	32,32,32,32	0
56	MG	1A	3484	1/1	0.96	0.24	22,22,22,22	0
56	MG	2A	3020	1/1	0.96	0.15	29,29,29,29	0
56	MG	1A	3891	1/1	0.96	0.10	33,33,33,33	0
56	MG	1A	3006	1/1	0.96	0.10	33,33,33,33	0
56	MG	1A	3245	1/1	0.96	0.46	28,28,28,28	0
56	MG	2A	3512	1/1	0.96	0.15	55,55,55,55	0
56	MG	1A	3070	1/1	0.96	0.17	23,23,23,23	0
56	MG	1I	105	1/1	0.96	0.11	32,32,32,32	0
56	MG	1A	3554	1/1	0.96	0.13	14,14,14,14	0
56	MG	2A	3553	1/1	0.96	0.09	57,57,57,57	0
56	MG	1A	3753	1/1	0.96	0.31	27,27,27,27	0
56	MG	1A	3240	1/1	0.96	0.15	38,38,38,38	0
56	MG	2X	3002	1/1	0.96	0.14	49,49,49,49	0
56	MG	2A	3700	1/1	0.96	0.06	61,61,61,61	0
56	MG	2U	206	1/1	0.96	0.13	42,42,42,42	0
56	MG	2A	3516	1/1	0.96	0.13	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	16	104	1/1	0.96	0.14	38,38,38,38	0
56	MG	1A	3446	1/1	0.96	0.11	43,43,43,43	0
56	MG	1A	3046	1/1	0.96	0.26	50,50,50,50	0
56	MG	1A	3037	1/1	0.96	0.26	22,22,22,22	0
56	MG	2A	3463	1/1	0.96	0.16	27,27,27,27	0
56	MG	2A	3272	1/1	0.96	0.09	33,33,33,33	0
56	MG	2A	3239	1/1	0.96	0.44	64,64,64,64	0
56	MG	1A	3525	1/1	0.96	0.13	9,9,9,9	0
56	MG	1a	3015	1/1	0.96	0.31	48,48,48,48	0
56	MG	15	103	1/1	0.96	0.46	25,25,25,25	0
56	MG	2A	3488	1/1	0.96	0.08	53,53,53,53	0
56	MG	1A	3862	1/1	0.96	0.11	52,52,52,52	0
56	MG	2a	1805	1/1	0.96	0.05	53,53,53,53	0
56	MG	2A	3729	1/1	0.96	0.20	43,43,43,43	0
56	MG	1A	3147	1/1	0.96	0.07	50,50,50,50	0
56	MG	2a	1753	1/1	0.96	0.15	45,45,45,45	0
56	MG	2a	1733	1/1	0.96	0.12	56,56,56,56	0
56	MG	1A	3866	1/1	0.96	0.23	20,20,20,20	0
56	MG	1A	3028	1/1	0.96	0.34	20,20,20,20	0
56	MG	1A	3498	1/1	0.96	0.15	39,39,39,39	0
56	MG	2a	1781	1/1	0.96	0.10	67,67,67,67	0
56	MG	1a	3041	1/1	0.96	0.05	51,51,51,51	0
56	MG	2A	3622	1/1	0.96	0.11	55,55,55,55	0
56	MG	2a	1619	1/1	0.96	0.34	53,53,53,53	0
56	MG	1A	3295	1/1	0.96	0.11	38,38,38,38	0
56	MG	1A	3477	1/1	0.96	0.23	32,32,32,32	0
56	MG	2A	3084	1/1	0.96	0.18	29,29,29,29	0
56	MG	1A	3702	1/1	0.96	0.07	23,23,23,23	0
56	MG	1A	3773	1/1	0.96	0.10	15,15,15,15	0
56	MG	2A	3398	1/1	0.96	0.24	26,26,26,26	0
56	MG	2A	3359	1/1	0.96	0.20	52,52,52,52	0
56	MG	1A	3752	1/1	0.96	0.45	36,36,36,36	0
56	MG	2y	3004	1/1	0.96	0.17	36,36,36,36	0
56	MG	1A	3725	1/1	0.96	0.17	30,30,30,30	0
56	MG	2A	3260	1/1	0.96	0.16	48,48,48,48	0
56	MG	1A	3066	1/1	0.96	0.06	22,22,22,22	0
56	MG	2D	303	1/1	0.96	0.34	41,41,41,41	0
56	MG	1A	3233	1/1	0.96	0.43	35,35,35,35	0
56	MG	2A	3541	1/1	0.96	0.14	32,32,32,32	0
56	MG	1A	3539	1/1	0.96	0.07	20,20,20,20	0
56	MG	1a	3085	1/1	0.96	0.21	33,33,33,33	0
56	MG	1A	3736	1/1	0.96	0.24	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3579	1/1	0.96	0.18	31,31,31,31	0
56	MG	2a	1717	1/1	0.96	0.08	66,66,66,66	0
56	MG	1A	3949	1/1	0.96	0.11	18,18,18,18	0
56	MG	1A	3206	1/1	0.96	0.13	30,30,30,30	0
56	MG	1W	3005	1/1	0.96	0.14	21,21,21,21	0
56	MG	2w	103	1/1	0.96	0.09	44,44,44,44	0
57	K	1A	4028	1/1	0.96	0.10	40,40,40,40	0
56	MG	1a	3195	1/1	0.96	0.06	45,45,45,45	0
56	MG	1A	3437	1/1	0.96	0.11	52,52,52,52	0
56	MG	1A	4032	1/1	0.96	0.49	30,30,30,30	0
56	MG	2A	3009	1/1	0.96	0.14	29,29,29,29	0
56	MG	2A	3341	1/1	0.96	0.17	39,39,39,39	0
56	MG	2A	3713	1/1	0.96	0.18	26,26,26,26	0
56	MG	1A	3126	1/1	0.96	0.48	21,21,21,21	0
56	MG	1D	306	1/1	0.96	0.10	17,17,17,17	0
56	MG	1A	3320	1/1	0.96	0.07	48,48,48,48	0
56	MG	1A	3822	1/1	0.96	0.10	45,45,45,45	0
56	MG	2A	3203	1/1	0.96	0.12	53,53,53,53	0
56	MG	2A	3403	1/1	0.96	0.26	29,29,29,29	0
56	MG	2A	3162	1/1	0.96	0.08	54,54,54,54	0
56	MG	2A	3711	1/1	0.96	0.07	37,37,37,37	0
56	MG	1B	206	1/1	0.96	0.07	36,36,36,36	0
56	MG	1A	3910	1/1	0.96	0.10	32,32,32,32	0
56	MG	1A	3010	1/1	0.96	0.21	33,33,33,33	0
56	MG	1A	3875	1/1	0.96	0.17	43,43,43,43	0
56	MG	2A	3284	1/1	0.96	0.08	37,37,37,37	0
56	MG	1A	3936	1/1	0.96	0.08	49,49,49,49	0
56	MG	2A	3451	1/1	0.96	0.09	44,44,44,44	0
56	MG	2A	3268	1/1	0.96	0.10	47,47,47,47	0
56	MG	1A	3489	1/1	0.96	0.22	30,30,30,30	0
56	MG	18	101	1/1	0.96	0.34	37,37,37,37	0
56	MG	1Q	201	1/1	0.96	0.36	33,33,33,33	0
56	MG	2A	3597	1/1	0.96	0.12	34,34,34,34	0
56	MG	1B	223	1/1	0.96	0.10	51,51,51,51	0
56	MG	1A	3419	1/1	0.96	0.14	42,42,42,42	0
56	MG	1A	3999	1/1	0.96	0.17	25,25,25,25	0
56	MG	2E	301	1/1	0.96	0.14	33,33,33,33	0
56	MG	2A	3525	1/1	0.96	0.27	52,52,52,52	0
56	MG	1A	3122	1/1	0.96	0.13	32,32,32,32	0
56	MG	1A	4051	1/1	0.96	0.22	13,13,13,13	0
56	MG	1A	3588	1/1	0.96	0.16	32,32,32,32	0
56	MG	2A	3150	1/1	0.96	0.21	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3229	1/1	0.96	0.15	28,28,28,28	0
56	MG	1A	3974	1/1	0.96	0.11	50,50,50,50	0
56	MG	1a	3080	1/1	0.96	0.23	46,46,46,46	0
56	MG	1A	3406	1/1	0.96	0.28	48,48,48,48	0
56	MG	1A	3033	1/1	0.96	0.12	21,21,21,21	0
56	MG	2A	3734	1/1	0.96	0.16	25,25,25,25	0
56	MG	2A	3496	1/1	0.96	0.11	37,37,37,37	0
56	MG	2A	3192	1/1	0.96	0.30	54,54,54,54	0
56	MG	1a	3125	1/1	0.96	0.12	42,42,42,42	0
56	MG	1a	3172	1/1	0.96	0.07	46,46,46,46	0
56	MG	1A	3157	1/1	0.96	0.08	50,50,50,50	0
56	MG	2A	3462	1/1	0.96	0.14	54,54,54,54	0
56	MG	2a	1810	1/1	0.96	0.15	81,81,81,81	0
56	MG	1A	3008	1/1	0.96	0.16	18,18,18,18	0
56	MG	2A	3165	1/1	0.96	0.18	40,40,40,40	0
56	MG	1A	3049	1/1	0.96	0.10	21,21,21,21	0
56	MG	1A	3139	1/1	0.96	0.19	21,21,21,21	0
56	MG	1a	3160	1/1	0.96	0.09	52,52,52,52	0
56	MG	1A	3688	1/1	0.96	0.20	21,21,21,21	0
56	MG	1A	3540	1/1	0.96	0.11	46,46,46,46	0
56	MG	1A	3717	1/1	0.96	0.10	45,45,45,45	0
56	MG	2a	1763	1/1	0.96	0.10	72,72,72,72	0
56	MG	1a	3082	1/1	0.96	0.47	41,41,41,41	0
56	MG	2A	3422	1/1	0.96	0.19	49,49,49,49	0
56	MG	2A	3143	1/1	0.96	0.13	41,41,41,41	0
56	MG	1A	3617	1/1	0.96	0.10	45,45,45,45	0
56	MG	2A	3303	1/1	0.96	0.17	35,35,35,35	0
56	MG	1A	3689	1/1	0.96	0.39	20,20,20,20	0
56	MG	1A	3180	1/1	0.96	0.14	42,42,42,42	0
56	MG	1A	3520	1/1	0.96	0.11	11,11,11,11	0
56	MG	1A	3394	1/1	0.96	0.23	37,37,37,37	0
56	MG	1a	3198	1/1	0.96	0.25	46,46,46,46	0
56	MG	2A	3418	1/1	0.96	0.06	46,46,46,46	0
56	MG	1A	3451	1/1	0.96	0.28	24,24,24,24	0
56	MG	1A	3149	1/1	0.96	0.60	28,28,28,28	0
56	MG	1A	4031	1/1	0.96	0.42	35,35,35,35	0
56	MG	2A	3412	1/1	0.96	0.14	47,47,47,47	0
56	MG	1A	3196	1/1	0.96	0.12	34,34,34,34	0
56	MG	2A	3405	1/1	0.96	0.15	35,35,35,35	0
56	MG	1A	3776	1/1	0.96	0.20	25,25,25,25	0
56	MG	2A	3508	1/1	0.96	0.18	57,57,57,57	0
56	MG	1E	311	1/1	0.96	0.46	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3124	1/1	0.96	0.07	33,33,33,33	0
56	MG	1A	3067	1/1	0.96	0.08	22,22,22,22	0
56	MG	1A	3095	1/1	0.96	0.43	28,28,28,28	0
56	MG	2a	1712	1/1	0.96	0.09	63,63,63,63	0
56	MG	2a	1668	1/1	0.96	0.17	55,55,55,55	0
56	MG	1A	3501	1/1	0.96	0.21	30,30,30,30	0
56	MG	1A	3543	1/1	0.96	0.14	20,20,20,20	0
56	MG	1a	3182	1/1	0.96	0.15	45,45,45,45	0
56	MG	2A	3521	1/1	0.96	0.07	63,63,63,63	0
56	MG	1a	3153	1/1	0.96	0.10	52,52,52,52	0
56	MG	1a	3173	1/1	0.96	0.18	39,39,39,39	0
56	MG	1A	3946	1/1	0.96	0.11	46,46,46,46	0
56	MG	2A	3270	1/1	0.96	0.33	34,34,34,34	0
56	MG	1A	3625	1/1	0.96	0.26	10,10,10,10	0
56	MG	1A	3874	1/1	0.96	0.16	36,36,36,36	0
56	MG	2A	3602	1/1	0.96	0.19	62,62,62,62	0
56	MG	1A	3930	1/1	0.96	0.23	33,33,33,33	0
56	MG	2A	3696	1/1	0.96	0.09	39,39,39,39	0
56	MG	1E	309	1/1	0.97	0.16	15,15,15,15	0
56	MG	2A	3072	1/1	0.97	0.29	32,32,32,32	0
56	MG	2A	3172	1/1	0.97	0.32	48,48,48,48	0
56	MG	1U	201	1/1	0.97	0.10	20,20,20,20	0
56	MG	1A	3676	1/1	0.97	0.17	31,31,31,31	0
56	MG	1A	3275	1/1	0.97	0.14	25,25,25,25	0
56	MG	1A	3268	1/1	0.97	0.16	31,31,31,31	0
56	MG	1A	4019	1/1	0.97	0.27	26,26,26,26	0
56	MG	1a	3031	1/1	0.97	0.06	54,54,54,54	0
56	MG	1a	3086	1/1	0.97	0.07	60,60,60,60	0
56	MG	1A	3567	1/1	0.97	0.21	13,13,13,13	0
56	MG	1Q	202	1/1	0.97	0.16	28,28,28,28	0
56	MG	2A	3368	1/1	0.97	0.13	36,36,36,36	0
56	MG	1A	3155	1/1	0.97	0.14	29,29,29,29	0
56	MG	2A	3453	1/1	0.97	0.18	34,34,34,34	0
56	MG	2A	3077	1/1	0.97	0.10	41,41,41,41	0
56	MG	1A	3742	1/1	0.97	0.14	28,28,28,28	0
56	MG	1A	3392	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	3040	1/1	0.97	0.06	30,30,30,30	0
56	MG	1A	3068	1/1	0.97	0.35	41,41,41,41	0
56	MG	1O	204	1/1	0.97	0.10	45,45,45,45	0
56	MG	2A	3235	1/1	0.97	0.18	40,40,40,40	0
56	MG	2A	3608	1/1	0.97	0.13	48,48,48,48	0
59	ZN	2Y	501	1/1	0.97	0.15	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3519	1/1	0.97	0.14	35,35,35,35	0
56	MG	1A	3538	1/1	0.97	0.06	45,45,45,45	0
56	MG	2A	3336	1/1	0.97	0.14	58,58,58,58	0
56	MG	2A	3016	1/1	0.97	0.20	32,32,32,32	0
56	MG	1A	3270	1/1	0.97	0.09	31,31,31,31	0
56	MG	1G	3002	1/1	0.97	0.15	39,39,39,39	0
56	MG	1a	3002	1/1	0.97	0.10	46,46,46,46	0
56	MG	1A	3184	1/1	0.97	0.14	14,14,14,14	0
56	MG	1a	3058	1/1	0.97	0.07	58,58,58,58	0
56	MG	2A	3627	1/1	0.97	0.14	50,50,50,50	0
56	MG	2A	3648	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	3850	1/1	0.97	0.40	43,43,43,43	0
56	MG	1A	3734	1/1	0.97	0.08	42,42,42,42	0
56	MG	1A	3870	1/1	0.97	0.09	55,55,55,55	0
56	MG	1b	3001	1/1	0.97	0.15	69,69,69,69	0
56	MG	1A	3454	1/1	0.97	0.37	30,30,30,30	0
56	MG	1A	3165	1/1	0.97	0.07	31,31,31,31	0
56	MG	1A	3927	1/1	0.97	0.29	37,37,37,37	0
56	MG	1Z	3004	1/1	0.97	0.14	41,41,41,41	0
56	MG	1O	202	1/1	0.97	0.24	56,56,56,56	0
56	MG	1A	3723	1/1	0.97	0.10	34,34,34,34	0
56	MG	1A	4017	1/1	0.97	0.41	37,37,37,37	0
56	MG	1A	3824	1/1	0.97	0.13	33,33,33,33	0
56	MG	1A	3906	1/1	0.97	0.17	60,60,60,60	0
56	MG	2A	3387	1/1	0.97	0.09	50,50,50,50	0
56	MG	2a	1660	1/1	0.97	0.13	59,59,59,59	0
56	MG	1A	3128	1/1	0.97	0.31	27,27,27,27	0
56	MG	2A	3063	1/1	0.97	0.14	43,43,43,43	0
56	MG	2A	3164	1/1	0.97	0.37	53,53,53,53	0
56	MG	1a	3202	1/1	0.97	0.06	45,45,45,45	0
56	MG	2A	3047	1/1	0.97	0.14	60,60,60,60	0
56	MG	1A	3663	1/1	0.97	0.13	43,43,43,43	0
56	MG	1A	3665	1/1	0.97	0.13	12,12,12,12	0
56	MG	2A	3575	1/1	0.97	0.12	46,46,46,46	0
56	MG	1A	3045	1/1	0.97	0.17	13,13,13,13	0
56	MG	2A	3388	1/1	0.97	0.17	25,25,25,25	0
56	MG	1A	3583	1/1	0.97	0.18	22,22,22,22	0
56	MG	1B	238	1/1	0.97	0.10	23,23,23,23	0
56	MG	2a	1787	1/1	0.97	0.06	53,53,53,53	0
56	MG	2E	302	1/1	0.97	0.09	44,44,44,44	0
56	MG	1D	304	1/1	0.97	0.68	43,43,43,43	0
56	MG	1A	3840	1/1	0.97	0.17	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2B	3020	1/1	0.97	0.14	54,54,54,54	0
56	MG	15	105	1/1	0.97	0.46	33,33,33,33	0
56	MG	1A	3552	1/1	0.97	0.14	23,23,23,23	0
59	ZN	1n	501	1/1	0.97	0.11	51,51,51,51	0
56	MG	1A	3220	1/1	0.97	0.08	24,24,24,24	0
56	MG	1A	3996	1/1	0.97	0.17	49,49,49,49	0
56	MG	1a	3035	1/1	0.97	0.22	49,49,49,49	0
56	MG	1A	3604	1/1	0.97	0.11	28,28,28,28	0
56	MG	1A	3716	1/1	0.97	0.10	45,45,45,45	0
56	MG	2A	3673	1/1	0.97	0.17	47,47,47,47	0
56	MG	2A	3647	1/1	0.97	0.11	51,51,51,51	0
56	MG	1A	3032	1/1	0.97	0.14	26,26,26,26	0
56	MG	1A	3863	1/1	0.97	0.11	56,56,56,56	0
56	MG	1f	3001	1/1	0.97	0.11	31,31,31,31	0
56	MG	1A	3656	1/1	0.97	0.19	25,25,25,25	0
56	MG	2a	1827	1/1	0.97	0.19	58,58,58,58	0
56	MG	1A	3077	1/1	0.97	0.44	21,21,21,21	0
56	MG	1A	3830	1/1	0.97	0.26	39,39,39,39	0
56	MG	2A	3144	1/1	0.97	0.10	33,33,33,33	0
56	MG	2A	3109	1/1	0.97	0.25	39,39,39,39	0
56	MG	1A	3856	1/1	0.97	0.06	62,62,62,62	0
56	MG	1A	3846	1/1	0.97	0.10	48,48,48,48	0
56	MG	2A	3589	1/1	0.97	0.26	45,45,45,45	0
56	MG	2A	3686	1/1	0.97	0.15	40,40,40,40	0
56	MG	2A	3540	1/1	0.97	0.09	37,37,37,37	0
56	MG	2A	3364	1/1	0.97	0.08	45,45,45,45	0
56	MG	2A	3511	1/1	0.97	0.14	39,39,39,39	0
56	MG	1A	3130	1/1	0.97	0.23	10,10,10,10	0
56	MG	1A	3358	1/1	0.97	0.13	44,44,44,44	0
56	MG	1A	3655	1/1	0.97	0.14	11,11,11,11	0
56	MG	1A	3163	1/1	0.97	0.08	24,24,24,24	0
56	MG	1A	3173	1/1	0.97	0.29	34,34,34,34	0
56	MG	2a	1699	1/1	0.97	0.05	58,58,58,58	0
56	MG	1A	3821	1/1	0.97	0.11	32,32,32,32	0
56	MG	1a	3098	1/1	0.97	0.16	39,39,39,39	0
56	MG	1A	3873	1/1	0.97	0.17	42,42,42,42	0
56	MG	1B	222	1/1	0.97	0.22	48,48,48,48	0
56	MG	2A	3694	1/1	0.97	0.09	54,54,54,54	0
56	MG	1A	3643	1/1	0.97	0.40	29,29,29,29	0
56	MG	2A	3704	1/1	0.97	0.14	37,37,37,37	0
56	MG	1A	3728	1/1	0.97	0.12	39,39,39,39	0
56	MG	1A	3090	1/1	0.97	0.24	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3518	1/1	0.97	0.11	41,41,41,41	0
56	MG	1A	3541	1/1	0.97	0.10	35,35,35,35	0
56	MG	1A	3868	1/1	0.97	0.14	24,24,24,24	0
56	MG	2a	1816	1/1	0.97	0.15	48,48,48,48	0
56	MG	2A	3633	1/1	0.97	0.13	66,66,66,66	0
56	MG	1D	305	1/1	0.97	0.24	28,28,28,28	0
56	MG	1A	3911	1/1	0.97	0.10	29,29,29,29	0
56	MG	2A	3078	1/1	0.97	0.11	54,54,54,54	0
56	MG	2A	3751	1/1	0.97	0.78	44,44,44,44	0
56	MG	1A	3442	1/1	0.97	0.22	36,36,36,36	0
56	MG	1A	3556	1/1	0.97	0.15	20,20,20,20	0
56	MG	1F	309	1/1	0.97	0.33	50,50,50,50	0
56	MG	1a	3215	1/1	0.97	0.07	39,39,39,39	0
56	MG	1A	3686	1/1	0.97	0.16	18,18,18,18	0
56	MG	2A	3068	1/1	0.97	0.04	35,35,35,35	0
56	MG	2A	3038	1/1	0.97	0.16	33,33,33,33	0
56	MG	1A	3764	1/1	0.97	0.15	24,24,24,24	0
56	MG	1A	3433	1/1	0.97	0.08	50,50,50,50	0
56	MG	2P	201	1/1	0.97	0.13	54,54,54,54	0
56	MG	1A	3678	1/1	0.97	0.16	22,22,22,22	0
56	MG	1X	106	1/1	0.97	0.15	21,21,21,21	0
56	MG	1a	3184	1/1	0.97	0.08	49,49,49,49	0
56	MG	1A	3962	1/1	0.97	0.08	23,23,23,23	0
56	MG	1A	3633	1/1	0.97	0.10	52,52,52,52	0
56	MG	2A	3344	1/1	0.97	0.11	24,24,24,24	0
56	MG	1A	3614	1/1	0.97	0.15	15,15,15,15	0
56	MG	1A	3236	1/1	0.97	0.21	35,35,35,35	0
56	MG	1A	3385	1/1	0.97	0.30	29,29,29,29	0
56	MG	1A	3496	1/1	0.97	0.09	35,35,35,35	0
56	MG	2A	3323	1/1	0.97	0.43	31,31,31,31	0
56	MG	1a	3054	1/1	0.97	0.06	46,46,46,46	0
56	MG	1a	3107	1/1	0.97	0.20	39,39,39,39	0
56	MG	1A	3964	1/1	0.97	0.27	45,45,45,45	0
56	MG	1A	3842	1/1	0.97	0.07	34,34,34,34	0
56	MG	1A	3589	1/1	0.97	0.12	23,23,23,23	0
56	MG	1N	205	1/1	0.97	0.49	48,48,48,48	0
56	MG	12	3002	1/1	0.97	0.19	35,35,35,35	0
56	MG	1A	4064	1/1	0.97	0.26	30,30,30,30	0
56	MG	2A	3275	1/1	0.97	0.09	37,37,37,37	0
56	MG	2a	1830	1/1	0.97	0.16	71,71,71,71	0
56	MG	1A	3162	1/1	0.97	0.13	24,24,24,24	0
56	MG	2a	1689	1/1	0.97	0.08	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4034	1/1	0.97	0.58	28,28,28,28	0
56	MG	1a	3079	1/1	0.97	0.14	47,47,47,47	0
56	MG	1A	3778	1/1	0.97	0.17	13,13,13,13	0
56	MG	2A	3148	1/1	0.97	0.06	34,34,34,34	0
56	MG	1R	203	1/1	0.97	0.49	34,34,34,34	0
56	MG	1A	3517	1/1	0.97	0.15	28,28,28,28	0
56	MG	1A	3017	1/1	0.97	0.11	19,19,19,19	0
56	MG	2a	1676	1/1	0.97	0.19	48,48,48,48	0
56	MG	2A	3029	1/1	0.97	0.14	36,36,36,36	0
56	MG	2A	3041	1/1	0.97	0.12	46,46,46,46	0
56	MG	1A	3022	1/1	0.97	0.13	22,22,22,22	0
56	MG	1A	3578	1/1	0.97	0.14	23,23,23,23	0
56	MG	1A	3729	1/1	0.97	0.18	49,49,49,49	0
56	MG	1a	3025	1/1	0.97	0.16	24,24,24,24	0
56	MG	2A	3209	1/1	0.97	0.08	35,35,35,35	0
56	MG	1A	3343	1/1	0.97	0.24	30,30,30,30	0
56	MG	1A	3164	1/1	0.97	0.17	12,12,12,12	0
56	MG	1A	3015	1/1	0.97	0.16	37,37,37,37	0
56	MG	2A	3119	1/1	0.97	0.12	41,41,41,41	0
56	MG	2a	1741	1/1	0.97	0.09	57,57,57,57	0
56	MG	2A	3693	1/1	0.97	0.05	68,68,68,68	0
56	MG	2A	3367	1/1	0.97	0.13	28,28,28,28	0
56	MG	1B	217	1/1	0.97	0.17	44,44,44,44	0
56	MG	2A	3091	1/1	0.97	0.30	38,38,38,38	0
56	MG	2A	3306	1/1	0.97	0.22	47,47,47,47	0
56	MG	1E	305	1/1	0.97	0.23	50,50,50,50	0
56	MG	2A	3428	1/1	0.97	0.17	43,43,43,43	0
56	MG	1A	3097	1/1	0.97	0.09	24,24,24,24	0
56	MG	15	102	1/1	0.97	0.19	22,22,22,22	0
59	ZN	29	501	1/1	0.97	0.07	63,63,63,63	0
56	MG	2a	1659	1/1	0.97	0.12	47,47,47,47	0
56	MG	1a	3127	1/1	0.97	0.08	48,48,48,48	0
56	MG	1A	3530	1/1	0.97	0.22	25,25,25,25	0
56	MG	2A	3060	1/1	0.97	0.20	32,32,32,32	0
56	MG	1A	3745	1/1	0.97	0.13	33,33,33,33	0
56	MG	1A	3502	1/1	0.97	0.33	20,20,20,20	0
56	MG	1A	3610	1/1	0.97	0.17	45,45,45,45	0
56	MG	1A	3404	1/1	0.97	0.26	28,28,28,28	0
56	MG	1a	3028	1/1	0.97	0.14	37,37,37,37	0
56	MG	1A	3615	1/1	0.97	0.11	12,12,12,12	0
56	MG	1A	3908	1/1	0.97	0.14	27,27,27,27	0
56	MG	2A	3611	1/1	0.97	0.13	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1B	219	1/1	0.97	0.12	27,27,27,27	0
56	MG	2A	3522	1/1	0.97	0.08	49,49,49,49	0
56	MG	1E	302	1/1	0.97	0.37	16,16,16,16	0
56	MG	1a	3078	1/1	0.97	0.11	48,48,48,48	0
56	MG	1a	3071	1/1	0.97	0.10	43,43,43,43	0
56	MG	1A	3829	1/1	0.97	0.17	43,43,43,43	0
56	MG	1A	3623	1/1	0.97	0.15	41,41,41,41	0
56	MG	1A	4020	1/1	0.97	0.30	50,50,50,50	0
56	MG	1A	3701	1/1	0.97	0.10	15,15,15,15	0
56	MG	2A	3548	1/1	0.97	0.13	51,51,51,51	0
56	MG	1A	3814	1/1	0.97	0.14	8,8,8,8	0
56	MG	1a	3106	1/1	0.97	0.13	52,52,52,52	0
56	MG	1A	3893	1/1	0.97	0.27	27,27,27,27	0
56	MG	2A	3407	1/1	0.97	0.15	35,35,35,35	0
56	MG	2A	3149	1/1	0.97	0.27	57,57,57,57	0
56	MG	2A	3423	1/1	0.97	0.12	22,22,22,22	0
56	MG	1A	3668	1/1	0.97	0.14	22,22,22,22	0
56	MG	1Y	503	1/1	0.97	0.40	42,42,42,42	0
56	MG	1a	3016	1/1	0.97	0.12	38,38,38,38	0
56	MG	1A	3260	1/1	0.97	0.15	18,18,18,18	0
56	MG	2A	3455	1/1	0.97	0.15	42,42,42,42	0
56	MG	2A	3717	1/1	0.97	0.11	57,57,57,57	0
56	MG	1I	101	1/1	0.97	0.11	28,28,28,28	0
56	MG	2E	304	1/1	0.97	0.20	49,49,49,49	0
56	MG	1E	304	1/1	0.97	0.33	22,22,22,22	0
56	MG	1A	3757	1/1	0.97	0.23	22,22,22,22	0
56	MG	2A	3362	1/1	0.97	0.09	58,58,58,58	0
56	MG	1A	3848	1/1	0.97	0.10	34,34,34,34	0
56	MG	2A	3085	1/1	0.97	0.18	48,48,48,48	0
56	MG	1A	3255	1/1	0.97	0.11	36,36,36,36	0
56	MG	2A	3452	1/1	0.97	0.22	32,32,32,32	0
56	MG	1x	107	1/1	0.97	0.20	46,46,46,46	0
56	MG	1A	3509	1/1	0.97	0.18	31,31,31,31	0
56	MG	1A	3021	1/1	0.97	0.13	29,29,29,29	0
56	MG	1A	3925	1/1	0.97	0.17	12,12,12,12	0
56	MG	2A	3411	1/1	0.97	0.14	27,27,27,27	0
56	MG	2A	3750	1/1	0.97	0.28	40,40,40,40	0
56	MG	2E	308	1/1	0.97	0.09	49,49,49,49	0
57	K	2A	3327	1/1	0.97	0.11	29,29,29,29	0
56	MG	1F	302	1/1	0.97	0.32	30,30,30,30	0
56	MG	2A	3324	1/1	0.97	0.06	40,40,40,40	0
56	MG	1A	3034	1/1	0.97	0.22	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3561	1/1	0.97	0.11	17,17,17,17	0
56	MG	2A	3669	1/1	0.97	0.20	27,27,27,27	0
56	MG	1a	3121	1/1	0.97	0.15	54,54,54,54	0
56	MG	2A	3151	1/1	0.97	0.09	47,47,47,47	0
56	MG	2r	3001	1/1	0.97	0.15	56,56,56,56	0
56	MG	1A	3634	1/1	0.97	0.12	28,28,28,28	0
56	MG	2E	310	1/1	0.97	0.09	50,50,50,50	0
56	MG	1A	3657	1/1	0.97	0.13	23,23,23,23	0
56	MG	1A	3784	1/1	0.97	0.12	57,57,57,57	0
56	MG	1A	3690	1/1	0.97	0.10	42,42,42,42	0
56	MG	1A	4010	1/1	0.97	0.13	23,23,23,23	0
56	MG	2A	3671	1/1	0.97	0.18	29,29,29,29	0
56	MG	1a	3114	1/1	0.97	0.10	68,68,68,68	0
56	MG	1A	3918	1/1	0.97	0.11	33,33,33,33	0
56	MG	1A	3337	1/1	0.97	0.60	27,27,27,27	0
56	MG	10	101	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3225	1/1	0.97	0.12	40,40,40,40	0
56	MG	1A	4044	1/1	0.97	0.27	29,29,29,29	0
56	MG	2A	3561	1/1	0.97	0.18	56,56,56,56	0
56	MG	1A	3186	1/1	0.97	0.20	27,27,27,27	0
56	MG	1A	3114	1/1	0.97	0.32	22,22,22,22	0
56	MG	1A	3051	1/1	0.97	0.17	22,22,22,22	0
56	MG	1A	3952	1/1	0.97	0.14	50,50,50,50	0
56	MG	2a	1726	1/1	0.97	0.13	64,64,64,64	0
56	MG	2A	3527	1/1	0.97	0.18	52,52,52,52	0
56	MG	2A	3090	1/1	0.97	0.15	32,32,32,32	0
56	MG	2A	3062	1/1	0.97	0.14	47,47,47,47	0
56	MG	1A	3755	1/1	0.97	0.20	21,21,21,21	0
56	MG	2B	3021	1/1	0.97	0.18	59,59,59,59	0
56	MG	1A	3748	1/1	0.97	0.10	38,38,38,38	0
56	MG	2A	3122	1/1	0.97	0.15	26,26,26,26	0
56	MG	1A	3452	1/1	0.97	0.28	30,30,30,30	0
56	MG	1A	3954	1/1	0.97	0.15	53,53,53,53	0
56	MG	2A	3401	1/1	0.97	0.19	32,32,32,32	0
57	K	2A	3745	1/1	0.97	0.08	53,53,53,53	0
56	MG	2A	3634	1/1	0.97	0.21	48,48,48,48	0
56	MG	1A	3132	1/1	0.97	0.15	37,37,37,37	0
56	MG	2A	3740	1/1	0.97	0.22	37,37,37,37	0
56	MG	2A	3500	1/1	0.97	0.13	49,49,49,49	0
56	MG	1a	3136	1/1	0.97	0.12	49,49,49,49	0
56	MG	1A	3448	1/1	0.97	0.18	37,37,37,37	0
56	MG	2A	3736	1/1	0.97	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3038	1/1	0.97	0.22	25,25,25,25	0
56	MG	1A	3858	1/1	0.97	0.17	54,54,54,54	0
56	MG	2a	1735	1/1	0.97	0.18	50,50,50,50	0
56	MG	1A	3599	1/1	0.97	0.11	15,15,15,15	0
56	MG	2A	3030	1/1	0.97	0.08	25,25,25,25	0
56	MG	1A	3871	1/1	0.97	0.05	59,59,59,59	0
56	MG	2A	3509	1/1	0.97	0.20	52,52,52,52	0
56	MG	1F	301	1/1	0.98	0.58	23,23,23,23	0
56	MG	2a	1703	1/1	0.98	0.12	41,41,41,41	0
56	MG	1A	3483	1/1	0.98	0.39	32,32,32,32	0
56	MG	1A	3577	1/1	0.98	0.13	54,54,54,54	0
56	MG	1A	4005	1/1	0.98	0.22	10,10,10,10	0
56	MG	2A	3712	1/1	0.98	0.15	35,35,35,35	0
56	MG	1A	3738	1/1	0.98	0.09	32,32,32,32	0
56	MG	2A	3032	1/1	0.98	0.12	41,41,41,41	0
56	MG	1A	3661	1/1	0.98	0.17	18,18,18,18	0
56	MG	2a	1665	1/1	0.98	0.15	49,49,49,49	0
56	MG	2a	1832	1/1	0.98	0.13	37,37,37,37	0
56	MG	1A	3685	1/1	0.98	0.22	21,21,21,21	0
56	MG	2A	3668	1/1	0.98	0.12	41,41,41,41	0
56	MG	1A	3667	1/1	0.98	0.18	31,31,31,31	0
56	MG	1a	3045	1/1	0.98	0.11	52,52,52,52	0
56	MG	1A	3654	1/1	0.98	0.14	37,37,37,37	0
56	MG	1A	3535	1/1	0.98	0.09	23,23,23,23	0
56	MG	1O	203	1/1	0.98	0.16	48,48,48,48	0
56	MG	1a	3070	1/1	0.98	0.05	30,30,30,30	0
56	MG	1A	3009	1/1	0.98	0.11	24,24,24,24	0
56	MG	1A	3917	1/1	0.98	0.14	31,31,31,31	0
57	K	1A	3486	1/1	0.98	0.07	19,19,19,19	0
56	MG	1A	3353	1/1	0.98	0.43	35,35,35,35	0
60	SF4	2d	501	8/8	0.98	0.15	58,60,69,79	0
56	MG	2A	3379	1/1	0.98	0.09	41,41,41,41	0
56	MG	1a	3095	1/1	0.98	0.11	55,55,55,55	0
56	MG	1a	3204	1/1	0.98	0.11	44,44,44,44	0
56	MG	1A	3632	1/1	0.98	0.29	27,27,27,27	0
56	MG	1A	4050	1/1	0.98	0.28	26,26,26,26	0
56	MG	2A	3674	1/1	0.98	0.22	23,23,23,23	0
56	MG	2A	3594	1/1	0.98	0.12	54,54,54,54	0
56	MG	1A	3662	1/1	0.98	0.19	32,32,32,32	0
56	MG	1A	3001	1/1	0.98	0.09	32,32,32,32	0
56	MG	2A	3330	1/1	0.98	0.20	42,42,42,42	0
56	MG	2v	3005	1/1	0.98	0.15	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	1812	1/1	0.98	0.11	64,64,64,64	0
56	MG	2A	3120	1/1	0.98	0.13	38,38,38,38	0
56	MG	1A	3580	1/1	0.98	0.07	18,18,18,18	0
56	MG	1A	3031	1/1	0.98	0.31	34,34,34,34	0
56	MG	1E	303	1/1	0.98	0.24	22,22,22,22	0
56	MG	1A	3507	1/1	0.98	0.19	24,24,24,24	0
56	MG	1A	3865	1/1	0.98	0.18	18,18,18,18	0
56	MG	2a	1649	1/1	0.98	0.22	41,41,41,41	0
56	MG	2A	3721	1/1	0.98	0.07	50,50,50,50	0
56	MG	1A	3645	1/1	0.98	0.11	25,25,25,25	0
56	MG	1A	3896	1/1	0.98	0.20	42,42,42,42	0
56	MG	1A	4026	1/1	0.98	0.52	35,35,35,35	0
56	MG	1A	3855	1/1	0.98	0.04	49,49,49,49	0
56	MG	1A	3131	1/1	0.98	0.12	35,35,35,35	0
56	MG	2a	1758	1/1	0.98	0.07	52,52,52,52	0
56	MG	2A	3003	1/1	0.98	0.19	49,49,49,49	0
56	MG	2A	3475	1/1	0.98	0.20	37,37,37,37	0
56	MG	1A	3266	1/1	0.98	0.14	24,24,24,24	0
56	MG	1Q	203	1/1	0.98	0.22	28,28,28,28	0
56	MG	1A	3250	1/1	0.98	0.31	20,20,20,20	0
56	MG	2A	3631	1/1	0.98	0.11	53,53,53,53	0
56	MG	1A	3791	1/1	0.98	0.34	23,23,23,23	0
56	MG	2a	1731	1/1	0.98	0.09	56,56,56,56	0
56	MG	1A	3289	1/1	0.98	0.15	41,41,41,41	0
56	MG	2A	3459	1/1	0.98	0.08	50,50,50,50	0
56	MG	2A	3315	1/1	0.98	0.20	42,42,42,42	0
56	MG	1A	3142	1/1	0.98	0.12	17,17,17,17	0
56	MG	2a	1814	1/1	0.98	0.14	63,63,63,63	0
56	MG	1A	3642	1/1	0.98	0.09	34,34,34,34	0
56	MG	2a	1801	1/1	0.98	0.09	63,63,63,63	0
56	MG	1A	3972	1/1	0.98	0.15	49,49,49,49	0
56	MG	1A	3994	1/1	0.98	0.27	21,21,21,21	0
56	MG	1A	3390	1/1	0.98	0.10	43,43,43,43	0
56	MG	1A	3966	1/1	0.98	0.08	41,41,41,41	0
56	MG	1A	3156	1/1	0.98	0.26	27,27,27,27	0
56	MG	1A	4056	1/1	0.98	0.32	33,33,33,33	0
56	MG	1A	3328	1/1	0.98	0.41	25,25,25,25	0
56	MG	1A	3007	1/1	0.98	0.10	12,12,12,12	0
56	MG	1A	3727	1/1	0.98	0.05	42,42,42,42	0
56	MG	1A	3854	1/1	0.98	0.12	46,46,46,46	0
56	MG	2A	3369	1/1	0.98	0.14	53,53,53,53	0
56	MG	1A	3153	1/1	0.98	0.16	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3499	1/1	0.98	0.14	23,23,23,23	0
56	MG	1A	3810	1/1	0.98	0.15	40,40,40,40	0
56	MG	1A	3310	1/1	0.98	0.17	24,24,24,24	0
56	MG	2A	3415	1/1	0.98	0.18	47,47,47,47	0
56	MG	2A	3236	1/1	0.98	0.21	49,49,49,49	0
56	MG	2a	1679	1/1	0.98	0.14	44,44,44,44	0
56	MG	1A	3490	1/1	0.98	0.15	26,26,26,26	0
56	MG	2A	3440	1/1	0.98	0.13	51,51,51,51	0
56	MG	1A	3651	1/1	0.98	0.12	22,22,22,22	0
56	MG	2A	3363	1/1	0.98	0.15	43,43,43,43	0
56	MG	1A	3770	1/1	0.98	0.16	12,12,12,12	0
56	MG	2A	3325	1/1	0.98	0.51	63,63,63,63	0
56	MG	1E	312	1/1	0.98	0.15	44,44,44,44	0
56	MG	1D	312	1/1	0.98	0.25	27,27,27,27	0
56	MG	1A	3864	1/1	0.98	0.23	20,20,20,20	0
56	MG	1A	3809	1/1	0.98	0.09	30,30,30,30	0
56	MG	1A	3364	1/1	0.98	0.14	23,23,23,23	0
56	MG	1A	3519	1/1	0.98	0.17	21,21,21,21	0
56	MG	2A	3059	1/1	0.98	0.16	35,35,35,35	0
56	MG	2A	3534	1/1	0.98	0.11	53,53,53,53	0
56	MG	1A	3257	1/1	0.98	0.10	34,34,34,34	0
56	MG	1A	3325	1/1	0.98	0.14	33,33,33,33	0
56	MG	1A	3035	1/1	0.98	0.20	24,24,24,24	0
56	MG	1A	3091	1/1	0.98	0.18	31,31,31,31	0
56	MG	1a	3131	1/1	0.98	0.10	38,38,38,38	0
56	MG	1A	3995	1/1	0.98	0.10	32,32,32,32	0
56	MG	2A	3292	1/1	0.98	0.16	31,31,31,31	0
56	MG	1A	3652	1/1	0.98	0.15	23,23,23,23	0
56	MG	1A	3529	1/1	0.98	0.09	34,34,34,34	0
56	MG	1A	3023	1/1	0.98	0.16	43,43,43,43	0
56	MG	2a	1790	1/1	0.98	0.21	50,50,50,50	0
56	MG	2A	3709	1/1	0.98	0.14	40,40,40,40	0
56	MG	2A	3393	1/1	0.98	0.19	44,44,44,44	0
56	MG	1A	3318	1/1	0.98	0.20	46,46,46,46	0
56	MG	1A	4024	1/1	0.98	0.35	43,43,43,43	0
56	MG	2a	1734	1/1	0.98	0.11	48,48,48,48	0
56	MG	17	103	1/1	0.98	0.47	33,33,33,33	0
56	MG	1A	3573	1/1	0.98	0.09	24,24,24,24	0
56	MG	1A	3041	1/1	0.98	0.11	32,32,32,32	0
56	MG	1A	4000	1/1	0.98	0.07	29,29,29,29	0
60	SF4	1d	501	8/8	0.98	0.16	52,54,61,66	0
56	MG	1A	3003	1/1	0.98	0.20	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3064	1/1	0.98	0.11	12,12,12,12	0
56	MG	2a	1687	1/1	0.98	0.05	40,40,40,40	0
56	MG	1A	3607	1/1	0.98	0.13	19,19,19,19	0
56	MG	1A	3892	1/1	0.98	0.20	33,33,33,33	0
56	MG	2A	3404	1/1	0.98	0.18	39,39,39,39	0
56	MG	1A	3807	1/1	0.98	0.11	28,28,28,28	0
56	MG	2x	105	1/1	0.98	0.14	47,47,47,47	0
56	MG	1A	3120	1/1	0.98	0.33	29,29,29,29	0
56	MG	2A	3291	1/1	0.98	0.12	55,55,55,55	0
56	MG	2A	3641	1/1	0.98	0.13	50,50,50,50	0
56	MG	1x	113	1/1	0.98	0.12	58,58,58,58	0
56	MG	1A	3884	1/1	0.98	0.08	30,30,30,30	0
56	MG	2a	1698	1/1	0.98	0.07	60,60,60,60	0
56	MG	1A	3375	1/1	0.98	0.37	34,34,34,34	0
56	MG	1A	3481	1/1	0.98	0.12	28,28,28,28	0
56	MG	1A	3069	1/1	0.98	0.26	27,27,27,27	0
56	MG	1A	3485	1/1	0.98	0.22	21,21,21,21	0
56	MG	2a	1601	1/1	0.98	0.24	46,46,46,46	0
56	MG	1A	3497	1/1	0.98	0.10	23,23,23,23	0
56	MG	1A	3221	1/1	0.98	0.28	21,21,21,21	0
56	MG	1A	3732	1/1	0.98	0.07	45,45,45,45	0
56	MG	1a	3034	1/1	0.98	0.14	44,44,44,44	0
56	MG	1A	3211	1/1	0.98	0.23	30,30,30,30	0
59	ZN	25	501	1/1	0.98	0.18	45,45,45,45	0
56	MG	1A	3515	1/1	0.98	0.21	11,11,11,11	0
56	MG	1A	3605	1/1	0.98	0.09	14,14,14,14	0
56	MG	1a	3199	1/1	0.98	0.19	47,47,47,47	0
56	MG	1A	3978	1/1	0.98	0.08	33,33,33,33	0
56	MG	2a	1813	1/1	0.98	0.05	54,54,54,54	0
59	ZN	19	501	1/1	0.98	0.17	42,42,42,42	0
56	MG	2A	3320	1/1	0.98	0.20	17,17,17,17	0
56	MG	2v	3001	1/1	0.98	0.07	49,49,49,49	0
56	MG	2w	107	1/1	0.98	0.14	55,55,55,55	0
56	MG	1A	3084	1/1	0.98	0.10	35,35,35,35	0
56	MG	2w	108	1/1	0.98	0.08	68,68,68,68	0
56	MG	1A	3587	1/1	0.98	0.10	12,12,12,12	0
56	MG	1B	216	1/1	0.98	0.17	42,42,42,42	0
56	MG	1a	3201	1/1	0.98	0.06	44,44,44,44	0
56	MG	1B	234	1/1	0.98	0.06	41,41,41,41	0
56	MG	2A	3739	1/1	0.98	0.23	29,29,29,29	0
56	MG	2A	3661	1/1	0.98	0.26	36,36,36,36	0
56	MG	2A	3328	1/1	0.98	0.23	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3880	1/1	0.98	0.26	23,23,23,23	0
56	MG	1X	104	1/1	0.98	0.20	31,31,31,31	0
56	MG	1A	3088	1/1	0.98	0.20	32,32,32,32	0
59	ZN	26	501	1/1	0.98	0.09	59,59,59,59	0
56	MG	2A	3343	1/1	0.98	0.28	36,36,36,36	0
56	MG	2A	3556	1/1	0.98	0.20	46,46,46,46	0
56	MG	1A	3948	1/1	0.98	0.09	14,14,14,14	0
56	MG	2A	3662	1/1	0.98	0.26	28,28,28,28	0
56	MG	1a	3208	1/1	0.98	0.11	42,42,42,42	0
56	MG	2A	3469	1/1	0.98	0.29	39,39,39,39	0
56	MG	2A	3473	1/1	0.98	0.10	29,29,29,29	0
56	MG	1A	3181	1/1	0.98	0.08	43,43,43,43	0
56	MG	1A	3334	1/1	0.98	0.21	22,22,22,22	0
56	MG	1A	3223	1/1	0.98	0.20	34,34,34,34	0
56	MG	1A	3154	1/1	0.98	0.44	31,31,31,31	0
56	MG	1U	206	1/1	0.98	0.21	16,16,16,16	0
56	MG	1A	3099	1/1	0.98	0.24	23,23,23,23	0
56	MG	2a	1776	1/1	0.98	0.11	47,47,47,47	0
56	MG	1A	3011	1/1	0.98	0.09	20,20,20,20	0
56	MG	1A	3602	1/1	0.98	0.09	48,48,48,48	0
56	MG	2A	3335	1/1	0.98	0.11	49,49,49,49	0
56	MG	1A	4038	1/1	0.98	0.49	31,31,31,31	0
56	MG	1A	3915	1/1	0.98	0.07	34,34,34,34	0
56	MG	1A	3176	1/1	0.98	0.44	25,25,25,25	0
56	MG	2a	1766	1/1	0.98	0.14	36,36,36,36	0
56	MG	2y	3002	1/1	0.98	0.14	51,51,51,51	0
56	MG	1A	3395	1/1	0.98	0.14	33,33,33,33	0
56	MG	1A	3074	1/1	0.98	0.32	24,24,24,24	0
56	MG	2A	3089	1/1	0.98	0.16	40,40,40,40	0
56	MG	1A	3053	1/1	0.98	0.07	43,43,43,43	0
56	MG	1A	3983	1/1	0.98	0.17	32,32,32,32	0
56	MG	1A	4063	1/1	0.98	0.40	31,31,31,31	0
56	MG	1A	3286	1/1	0.98	0.15	34,34,34,34	0
56	MG	1A	3348	1/1	0.98	0.13	44,44,44,44	0
56	MG	1A	3693	1/1	0.98	0.12	40,40,40,40	0
56	MG	1A	3136	1/1	0.98	0.08	21,21,21,21	0
56	MG	2A	3754	1/1	0.98	0.26	43,43,43,43	0
56	MG	2A	3397	1/1	0.98	0.12	37,37,37,37	0
56	MG	2A	3557	1/1	0.98	0.24	27,27,27,27	0
56	MG	1A	3699	1/1	0.98	0.08	25,25,25,25	0
56	MG	2A	3243	1/1	0.98	0.18	49,49,49,49	0
56	MG	2A	3096	1/1	0.98	0.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3677	1/1	0.98	0.17	18,18,18,18	0
56	MG	2A	3026	1/1	0.98	0.09	43,43,43,43	0
56	MG	2A	3555	1/1	0.98	0.15	38,38,38,38	0
56	MG	2A	3437	1/1	0.98	0.24	39,39,39,39	0
56	MG	17	104	1/1	0.98	0.08	27,27,27,27	0
56	MG	1A	4057	1/1	0.98	0.21	27,27,27,27	0
56	MG	1A	4066	1/1	0.98	0.23	35,35,35,35	0
56	MG	1A	3013	1/1	0.98	0.10	14,14,14,14	0
56	MG	2A	3138	1/1	0.98	0.23	34,34,34,34	0
56	MG	1A	3116	1/1	0.98	0.17	26,26,26,26	0
56	MG	1A	3012	1/1	0.98	0.19	13,13,13,13	0
56	MG	2q	201	1/1	0.98	0.07	46,46,46,46	0
56	MG	1A	3932	1/1	0.98	0.23	13,13,13,13	0
56	MG	1A	3470	1/1	0.98	0.17	33,33,33,33	0
56	MG	2a	1706	1/1	0.98	0.05	54,54,54,54	0
56	MG	1A	3601	1/1	0.98	0.08	24,24,24,24	0
56	MG	2A	3043	1/1	0.98	0.10	40,40,40,40	0
56	MG	2A	3629	1/1	0.98	0.18	62,62,62,62	0
56	MG	1A	3754	1/1	0.98	0.22	22,22,22,22	0
56	MG	1A	3820	1/1	0.98	0.12	35,35,35,35	0
56	MG	2A	3051	1/1	0.99	0.05	46,46,46,46	0
56	MG	1W	3002	1/1	0.99	0.16	29,29,29,29	0
56	MG	1A	3800	1/1	0.99	0.20	54,54,54,54	0
56	MG	2A	3288	1/1	0.99	0.25	30,30,30,30	0
56	MG	1A	3267	1/1	0.99	0.12	24,24,24,24	0
56	MG	2a	1749	1/1	0.99	0.05	55,55,55,55	0
56	MG	1A	3585	1/1	0.99	0.16	30,30,30,30	0
56	MG	1A	3669	1/1	0.99	0.11	35,35,35,35	0
56	MG	2A	3114	1/1	0.99	0.28	29,29,29,29	0
56	MG	2A	3465	1/1	0.99	0.28	42,42,42,42	0
56	MG	1A	3635	1/1	0.99	0.22	25,25,25,25	0
56	MG	1A	3612	1/1	0.99	0.09	24,24,24,24	0
56	MG	1A	3639	1/1	0.99	0.09	39,39,39,39	0
56	MG	2A	3355	1/1	0.99	0.21	23,23,23,23	0
56	MG	1A	3254	1/1	0.99	0.29	11,11,11,11	0
56	MG	1A	3150	1/1	0.99	0.25	27,27,27,27	0
56	MG	2A	3395	1/1	0.99	0.21	33,33,33,33	0
56	MG	1W	3004	1/1	0.99	0.20	21,21,21,21	0
56	MG	1a	3185	1/1	0.99	0.10	26,26,26,26	0
56	MG	1a	3102	1/1	0.99	0.16	39,39,39,39	0
56	MG	2E	309	1/1	0.99	0.06	41,41,41,41	0
56	MG	1B	205	1/1	0.99	0.30	45,45,45,45	0

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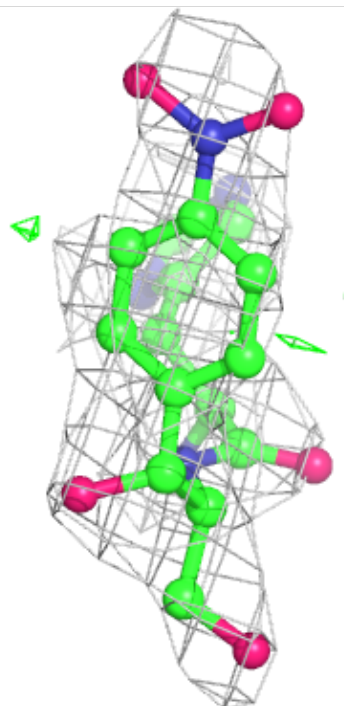
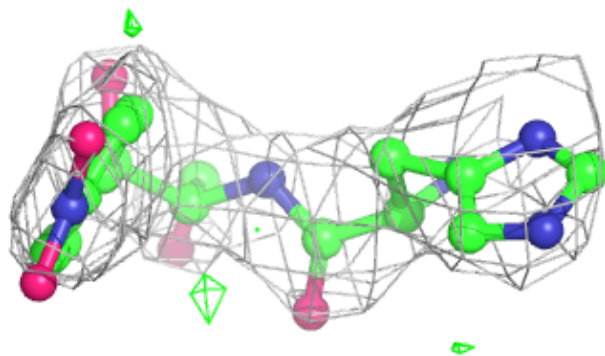
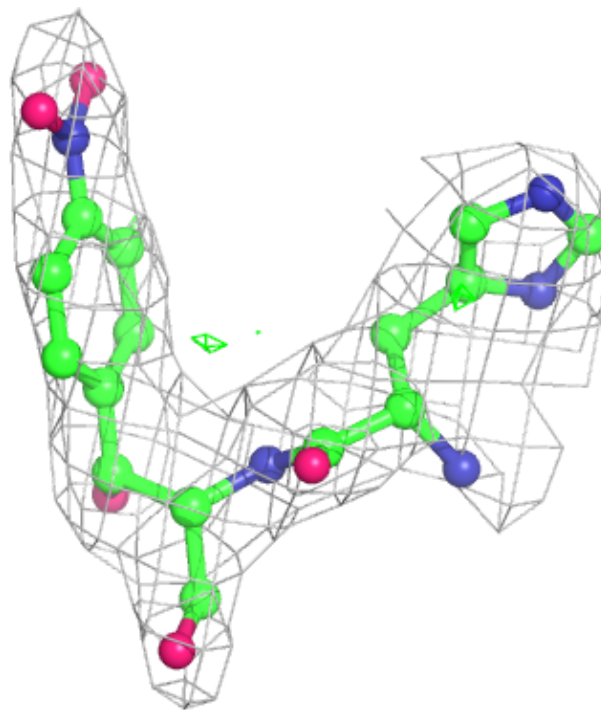
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3696	1/1	0.99	0.23	46,46,46,46	0
56	MG	1A	3544	1/1	0.99	0.08	12,12,12,12	0
56	MG	1A	3793	1/1	0.99	0.25	26,26,26,26	0
56	MG	1D	308	1/1	0.99	0.32	26,26,26,26	0
59	ZN	14	501	1/1	0.99	0.13	70,70,70,70	0
56	MG	1A	3557	1/1	0.99	0.08	25,25,25,25	0
56	MG	2A	3450	1/1	0.99	0.14	37,37,37,37	0
56	MG	1A	3161	1/1	0.99	0.24	20,20,20,20	0
59	ZN	1Y	501	1/1	0.99	0.14	58,58,58,58	0
56	MG	2A	3504	1/1	0.99	0.08	29,29,29,29	0
56	MG	1A	3522	1/1	0.99	0.15	30,30,30,30	0
56	MG	1A	3660	1/1	0.99	0.09	26,26,26,26	0
59	ZN	15	104	1/1	0.99	0.20	42,42,42,42	0
56	MG	2A	3129	1/1	0.99	0.19	54,54,54,54	0
56	MG	2A	3482	1/1	0.99	0.17	38,38,38,38	0
56	MG	1A	3214	1/1	0.99	0.31	32,32,32,32	0
56	MG	1a	3179	1/1	0.99	0.13	39,39,39,39	0
56	MG	1A	3258	1/1	0.99	0.20	33,33,33,33	0
56	MG	1A	3042	1/1	0.99	0.21	19,19,19,19	0
56	MG	1A	3115	1/1	0.99	0.20	39,39,39,39	0
56	MG	1U	204	1/1	0.99	0.26	23,23,23,23	0
56	MG	2A	3732	1/1	0.99	0.31	24,24,24,24	0
56	MG	2A	3505	1/1	0.99	0.08	42,42,42,42	0
56	MG	1w	109	1/1	0.99	0.41	37,37,37,37	0
56	MG	1A	3178	1/1	0.99	0.29	21,21,21,21	0
56	MG	2A	3171	1/1	0.99	0.05	51,51,51,51	0
56	MG	2A	3424	1/1	0.99	0.09	24,24,24,24	0
56	MG	1A	3393	1/1	0.99	0.22	24,24,24,24	0
56	MG	2A	3741	1/1	0.99	0.12	39,39,39,39	0
56	MG	2A	3649	1/1	0.99	0.13	21,21,21,21	0
56	MG	1A	3636	1/1	0.99	0.16	21,21,21,21	0
56	MG	1A	3894	1/1	0.99	0.09	37,37,37,37	0
56	MG	2A	3019	1/1	0.99	0.19	50,50,50,50	0
56	MG	2A	3660	1/1	0.99	0.13	37,37,37,37	0
56	MG	1A	3987	1/1	0.99	0.22	36,36,36,36	0
56	MG	1A	3338	1/1	0.99	0.22	19,19,19,19	0
59	ZN	16	102	1/1	0.99	0.17	38,38,38,38	0
56	MG	1a	3213	1/1	0.99	0.15	33,33,33,33	0
56	MG	2A	3370	1/1	1.00	0.17	44,44,44,44	0
56	MG	1A	3189	1/1	1.00	0.11	23,23,23,23	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

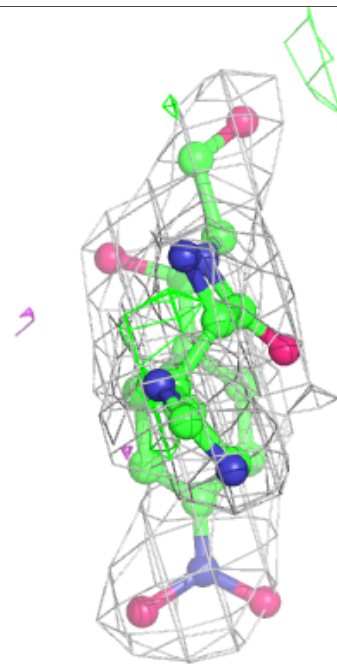
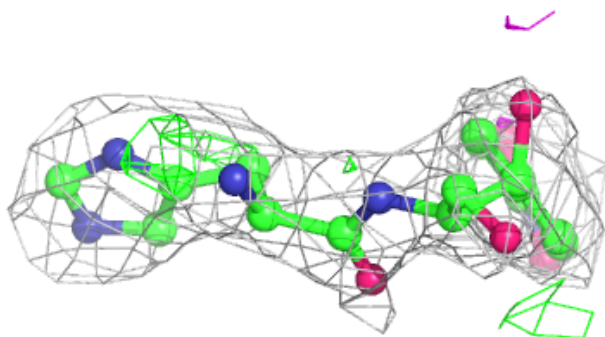
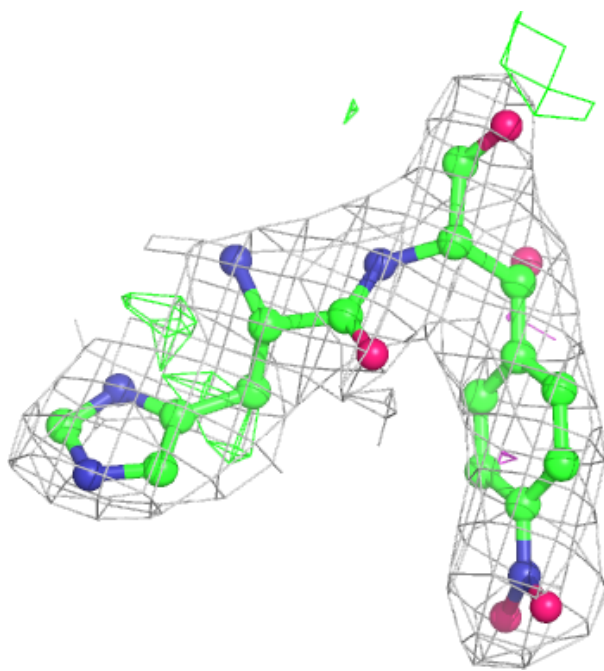
Electron density around EZG 2A 3746:

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



Electron density around EZG 1A 4030:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.