



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 04:54 pm BST

PDB ID : 5WIT
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with pikromycin and bound to mRNA and A-, P- and E-site tRNAs at 2.6Å resolution
Authors : Almutairi, M.M.; Svetlov, M.S.; Hansen, D.A.; Khabibullina, N.F.; Klepacki, D.; Kang, H.Y.; Sherman, D.H.; Vazquez-Laslop, N.; Polikanov, Y.S.; Mankin, A.S.
Deposited on : 2017-07-20
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

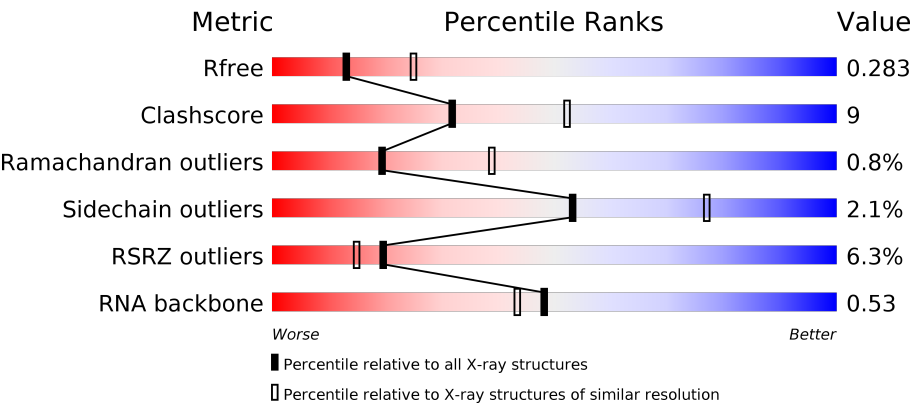
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.60 Å.

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



























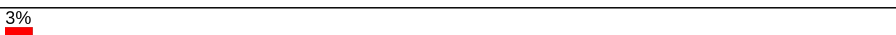
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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>4%</div><div><div></div><div>63%</div><div>28%</div><div>7%</div><div></div></div><div></div></div>
1	2A	2915	<div><div>2%</div><div><div></div><div>55%</div><div>34%</div><div>7%</div><div></div></div><div></div></div>
2	1B	121	<div><div></div><div><div></div><div>78%</div><div>17%</div><div></div></div><div></div></div>
2	2B	121	<div><div>4%</div><div><div></div><div>40%</div><div>47%</div><div>12%</div><div></div></div><div></div></div>

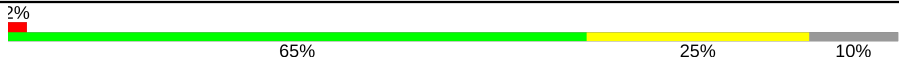















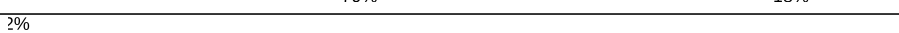

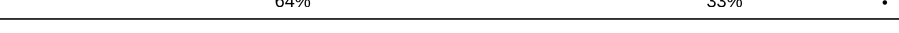
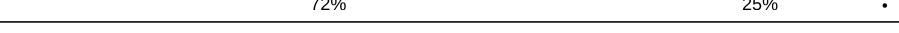
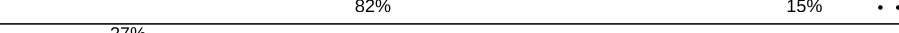




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Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118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






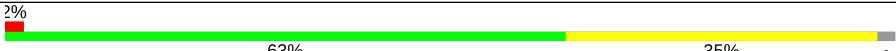
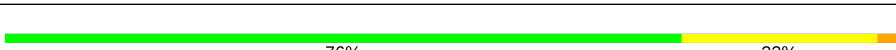

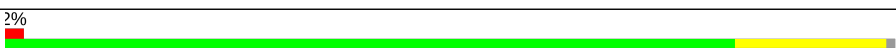

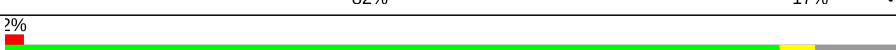
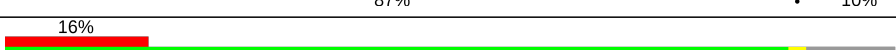

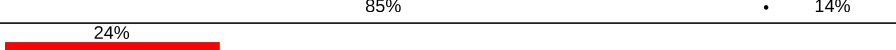
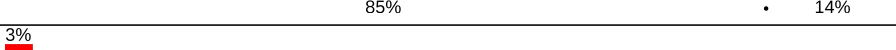
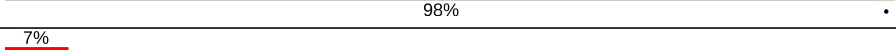
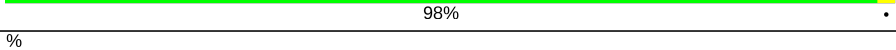
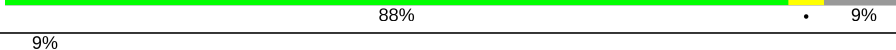

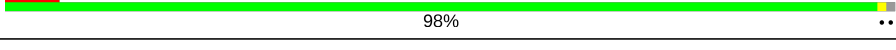
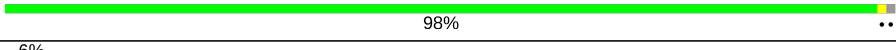
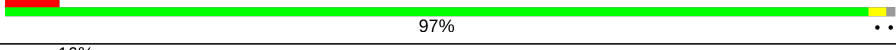
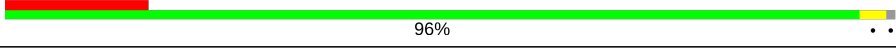
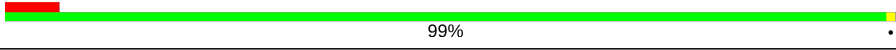
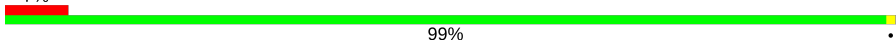
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Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25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

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

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

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Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	2y	76	

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	MIA	2y	37	-	-	-	X
56	5MU	2y	54	-	-	-	X
57	MG	1O	202	-	-	-	X
57	MG	2A	3052	-	-	-	X
57	MG	2A	3121	-	-	-	X
57	MG	2A	3189	-	-	-	X
57	MG	2A	3200	-	-	-	X
57	MG	2A	3305	-	-	-	X
57	MG	2A	3670	-	-	-	X
57	MG	2j	8002	-	-	-	X

2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 298900 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1429	916	256	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

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

- Molecule 54 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0
			1603	722	287	518	74	2		
54	2w	72	Total	C	N	O	P	S	0	0
			1555	699	280	502	72	2		

- 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
			1625	725	294	529	76	1		
55	2x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 56 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1y	74	Total	C	N	O	P	S	0	0
			1585	707	285	518	74	1		
56	2y	73	Total	C	N	O	P	S	0	0
			1565	698	283	510	73	1		

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2E	6	Total	Mg	0	0
			6	6		
57	17	2	Total	Mg	0	0
			2	2		
57	2d	2	Total	Mg	0	0
			2	2		
57	1T	2	Total	Mg	0	0
			2	2		
57	1N	7	Total	Mg	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	20	3	Total 3	Mg 3	0	0
57	18	4	Total 4	Mg 4	0	0
57	2W	1	Total 1	Mg 1	0	0
57	1Y	4	Total 4	Mg 4	0	0
57	13	1	Total 1	Mg 1	0	0
57	1f	1	Total 1	Mg 1	0	0
57	2h	1	Total 1	Mg 1	0	0
57	1P	4	Total 4	Mg 4	0	0
57	2B	21	Total 21	Mg 21	0	0
57	1q	1	Total 1	Mg 1	0	0
57	2a	201	Total 201	Mg 201	0	0
57	1E	10	Total 10	Mg 10	0	0
57	1b	2	Total 2	Mg 2	0	0
57	2l	2	Total 2	Mg 2	0	0
57	2F	6	Total 6	Mg 6	0	0
57	16	1	Total 1	Mg 1	0	0
57	28	2	Total 2	Mg 2	0	0
57	2e	1	Total 1	Mg 1	0	0
57	1W	6	Total 6	Mg 6	0	0
57	1A	1001	Total 1001	Mg 1001	0	0
57	1t	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1n	2	Total 2	Mg 2	0	0
57	2P	1	Total 1	Mg 1	0	0
57	1X	7	Total 7	Mg 7	0	0
57	12	2	Total 2	Mg 2	0	0
57	1y	2	Total 2	Mg 2	0	0
57	1S	3	Total 3	Mg 3	0	0
57	25	3	Total 3	Mg 3	0	0
57	1D	12	Total 12	Mg 12	0	0
57	1e	1	Total 1	Mg 1	0	0
57	2G	1	Total 1	Mg 1	0	0
57	1I	1	Total 1	Mg 1	0	0
57	2f	2	Total 2	Mg 2	0	0
57	1V	3	Total 3	Mg 3	0	0
57	2X	2	Total 2	Mg 2	0	0
57	1w	4	Total 4	Mg 4	0	0
57	1a	231	Total 231	Mg 231	0	0
57	2Q	3	Total 3	Mg 3	0	0
57	15	4	Total 4	Mg 4	0	0
57	1x	11	Total 11	Mg 11	0	0
57	2j	2	Total 2	Mg 2	0	0
57	1R	3	Total 3	Mg 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2v	2	Total Mg 2 2	0	0
57	2U	2	Total Mg 2 2	0	0
57	1G	5	Total Mg 5 5	0	0
57	2O	1	Total Mg 1 1	0	0
57	1l	3	Total Mg 3 3	0	0
57	2r	1	Total Mg 1 1	0	0
57	2q	3	Total Mg 3 3	0	0
57	2g	1	Total Mg 1 1	0	0
57	2Y	1	Total Mg 1 1	0	0
57	23	1	Total Mg 1 1	0	0
57	2x	5	Total Mg 5 5	0	0
57	2R	2	Total Mg 2 2	0	0
57	1Z	3	Total Mg 3 3	0	0
57	2D	8	Total Mg 8 8	0	0
57	14	1	Total Mg 1 1	0	0
57	1U	4	Total Mg 4 4	0	0
57	1O	7	Total Mg 7 7	0	0
57	1r	1	Total Mg 1 1	0	0
57	19	1	Total Mg 1 1	0	0
57	1l	2	Total Mg 2 2	0	0
57	2V	2	Total Mg 2 2	0	0

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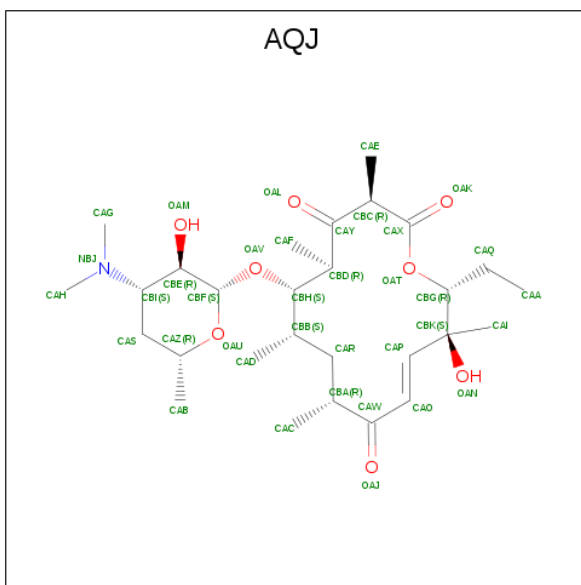
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1F	9	Total	Mg	0	0
			9	9		
57	10	5	Total	Mg	0	0
			5	5		
57	2t	1	Total	Mg	0	0
			1	1		
57	1Q	6	Total	Mg	0	0
			6	6		
57	2A	687	Total	Mg	0	0
			687	687		
57	2Z	1	Total	Mg	0	0
			1	1		
57	1B	31	Total	Mg	0	0
			31	31		
57	2w	4	Total	Mg	0	0
			4	4		

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

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

- Molecule 59 is (3R,5R,6S,7S,9R,11E,13S,14R)-14-ethyl-13-hydroxy-3,5,7,9,13-pentamethyl-2,4,10-trioxo-1-oxacyclotetradec-11-en-6-yl 3,4,6-trideoxy-3-(dimethylamino)-beta-D-xylo-hexopyranoside (three-letter code: AQJ) (formula: C₂₈H₄₇NO₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	1A	1	Total 37	C 28	N 1	O 8	0	0
59	2A	1	Total 37	C 28	N 1	O 8	0	0

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

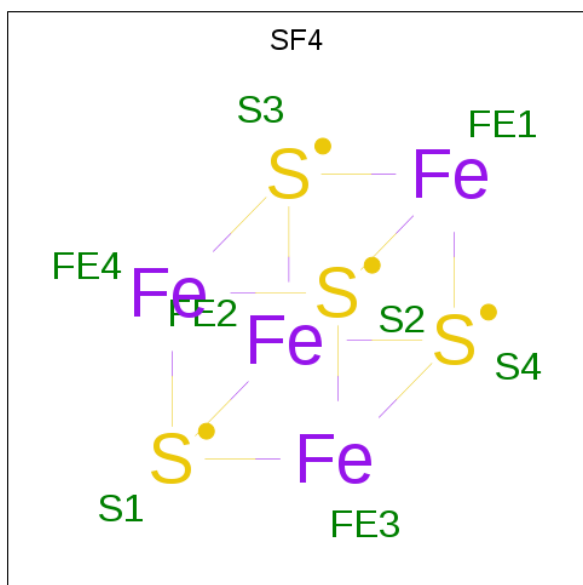
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1Y	1	Total Zn 1 1	0	0
60	14	1	Total Zn 1 1	0	0
60	1n	1	Total Zn 1 1	0	0
60	15	1	Total Zn 1 1	0	0
60	29	1	Total Zn 1 1	0	0
60	19	1	Total Zn 1 1	0	0
60	26	1	Total Zn 1 1	0	0
60	25	1	Total Zn 1 1	0	0
60	24	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2Y	1	Total	Zn	0	0
			1	1		
60	16	1	Total	Zn	0	0
			1	1		

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
61	1d	1	Total	Fe	S	0	0
			8	4	4		
61	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	1610	Total	O	0	0
			1610	1610		
62	1B	40	Total	O	0	0
			40	40		
62	1D	21	Total	O	0	0
			21	21		
62	1E	19	Total	O	0	0
			19	19		
62	1F	14	Total	O	0	0
			14	14		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1G	5	Total 5	O 5	0	0
62	1H	1	Total 1	O 1	0	0
62	1I	2	Total 2	O 2	0	0
62	1N	2	Total 2	O 2	0	0
62	1O	5	Total 5	O 5	0	0
62	1P	18	Total 18	O 18	0	0
62	1Q	3	Total 3	O 3	0	0
62	1R	6	Total 6	O 6	0	0
62	1S	5	Total 5	O 5	0	0
62	1T	6	Total 6	O 6	0	0
62	1U	9	Total 9	O 9	0	0
62	1V	4	Total 4	O 4	0	0
62	1W	4	Total 4	O 4	0	0
62	1X	5	Total 5	O 5	0	0
62	1Y	3	Total 3	O 3	0	0
62	1Z	1	Total 1	O 1	0	0
62	10	7	Total 7	O 7	0	0
62	11	2	Total 2	O 2	0	0
62	12	4	Total 4	O 4	0	0
62	13	3	Total 3	O 3	0	0
62	14	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	15	4	Total 4	O 4	0	0
62	17	4	Total 4	O 4	0	0
62	18	8	Total 8	O 8	0	0
62	19	1	Total 1	O 1	0	0
62	1a	276	Total 276	O 276	0	0
62	1b	1	Total 1	O 1	0	0
62	1e	1	Total 1	O 1	0	0
62	1j	1	Total 1	O 1	0	0
62	1k	1	Total 1	O 1	0	0
62	1l	3	Total 3	O 3	0	0
62	1q	1	Total 1	O 1	0	0
62	1v	3	Total 3	O 3	0	0
62	1w	6	Total 6	O 6	0	0
62	1x	9	Total 9	O 9	0	0
62	1y	1	Total 1	O 1	0	0
62	2A	926	Total 926	O 926	0	0
62	2B	10	Total 10	O 10	0	0
62	2D	16	Total 16	O 16	0	0
62	2E	10	Total 10	O 10	0	0
62	2F	5	Total 5	O 5	0	0
62	2I	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2N	1	Total 1	O 1	0	0
62	2O	1	Total 1	O 1	0	0
62	2P	10	Total 10	O 10	0	0
62	2Q	1	Total 1	O 1	0	0
62	2R	2	Total 2	O 2	0	0
62	2T	2	Total 2	O 2	0	0
62	2U	3	Total 3	O 3	0	0
62	2V	1	Total 1	O 1	0	0
62	2W	1	Total 1	O 1	0	0
62	2X	3	Total 3	O 3	0	0
62	2Z	2	Total 2	O 2	0	0
62	20	3	Total 3	O 3	0	0
62	21	3	Total 3	O 3	0	0
62	22	1	Total 1	O 1	0	0
62	25	3	Total 3	O 3	0	0
62	27	4	Total 4	O 4	0	0
62	28	4	Total 4	O 4	0	0
62	29	1	Total 1	O 1	0	0
62	2a	230	Total 230	O 230	0	0
62	2d	2	Total 2	O 2	0	0
62	2e	1	Total 1	O 1	0	0

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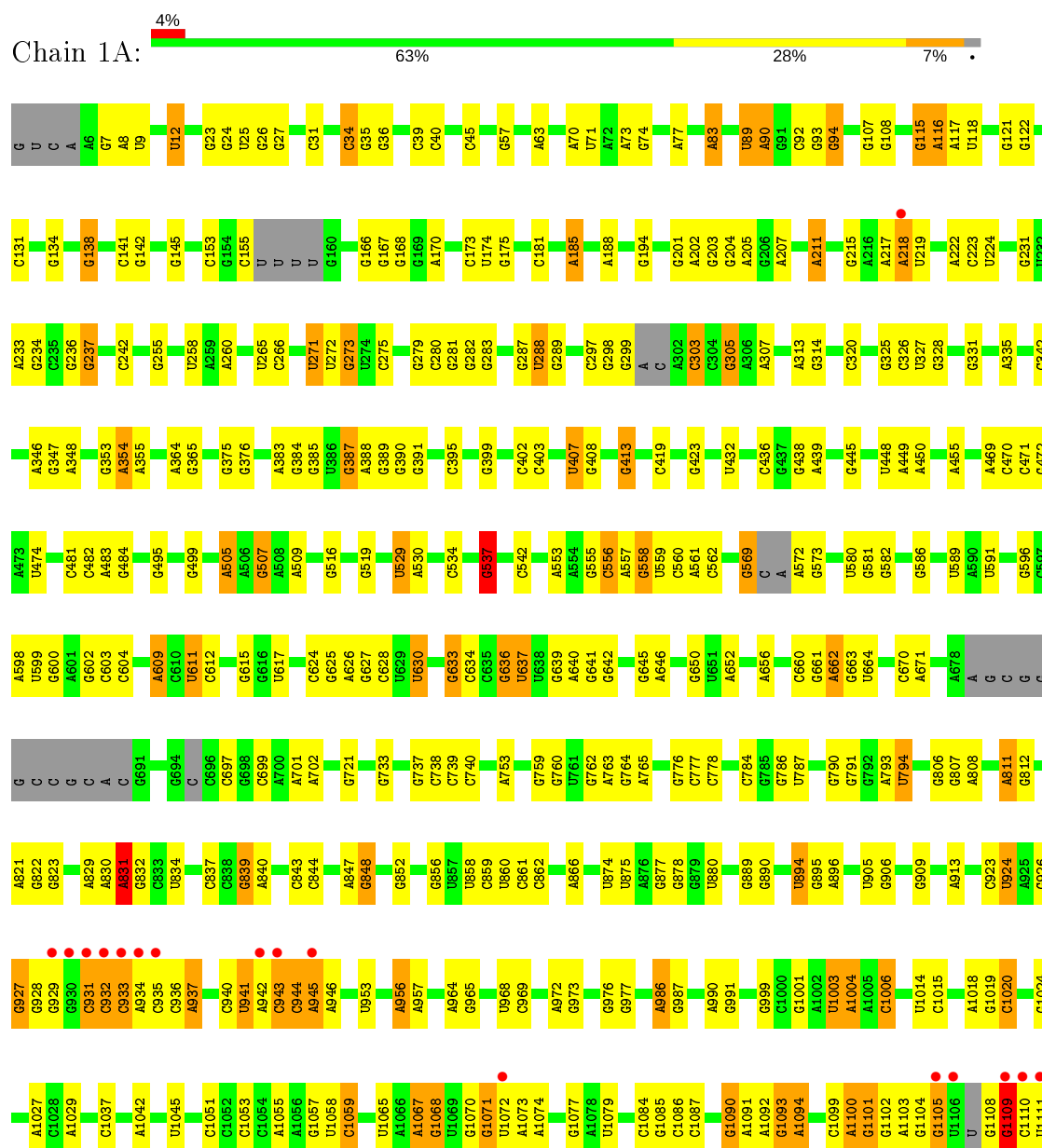
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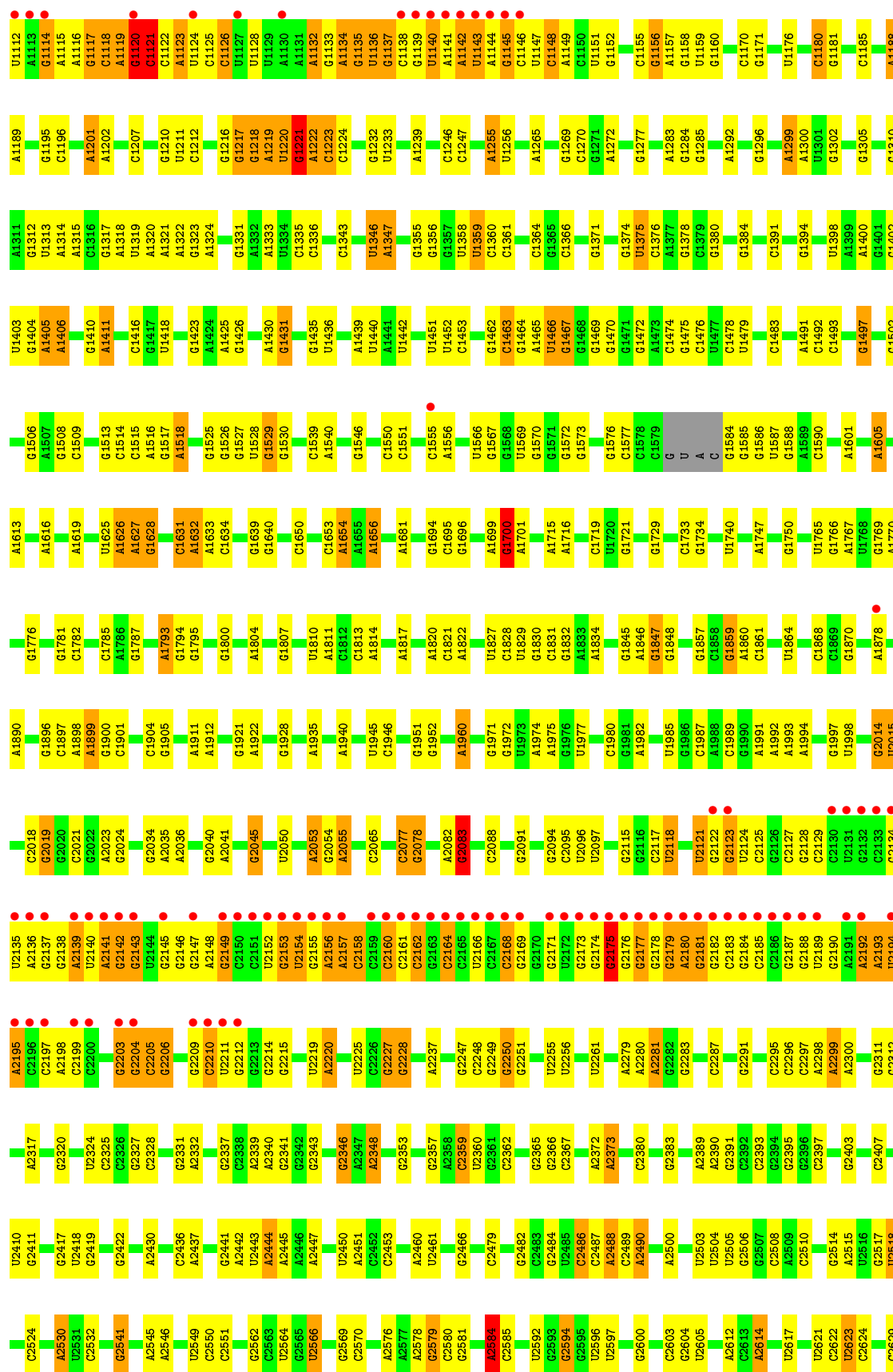
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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62	2g	1	Total 1	O 1	0	0
62	2i	2	Total 2	O 2	0	0
62	2j	4	Total 4	O 4	0	0
62	2l	3	Total 3	O 3	0	0
62	2n	1	Total 1	O 1	0	0
62	2o	1	Total 1	O 1	0	0
62	2v	2	Total 2	O 2	0	0
62	2w	1	Total 1	O 1	0	0
62	2x	5	Total 5	O 5	0	0

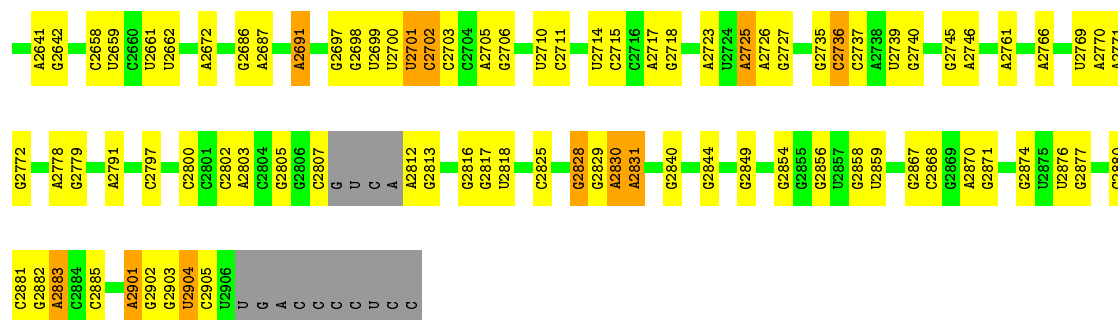
3 Residue-property plots

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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

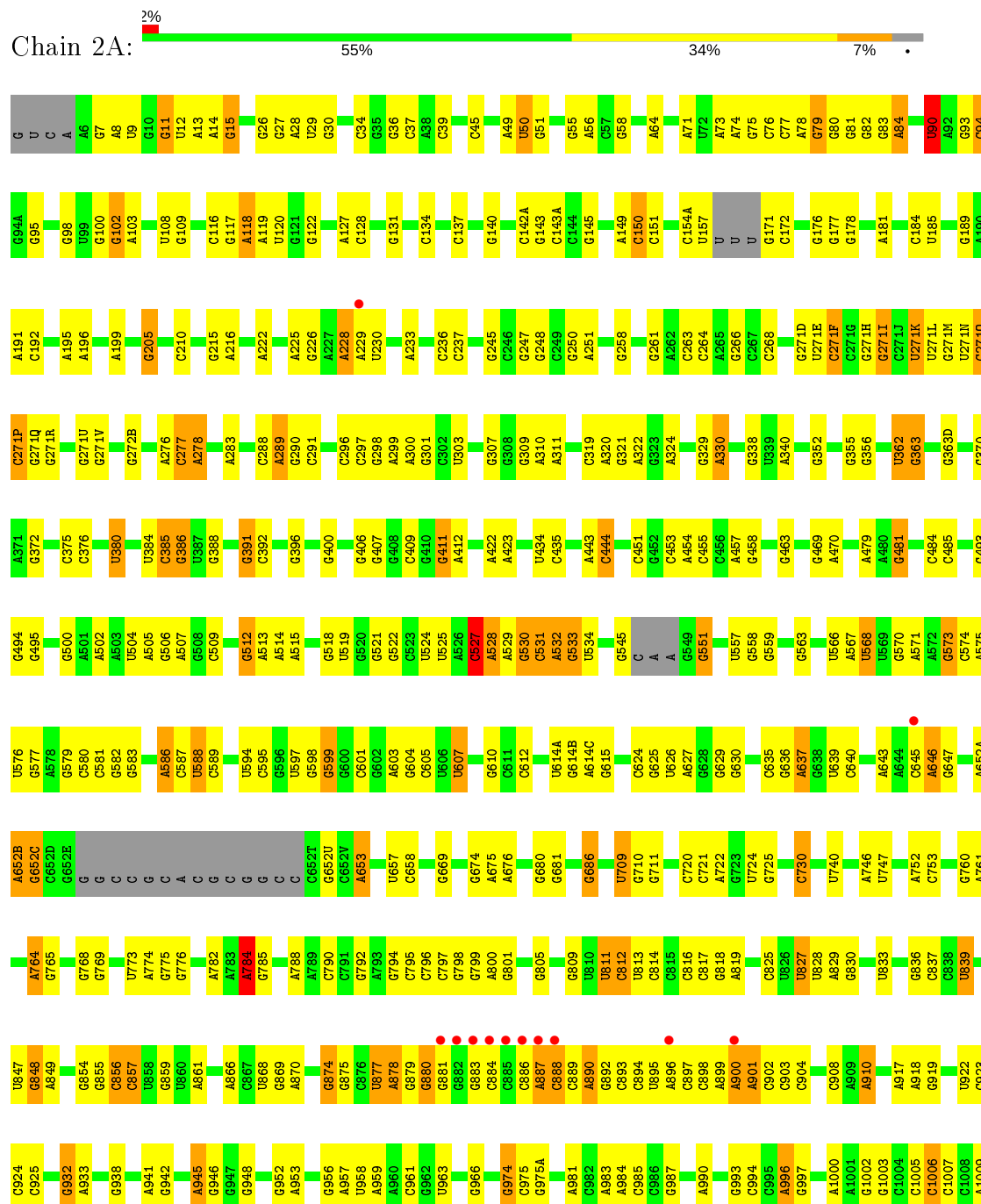
- Molecule 1: 23S Ribosomal RNA



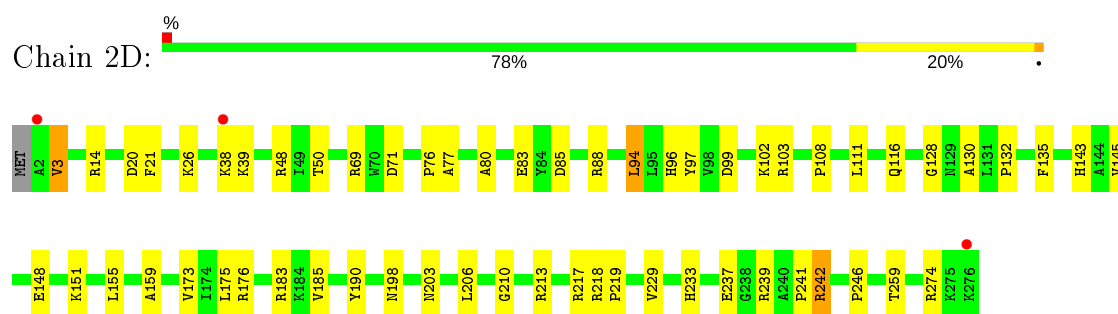




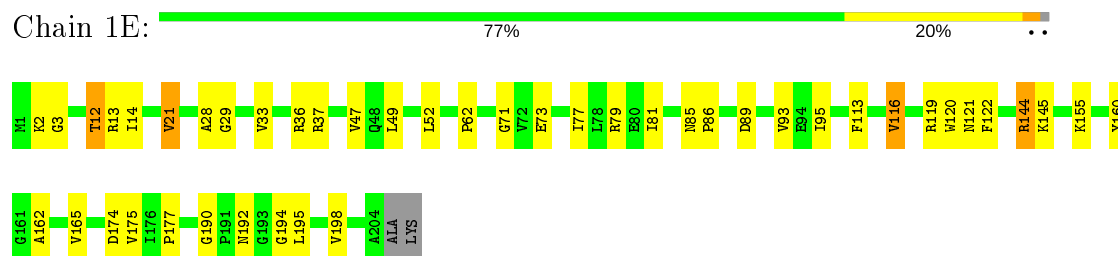
• Molecule 1: 23S Ribosomal RNA



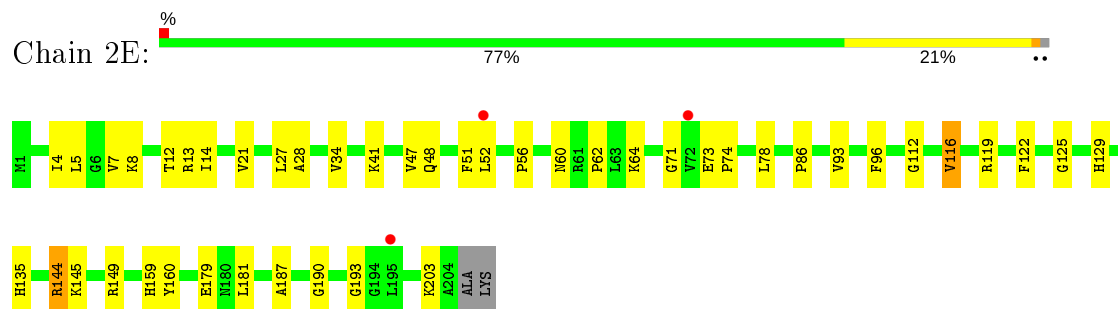




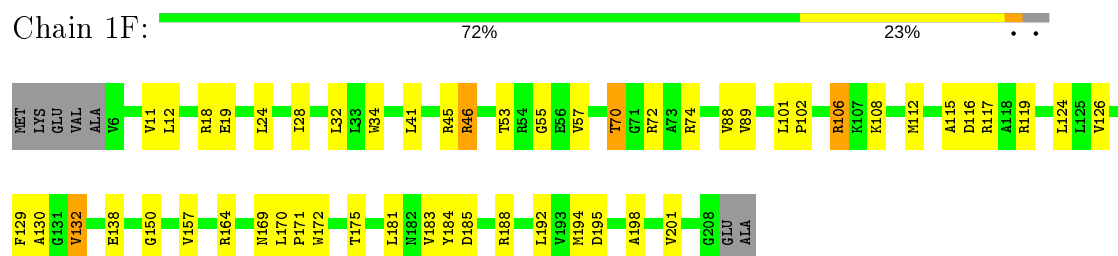
- Molecule 4: 50S ribosomal protein L3



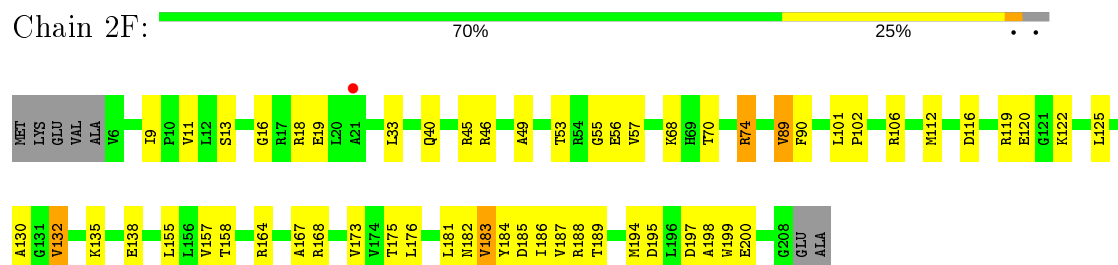
- Molecule 4: 50S ribosomal protein L3



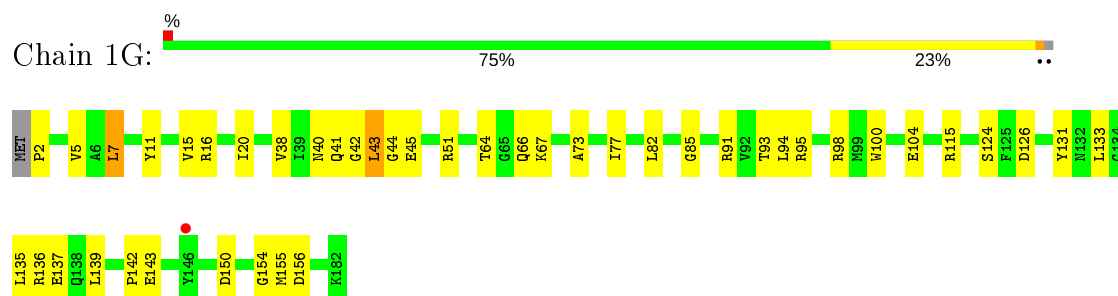
- Molecule 5: 50S ribosomal protein L4



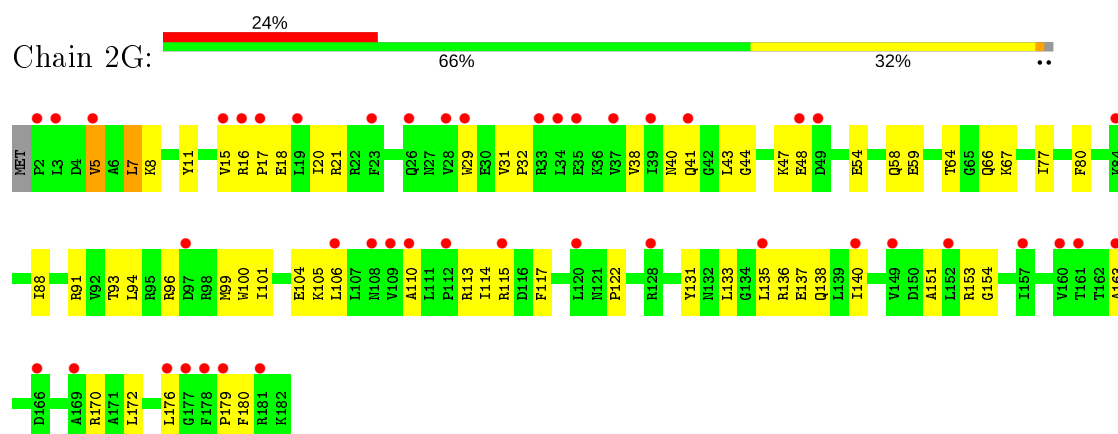
- Molecule 5: 50S ribosomal protein L4



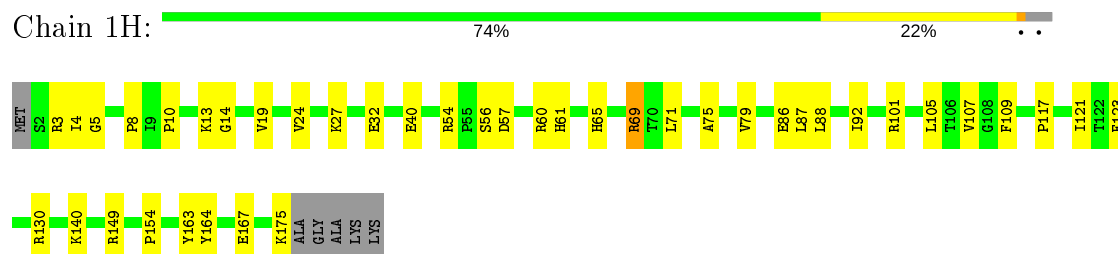
- Molecule 6: 50S ribosomal protein L5



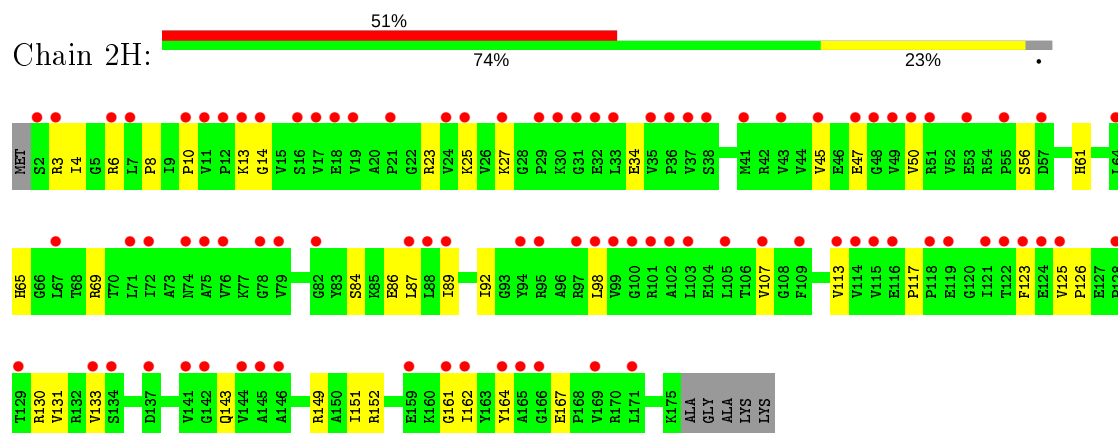
- Molecule 6: 50S ribosomal protein L5



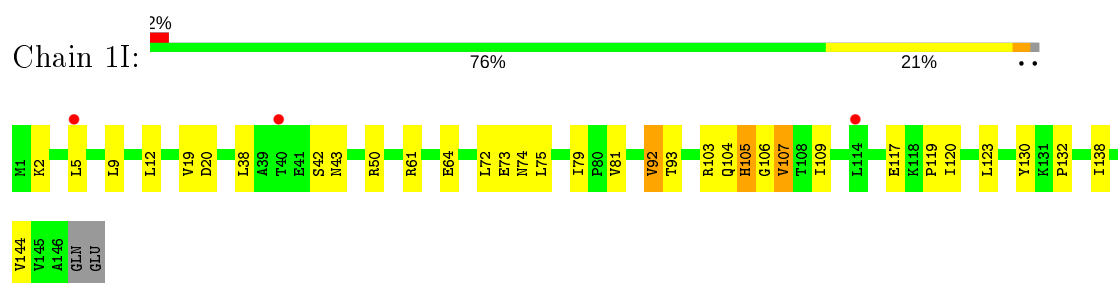
- Molecule 7: 50S ribosomal protein L6



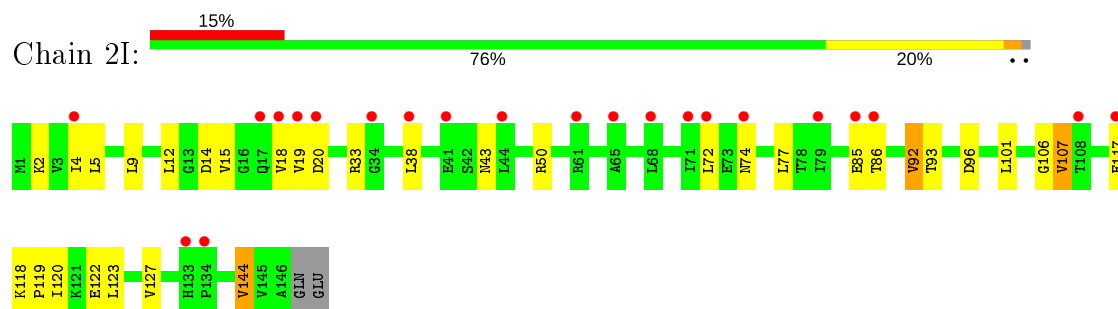
- Molecule 7: 50S ribosomal protein L6



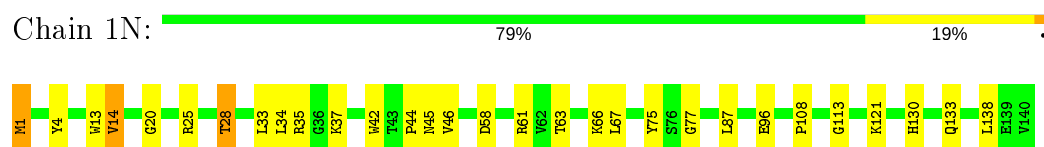
- Molecule 8: 50S ribosomal protein L9



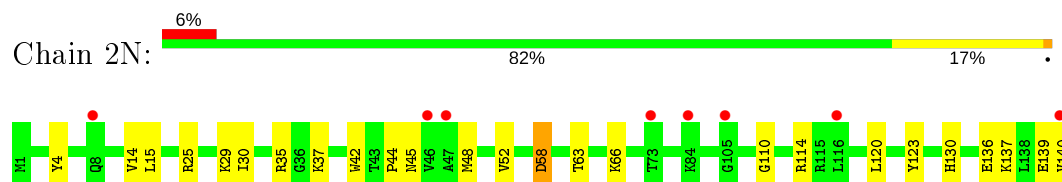
- Molecule 8: 50S ribosomal protein L9



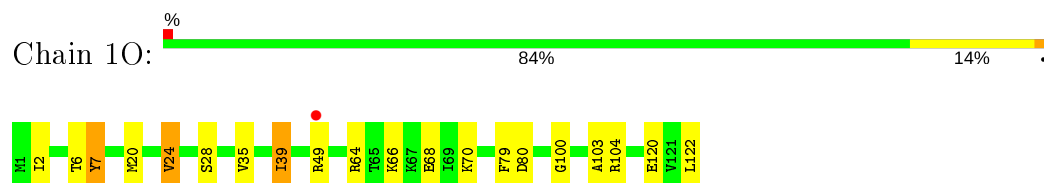
- Molecule 9: 50S ribosomal protein L13



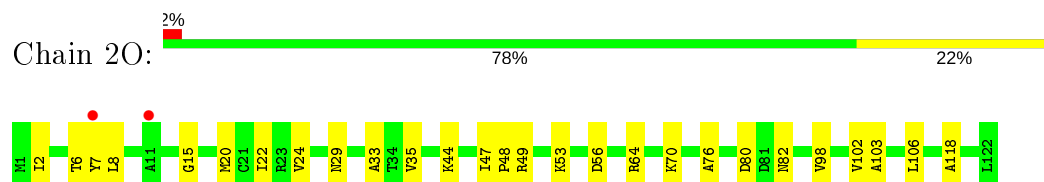
- Molecule 9: 50S ribosomal protein L13



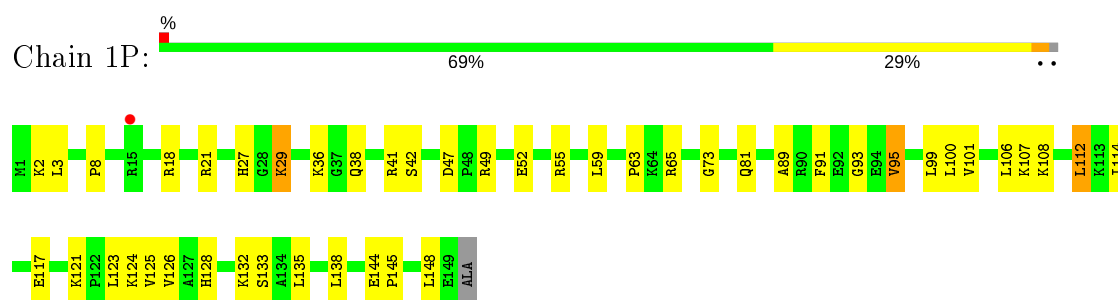
- Molecule 10: 50S ribosomal protein L14



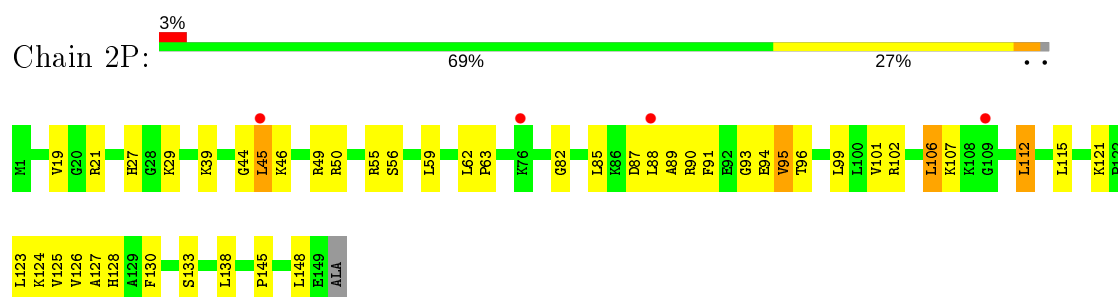
- Molecule 10: 50S ribosomal protein L14



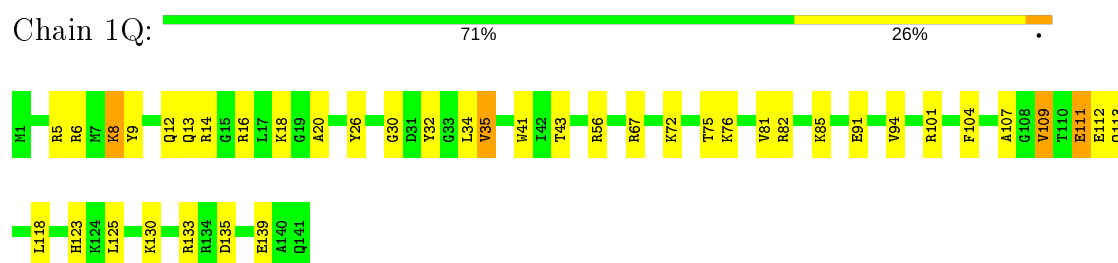
- Molecule 11: 50S ribosomal protein L15



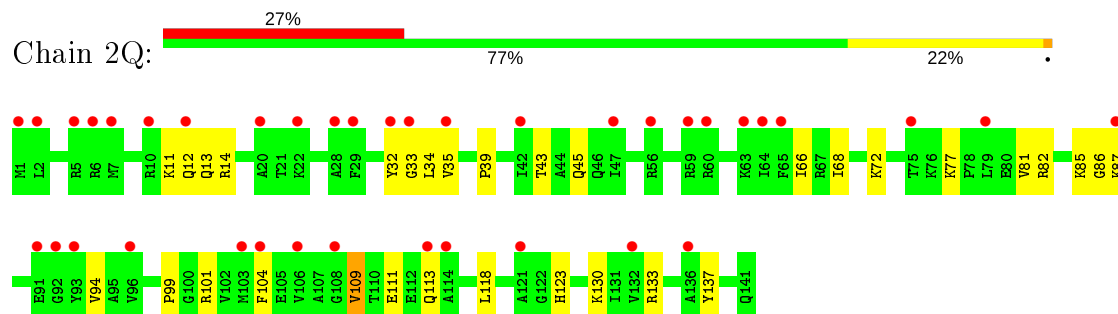
- Molecule 11: 50S ribosomal protein L15



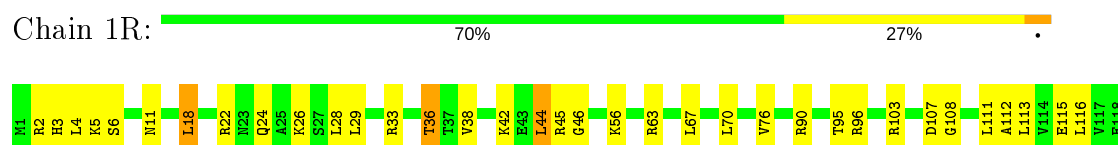
- Molecule 12: 50S ribosomal protein L16



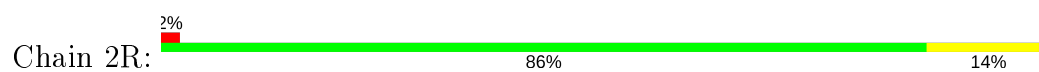
- Molecule 12: 50S ribosomal protein L16



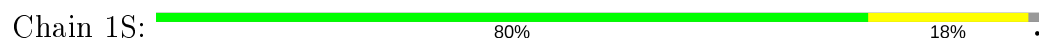
- Molecule 13: 50S ribosomal protein L17



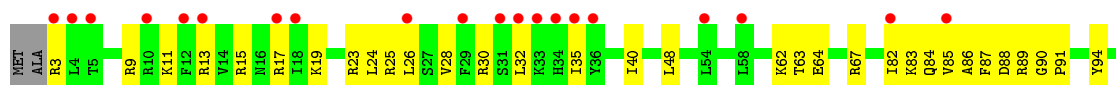
- Molecule 13: 50S ribosomal protein L17



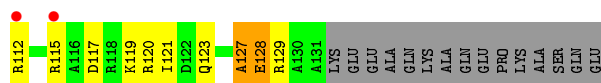
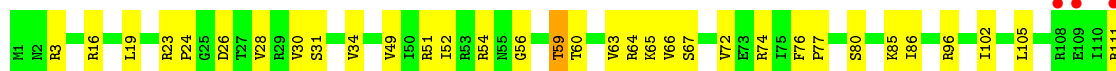
- Molecule 14: 50S ribosomal protein L18



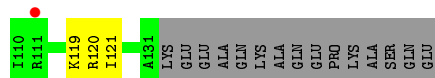
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19

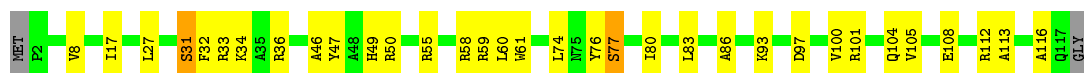


- Molecule 15: 50S ribosomal protein L19

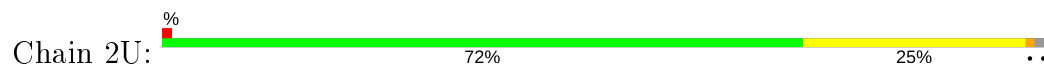


- Molecule 16: 50S ribosomal protein L20

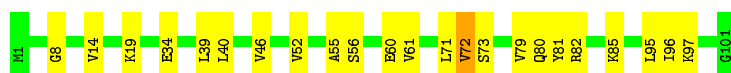
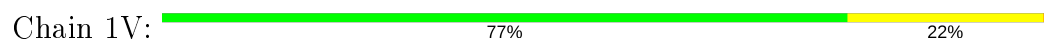




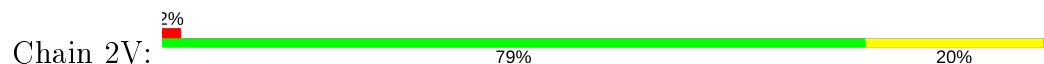
- Molecule 16: 50S ribosomal protein L20



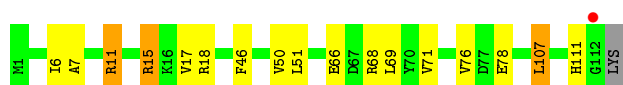
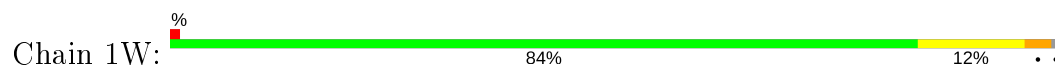
- Molecule 17: 50S ribosomal protein L21



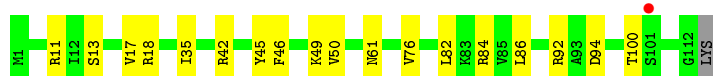
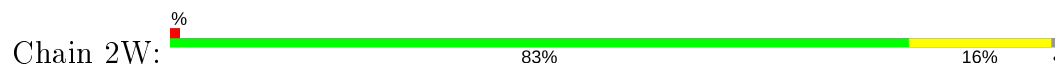
- Molecule 17: 50S ribosomal protein L21



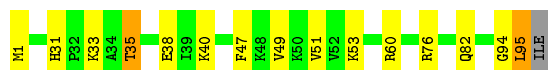
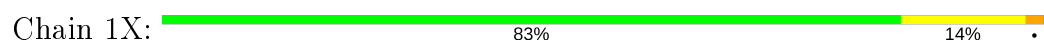
- Molecule 18: 50S ribosomal protein L22



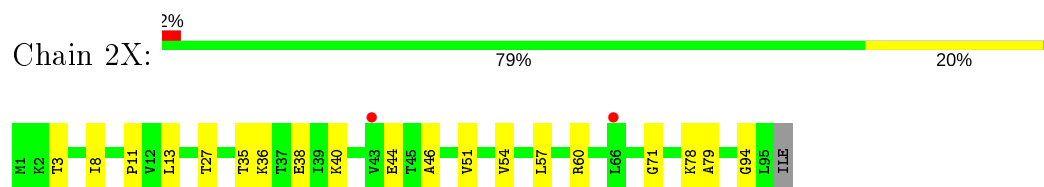
- Molecule 18: 50S ribosomal protein L22



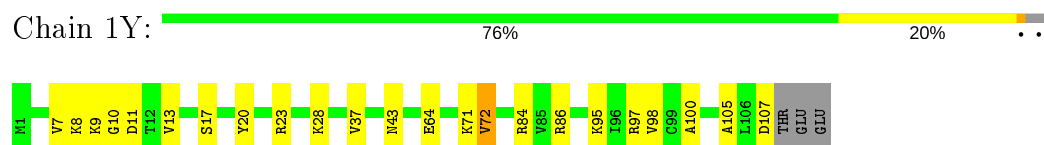
- Molecule 19: 50S ribosomal protein L23



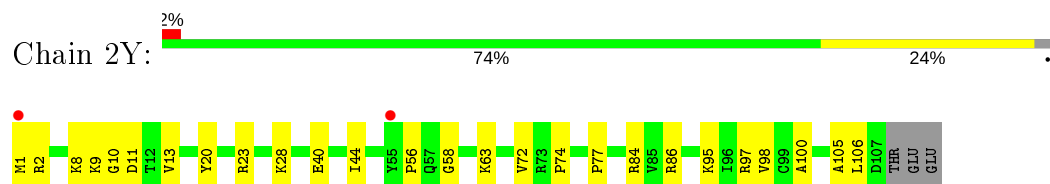
- Molecule 19: 50S ribosomal protein L23



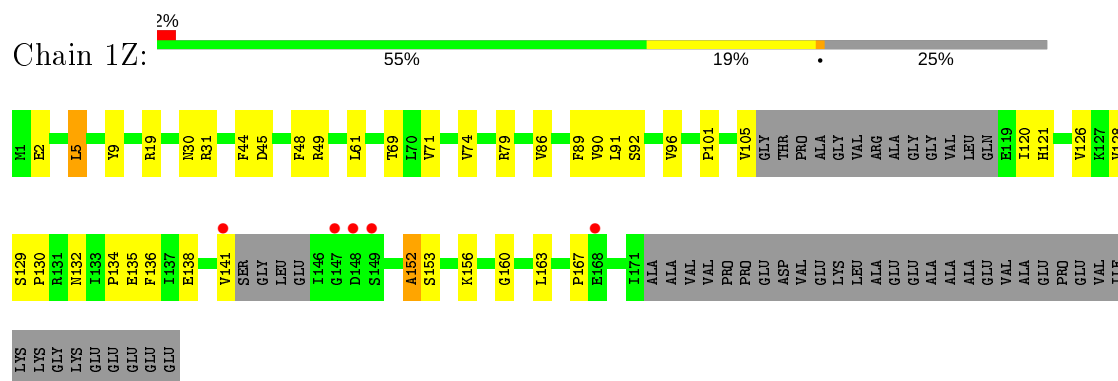
- Molecule 20: 50S ribosomal protein L24



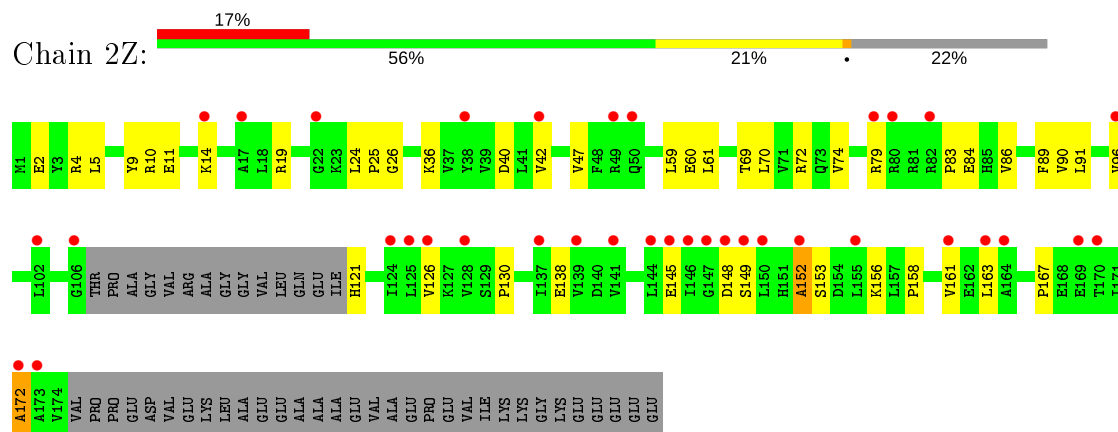
- Molecule 20: 50S ribosomal protein L24




- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25




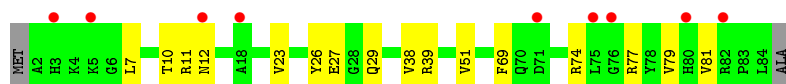
- Molecule 22: 50S ribosomal protein L27

Chain 10:  81% 16%




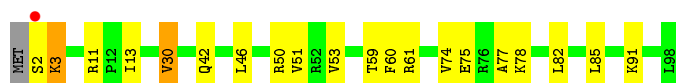
- Molecule 22: 50S ribosomal protein L27

Chain 20:  11% 79% 19%




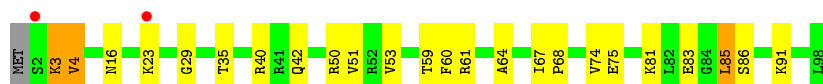
- Molecule 23: 50S ribosomal protein L28

Chain 11:  % 79% 18%



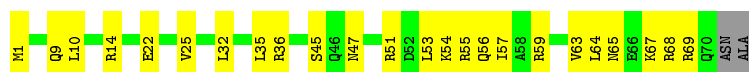
- Molecule 23: 50S ribosomal protein L28

Chain 21:  2% 74% 21%



- Molecule 24: 50S ribosomal protein L29

Chain 12:  64% 33%




- Molecule 24: 50S ribosomal protein L29

Chain 22:  72% 25%



- Molecule 25: 50S ribosomal protein L30

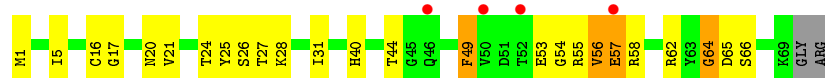
Chain 13:  82% 15%



- Molecule 25: 50S ribosomal protein L30



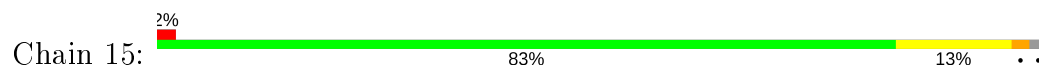
- Molecule 26: 50S ribosomal protein L31



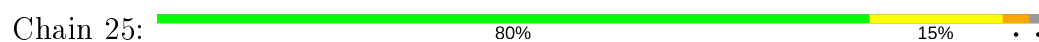
- Molecule 26: 50S ribosomal protein L31



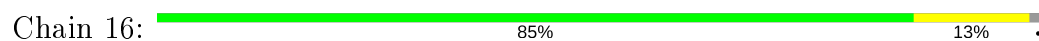
- Molecule 27: 50S ribosomal protein L32



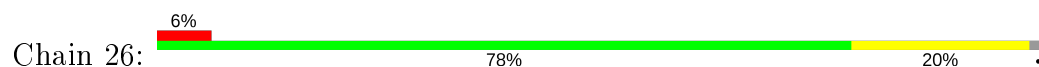
- Molecule 27: 50S ribosomal protein L32



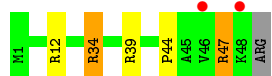
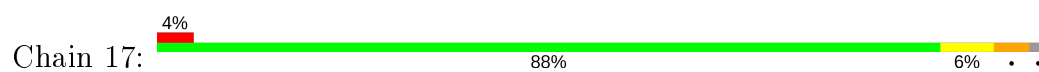
- Molecule 28: 50S ribosomal protein L33



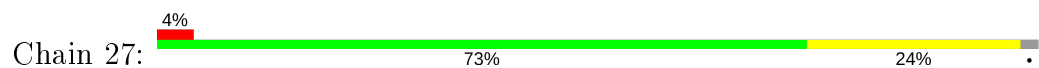
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



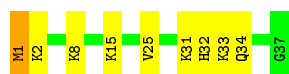
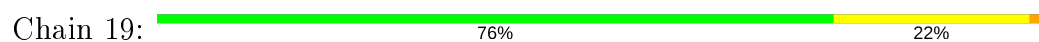
- Molecule 30: 50S ribosomal protein L35



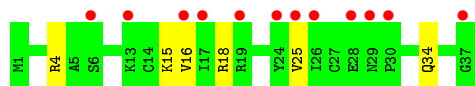
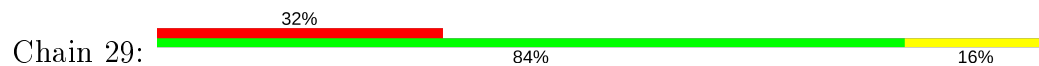
- Molecule 30: 50S ribosomal protein L35



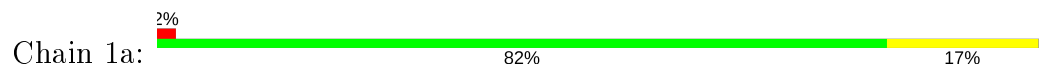
- Molecule 31: 50S ribosomal protein L36

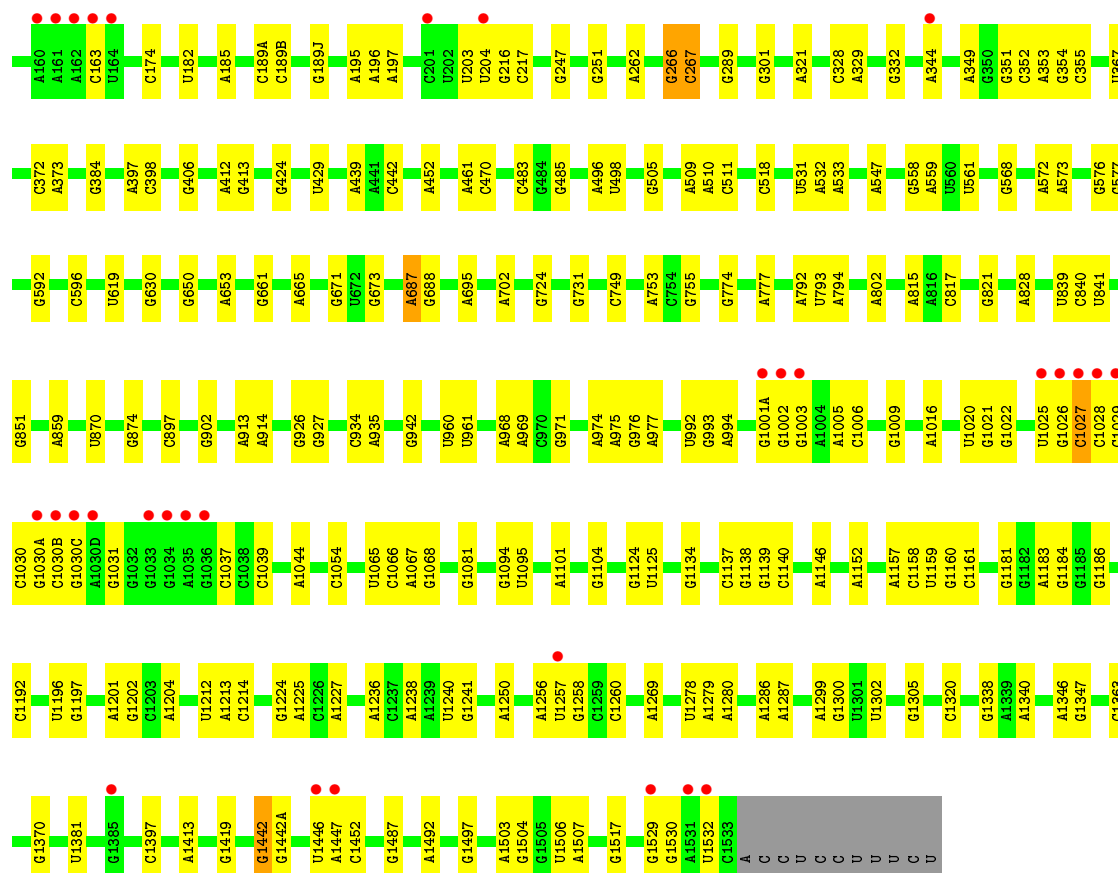


- Molecule 31: 50S ribosomal protein L36

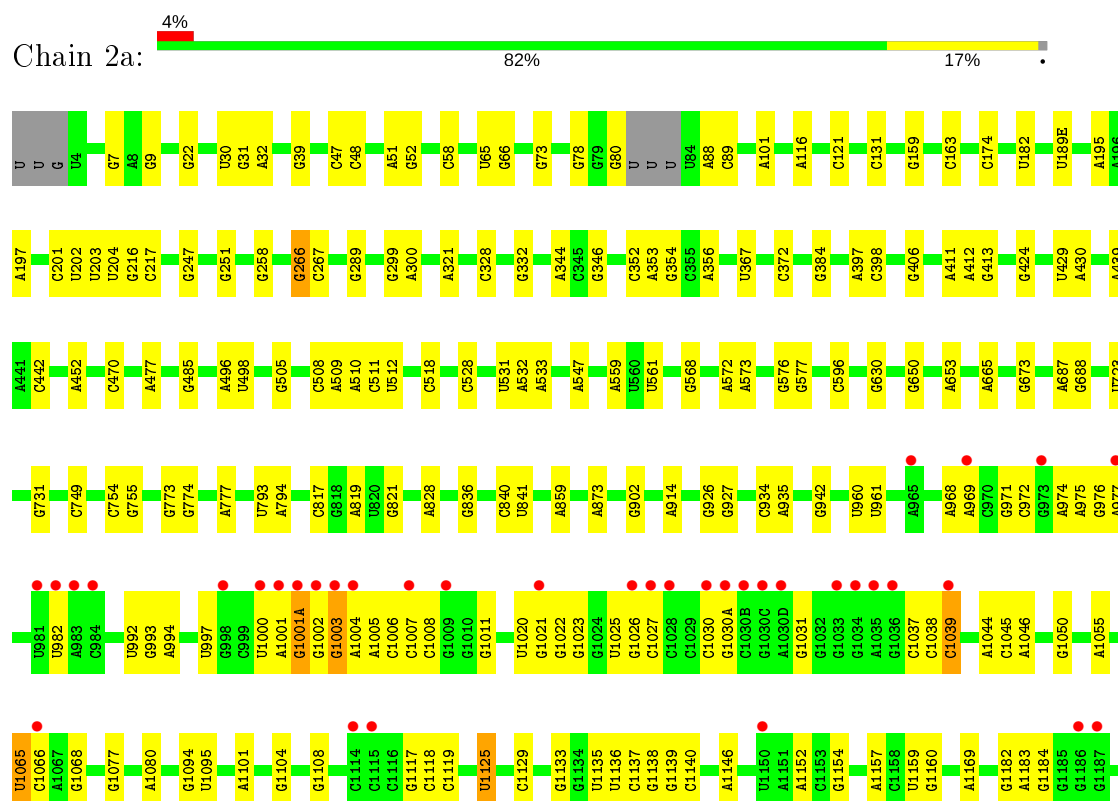


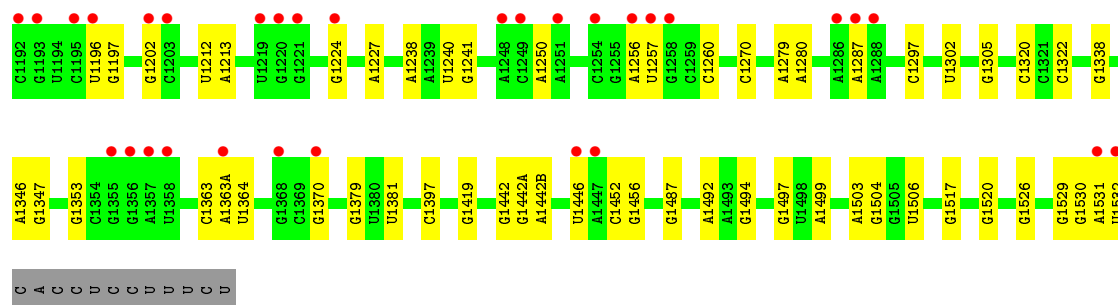
- Molecule 32: 16S Ribosomal RNA



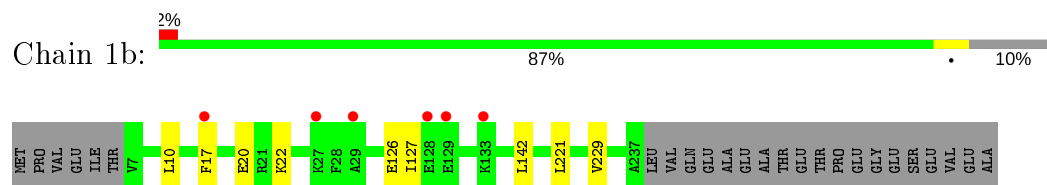


- Molecule 32: 16S Ribosomal RNA

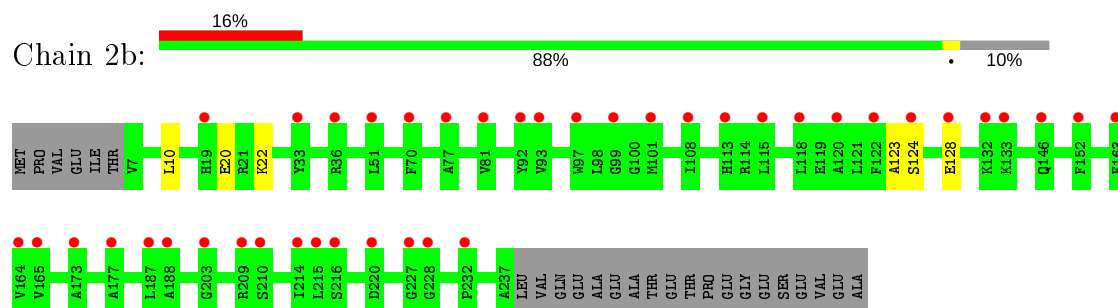




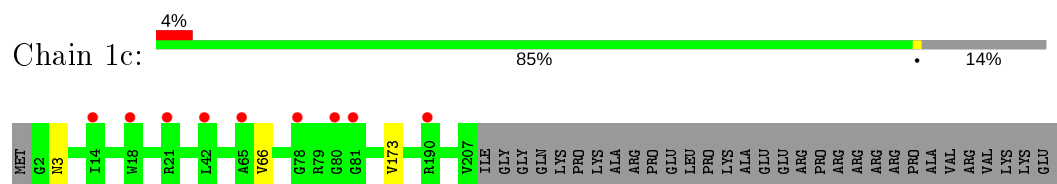
- Molecule 33: 30S ribosomal protein S2



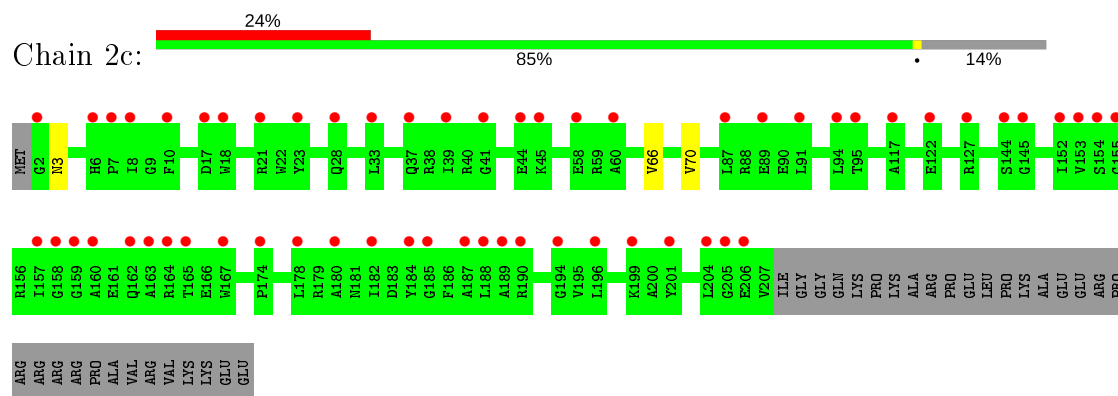
- Molecule 33: 30S ribosomal protein S2



- Molecule 34: 30S ribosomal protein S3



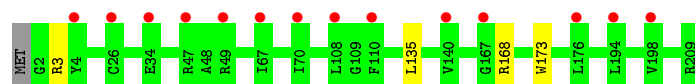
- Molecule 34: 30S ribosomal protein S3



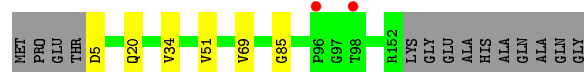
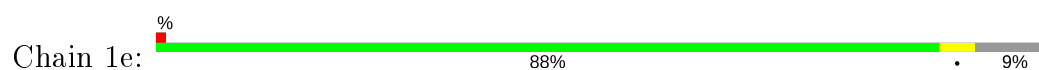
- Molecule 35: 30S ribosomal protein S4



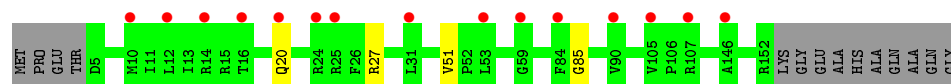
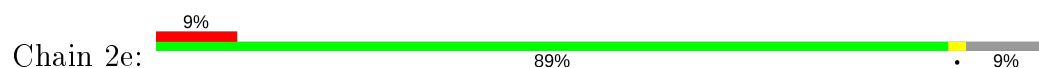
- Molecule 35: 30S ribosomal protein S4



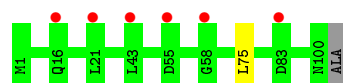
- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



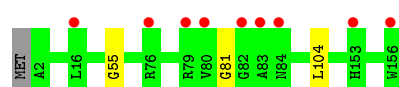
- Molecule 37: 30S ribosomal protein S6



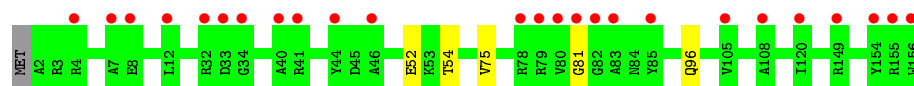
- Molecule 37: 30S ribosomal protein S6



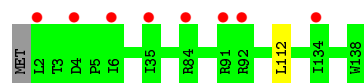
- Molecule 38: 30S ribosomal protein S7



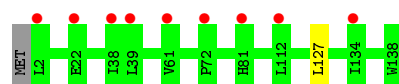
- Molecule 38: 30S ribosomal protein S7



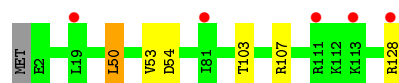
- Molecule 39: 30S ribosomal protein S8



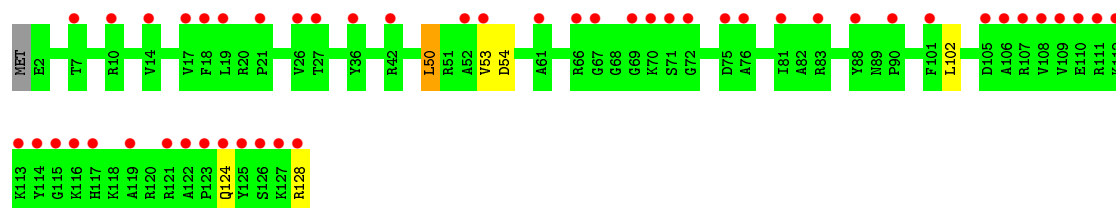
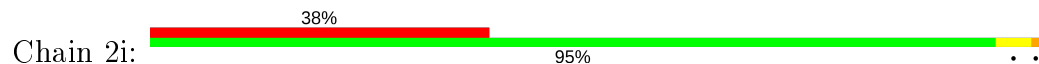
- Molecule 39: 30S ribosomal protein S8



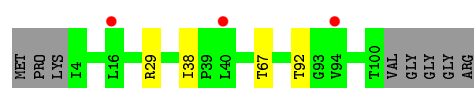
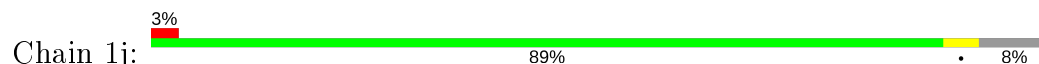
- Molecule 40: 30S ribosomal protein S9



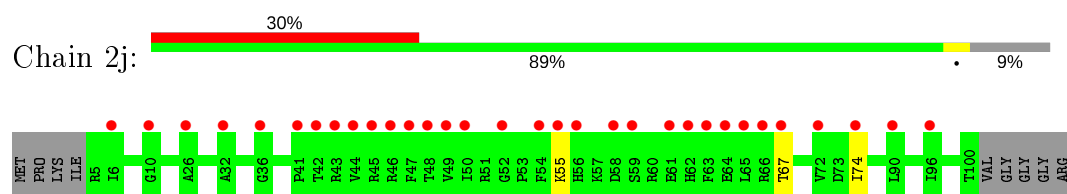
- Molecule 40: 30S ribosomal protein S9



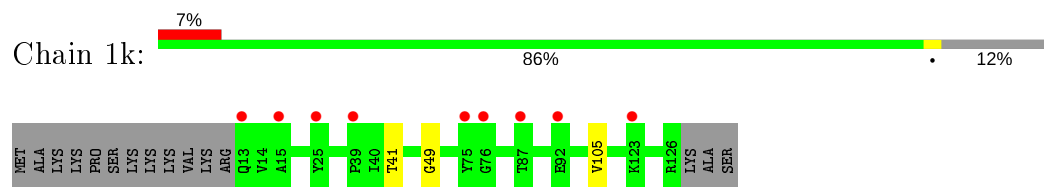
- Molecule 41: 30S ribosomal protein S10



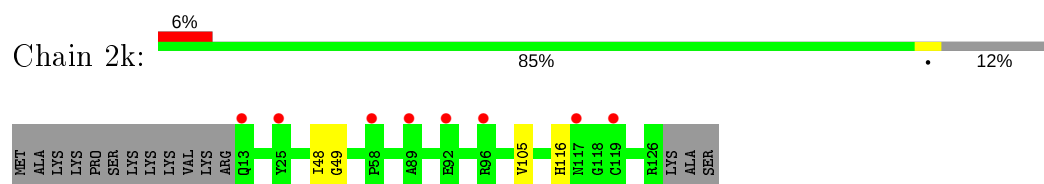
- Molecule 41: 30S ribosomal protein S10



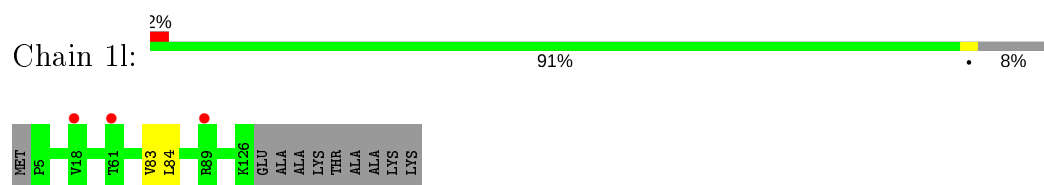
- Molecule 42: 30S ribosomal protein S11



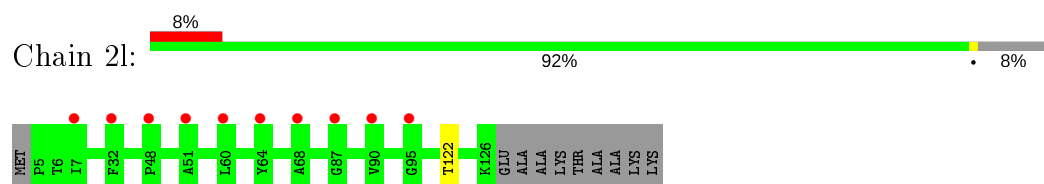
- Molecule 42: 30S ribosomal protein S11



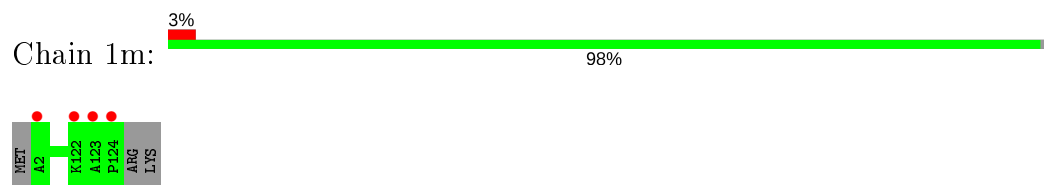
- Molecule 43: 30S ribosomal protein S12



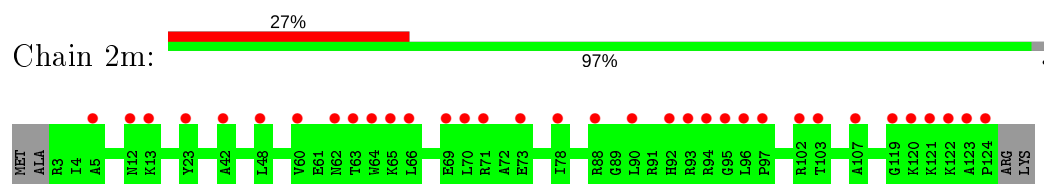
- Molecule 43: 30S ribosomal protein S12



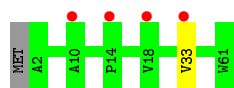
- Molecule 44: 30S ribosomal protein S13



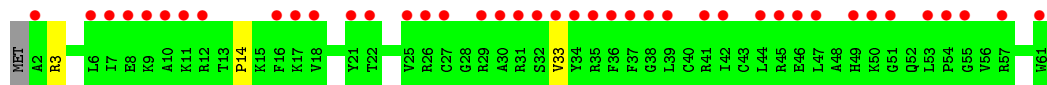
- Molecule 44: 30S ribosomal protein S13



- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



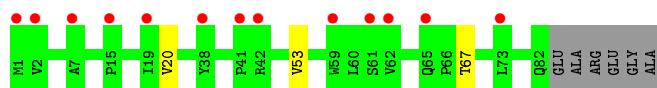
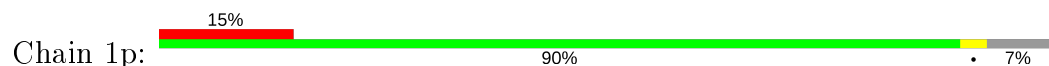
- Molecule 46: 30S ribosomal protein S15



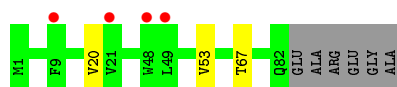
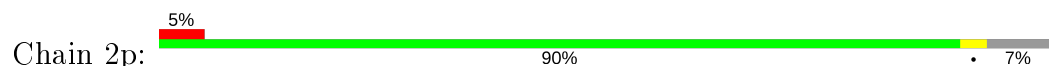
- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16

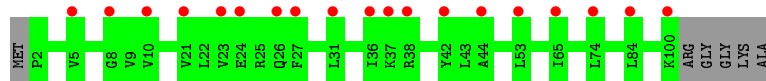


- Molecule 48: 30S ribosomal protein S17

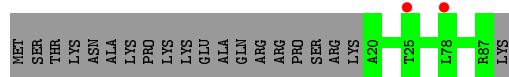
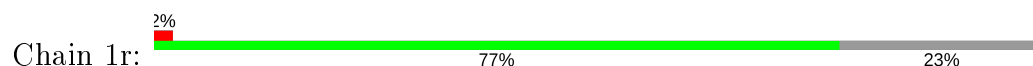




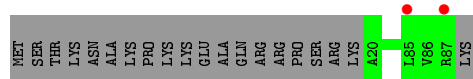
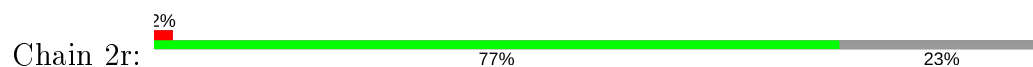
- Molecule 48: 30S ribosomal protein S17



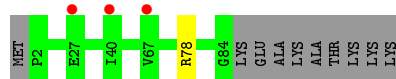
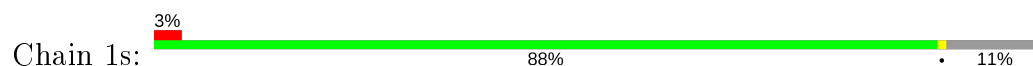
- Molecule 49: 30S ribosomal protein S18



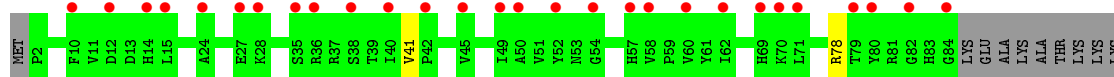
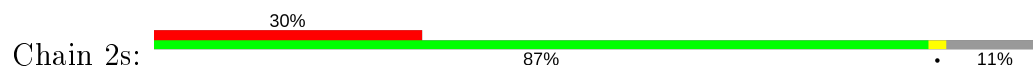
- Molecule 49: 30S ribosomal protein S18



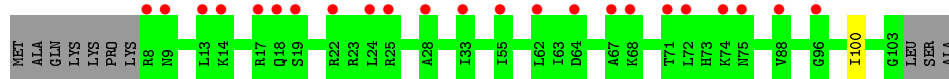
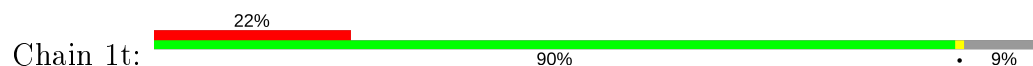
- Molecule 50: 30S ribosomal protein S19



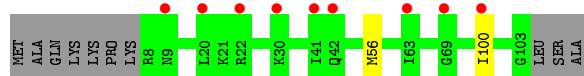
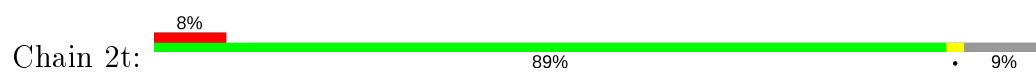
- Molecule 50: 30S ribosomal protein S19



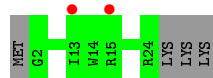
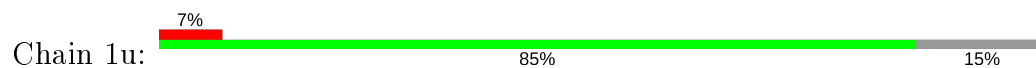
- Molecule 51: 30S ribosomal protein S20



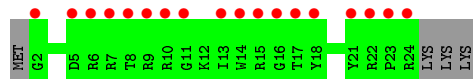
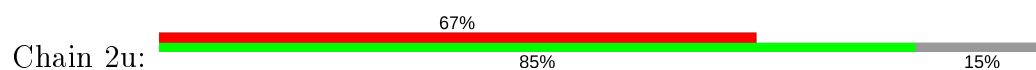
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



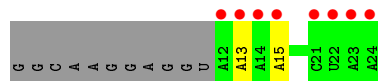
- Molecule 52: 30S ribosomal protein Thx



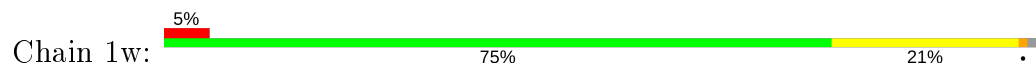
- Molecule 53: mRNA



- Molecule 53: mRNA



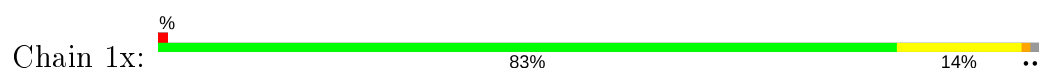
- Molecule 54: A-site tRNA



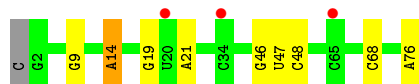
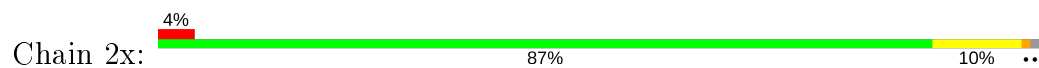
- Molecule 54: A-site tRNA



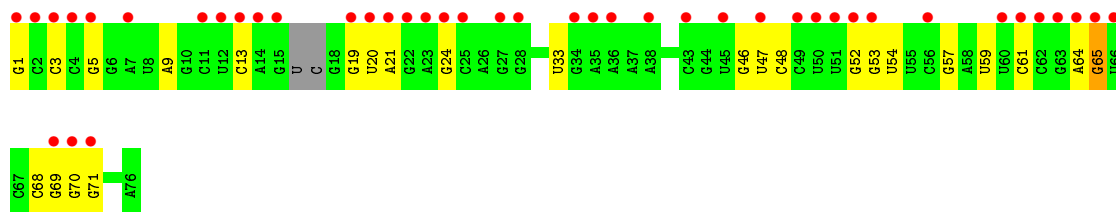
- Molecule 55: P-site tRNA



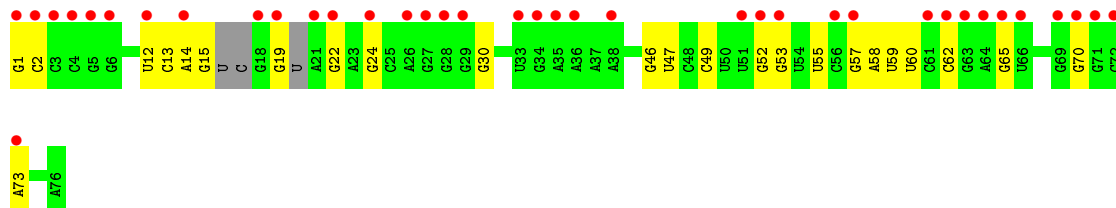
• Molecule 55: P-site tRNA



• Molecule 56: E-site tRNA



• Molecule 56: E-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	209.34Å 447.21Å 620.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.82 – 2.60 189.60 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (152.82-2.60) 98.3 (189.60-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.238 , 0.283 0.239 , 0.283	Depositor DCC
R_{free} test set	86837 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	298900	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% 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, F3N, PSU, 2MA, 2MG, 5MC, UR3, MA6, 4OC, M2G, 7MG, K, AQJ

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	0.49	0/69009	0.98	69/107712 (0.1%)
1	2A	0.38	0/67293	0.87	36/105034 (0.0%)
2	1B	0.47	1/2882 (0.0%)	0.89	0/4494
2	2B	0.39	1/2879 (0.0%)	0.87	1/4487 (0.0%)
3	1D	0.36	0/2186	0.58	0/2944
3	2D	0.31	0/2186	0.53	0/2944
4	1E	0.34	0/1592	0.56	0/2149
4	2E	0.29	0/1592	0.51	0/2149
5	1F	0.34	0/1619	0.54	0/2193
5	2F	0.30	0/1615	0.48	0/2188
6	1G	0.30	0/1454	0.51	0/1964
6	2G	0.29	0/1453	0.47	0/1963
7	1H	0.34	0/1356	0.49	0/1834
7	2H	0.28	0/1356	0.46	0/1834
8	1I	0.28	0/1112	0.50	0/1514
8	2I	0.28	0/1079	0.50	0/1475
9	1N	0.34	0/1144	0.51	0/1543
9	2N	0.29	0/1144	0.47	0/1543
10	1O	0.34	0/943	0.54	0/1269
10	2O	0.32	0/943	0.51	0/1269
11	1P	0.33	0/1152	0.55	0/1533
11	2P	0.31	0/1152	0.49	0/1533
12	1Q	0.36	0/1143	0.51	0/1527
12	2Q	0.30	0/1143	0.48	0/1527
13	1R	0.32	0/982	0.56	0/1312
13	2R	0.29	0/982	0.50	0/1312
14	1S	0.30	0/883	0.51	0/1176
14	2S	0.29	0/880	0.48	0/1172
15	1T	0.34	0/1105	0.52	0/1477
15	2T	0.30	0/1097	0.49	0/1468
16	1U	0.34	0/977	0.49	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.29	0/977	0.44	0/1301
17	1V	0.37	0/782	0.55	0/1049
17	2V	0.29	0/782	0.52	0/1049
18	1W	0.32	0/897	0.54	0/1205
18	2W	0.30	0/897	0.49	0/1205
19	1X	0.35	0/764	0.55	0/1025
19	2X	0.31	0/764	0.50	0/1025
20	1Y	0.34	0/819	0.56	0/1095
20	2Y	0.31	0/819	0.51	0/1095
21	1Z	0.30	0/1267	0.50	0/1717
21	2Z	0.29	0/1299	0.51	0/1763
22	10	0.35	0/662	0.55	0/881
22	20	0.30	0/662	0.50	0/881
23	11	0.32	0/762	0.51	0/1014
23	21	0.31	0/762	0.49	0/1014
24	12	0.31	0/590	0.48	0/781
24	22	0.27	0/590	0.42	0/781
25	13	0.32	0/474	0.48	0/635
25	23	0.28	0/469	0.45	0/630
26	14	0.32	0/565	0.57	0/761
26	24	0.32	0/545	0.53	0/737
27	15	0.34	0/469	0.57	0/635
27	25	0.31	0/469	0.51	0/635
28	16	0.32	0/460	0.51	0/613
28	26	0.29	0/456	0.52	0/608
29	17	0.33	0/426	0.54	0/561
29	27	0.29	0/426	0.48	0/561
30	18	0.33	0/525	0.52	0/691
30	28	0.30	0/525	0.47	0/691
31	19	0.35	0/310	0.55	0/407
31	29	0.27	0/310	0.50	0/407
32	1a	0.36	0/35795	0.88	25/55864 (0.0%)
32	2a	0.34	0/35886	0.87	28/56005 (0.0%)
33	1b	0.30	0/1881	0.48	0/2542
33	2b	0.29	0/1860	0.48	0/2518
34	1c	0.33	1/1572 (0.1%)	0.47	0/2126
34	2c	0.28	0/1566	0.47	0/2119
35	1d	0.28	0/1685	0.47	0/2262
35	2d	0.30	0/1704	0.48	0/2284
36	1e	0.29	0/1145	0.49	0/1543
36	2e	0.29	0/1149	0.49	0/1548
37	1f	0.30	0/823	0.48	0/1115
37	2f	0.29	0/829	0.47	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.28	0/1250	0.43	0/1679
38	2g	0.27	0/1254	0.42	0/1683
39	1h	0.27	0/1108	0.47	0/1494
39	2h	0.28	0/1108	0.46	0/1494
40	1i	0.28	0/1002	0.52	1/1346 (0.1%)
40	2i	0.29	0/997	0.50	1/1343 (0.1%)
41	1j	0.28	0/722	0.50	0/982
41	2j	0.27	0/727	0.47	0/988
42	1k	0.29	0/844	0.48	0/1145
42	2k	0.27	0/848	0.45	0/1149
43	1l	0.30	0/937	0.52	0/1260
43	2l	0.30	0/937	0.50	0/1260
44	1m	0.30	0/969	0.49	0/1302
44	2m	0.29	0/961	0.48	0/1291
45	1n	0.30	0/501	0.45	0/664
45	2n	0.27	0/501	0.46	0/664
46	1o	0.27	0/739	0.43	0/985
46	2o	0.27	0/739	0.43	0/985
47	1p	0.28	0/697	0.49	0/939
47	2p	0.28	0/693	0.49	0/935
48	1q	0.28	0/836	0.47	0/1117
48	2q	0.29	0/836	0.47	0/1117
49	1r	0.28	0/560	0.45	0/746
49	2r	0.26	0/560	0.46	0/746
50	1s	0.27	0/667	0.53	0/900
50	2s	0.28	0/661	0.50	0/893
51	1t	0.27	0/730	0.41	0/965
51	2t	0.27	0/729	0.44	0/965
52	1u	0.26	0/203	0.48	0/266
52	2u	0.27	0/203	0.46	0/266
53	1v	0.38	0/310	0.84	0/480
53	2v	0.46	0/310	0.95	0/480
54	1w	0.46	1/1581 (0.1%)	1.01	2/2458 (0.1%)
54	2w	0.40	0/1531	1.01	1/2379 (0.0%)
55	1x	0.48	0/1725	1.08	10/2689 (0.4%)
55	2x	0.42	0/1725	1.01	4/2689 (0.1%)
56	1y	0.56	1/1606 (0.1%)	1.16	7/2497 (0.3%)
56	2y	0.55	1/1583 (0.1%)	1.12	3/2459 (0.1%)
All	All	0.39	6/316642 (0.0%)	0.83	188/474042 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	2P	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	1	G	OP3-P	-10.56	1.48	1.61
2	2B	1	U	OP3-P	-10.29	1.48	1.61
56	1y	1	G	OP3-P	-10.26	1.48	1.61
54	1w	1	G	OP3-P	-10.18	1.49	1.61
2	1B	1	U	OP3-P	-10.14	1.49	1.61
34	1c	173	VAL	C-N	7.38	1.48	1.34

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2083	G	O5'-P-OP2	-10.61	96.15	105.70
1	2A	1178	C	N1-C2-O2	9.82	124.79	118.90
32	1a	1030(B)	C	N1-C2-O2	9.10	124.36	118.90
32	2a	299	G	C5-C6-O6	-9.01	123.19	128.60
32	1a	558	G	O5'-P-OP1	-8.91	97.69	105.70
1	2A	2152	G	C5-C6-O6	-8.48	123.51	128.60
1	2A	2152	G	N1-C6-O6	8.47	124.98	119.90
55	2x	14	A	C4-C5-C6	8.43	121.21	117.00
32	2a	1001(A)	G	N3-C4-N9	8.40	131.04	126.00
1	2A	2136	C	N1-C2-O2	8.27	123.86	118.90
32	1a	1030(B)	C	C2-N1-C1'	8.22	127.85	118.80
1	1A	1020	C	N1-C2-O2	-8.16	114.00	118.90
56	1y	33	U	N1-C2-O2	8.12	128.48	122.80
1	1A	848	G	O5'-P-OP2	-8.10	98.41	105.70
1	1A	12	U	C2-N1-C1'	8.05	127.36	117.70
1	1A	1137	G	N3-C4-N9	7.94	130.76	126.00
55	1x	14	A	C4-C5-C6	7.89	120.94	117.00
56	1y	68	C	N1-C2-O2	7.74	123.54	118.90
1	2A	1178	C	N3-C2-O2	-7.73	116.49	121.90
32	1a	1030(B)	C	N3-C2-O2	-7.66	116.53	121.90
56	1y	33	U	N3-C2-O2	-7.58	116.89	122.20
1	1A	834	U	O5'-P-OP1	-7.57	98.89	105.70
1	2A	2139	C	N1-C2-O2	7.56	123.44	118.90
1	1A	1121	C	N1-C2-O2	7.56	123.44	118.90
56	1y	33	U	C2-N1-C1'	7.56	126.77	117.70
1	2A	2139	C	C2-N1-C1'	7.54	127.09	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2189	U	C2-N1-C1'	7.47	126.67	117.70
55	1x	46	G	C6-N1-C2	-7.39	120.67	125.10
1	1A	1143	U	C2-N1-C1'	7.29	126.45	117.70
1	1A	1109	G	C5-C6-O6	7.21	132.93	128.60
1	1A	611	U	O5'-P-OP2	-7.15	99.26	105.70
1	1A	2014	G	P-O3'-C3'	7.15	128.28	119.70
1	1A	1146	C	C2-N1-C1'	7.15	126.66	118.80
1	1A	1121	C	C2-N3-C4	7.10	123.45	119.90
32	2a	754	C	C2-N1-C1'	7.09	126.60	118.80
32	1a	1030(B)	C	C6-N1-C2	-6.94	117.53	120.30
32	2a	299	G	C4-C5-N7	6.93	113.57	110.80
1	2A	2152	G	C6-C5-N7	-6.81	126.32	130.40
1	2A	2174	C	C2-N1-C1'	6.79	126.26	118.80
54	1w	47	U	C2-N1-C1'	6.73	125.78	117.70
56	1y	64	A	C5-C6-N6	6.64	129.01	123.70
1	1A	1132	A	N1-C6-N6	-6.62	114.63	118.60
55	2x	46	G	C6-N1-C2	-6.58	121.15	125.10
1	1A	1374	G	N1-C6-O6	-6.56	115.96	119.90
56	1y	64	A	N1-C6-N6	-6.55	114.67	118.60
32	2a	299	G	N1-C6-O6	6.55	123.83	119.90
1	1A	2210	C	N1-C2-O2	6.52	122.81	118.90
1	1A	1137	G	N9-C4-C5	-6.50	102.80	105.40
1	1A	537	G	O4'-C1'-N9	6.44	113.35	108.20
1	1A	831	A	O4'-C1'-N9	6.43	113.34	108.20
32	2a	299	G	N9-C4-C5	-6.41	102.83	105.40
55	1x	22	G	N1-C6-O6	-6.39	116.06	119.90
55	1x	14	A	C5-N7-C8	6.34	107.07	103.90
32	2a	1001(A)	G	C6-C5-N7	-6.34	126.59	130.40
32	2a	1001(A)	G	C4-N9-C1'	6.34	134.74	126.50
1	2A	1178	C	C2-N1-C1'	6.33	125.77	118.80
32	2a	266	G	P-O3'-C3'	6.28	127.24	119.70
40	1i	50	LEU	CA-CB-CG	6.28	129.74	115.30
1	2A	2139	C	C6-N1-C1'	-6.28	113.27	120.80
1	1A	1418	U	N3-C4-O4	6.26	123.78	119.40
32	1a	1002	G	C4-N9-C1'	6.25	134.63	126.50
1	1A	2503	U	OP1-P-O3'	6.25	118.95	105.20
32	1a	1002	G	N3-C4-N9	6.21	129.73	126.00
32	2a	754	C	N1-C2-O2	6.21	122.62	118.90
1	2A	2152	G	N3-C4-N9	6.14	129.69	126.00
32	2a	1039	C	C5-C4-N4	-6.14	115.90	120.20
2	2B	80	U	O4'-C1'-N1	6.12	113.10	108.20
1	1A	2055	A	O5'-P-OP1	-6.12	100.20	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1001(A)	G	C8-N9-C1'	-6.10	119.07	127.00
1	1A	1137	G	C8-N9-C1'	-6.08	119.09	127.00
32	2a	1004	A	O4'-C1'-N9	6.05	113.04	108.20
1	1A	1143	U	N3-C2-O2	-5.99	118.01	122.20
1	1A	1418	U	C5-C4-O4	-5.99	122.31	125.90
1	1A	2261	U	C6-N1-C2	5.97	124.58	121.00
1	1A	1137	G	C6-C5-N7	-5.93	126.84	130.40
1	1A	637	U	C2-N1-C1'	5.92	124.81	117.70
1	1A	2189	U	N1-C2-O2	5.92	126.94	122.80
1	1A	2189	U	N3-C2-O2	-5.90	118.07	122.20
1	1A	1374	G	C5-C6-O6	5.87	132.12	128.60
32	1a	1002	G	C8-N9-C1'	-5.87	119.37	127.00
55	1x	22	G	C4-C5-C6	-5.85	115.29	118.80
1	1A	1146	C	C6-N1-C1'	-5.84	113.79	120.80
1	1A	1359	U	C2-N1-C1'	5.84	124.71	117.70
32	1a	1158	C	C2-N1-C1'	5.83	125.21	118.80
1	1A	894	U	C2-N1-C1'	5.82	124.68	117.70
1	2A	2061	G	O5'-P-OP2	-5.81	100.47	105.70
1	1A	1143	U	N1-C2-O2	5.80	126.86	122.80
1	1A	2050	U	N3-C4-O4	-5.79	115.35	119.40
32	2a	1001(A)	G	N9-C4-C5	-5.78	103.09	105.40
1	1A	2723	A	O5'-P-OP2	-5.77	100.51	105.70
1	2A	2174	C	N1-C2-O2	5.75	122.35	118.90
1	1A	1137	G	C4-N9-C1'	5.75	133.97	126.50
54	1w	47	U	N1-C2-O2	5.73	126.81	122.80
1	2A	512	G	O4'-C1'-N9	5.72	112.78	108.20
32	1a	267	C	O5'-P-OP1	-5.64	100.63	105.70
32	2a	1026	G	N3-C4-C5	-5.63	125.78	128.60
32	1a	839	U	P-O3'-C3'	5.63	126.46	119.70
40	2i	50	LEU	CA-CB-CG	5.63	128.25	115.30
55	2x	14	A	C5-C6-N1	-5.61	114.90	117.70
1	1A	1020	C	C2-N1-C1'	-5.60	112.64	118.80
1	1A	1700	G	C8-N9-C4	-5.60	104.16	106.40
1	1A	2584	A	C8-N9-C4	5.60	108.04	105.80
32	2a	299	G	C6-C5-N7	-5.59	127.05	130.40
1	1A	1020	C	C6-N1-C1'	5.58	127.50	120.80
1	1A	1221	G	P-O3'-C3'	5.58	126.40	119.70
1	1A	2858	G	O4'-C1'-N9	5.58	112.67	108.20
1	2A	1022	G	N3-C4-N9	-5.58	122.65	126.00
56	1y	65	G	N3-C2-N2	5.56	123.79	119.90
32	1a	1067	A	P-O3'-C3'	5.55	126.36	119.70
56	2y	12	U	C5-C4-O4	5.55	129.23	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1105	G	C5-C6-O6	5.50	131.90	128.60
1	1A	1221	G	OP1-P-O3'	5.50	117.31	105.20
1	1A	1109	G	N3-C2-N2	5.49	123.74	119.90
32	2a	1003	G	C4-N9-C1'	5.47	133.61	126.50
1	1A	1006	C	N1-C2-O2	-5.47	115.62	118.90
1	2A	2155	G	N9-C4-C5	-5.47	103.21	105.40
32	1a	1225	A	N1-C6-N6	-5.46	115.32	118.60
1	1A	201	G	C4-N9-C1'	-5.46	119.40	126.50
32	2a	1001(A)	G	N3-C4-C5	-5.46	125.87	128.60
1	2A	2155	G	N3-C2-N2	5.45	123.72	119.90
1	2A	784	A	O4'-C1'-N9	5.45	112.56	108.20
55	1x	14	A	C5-C6-N1	-5.45	114.98	117.70
1	1A	1109	G	C6-N1-C2	5.44	128.36	125.10
32	1a	1027	C	C2-N1-C1'	5.43	124.78	118.80
1	2A	527	C	N1-C2-O2	5.43	122.16	118.90
1	2A	1313	U	C2-N1-C1'	5.41	124.19	117.70
32	2a	1001(A)	G	C4-C5-N7	5.41	112.96	110.80
32	1a	266	G	P-O3'-C3'	5.40	126.19	119.70
32	2a	1003	G	N3-C4-N9	5.40	129.24	126.00
1	1A	2883	A	O4'-C1'-N9	5.40	112.52	108.20
32	2a	1007	C	C2-N3-C4	5.40	122.60	119.90
56	2y	22	G	N3-C4-N9	5.39	129.23	126.00
1	1A	740	C	N3-C2-O2	-5.38	118.13	121.90
1	2A	90	U	N3-C2-O2	-5.38	118.44	122.20
1	2A	2155	G	N3-C4-N9	5.36	129.22	126.00
1	2A	2152	G	N9-C4-C5	-5.36	103.26	105.40
32	2a	1003	G	N3-C4-C5	-5.35	125.92	128.60
1	1A	1146	C	N1-C2-O2	5.34	122.11	118.90
32	1a	1158	C	N1-C2-O2	5.34	122.10	118.90
55	1x	22	G	C5-N7-C8	-5.34	101.63	104.30
1	1A	2261	U	N3-C4-C5	5.33	117.80	114.60
55	1x	22	G	N3-C4-N9	-5.33	122.80	126.00
32	1a	687	A	P-O3'-C3'	5.32	126.08	119.70
1	2A	1779	U	C2-N1-C1'	5.31	124.07	117.70
32	1a	115	G	P-O3'-C3'	5.30	126.07	119.70
1	2A	1992	G	P-O3'-C3'	5.29	126.05	119.70
1	1A	1120	G	P-O3'-C3'	5.28	126.04	119.70
55	1x	22	G	C8-N9-C1'	5.27	133.85	127.00
1	2A	2152	G	C4-C5-N7	5.27	112.91	110.80
1	1A	860	U	O5'-P-OP1	-5.26	100.96	105.70
32	2a	754	C	C6-N1-C1'	-5.26	114.48	120.80
1	1A	2605	U	C5-C4-O4	5.25	129.05	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2155	G	C6-C5-N7	-5.24	127.26	130.40
55	1x	22	G	C5-C6-N1	5.23	114.11	111.50
1	1A	2015	U	O5'-P-OP1	-5.21	101.01	105.70
1	1A	2175	G	N3-C4-N9	-5.21	122.88	126.00
32	1a	1225	A	C5-C6-N6	5.21	127.87	123.70
1	1A	1371	G	N1-C6-O6	-5.20	116.78	119.90
32	1a	1030(B)	C	C6-N1-C1'	-5.20	114.56	120.80
1	2A	1653	G	P-O3'-C3'	5.20	125.94	119.70
1	2A	2689	U	N3-C2-O2	-5.19	118.57	122.20
1	1A	2605	U	N3-C4-O4	-5.17	115.78	119.40
1	1A	1137	G	C4-C5-N7	5.17	112.87	110.80
1	1A	1374	G	N3-C2-N2	5.15	123.51	119.90
1	1A	637	U	O4'-C1'-N1	5.14	112.31	108.20
1	2A	1395	A	O4'-C1'-N9	5.14	112.31	108.20
1	1A	1270	C	C6-N1-C2	-5.12	118.25	120.30
32	2a	1065	U	P-O3'-C3'	5.12	125.84	119.70
54	2w	3	C	N1-C2-O2	5.12	121.97	118.90
56	2y	47	U	C2-N1-C1'	5.12	123.84	117.70
32	1a	1442	G	P-O3'-C3'	5.11	125.84	119.70
32	2a	1224	G	C5-C6-O6	5.11	131.67	128.60
1	2A	2897	U	C2-N1-C1'	5.11	123.83	117.70
1	1A	12	U	C6-N1-C1'	-5.10	114.06	121.20
32	1a	1201	A	P-O3'-C3'	5.10	125.82	119.70
1	1A	31	C	O5'-P-OP1	-5.10	101.11	105.70
32	1a	1002	G	N3-C4-C5	-5.08	126.06	128.60
1	2A	2139	C	N3-C4-C5	5.08	123.93	121.90
32	2a	1039	C	N1-C2-O2	5.08	121.94	118.90
55	2x	14	A	C5-N7-C8	5.08	106.44	103.90
1	2A	228	A	P-O3'-C3'	5.07	125.78	119.70
1	1A	1371	G	O4'-C1'-N9	5.06	112.25	108.20
1	2A	527	C	N3-C2-O2	-5.04	118.37	121.90
32	1a	913	A	P-O3'-C3'	5.03	125.74	119.70
32	2a	1125	U	C2-N1-C1'	5.03	123.74	117.70
1	2A	2136	C	N3-C2-O2	-5.01	118.39	121.90
32	2a	65	U	P-O3'-C3'	5.01	125.72	119.70
32	1a	1027	C	C5-C6-N1	5.00	123.50	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	2P	44	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31190	652	0
1	2A	60322	0	30415	739	0
2	1B	2577	0	1304	22	0
2	2B	2575	0	1302	44	0
3	1D	2136	0	2218	47	0
3	2D	2136	0	2218	45	0
4	1E	1559	0	1618	31	0
4	2E	1559	0	1618	32	0
5	1F	1584	0	1625	35	0
5	2F	1580	0	1619	38	0
6	1G	1429	0	1447	28	0
6	2G	1428	0	1438	52	0
7	1H	1330	0	1407	27	0
7	2H	1330	0	1407	24	0
8	1I	1097	0	1140	26	0
8	2I	1064	0	1082	19	0
9	1N	1117	0	1184	20	0
9	2N	1117	0	1184	17	0
10	1O	933	0	996	17	0
10	2O	933	0	996	25	0
11	1P	1135	0	1212	44	0
11	2P	1135	0	1211	32	0
12	1Q	1122	0	1179	30	0
12	2Q	1122	0	1179	25	0
13	1R	968	0	1033	24	0
13	2R	968	0	1033	11	0
14	1S	873	0	927	15	0
14	2S	870	0	923	29	0
15	1T	1091	0	1151	36	0
15	2T	1083	0	1136	29	0
16	1U	959	0	1019	25	0
16	2U	959	0	1018	23	0
17	1V	771	0	830	17	0
17	2V	771	0	830	13	0
18	1W	886	0	939	10	0
18	2W	886	0	940	12	0
19	1X	750	0	814	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2X	750	0	813	13	0
20	1Y	806	0	881	17	0
20	2Y	806	0	881	18	0
21	1Z	1240	0	1240	25	0
21	2Z	1271	0	1273	29	0
22	10	653	0	674	14	0
22	20	653	0	674	15	0
23	11	755	0	826	17	0
23	21	755	0	826	18	0
24	12	588	0	643	16	0
24	22	588	0	643	13	0
25	13	469	0	518	5	0
25	23	464	0	514	13	0
26	14	552	0	533	15	0
26	24	532	0	503	16	0
27	15	455	0	465	11	0
27	25	455	0	465	9	0
28	16	453	0	473	5	0
28	26	449	0	469	9	0
29	17	418	0	466	4	0
29	27	418	0	467	7	0
30	18	517	0	582	21	0
30	28	517	0	582	21	0
31	19	307	0	335	7	0
31	29	307	0	335	5	0
32	1a	32246	0	16295	0	0
32	2a	32327	0	16340	0	0
33	1b	1846	0	1867	0	0
33	2b	1825	0	1828	0	0
34	1c	1548	0	1535	0	0
34	2c	1542	0	1517	0	0
35	1d	1655	0	1672	0	0
35	2d	1674	0	1714	0	0
36	1e	1129	0	1185	0	0
36	2e	1133	0	1191	0	0
37	1f	810	0	804	0	0
37	2f	816	0	808	0	0
38	1g	1231	0	1238	0	0
38	2g	1235	0	1249	0	0
39	1h	1088	0	1126	0	0
39	2h	1088	0	1126	0	0
40	1i	983	0	986	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1603	0	829	0	0
54	2w	1555	0	797	0	0
55	1x	1625	0	828	0	0
55	2x	1625	0	828	0	0
56	1y	1585	0	804	0	0
56	2y	1565	0	795	0	0
57	10	5	0	0	0	0
57	11	3	0	0	0	0
57	12	2	0	0	0	0
57	13	1	0	0	0	0
57	14	1	0	0	0	0
57	15	4	0	0	0	0
57	16	1	0	0	0	0
57	17	2	0	0	0	0
57	18	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	19	1	0	0	0	0
57	1A	1001	0	0	0	0
57	1B	31	0	0	0	0
57	1D	12	0	0	0	0
57	1E	10	0	0	0	0
57	1F	9	0	0	0	0
57	1G	5	0	0	0	0
57	1I	1	0	0	0	0
57	1N	7	0	0	0	0
57	1O	7	0	0	0	0
57	1P	4	0	0	0	0
57	1Q	6	0	0	0	0
57	1R	3	0	0	0	0
57	1S	3	0	0	0	0
57	1T	2	0	0	0	0
57	1U	4	0	0	0	0
57	1V	3	0	0	0	0
57	1W	6	0	0	0	0
57	1X	7	0	0	0	0
57	1Y	4	0	0	0	0
57	1Z	3	0	0	0	0
57	1a	231	0	0	0	0
57	1b	2	0	0	0	0
57	1e	1	0	0	0	0
57	1f	1	0	0	0	0
57	1l	2	0	0	0	0
57	1n	2	0	0	0	0
57	1q	1	0	0	0	0
57	1r	1	0	0	0	0
57	1t	1	0	0	0	0
57	1w	4	0	0	0	0
57	1x	11	0	0	0	0
57	1y	2	0	0	0	0
57	20	3	0	0	0	0
57	23	1	0	0	0	0
57	25	3	0	0	0	0
57	28	2	0	0	0	0
57	2A	687	0	0	0	0
57	2B	21	0	0	0	0
57	2D	8	0	0	0	0
57	2E	6	0	0	0	0
57	2F	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2G	1	0	0	0	0
57	2O	1	0	0	0	0
57	2P	1	0	0	0	0
57	2Q	3	0	0	0	0
57	2R	2	0	0	0	0
57	2U	2	0	0	0	0
57	2V	2	0	0	0	0
57	2W	1	0	0	0	0
57	2X	2	0	0	0	0
57	2Y	1	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	201	0	0	0	0
57	2d	2	0	0	0	0
57	2e	1	0	0	0	0
57	2f	2	0	0	0	0
57	2g	1	0	0	0	0
57	2h	1	0	0	0	0
57	2j	2	0	0	0	0
57	2l	2	0	0	0	0
57	2q	3	0	0	0	0
57	2r	1	0	0	0	0
57	2t	1	0	0	0	0
57	2v	2	0	0	0	0
57	2w	4	0	0	0	0
57	2x	5	0	0	0	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	1A	37	0	0	0	0
59	2A	37	0	0	0	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2d	8	0	0	0	0
62	10	7	0	0	0	0
62	11	2	0	0	1	0
62	12	4	0	0	1	0
62	13	3	0	0	0	0
62	14	1	0	0	0	0
62	15	4	0	0	0	0
62	17	4	0	0	0	0
62	18	8	0	0	0	0
62	19	1	0	0	0	0
62	1A	1610	0	0	79	0
62	1B	40	0	0	1	0
62	1D	21	0	0	1	0
62	1E	19	0	0	5	0
62	1F	14	0	0	3	0
62	1G	5	0	0	0	0
62	1H	1	0	0	1	0
62	1I	2	0	0	0	0
62	1N	2	0	0	0	0
62	1O	5	0	0	0	0
62	1P	18	0	0	2	0
62	1Q	3	0	0	0	0
62	1R	6	0	0	0	0
62	1S	5	0	0	0	0
62	1T	6	0	0	0	0
62	1U	9	0	0	1	0
62	1V	4	0	0	0	0
62	1W	4	0	0	0	0
62	1X	5	0	0	0	0
62	1Y	3	0	0	0	0
62	1Z	1	0	0	0	0
62	1a	276	0	0	0	0
62	1b	1	0	0	0	0
62	1e	1	0	0	0	0
62	1j	1	0	0	0	0
62	1k	1	0	0	0	0
62	1l	3	0	0	0	0
62	1q	1	0	0	0	0
62	1v	3	0	0	0	0
62	1w	6	0	0	0	0
62	1x	9	0	0	0	0
62	1y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	20	3	0	0	0	0
62	21	3	0	0	0	0
62	22	1	0	0	0	0
62	25	3	0	0	0	0
62	27	4	0	0	1	0
62	28	4	0	0	1	0
62	29	1	0	0	0	0
62	2A	926	0	0	41	0
62	2B	10	0	0	0	0
62	2D	16	0	0	3	0
62	2E	10	0	0	3	0
62	2F	5	0	0	0	0
62	2I	3	0	0	0	0
62	2N	1	0	0	0	0
62	2O	1	0	0	0	0
62	2P	10	0	0	0	0
62	2Q	1	0	0	0	0
62	2R	2	0	0	0	0
62	2T	2	0	0	0	0
62	2U	3	0	0	0	0
62	2V	1	0	0	1	0
62	2W	1	0	0	0	0
62	2X	3	0	0	1	0
62	2Z	2	0	0	0	0
62	2a	230	0	0	0	0
62	2d	2	0	0	0	0
62	2e	1	0	0	0	0
62	2f	1	0	0	0	0
62	2g	1	0	0	0	0
62	2i	2	0	0	0	0
62	2j	4	0	0	0	0
62	2l	3	0	0	0	0
62	2n	1	0	0	0	0
62	2o	1	0	0	0	0
62	2v	2	0	0	0	0
62	2w	1	0	0	0	0
62	2x	5	0	0	0	0
All	All	298900	0	196701	2311	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 (2311) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1128:U:H3	1:1A:1132:A:N6	1.45	1.13
1:1A:2160:C:N4	1:1A:2175:G:H1	1.57	1.02
1:1A:1099:C:N4	1:1A:1152:G:H1	1.59	0.99
1:2A:1422:G:H5''	10:2O:48:PRO:HB3	99.99	0.96
1:1A:1128:U:O4	1:1A:1132:A:N1	1.96	0.96
1:2A:2138:C:H42	1:2A:2153:G:H1	1.01	0.96
1:2A:2139:C:H42	1:2A:2152:G:H1	0.97	0.95
1:2A:2139:C:N4	1:2A:2152:G:H1	1.64	0.94
12:1Q:12:GLN:HE21	12:1Q:72:LYS:HG3	1.36	0.91
22:10:10:THR:HG22	22:10:12:ASN:H	1.34	0.91
1:1A:2122:G:H1	1:1A:2211:U:H3	0.92	0.91
1:1A:2143:G:H1	1:1A:2199:C:H42	1.19	0.91
1:2A:2138:C:N4	1:2A:2153:G:H1	1.69	0.90
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.36	0.89
4:1E:36:ARG:NH1	4:1E:85:ASN:OD1	2.09	0.86
1:2A:2319:G:H22	14:2S:3:ARG:HD2	1.41	0.85
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.22	0.85
1:2A:1309:G:HO2'	1:2A:1611:C:HO2'	1.24	0.85
1:1A:1118:C:O2	1:1A:1138:C:N4	2.09	0.84
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.24	0.84
9:1N:20:GLY:HA2	9:1N:61:ARG:HD2	1.57	0.84
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.60	0.84
1:2A:1689:A:H62	1:2A:1698:A:H2	1.20	0.84
1:1A:1099:C:H42	1:1A:1152:G:H1	0.84	0.83
13:2R:24:GLN:HB3	13:2R:44:LEU:HD11	1.61	0.83
10:2O:64:ARG:HH12	15:2T:70:VAL:HG21	1.44	0.82
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.13	0.82
30:28:6:THR:HG22	30:28:63:PRO:HD2	1.62	0.82
1:2A:271(K):U:O2	8:2I:50:ARG:NH2	2.13	0.81
21:1Z:153:SER:HB3	21:1Z:167:PRO:HB3	1.63	0.81
1:2A:2138:C:N3	1:2A:2153:G:N2	2.28	0.81
1:1A:1070:G:OP2	62:1A:4144:HOH:O	1.99	0.81
1:1A:1018:A:OP2	62:1A:4152:HOH:O	1.97	0.80
2:2B:22:U:H3	2:2B:61:G:H1	1.28	0.80
1:2A:1529:G:H1	1:2A:1540:U:H3	1.29	0.80
2:1B:42:C:N4	6:1G:91:ARG:HH12	1.80	0.79
1:2A:987:G:H1	1:2A:1218:C:H42	46.26	0.79
1:1A:2160:C:N3	1:1A:2175:G:N2	2.30	0.79
22:10:11:ARG:O	22:10:14:ARG:NH2	2.13	0.79
1:1A:2121:U:H3	1:1A:2212:G:H1	1.30	0.79
1:1A:2331:G:H22	14:1S:3:ARG:HD2	1.48	0.79
1:1A:661:G:HO2'	1:1A:663:G:HO2'	1.29	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2785:C:OP1	4:2E:41:LYS:NZ	2.15	0.78
11:2P:87:ASP:O	11:2P:90:ARG:NH1	2.16	0.78
12:2Q:77:LYS:NZ	12:2Q:86:GLY:O	2.17	0.78
1:2A:370:G:OP2	62:2A:3776:HOH:O	2.02	0.78
23:21:51:VAL:HG11	23:21:74:VAL:HG21	1.64	0.78
6:1G:41:GLN:NE2	6:1G:154:GLY:O	2.17	0.77
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.66	0.77
3:1D:69:ARG:NH2	3:1D:128:GLY:O	2.18	0.77
1:1A:211:A:OP1	62:1A:4155:HOH:O	2.02	0.77
2:2B:54:G:H21	6:2G:29:TRP:HZ2	1.31	0.77
1:2A:2753:A:N3	31:29:15:LYS:NZ	2.32	0.77
1:2A:1204:A:H2	1:2A:1241:A:H62	1.32	0.77
1:2A:765:G:H1	1:2A:812:C:HO2'	84.66	0.77
1:2A:1852:C:O2	1:2A:1890:A:N6	2.18	0.76
1:1A:2158:C:N4	1:1A:2177:G:C6	2.54	0.76
2:2B:15:A:OP2	2:2B:69:G:N2	2.18	0.76
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.19	0.76
1:1A:2123:G:H1	1:1A:2210:C:N4	1.83	0.76
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.66	0.76
21:2Z:10:ARG:NH2	21:2Z:26:GLY:O	2.18	0.76
1:1A:1099:C:N3	1:1A:1152:G:N2	2.32	0.76
1:1A:1310:G:OP1	27:15:19:ARG:NH2	2.19	0.76
1:1A:1361:C:OP2	62:1A:4154:HOH:O	2.02	0.76
1:1A:2614:A:OP1	62:1A:4153:HOH:O	2.02	0.76
3:2D:38:LYS:NZ	3:2D:39:LYS:O	2.18	0.76
1:1A:2123:G:N1	1:1A:2210:C:N4	2.34	0.75
1:2A:76:C:H42	1:2A:93:G:H1	26.58	0.75
1:2A:856:C:H2'	1:2A:857:C:H6	1.52	0.75
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.68	0.75
1:2A:195:A:N7	62:2A:3705:HOH:O	2.18	0.75
1:2A:2807:G:N1	1:2A:2893:G:O6	2.18	0.75
21:1Z:138:GLU:H	21:1Z:156:LYS:HZ1	1.34	0.75
1:1A:1093:G:H2'	1:1A:1156:G:H22	1.52	0.75
1:1A:1120:G:O2'	1:1A:1121:C:OP1	2.05	0.75
1:1A:2160:C:H42	1:1A:2175:G:H1	0.79	0.75
1:1A:7:G:H1	1:1A:2905:C:H42	1.35	0.75
1:2A:2793:G:H1	1:2A:2803:C:H42	1.33	0.74
1:2A:2867:G:OP2	15:2T:119:LYS:NZ	2.18	0.74
1:1A:1139:G:H3'	1:1A:1140:U:H5''	1.70	0.74
3:2D:237:GLU:OE2	62:2D:401:HOH:O	2.05	0.74
21:2Z:156:LYS:HE3	21:2Z:158:PRO:HD3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2152:U:O2'	1:1A:2180:A:N1	2.21	0.74
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.69	0.74
1:1A:591:U:O4	62:1A:4152:HOH:O	2.05	0.74
1:1A:929:G:H1	1:1A:940:C:H42	1.34	0.73
1:1A:2205:C:H2'	1:1A:2206:G:H8	1.53	0.73
1:1A:71:U:OP1	62:1A:4156:HOH:O	2.05	0.73
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.70	0.73
1:1A:1829:U:H5'	3:1D:259:THR:HG22	1.69	0.73
1:2A:740:U:OP2	62:2A:3777:HOH:O	2.06	0.73
1:1A:2419:G:OP1	62:1A:4130:HOH:O	2.05	0.73
1:1A:599:U:OP1	62:1A:4157:HOH:O	2.06	0.73
17:1V:72:VAL:HG13	17:1V:85:LYS:HB3	1.71	0.73
1:2A:599:G:N7	62:2A:3801:HOH:O	2.21	0.73
2:1B:77:U:OP1	21:1Z:19:ARG:NH2	2.22	0.73
7:1H:86:GLU:OE2	7:1H:130:ARG:NH1	2.21	0.73
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.22	0.73
1:2A:1332:G:OP1	62:2A:3778:HOH:O	2.07	0.73
1:2A:2299:G:H2'	1:2A:2300:G:H8	1.54	0.73
1:2A:1568:G:N7	62:2A:3799:HOH:O	2.21	0.72
1:1A:973:G:N7	62:1A:4194:HOH:O	2.21	0.72
17:2V:78:LYS:O	62:2V:301:HOH:O	2.07	0.72
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.70	0.72
20:2Y:20:TYR:HB3	20:2Y:23:ARG:HD2	1.71	0.72
1:2A:1428:C:N4	1:2A:1570:A:OP2	2.20	0.71
1:1A:2123:G:N2	1:1A:2210:C:N3	2.36	0.71
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.23	0.71
1:1A:1114:G:N1	1:1A:1141:A:O2'	2.24	0.71
1:1A:2701:U:H4'	1:1A:2702:C:H5'	1.72	0.71
1:2A:527:C:N4	1:2A:2779:U:OP2	2.23	0.71
1:2A:83:G:H1	1:2A:102:G:HO2'	1.38	0.71
1:1A:131:C:O2	1:1A:231:G:N2	72.27	0.71
4:2E:8:LYS:NZ	4:2E:190:GLY:O	2.22	0.71
1:2A:987:G:H1	1:2A:1218:C:N4	45.99	0.70
1:2A:1002:G:H2'	1:2A:1003:G:H8	3.14	0.70
1:2A:1951:U:OP1	62:2A:3779:HOH:O	2.09	0.70
17:1V:40:LEU:HB2	17:1V:46:VAL:HG22	1.73	0.70
1:1A:1116:A:N7	1:1A:1142:A:O2'	2.25	0.70
1:2A:2849:U:OP2	15:2T:95:ARG:NH1	2.24	0.70
1:1A:889:G:N7	62:1A:4219:HOH:O	2.24	0.70
1:2A:2166:G:O6	1:2A:2171:A:N6	2.25	0.70
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2725:A:N3	62:1A:4217:HOH:O	2.24	0.70
4:1E:119:ARG:HD2	4:1E:160:TYR:HB2	1.73	0.70
1:1A:2143:G:H1	1:1A:2199:C:N4	1.90	0.69
1:1A:2158:C:N3	1:1A:2177:G:C2	2.60	0.69
1:2A:1269:A:OP1	62:2A:3780:HOH:O	2.10	0.69
7:2H:25:LYS:HB3	7:2H:27:LYS:HZ1	1.57	0.69
22:20:51:VAL:HG22	22:20:81:VAL:HG23	1.74	0.69
11:1P:52:GLU:OE1	11:1P:55:ARG:NH1	2.26	0.69
1:2A:276:A:H5''	1:2A:277:C:H5'	1.74	0.69
1:2A:463:G:N7	62:2A:3816:HOH:O	2.26	0.69
1:1A:894:U:OP2	62:1A:4159:HOH:O	2.09	0.69
1:2A:2097:C:N3	1:2A:2192:G:O6	2.26	0.69
1:2A:2343:C:HO2'	1:2A:2373:G:HO2'	1.36	0.69
6:1G:7:LEU:HD13	6:1G:104:GLU:HA	1.75	0.69
1:2A:890:A:H2'	1:2A:892:G:C8	2.28	0.69
1:1A:1003:U:OP2	12:1Q:14:ARG:NH1	2.25	0.68
1:2A:1537:G:H2'	1:2A:1538:G:H8	1.56	0.68
4:2E:125:GLY:O	62:2E:401:HOH:O	2.11	0.68
1:1A:231:G:OP1	62:1A:4160:HOH:O	2.10	0.68
5:1F:101:LEU:O	5:1F:106:ARG:NH1	2.27	0.68
7:1H:101:ARG:NH2	7:1H:121:ILE:O	2.25	0.68
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.75	0.68
1:2A:2355:C:H1'	22:20:39:ARG:HH21	1.58	0.68
1:1A:1114:G:O2'	1:1A:1116:A:N7	2.27	0.68
11:1P:138:LEU:HD23	11:1P:145:PRO:HG3	1.76	0.68
3:2D:85:ASP:OD2	3:2D:88:ARG:NH1	2.26	0.68
1:1A:2718:G:N7	62:1A:4234:HOH:O	2.26	0.68
1:2A:1423:G:H5'	10:2O:49:ARG:HH22	96.71	0.68
12:2Q:68:ILE:HG22	12:2Q:101:ARG:HE	1.59	0.68
1:1A:928:G:H3'	1:1A:929:G:H8	1.57	0.68
4:2E:56:PRO:HG3	4:2E:74:PRO:HG2	1.75	0.68
1:2A:2287:A:H62	1:2A:2344:U:H3	1.39	0.68
19:2X:44:GLU:OE1	62:2X:3101:HOH:O	2.12	0.68
30:18:28:GLY:O	30:18:36:LYS:NZ	2.27	0.67
1:1A:2530:A:OP2	62:1A:4161:HOH:O	2.10	0.67
31:29:16:VAL:HG22	31:29:25:VAL:HG22	1.75	0.67
1:2A:1153:C:OP2	62:2A:3784:HOH:O	2.12	0.67
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.27	0.67
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.28	0.67
1:2A:2022:U:OP1	62:2A:3782:HOH:O	2.11	0.67
10:1O:64:ARG:HH12	10:1O:100:GLY:HA3	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:96:U:OP1	21:2Z:14:LYS:NZ	2.27	0.67
1:1A:2205:C:H2'	1:1A:2206:G:C8	2.29	0.67
13:1R:24:GLN:HE22	13:1R:36:THR:HG21	1.59	0.67
1:2A:817:C:N4	1:2A:1529:G:O6	111.40	0.67
17:2V:40:LEU:HB2	17:2V:46:VAL:HG22	1.75	0.67
1:2A:1385:G:O2'	1:2A:1396:U:O2	2.11	0.67
1:1A:556:C:OP2	62:1A:4166:HOH:O	2.13	0.67
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.28	0.67
1:2A:730:C:OP2	62:2A:3785:HOH:O	2.13	0.67
3:2D:76:PRO:HB2	3:2D:116:GLN:HE21	1.59	0.67
1:1A:778:C:OP1	62:1A:4164:HOH:O	2.12	0.67
1:2A:2104:G:H1	1:2A:2185:C:H42	1.43	0.67
1:2A:2531:A:H61	1:2A:2662:A:H61	1.43	0.67
1:1A:1729:G:OP1	62:1A:4163:HOH:O	2.12	0.67
1:1A:2817:G:N1	1:1A:2902:G:O6	2.19	0.67
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.76	0.67
7:2H:23:ARG:NH1	7:2H:34:GLU:OE1	2.27	0.67
1:2A:1266:G:N2	1:2A:1269:A:OP2	13.25	0.67
1:2A:271(H):G:HO2'	1:2A:271(I):G:H8	1.42	0.67
8:1I:5:LEU:HD23	8:1I:9:LEU:HD13	1.77	0.67
1:1A:2518:U:OP1	4:1E:144:ARG:NH2	2.28	0.66
1:2A:469:G:OP2	62:2A:3781:HOH:O	2.11	0.66
4:2E:119:ARG:HD2	4:2E:160:TYR:HB2	1.76	0.66
6:2G:131:TYR:HE2	6:2G:133:LEU:HD23	1.58	0.66
11:1P:42:SER:O	62:1P:3101:HOH:O	2.14	0.66
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.31	0.66
1:1A:331:G:N7	62:1A:4243:HOH:O	2.28	0.66
1:1A:2797:C:H1'	4:1E:37:ARG:HH12	1.59	0.66
1:2A:277:C:H4'	1:2A:278:A:H8	1.60	0.66
6:2G:7:LEU:HD13	6:2G:104:GLU:HA	1.77	0.66
8:2I:12:LEU:HD21	8:2I:19:VAL:HG21	1.78	0.66
1:1A:2164:C:N3	1:1A:2171:G:O6	2.29	0.66
25:23:18:ASP:OD1	25:23:19:GLN:N	2.29	0.66
6:2G:59:GLU:OE2	6:2G:153:ARG:NH1	2.27	0.66
1:1A:2717:A:N3	62:1A:4240:HOH:O	2.28	0.66
1:2A:963:U:OP2	62:2A:3713:HOH:O	2.13	0.66
6:2G:122:PRO:HG3	6:2G:180:PHE:HB3	1.76	0.66
1:2A:2744:G:N2	7:2H:143:GLN:OE1	2.29	0.66
10:1O:120:GLU:OE1	15:1T:67:SER:OG	2.13	0.66
30:28:30:ARG:O	62:28:201:HOH:O	2.13	0.66
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2127:G:N1	1:2A:2161:C:C2	2.63	0.66
1:2A:856:C:H2'	1:2A:857:C:C6	2.30	0.66
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.31	0.66
1:2A:956:G:OP2	12:2Q:14:ARG:NH2	2.27	0.66
23:21:85:LEU:HD22	23:21:86:SER:H	1.61	0.66
2:2B:48:A:OP2	14:2S:30:ARG:NH2	2.29	0.66
1:2A:2518:A:OP2	62:2A:3786:HOH:O	2.13	0.65
13:1R:33:ARG:HH21	13:1R:113:LEU:HD22	1.60	0.65
26:24:64:GLY:O	26:24:66:SER:N	2.29	0.65
1:2A:2319:G:N2	14:2S:3:ARG:HD2	2.12	0.65
1:1A:943:C:N3	1:1A:944:C:N4	2.43	0.65
1:1A:572:A:H61	17:1V:19:LYS:H	1.43	0.65
18:1W:71:VAL:HA	18:1W:107:LEU:HD12	1.78	0.65
19:1X:35:THR:HG22	19:1X:38:GLU:HB2	1.78	0.65
16:2U:6:THR:HG21	16:2U:10:ARG:HD3	1.77	0.65
1:1A:2812:A:H1'	1:1A:2904:U:H1'	1.79	0.65
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	1.79	0.65
1:2A:1009:A:OP2	9:2N:37:LYS:NZ	2.28	0.65
1:2A:601:C:N4	62:2A:3834:HOH:O	2.30	0.65
4:2E:27:LEU:HD12	15:2T:6:LEU:HD21	1.79	0.65
5:1F:11:VAL:HB	5:1F:18:ARG:HB3	1.79	0.65
12:1Q:109:VAL:HG13	12:1Q:113:GLN:HB2	1.78	0.65
1:1A:1140:U:H1'	1:1A:1143:U:C5	2.32	0.65
1:1A:1896:G:N2	1:1A:1899:A:OP2	2.27	0.65
1:2A:2036:C:OP1	62:2A:3788:HOH:O	2.15	0.65
1:2A:848:G:C2	1:2A:933:A:H1'	2.32	0.65
5:2F:40:GLN:NE2	5:2F:182:ASN:HB2	2.11	0.65
1:1A:1740:U:H1'	3:1D:14:ARG:NH2	2.12	0.64
1:2A:1426:G:O2'	1:2A:1572:A:N6	2.28	0.64
1:1A:1405:A:H2'	1:1A:1406:A:H5'	1.78	0.64
11:2P:93:GLY:H	11:2P:123:LEU:HD22	1.62	0.64
1:2A:1434:A:H61	1:2A:1558:A:H62	1.43	0.64
1:2A:856:C:N4	62:2A:3706:HOH:O	2.25	0.64
1:1A:946:A:O2'	1:1A:1333:A:N3	124.57	0.64
1:2A:1783:A:OP1	62:2A:3777:HOH:O	2.15	0.64
1:1A:1133:G:H2'	1:1A:1135:G:C8	2.33	0.64
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.80	0.64
14:2S:83:LYS:HG3	14:2S:84:GLN:H	1.63	0.64
1:1A:1827:U:H2'	1:1A:1828:C:C6	2.32	0.64
1:1A:2040:G:N3	16:1U:34:LYS:NZ	2.46	0.64
1:2A:2193:G:H2'	1:2A:2194:G:C8	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:880:G:H2'	1:2A:881:G:H8	1.63	0.64
1:1A:1105:G:N2	1:1A:1126:C:O2	2.31	0.64
1:1A:242:C:OP2	30:18:5:LYS:NZ	2.21	0.64
1:1A:2772:G:N7	62:1A:4249:HOH:O	2.29	0.64
1:1A:288:U:OP2	62:1A:4170:HOH:O	2.15	0.64
1:2A:1002:G:H1	1:2A:1038:C:H42	43.14	0.64
1:1A:1108:G:H1'	1:1A:1134:A:N7	2.12	0.64
1:1A:625:G:O6	62:1A:4162:HOH:O	2.12	0.64
1:2A:1632:A:OP2	62:2A:3787:HOH:O	2.14	0.64
1:1A:2127:C:H2'	1:1A:2128:G:H8	1.62	0.64
1:1A:2849:G:H5'	13:1R:46:GLY:HA2	1.80	0.64
1:2A:1007:C:N3	1:2A:1022:G:O6	16.55	0.64
1:2A:1971:A:OP1	62:2A:3789:HOH:O	2.15	0.63
1:1A:1128:U:H3	1:1A:1132:A:H61	0.71	0.63
1:1A:1681:A:OP2	62:1A:4168:HOH:O	2.15	0.63
1:1A:2740:G:O2'	10:1O:70:LYS:NZ	2.31	0.63
22:20:10:THR:HG22	22:20:12:ASN:H	1.63	0.63
1:2A:2150:U:H2'	1:2A:2151:G:H8	1.63	0.63
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.32	0.63
21:2Z:153:SER:HB3	21:2Z:167:PRO:HB3	1.79	0.63
26:14:64:GLY:O	26:14:66:SER:N	2.31	0.63
1:1A:23:G:OP1	1:1A:529:U:N3	2.27	0.63
4:1E:77:ILE:HD13	4:1E:195:LEU:HD22	1.80	0.63
1:2A:1778:U:OP1	62:2A:3790:HOH:O	2.15	0.63
15:1T:49:VAL:HG12	15:1T:63:VAL:HG22	1.80	0.63
1:1A:1114:G:H1	1:1A:1141:A:HO2'	1.43	0.63
11:2P:138:LEU:HD23	11:2P:145:PRO:HG3	1.81	0.63
1:1A:2083:G:H5''	1:1A:2515:2MA:C2	2.29	0.63
1:2A:1466:G:HO2'	1:2A:1546:C:HO2'	1.42	0.63
1:2A:1803:A:O2'	3:2D:259:THR:HG21	1.98	0.63
1:2A:39:C:O2	5:2F:46:ARG:NH2	2.32	0.63
1:1A:1202:A:OP1	16:1U:55:ARG:NH1	2.32	0.63
11:1P:106:LEU:HD13	11:1P:112:LEU:HD23	1.80	0.63
1:2A:2167:U:H2'	1:2A:2168:G:H21	1.64	0.63
1:2A:2299:G:H2'	1:2A:2300:G:C8	2.34	0.63
1:2A:1470:G:N2	1:2A:1520:G:OP2	2.32	0.62
1:2A:2011:U:O4	62:2A:3783:HOH:O	2.12	0.62
1:1A:181:C:OP1	62:1A:4172:HOH:O	2.16	0.62
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.80	0.62
13:1R:24:GLN:HB3	13:1R:44:LEU:HD11	1.80	0.62
1:2A:974:G:OP1	1:2A:1187:G:O2'	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2877:G:OP2	15:1T:119:LYS:NZ	2.30	0.62
24:22:8:LYS:NZ	24:22:12:GLU:OE2	2.27	0.62
5:1F:32:LEU:HD13	5:1F:112:MET:HE1	1.82	0.62
1:1A:2594:G:OP2	62:1A:4169:HOH:O	2.15	0.62
1:1A:2766:A:N3	31:19:15:LYS:NZ	2.47	0.62
1:1A:976:G:OP2	1:1A:1358:U:O2'	102.29	0.62
1:2A:83:G:N1	1:2A:102:G:O2'	2.26	0.62
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.80	0.62
1:1A:1108:G:H2'	1:1A:1109:G:C8	2.34	0.62
1:1A:1087:C:H42	1:1A:1160:G:H1	1.48	0.62
5:1F:164:ARG:HG3	5:1F:175:THR:OG1	1.99	0.62
1:2A:2300:G:N1	1:2A:2317:C:N3	2.48	0.62
8:1I:43:ASN:ND2	23:11:75:GLU:OE2	2.33	0.62
1:1A:313:A:N6	1:1A:375:G:O2'	2.33	0.62
1:2A:1721:G:N1	1:2A:1739:U:OP2	2.33	0.62
1:2A:2875:C:OP1	15:2T:3:ARG:NH1	2.25	0.62
5:2F:101:LEU:HD12	5:2F:102:PRO:HD2	1.82	0.62
1:1A:24:G:O2'	18:1W:78:GLU:O	2.17	0.62
1:1A:2178:G:H2'	1:1A:2179:G:C4	2.35	0.62
2:1B:33:G:H5'	6:1G:2:PRO:HD3	1.82	0.62
21:1Z:129:SER:HB3	21:1Z:132:ASN:HD22	1.65	0.62
3:2D:132:PRO:HG2	3:2D:135:PHE:HD2	1.65	0.62
26:14:24:THR:OG1	26:14:25:TYR:N	2.33	0.61
1:1A:1466:U:O2'	1:1A:1467:G:OP1	2.16	0.61
1:2A:2572:A:C8	4:2E:144:ARG:HD2	2.34	0.61
1:1A:1785:C:H5	15:1T:96:ARG:HH21	1.46	0.61
15:1T:24:PRO:HA	15:1T:49:VAL:HG23	1.82	0.61
11:2P:91:PHE:O	11:2P:121:LYS:NZ	2.31	0.61
21:1Z:138:GLU:H	21:1Z:156:LYS:NZ	1.98	0.61
1:2A:453:C:OP1	62:2A:3792:HOH:O	2.16	0.61
1:1A:611:U:H2'	1:1A:612:C:C6	2.35	0.61
1:1A:1834:A:O2'	3:1D:259:THR:HG21	2.00	0.61
8:1I:38:LEU:HD12	8:1I:38:LEU:H	1.64	0.61
21:2Z:138:GLU:H	21:2Z:156:LYS:HZ1	1.49	0.61
1:1A:484:G:O2'	1:1A:495:G:O6	2.17	0.61
16:1U:33:ARG:NH2	62:1U:301:HOH:O	2.34	0.61
21:1Z:91:LEU:HD23	21:1Z:130:PRO:HB3	1.83	0.61
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.35	0.61
1:2A:2815:C:H5'	27:25:29:THR:HG21	1.82	0.61
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.82	0.61
1:2A:300:A:OP1	20:2Y:86:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1440:U:OP1	62:1A:4174:HOH:O	2.16	0.61
1:2A:2199:A:H5''	23:21:50:ARG:HH21	1.66	0.61
1:2A:82:G:N1	1:2A:103:A:OP2	2.27	0.61
1:1A:1861:C:OP2	62:1A:4176:HOH:O	2.16	0.61
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.83	0.61
20:1Y:20:TYR:HB3	20:1Y:23:ARG:HD2	1.82	0.61
1:2A:2114:A:N6	1:2A:2119:A:H62	1.99	0.61
2:2B:24:G:N7	2:2B:56:G:H2'	2.16	0.61
5:2F:40:GLN:HE22	5:2F:182:ASN:HB2	1.65	0.61
6:2G:54:GLU:O	6:2G:58:GLN:N	2.29	0.61
1:2A:1422:G:O2'	10:2O:49:ARG:NH2	100.78	0.61
11:2P:95:VAL:HG13	11:2P:125:VAL:HA	1.83	0.61
1:1A:233:A:OP2	30:18:11:LYS:NZ	2.33	0.61
1:1A:1451:U:H2'	1:1A:1452:U:C6	2.36	0.61
1:1A:2383:G:O6	62:1A:4167:HOH:O	2.14	0.61
1:2A:2142:C:N3	1:2A:2149:G:O6	2.33	0.61
1:2A:910:A:N3	1:2A:2264:C:O2'	2.33	0.61
1:1A:1313:U:OP1	62:1A:4171:HOH:O	2.16	0.61
1:2A:551:G:O2'	1:2A:1220:A:N3	2.29	0.61
1:2A:2313:C:O4'	6:2G:40:ASN:ND2	2.34	0.61
1:1A:964:A:N3	2:1B:80:U:O2'	2.33	0.60
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.82	0.60
1:2A:2136:C:H1'	1:2A:2137:C:H5'	1.83	0.60
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.82	0.60
1:2A:625:G:N7	11:2P:107:LYS:NZ	2.43	0.60
2:2B:28:C:H2'	2:2B:29:A:H8	1.66	0.60
1:1A:2129:C:N4	1:1A:2204:G:H1	1.99	0.60
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.82	0.60
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.37	0.60
1:2A:880:G:H2'	1:2A:881:G:C8	2.37	0.60
1:2A:76:C:N4	1:2A:93:G:H1	25.79	0.60
5:2F:101:LEU:O	5:2F:106:ARG:NH1	2.34	0.60
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.83	0.60
15:2T:85:LYS:NZ	15:2T:87:ASP:OD2	2.34	0.60
1:1A:1101:G:N2	1:1A:1151:U:O2	2.34	0.60
1:1A:1123:A:H2	1:1A:1134:A:C2	2.18	0.60
1:1A:1475:G:H2'	1:1A:1476:C:C6	2.35	0.60
1:1A:2164:C:O2	1:1A:2171:G:N1	2.29	0.60
6:1G:67:LYS:HE3	26:14:5:ILE:HD12	1.83	0.60
1:1A:1151:U:H2'	1:1A:1152:G:H8	1.66	0.60
1:1A:39:C:O2	5:1F:46:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2193:G:H2'	1:2A:2194:G:H8	1.67	0.60
1:1A:1584:G:H2'	1:1A:1585:G:H8	1.66	0.60
1:2A:330:A:H2	1:2A:1210:A:HO2'	1.49	0.60
1:2A:409:C:OP1	62:2A:3791:HOH:O	2.16	0.60
12:2Q:12:GLN:HE21	12:2Q:72:LYS:HG3	1.67	0.60
21:2Z:152:ALA:HB1	21:2Z:163:LEU:HD21	1.84	0.60
1:1A:1223:C:H2'	1:1A:1224:C:H6	1.67	0.60
1:2A:1190:G:N7	62:2A:3722:HOH:O	2.32	0.60
24:12:59:ARG:NH2	62:12:3101:HOH:O	2.34	0.60
1:1A:1285:G:OP1	62:1A:4177:HOH:O	2.17	0.60
1:1A:2339:A:H2'	1:1A:2340:A:C8	2.37	0.60
21:2Z:74:VAL:HG22	21:2Z:86:VAL:HG12	1.83	0.60
5:1F:132:VAL:HA	5:1F:138:GLU:HB3	1.82	0.60
1:2A:2139:C:N3	1:2A:2152:G:N2	2.43	0.60
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.37	0.60
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.84	0.60
1:1A:1639:G:H2'	1:1A:1640:G:C8	2.37	0.60
22:20:23:VAL:HG22	22:20:38:VAL:HG22	1.83	0.60
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.35	0.60
9:2N:58:ASP:N	9:2N:58:ASP:OD1	2.31	0.60
13:2R:24:GLN:HE22	13:2R:36:THR:HG21	1.67	0.60
19:2X:57:LEU:HD11	19:2X:78:LYS:HE2	1.84	0.60
1:1A:1210:G:H2'	1:1A:1211:U:C6	2.37	0.59
30:18:6:THR:HG22	30:18:63:PRO:HD2	1.84	0.59
1:1A:1232:G:H5''	17:1V:81:TYR:CE1	2.37	0.59
1:1A:260:A:N3	1:1A:395:C:O2'	2.32	0.59
1:1A:848:G:O6	5:1F:53:THR:OG1	2.20	0.59
12:1Q:85:LYS:HD3	22:10:7:LEU:HD13	1.84	0.59
1:2A:2150:U:H2'	1:2A:2151:G:C8	2.38	0.59
1:1A:145:G:O6	62:1A:4165:HOH:O	2.12	0.59
1:1A:89:U:H1'	1:1A:90:A:C8	2.36	0.59
11:1P:89:ALA:O	11:1P:121:LYS:NZ	2.33	0.59
1:2A:2552:2MU:H6	1:2A:2552:2MU:O5'	2.02	0.59
1:2A:385:C:O2'	1:2A:388:G:N2	2.35	0.59
1:2A:1002:G:H1	1:2A:1038:C:N4	42.79	0.59
1:2A:764:A:H5'	3:2D:210:GLY:HA2	1.83	0.59
8:1I:72:LEU:C	8:1I:74:ASN:H	2.05	0.59
1:2A:1593:G:H2'	1:2A:1594:G:H8	1.67	0.59
1:1A:786:G:OP1	62:1A:4173:HOH:O	2.16	0.59
9:2N:15:LEU:N	9:2N:136:GLU:O	2.34	0.59
1:1A:1233:U:H5'	17:1V:79:VAL:HG13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:115:ARG:HB3	6:1G:136:ARG:HH21	1.67	0.59
1:2A:1123:C:H1'	31:29:18:ARG:HH21	1.66	0.59
1:2A:2323:G:O6	1:2A:2332:U:N3	2.19	0.59
6:2G:41:GLN:HG3	6:2G:43:LEU:HD13	1.85	0.59
7:2H:3:ARG:NH2	7:2H:65:HIS:HB3	2.16	0.59
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.36	0.59
1:1A:2800:C:H1'	4:1E:62:PRO:HG3	1.85	0.59
7:1H:56:SER:HB3	7:1H:61:HIS:ND1	2.18	0.59
1:1A:2331:G:N2	14:1S:3:ARG:HD2	2.16	0.59
1:1A:2162:C:O2	1:1A:2174:G:N2	2.35	0.58
1:2A:210:C:OP2	29:27:29:LYS:NZ	2.34	0.58
1:2A:2137:C:H2'	1:2A:2138:C:C6	2.38	0.58
3:2D:80:ALA:HB3	3:2D:94:LEU:HD23	1.84	0.58
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	1.84	0.58
1:1A:2156:A:H2	1:1A:2181:G:H4'	1.67	0.58
1:1A:387:G:H2'	1:1A:388:A:C8	2.38	0.58
21:2Z:91:LEU:HD23	21:2Z:130:PRO:HB3	1.85	0.58
5:2F:132:VAL:HA	5:2F:138:GLU:HB3	1.84	0.58
18:2W:35:ILE:HG23	27:25:28:PRO:HD2	1.85	0.58
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	1.85	0.58
3:2D:69:ARG:HE	3:2D:130:ALA:HB2	1.68	0.58
6:2G:41:GLN:NE2	6:2G:154:GLY:O	2.36	0.58
1:2A:2313:C:H5''	6:2G:91:ARG:HD3	1.85	0.58
1:2A:987:G:O2'	1:2A:1000:A:N3	2.32	0.58
1:2A:2756:U:H1'	1:2A:2757:A:H5''	1.85	0.58
13:1R:95:THR:HG22	13:1R:116:LEU:HD23	1.85	0.58
1:1A:1785:C:OP1	15:1T:96:ARG:NH1	2.37	0.58
12:2Q:82:ARG:HB2	22:20:7:LEU:HD11	1.84	0.58
1:2A:1671:U:OP2	62:2A:3793:HOH:O	2.17	0.58
2:2B:14:U:O3'	2:2B:108:U:O2'	2.22	0.58
7:1H:149:ARG:NH2	7:1H:167:GLU:OE2	2.35	0.58
1:2A:2287:A:N6	1:2A:2344:U:H3	2.01	0.58
2:2B:49:C:H2'	2:2B:50:G:C8	2.39	0.58
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.39	0.58
1:2A:307:G:N1	1:2A:310:A:OP2	2.37	0.58
1:1A:1108:G:H2'	1:1A:1109:G:H8	1.67	0.58
1:1A:1940:A:N6	62:1A:4283:HOH:O	2.34	0.58
1:1A:2346:G:H5'	14:1S:9:ARG:HG2	1.85	0.58
1:1A:790:G:N7	62:1A:4266:HOH:O	2.33	0.58
3:1D:85:ASP:OD2	3:1D:88:ARG:NH1	2.34	0.58
1:2A:987:G:N2	1:2A:1218:C:N3	46.42	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:574:C:N3	4:2E:145:LYS:NZ	2.52	0.58
1:2A:709:U:H2'	1:2A:710:G:C8	2.39	0.58
3:2D:71:ASP:HB2	3:2D:103:ARG:HH12	1.68	0.58
7:2H:25:LYS:HG2	7:2H:34:GLU:HG2	1.85	0.58
1:1A:1170:C:OP1	62:1A:4179:HOH:O	2.17	0.57
4:1E:174:ASP:OD1	4:1E:175:VAL:N	2.37	0.57
11:1P:89:ALA:HA	11:1P:121:LYS:HD3	1.85	0.57
12:2Q:81:VAL:HB	22:20:7:LEU:HD21	1.86	0.57
1:2A:2375:G:O2'	1:2A:2377:A:N7	2.28	0.57
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.39	0.57
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.86	0.57
1:1A:1452:U:H2'	1:1A:1453:C:C6	2.39	0.57
1:1A:153:C:H42	1:1A:168:G:H1	25.22	0.57
1:1A:2157:A:N6	1:1A:2178:G:O2'	2.37	0.57
1:1A:2227:G:H3'	1:1A:2228:G:C8	2.40	0.57
1:1A:630:U:OP1	5:1F:102:PRO:HA	2.04	0.57
1:1A:1053:C:OP1	9:1N:35:ARG:NH1	2.37	0.57
11:1P:47:ASP:OD2	11:1P:49:ARG:NH2	2.38	0.57
1:2A:1717:G:H1	1:2A:1745:C:H42	1.52	0.57
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.40	0.57
10:2O:2:ILE:HB	10:2O:33:ALA:HB3	1.86	0.57
10:2O:8:LEU:HD23	10:2O:82:ASN:HB3	1.86	0.57
26:14:57:GLU:HB3	26:14:58:ARG:HD2	1.87	0.57
1:1A:2296:C:P	28:16:6:ARG:HG3	2.43	0.57
2:1B:28:C:OP1	14:1S:36:TYR:OH	2.17	0.57
11:1P:126:VAL:HG12	11:1P:148:LEU:HD23	1.85	0.57
6:2G:32:PRO:HB2	6:2G:172:LEU:HD22	1.85	0.57
1:1A:660:C:O2'	1:1A:664:U:OP1	2.21	0.57
1:2A:296:C:O3'	20:2Y:95:LYS:NZ	2.38	0.57
1:2A:521:G:H2'	1:2A:522:G:H8	1.70	0.57
11:2P:85:LEU:HA	11:2P:88:LEU:HD12	1.86	0.57
12:2Q:11:LYS:HD3	12:2Q:87:LYS:HD3	1.86	0.57
1:1A:1814:A:N7	62:1A:4261:HOH:O	2.32	0.57
1:1A:2856:G:OP1	62:1A:4178:HOH:O	2.17	0.57
6:1G:150:ASP:OD1	6:1G:150:ASP:N	2.38	0.57
1:2A:1791:A:H5'	3:2D:206:LEU:HD12	1.86	0.57
1:2A:1693:U:H1'	3:2D:14:ARG:NH2	2.20	0.57
1:1A:2127:C:H2'	1:1A:2128:G:C8	2.39	0.57
1:1A:880:U:O2	11:1P:55:ARG:NH2	2.33	0.57
1:2A:2033:A:OP1	62:2A:3737:HOH:O	2.18	0.57
1:1A:2209:G:H2'	1:1A:2210:C:O4'	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2298:A:H4'	1:1A:2299:A:O4'	2.05	0.57
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.86	0.57
1:2A:118:A:N3	1:2A:178:G:H1'	2.19	0.57
1:2A:288:C:H2'	1:2A:289:A:C8	2.40	0.57
1:1A:542:C:OP1	27:15:16:ARG:NH2	2.37	0.57
4:1E:29:GLY:HA3	62:1E:401:HOH:O	2.05	0.57
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.87	0.57
1:2A:2398:U:H2'	1:2A:2399:G:C8	2.40	0.57
1:1A:1475:G:H2'	1:1A:1476:C:H6	1.69	0.56
3:1D:80:ALA:HB3	3:1D:94:LEU:HD23	1.86	0.56
15:2T:9:LEU:O	15:2T:12:SER:OG	2.14	0.56
1:1A:202:A:H2'	1:1A:203:G:O4'	2.05	0.56
1:2A:1827:C:C2'	1:2A:1828:G:H5'	2.35	0.56
1:2A:2171:A:H1'	1:2A:2172:U:C6	2.39	0.56
28:26:10:LEU:HG	28:26:54:ILE:HG13	1.86	0.56
5:2F:18:ARG:HG2	5:2F:19:GLU:H	1.70	0.56
17:2V:72:VAL:HG13	17:2V:85:LYS:HB3	1.86	0.56
1:1A:1633:A:H2'	1:1A:1634:C:C6	2.40	0.56
1:2A:1219:G:H1	1:2A:1230:C:H42	1.54	0.56
1:2A:2576:G:O2'	1:2A:2579:C:OP2	2.19	0.56
2:1B:1:U:O2'	2:1B:2:C:OP1	2.20	0.56
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.41	0.56
1:2A:646:A:H2'	1:2A:647:G:O4'	2.06	0.56
1:2A:271(H):G:O2'	1:2A:271(I):G:H8	1.88	0.56
1:1A:1410:G:OP1	23:11:2:SER:HA	2.06	0.56
1:1A:2816:G:H2'	1:1A:2817:G:H8	1.71	0.56
1:1A:933:C:H4'	1:1A:933:C:OP1	2.06	0.56
1:1A:968:U:H2'	1:1A:969:C:C6	2.41	0.56
20:1Y:17:SER:OG	20:1Y:71:LYS:NZ	2.39	0.56
1:2A:1142(A):A:H4'	9:2N:25:ARG:HH22	1.71	0.56
6:1G:143:GLU:O	26:14:28:LYS:NZ	2.38	0.56
1:1A:1128:U:C4	1:1A:1132:A:N1	2.74	0.56
1:1A:1451:U:H2'	1:1A:1452:U:H6	1.71	0.56
1:1A:1492:C:H2'	1:1A:1493:C:H6	1.71	0.56
1:1A:287:G:N7	1:1A:448:U:H2'	2.20	0.56
3:1D:26:LYS:HB3	3:1D:83:GLU:HG2	1.88	0.56
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.87	0.56
19:1X:1:MET:HE1	24:12:22:GLU:HA	1.87	0.56
1:1A:2311:G:H2'	1:1A:2312:G:H8	1.70	0.56
1:2A:1038:C:H42	1:2A:1117:G:H1	1.52	0.56
1:2A:1541:G:H3'	1:2A:1542:A:H2'	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2750:A:O2'	1:2A:2752:C:N4	2.35	0.56
1:2A:984:A:H5''	1:2A:985:C:H5	1.70	0.56
1:2A:990:A:OP2	62:2A:3734:HOH:O	2.17	0.56
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.87	0.56
1:1A:280:C:H2'	1:1A:281:G:H8	1.71	0.56
23:21:60:PHE:HE1	23:21:91:LYS:HG3	1.71	0.56
8:2I:43:ASN:ND2	23:21:75:GLU:OE2	2.39	0.56
5:2F:164:ARG:HG3	5:2F:175:THR:OG1	2.06	0.56
26:14:53:GLU:O	26:14:56:VAL:HG13	2.06	0.56
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.87	0.56
1:1A:469:A:H1'	1:1A:1246:C:O4'	2.06	0.56
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.41	0.56
1:1A:325:G:OP2	20:1Y:84:ARG:NH2	2.39	0.56
1:2A:518:G:H2'	1:2A:519:U:C6	2.41	0.56
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.41	0.56
15:2T:105:LEU:HD22	15:2T:109:GLU:HB3	1.87	0.56
4:2E:179:GLU:HG3	15:2T:9:LEU:HD21	1.88	0.56
24:12:51:ARG:HE	24:12:55:ARG:NH1	2.04	0.55
24:12:64:LEU:HD21	24:12:68:ARG:HE	1.70	0.55
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.41	0.55
1:1A:2825:C:H5'	27:15:29:THR:HG21	1.88	0.55
1:1A:2686:G:H2'	1:1A:2687:A:C8	2.40	0.55
1:1A:436:C:OP1	62:1A:4180:HOH:O	2.18	0.55
15:1T:77:PRO:HB2	15:1T:80:SER:HB2	1.87	0.55
20:1Y:86:ARG:HB2	20:1Y:98:VAL:HG23	1.88	0.55
6:2G:138:GLN:NE2	6:2G:151:ALA:O	2.37	0.55
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.71	0.55
12:2Q:85:LYS:HG2	22:20:7:LEU:HB3	1.88	0.55
1:1A:1102:G:N2	1:1A:1148:C:OP2	2.32	0.55
1:1A:2699:U:H2'	1:1A:2700:U:O4'	2.06	0.55
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.71	0.55
1:2A:861:A:N3	2:2B:79:C:O2'	2.36	0.55
1:1A:1211:U:H2'	1:1A:1212:C:C6	2.42	0.55
1:1A:2129:C:H42	1:1A:2204:G:H1	1.54	0.55
1:1A:965:G:N2	1:1A:2281:A:OP2	2.39	0.55
28:26:2:ALA:HB1	28:26:6:ARG:O	2.06	0.55
1:1A:2410:U:H2'	1:1A:2411:G:H8	1.72	0.55
1:2A:994:C:O2'	1:2A:996:A:OP1	2.18	0.55
5:2F:195:ASP:HB2	5:2F:198:ALA:H	1.72	0.55
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.06	0.55
25:13:8:LEU:HD13	25:13:31:LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1305:G:N2	1:1A:1331:G:H1'	40.23	0.55
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.42	0.55
14:2S:15:ARG:HB3	14:2S:19:LYS:NZ	2.21	0.55
1:1A:1586:G:H2'	1:1A:1587:U:O4'	2.07	0.55
1:2A:2285:C:OP2	28:26:6:ARG:HD3	2.07	0.55
1:2A:2138:C:N4	1:2A:2153:G:N1	2.33	0.55
1:2A:422:A:H2'	1:2A:423:A:C8	2.42	0.55
6:2G:5:VAL:HG13	6:2G:8:LYS:HB3	1.89	0.55
7:1H:121:ILE:HD11	7:1H:140:LYS:HG2	1.89	0.55
8:1I:61:ARG:NH1	8:1I:64:GLU:OE1	2.40	0.55
2:2B:54:G:N2	6:2G:29:TRP:HZ2	2.02	0.55
15:2T:59:THR:HG23	15:2T:78:LEU:HB3	1.86	0.55
1:1A:662:A:OP1	11:1P:133:SER:OG	2.21	0.55
1:2A:1425:G:H2'	1:2A:1426:G:O4'	2.07	0.55
1:2A:1671:U:HO2'	1:2A:1673:U:H5	1.53	0.55
1:2A:1918:A:O2'	1:2A:1920:4OC:N4	2.40	0.55
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.89	0.55
6:2G:47:LYS:HG3	6:2G:48:GLU:N	2.21	0.55
1:1A:1055:A:OP2	9:1N:37:LYS:NZ	2.34	0.55
1:1A:1782:C:HO2'	1:1A:2871:G:HO2'	1.53	0.55
1:1A:2325:C:H4'	6:1G:91:ARG:HD3	1.89	0.55
1:2A:922:U:O2'	22:20:29:GLN:NE2	2.40	0.55
1:1A:1378:G:OP1	62:1A:4154:HOH:O	2.18	0.54
1:1A:1817:A:H1'	1:1A:1960:A:N6	2.21	0.54
1:1A:2874:G:OP1	15:1T:119:LYS:HD2	2.06	0.54
1:1A:791:G:OP1	62:1A:4183:HOH:O	2.18	0.54
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.42	0.54
1:2A:830:G:N2	1:2A:856:C:O2	52.22	0.54
9:2N:137:LYS:NZ	9:2N:139:GLU:OE2	2.40	0.54
1:1A:1515:C:H2'	1:1A:1516:A:H8	1.73	0.54
1:1A:2054:G:OP2	1:1A:2466:G:O2'	2.21	0.54
1:1A:839:G:N3	1:1A:2094:G:O2'	2.33	0.54
15:1T:30:VAL:HG22	15:1T:86:ILE:HG12	1.88	0.54
17:1V:52:VAL:HG23	17:1V:55:ALA:HB3	1.89	0.54
1:2A:2297:C:O2	1:2A:2333:A:N6	2.39	0.54
4:2E:149:ARG:O	62:2E:402:HOH:O	2.18	0.54
7:2H:25:LYS:NZ	7:2H:34:GLU:OE2	2.39	0.54
19:2X:40:LYS:HG3	19:2X:51:VAL:HB	1.90	0.54
1:2A:652(C):G:N2	1:2A:653:A:H1'	2.23	0.54
1:1A:2158:C:N4	1:1A:2177:G:N1	2.55	0.54
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.21	0.54
1:2A:7:G:H2'	1:2A:8:A:C8	2.42	0.54
1:2A:8:A:H2'	1:2A:9:U:H6	1.71	0.54
14:2S:11:LYS:HG3	14:2S:91:PRO:HD3	1.90	0.54
1:1A:1221:G:H1'	1:1A:1222:A:H5''	1.89	0.54
1:1A:1694:G:OP1	62:1A:4127:HOH:O	2.18	0.54
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.43	0.54
1:1A:2297:C:OP2	28:16:6:ARG:HD3	2.06	0.54
1:2A:1827:C:H2'	1:2A:1828:G:H5'	1.89	0.54
1:2A:2129:C:N4	1:2A:2159:G:H1	2.06	0.54
12:2Q:109:VAL:HG13	12:2Q:113:GLN:HB2	1.88	0.54
1:1A:1827:U:H2'	1:1A:1828:C:H6	1.72	0.54
1:1A:2410:U:H2'	1:1A:2411:G:C8	2.42	0.54
1:1A:2854:G:O6	62:1A:4175:HOH:O	2.16	0.54
1:1A:407:U:H2'	1:1A:408:G:H8	1.73	0.54
9:1N:13:TRP:CE2	9:1N:133:GLN:HG2	2.42	0.54
25:23:6:VAL:HG22	25:23:56:VAL:HG13	1.89	0.54
1:2A:122:G:OP1	1:2A:149:A:O2'	2.26	0.54
1:2A:878:A:N6	1:2A:899:A:O2'	2.40	0.54
2:2B:94:C:H2'	2:2B:95:C:H6	1.71	0.54
10:2O:7:TYR:CE1	10:2O:20:MET:HB2	2.42	0.54
23:21:3:LYS:HB2	23:21:61:ARG:HH22	1.73	0.54
1:2A:1920:4OC:HM22	1:2A:1921:G:H5'	1.89	0.54
8:2I:117:GLU:HG3	8:2I:118:LYS:H	1.73	0.54
15:1T:54:ARG:HA	15:1T:59:THR:HB	1.89	0.54
19:1X:60:ARG:NH1	29:17:47:ARG:HH22	2.05	0.54
1:2A:307:G:H21	1:2A:330:A:N6	2.05	0.54
1:2A:816:C:O2'	1:2A:932:G:O6	2.26	0.54
8:2I:72:LEU:C	8:2I:74:ASN:H	2.10	0.54
1:1A:273:G:N2	8:1I:50:ARG:HH12	2.06	0.53
12:1Q:16:ARG:HH21	12:1Q:18:LYS:HD3	1.73	0.53
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.89	0.53
1:2A:1688:U:H1'	1:2A:1701:A:C6	2.43	0.53
1:2A:2347:C:HO2'	28:26:21:TYR:HH	1.56	0.53
1:2A:637:A:OP1	11:2P:133:SER:OG	2.22	0.53
5:2F:155:LEU:HB2	5:2F:189:THR:HG21	1.90	0.53
31:19:1:MET:HE2	31:19:33:LYS:HE3	1.90	0.53
1:1A:1492:C:H2'	1:1A:1493:C:C6	2.44	0.53
5:1F:74:ARG:HG2	62:1F:410:HOH:O	2.08	0.53
28:26:14:THR:O	28:26:17:LYS:NZ	2.42	0.53
23:11:50:ARG:NH1	62:11:201:HOH:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2359:C:H2'	1:1A:2360:U:C6	2.43	0.53
1:1A:932:C:C4	1:1A:933:C:H1'	2.43	0.53
1:2A:1826:G:H4'	3:2D:242:ARG:NH2	2.23	0.53
1:2A:2109:U:H5''	1:2A:2149:G:H21	1.73	0.53
3:2D:108:PRO:HG2	3:2D:111:LEU:HG	1.91	0.53
21:2Z:11:GLU:O	21:2Z:36:LYS:NZ	2.38	0.53
1:1A:1800:G:O2'	1:1A:1980:C:OP1	2.18	0.53
5:1F:28:ILE:HD13	5:1F:119:ARG:HH21	1.74	0.53
1:2A:2155:G:H2'	1:2A:2156:G:H5'	1.91	0.53
1:1A:2365:G:N7	62:1A:4285:HOH:O	2.34	0.53
1:1A:2603:C:H2'	1:1A:2604:G:C8	2.43	0.53
1:2A:1587:A:H2'	1:2A:1588:C:C6	2.44	0.53
1:2A:13:A:O2'	1:2A:15:G:N7	2.34	0.53
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.44	0.53
1:2A:2645:G:N2	1:2A:2767:C:OP2	2.42	0.53
2:2B:92:C:OP1	21:2Z:79:ARG:NH1	2.41	0.53
1:1A:1077:G:H5''	31:19:8:LYS:HE3	1.90	0.53
1:1A:1911:A:H2'	1:1A:1912:A:C8	2.44	0.53
1:1A:2096:U:H2'	1:1A:2097:U:C6	2.43	0.53
1:1A:2450:U:OP1	62:1A:4181:HOH:O	2.18	0.53
21:1Z:74:VAL:HG22	21:1Z:86:VAL:HG12	1.89	0.53
6:2G:179:PRO:HG3	26:24:43:TYR:CZ	2.44	0.53
10:2O:7:TYR:HE1	10:2O:20:MET:HB2	1.73	0.53
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.23	0.53
1:2A:776:G:N2	1:2A:2241:A:OP1	2.40	0.53
1:2A:568:U:H5'	1:2A:945:A:N1	2.24	0.53
1:2A:945:A:OP2	62:2A:3795:HOH:O	2.19	0.53
1:2A:586:A:H5'	5:2F:89:VAL:HG21	1.90	0.53
1:1A:174:U:H2'	1:1A:175:G:C8	2.44	0.53
1:1A:1785:C:H5	15:1T:96:ARG:NH2	2.05	0.53
1:1A:1296:G:N7	11:1P:18:ARG:NH2	2.57	0.53
22:20:27:GLU:HB2	22:20:69:PHE:HD2	1.74	0.53
13:1R:2:ARG:HG2	13:1R:5:LYS:HB2	1.90	0.53
1:2A:1533:G:H2'	1:2A:1536:C:H42	1.73	0.53
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.09	0.53
6:2G:131:TYR:CE2	6:2G:133:LEU:HD23	2.43	0.53
6:2G:77:ILE:HG22	6:2G:80:PHE:H	1.74	0.53
1:1A:561:A:H2'	1:1A:562:C:C6	2.44	0.53
1:2A:384:U:H2'	1:2A:385:C:H6	1.74	0.53
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.74	0.53
1:1A:2018:C:H4'	1:1A:2019:G:OP1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.44	0.52
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.27	0.52
1:2A:2823:A:OP1	4:2E:159:HIS:NE2	2.40	0.52
1:2A:8:A:H2'	1:2A:9:U:C6	2.44	0.52
1:2A:300:A:H1'	1:2A:319:C:H1'	1.91	0.52
1:2A:2467:C:H4'	12:2Q:123:HIS:CD2	2.44	0.52
1:1A:969:C:C4'	22:10:29:GLN:HE21	2.21	0.52
1:1A:2185:C:OP1	1:1A:2187:G:N1	2.42	0.52
1:1A:2816:G:H2'	1:1A:2817:G:C8	2.43	0.52
1:1A:791:G:N2	1:1A:1497:G:O3'	58.55	0.52
9:1N:4:TYR:HB2	16:1U:101:ARG:HH12	1.74	0.52
24:22:63:VAL:O	24:22:67:LYS:HG2	2.09	0.52
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.14	0.52
1:2A:2151:G:H2'	1:2A:2152:G:C8	2.44	0.52
1:2A:2375:G:N2	1:2A:2378:A:OP2	2.35	0.52
5:2F:13:SER:OG	5:2F:16:GLY:O	2.27	0.52
9:2N:4:TYR:HB2	16:2U:101:ARG:HH12	1.75	0.52
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.91	0.52
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.44	0.52
11:1P:100:LEU:HD12	11:1P:112:LEU:HD11	1.89	0.52
23:21:53:VAL:HG22	23:21:74:VAL:HG13	1.90	0.52
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.25	0.52
1:2A:1670:C:O2	4:2E:129:HIS:NE2	2.35	0.52
1:2A:997:G:OP2	16:2U:58:ARG:NH1	2.42	0.52
4:2E:135:HIS:NE2	62:2E:404:HOH:O	2.34	0.52
21:2Z:4:ARG:NH2	21:2Z:60:GLU:OE2	2.42	0.52
1:1A:1355:G:H2'	1:1A:1356:G:H8	3.17	0.52
1:1A:650:G:O6	11:1P:107:LYS:NZ	2.39	0.52
1:1A:7:G:H2'	1:1A:8:A:C8	2.44	0.52
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.91	0.52
13:1R:38:VAL:HG22	13:1R:112:ALA:HB2	1.91	0.52
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.23	0.52
1:2A:571:A:N6	1:2A:2499:C:O3'	2.43	0.52
1:1A:1716:A:H5''	1:1A:2562:G:OP1	2.09	0.52
1:1A:2175:G:H2'	1:1A:2176:G:H8	1.75	0.52
1:1A:519:G:H4'	18:1W:6:ILE:HB	1.92	0.52
1:1A:721:G:O2'	5:1F:74:ARG:HD3	2.10	0.52
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.45	0.52
1:2A:2144:U:O2'	1:2A:2147:G:O6	2.21	0.52
1:2A:2564:A:C2	1:2A:2647:U:H4'	2.45	0.52
1:2A:307:G:H21	1:2A:330:A:H62	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:900:A:O2'	1:2A:901:A:OP1	2.26	0.52
3:2D:132:PRO:HG2	3:2D:135:PHE:CD2	2.45	0.52
8:2I:9:LEU:HD23	8:2I:12:LEU:HD13	1.92	0.52
1:1A:1144:A:H2'	1:1A:1145:G:H5'	1.91	0.52
1:1A:1218:G:O2'	1:1A:1219:A:O5'	2.27	0.52
1:1A:1355:G:H2'	1:1A:1356:G:C8	3.77	0.52
1:1A:303:C:H42	1:1A:385:G:H1	1.58	0.52
3:1D:132:PRO:HD3	3:1D:190:TYR:CZ	2.45	0.52
1:2A:2206:G:H5''	1:2A:2207:G:C5	2.45	0.52
1:2A:2502:G:H5''	1:2A:2503:2MA:H5''	1.92	0.52
11:2P:126:VAL:HG12	11:2P:148:LEU:HD23	1.91	0.52
8:1I:12:LEU:HD21	8:1I:19:VAL:HG21	1.92	0.52
12:1Q:76:LYS:HB3	12:1Q:91:GLU:HG3	1.90	0.52
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.45	0.52
1:2A:2130:U:H4'	1:2A:2133:G:H4'	1.91	0.52
1:2A:2129:C:H5'	1:2A:2130:U:OP2	2.10	0.52
6:1G:38:VAL:HG22	6:1G:93:THR:HG23	1.92	0.52
19:1X:94:GLY:HA3	19:1X:95:LEU:HG	1.92	0.52
26:24:24:THR:OG1	26:24:25:TYR:N	2.41	0.52
1:2A:1007:C:O2	1:2A:1022:G:N1	17.95	0.52
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.45	0.52
1:2A:134:C:H42	1:2A:145:G:H1	1.58	0.52
2:1B:87:G:N2	2:1B:90:A:OP2	2.34	0.52
1:2A:2033:A:O2'	1:2A:2035:G:OP2	2.23	0.52
1:2A:2474:C:H5''	1:2A:2475:C:OP2	2.10	0.52
9:2N:63:THR:OG1	9:2N:66:LYS:NZ	2.41	0.52
2:1B:88:C:H2'	2:1B:89:G:O4'	2.09	0.51
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.45	0.51
1:2A:2104:G:H1	1:2A:2185:C:N4	2.08	0.51
10:2O:2:ILE:HD12	10:2O:6:THR:HG21	1.92	0.51
1:1A:1384:G:O2'	1:1A:1439:A:N1	2.39	0.51
1:1A:2247:G:H2'	1:1A:2248:C:C6	2.45	0.51
1:1A:2840:G:N7	62:1A:4287:HOH:O	2.34	0.51
1:2A:1409:C:H2'	1:2A:1410:G:C8	2.45	0.51
1:2A:2117:A:N6	1:2A:2166:G:O6	2.42	0.51
1:2A:2206:G:H5''	1:2A:2207:G:C6	2.45	0.51
1:2A:2612:C:OP2	27:25:2:ALA:N	2.43	0.51
1:1A:2576:A:C2	1:1A:2659:U:H4'	2.46	0.51
12:1Q:5:ARG:HG3	12:1Q:6:ARG:HG2	1.91	0.51
1:2A:245:G:O6	30:28:8:LYS:NZ	2.44	0.51
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:976:G:H5'	1:1A:1358:U:O2'	103.39	0.51
3:1D:71:ASP:HB2	3:1D:103:ARG:HH12	1.74	0.51
9:1N:58:ASP:OD1	9:1N:58:ASP:N	2.41	0.51
13:1R:24:GLN:NE2	13:1R:36:THR:HG21	2.24	0.51
1:2A:1251:C:OP1	16:2U:10:ARG:HG3	2.10	0.51
1:2A:1315:C:OP2	62:2A:3778:HOH:O	2.19	0.51
1:2A:289:A:H2'	1:2A:290:G:O4'	2.11	0.51
1:2A:639:U:H2'	1:2A:640:C:C6	2.45	0.51
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.46	0.51
11:2P:62:LEU:O	30:28:13:ARG:NH1	2.36	0.51
20:2Y:11:ASP:OD2	20:2Y:97:ARG:NH2	2.43	0.51
1:1A:2153:G:H5''	1:1A:2154:U:H3'	1.91	0.51
5:1F:126:VAL:HG21	5:1F:129:PHE:CZ	2.45	0.51
11:1P:91:PHE:O	11:1P:121:LYS:NZ	2.43	0.51
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.91	0.51
1:2A:1466:G:O2'	1:2A:1546:C:O2'	2.14	0.51
1:2A:854:G:H2'	1:2A:855:G:H8	1.75	0.51
29:17:12:ARG:NH2	29:17:44:PRO:HB3	2.26	0.51
1:1A:1093:G:O2'	1:1A:1094:A:O5'	2.25	0.51
1:1A:1219:A:H4'	1:1A:1220:U:OP1	2.11	0.51
1:1A:2604:G:OP1	62:1A:4187:HOH:O	2.19	0.51
1:1A:936:C:O2'	1:1A:937:A:O4'	2.28	0.51
6:1G:66:GLN:OE1	6:1G:98:ARG:NE	2.39	0.51
1:2A:1341:U:OP1	1:2A:1397:U:N3	2.41	0.51
1:2A:271(F):C:H42	1:2A:271(R):G:H1	1.57	0.51
1:1A:1102:G:H5''	1:1A:1103:A:O4'	2.08	0.51
1:1A:1120:G:HO2'	1:1A:1121:C:P	2.32	0.51
1:1A:1218:G:H22	1:1A:1222:A:P	2.33	0.51
1:1A:2564:2MU:H2'	1:1A:2566:U:OP2	2.10	0.51
2:1B:1:U:H2'	2:1B:2:C:H6	1.76	0.51
1:2A:400:G:N7	62:2A:3861:HOH:O	2.34	0.51
1:2A:784:A:OP1	62:2A:3756:HOH:O	2.18	0.51
2:2B:13:A:N1	2:2B:69:G:O2'	2.42	0.51
2:2B:28:C:H2'	2:2B:29:A:C8	2.45	0.51
3:2D:69:ARG:NH2	3:2D:128:GLY:O	2.44	0.51
6:2G:136:ARG:HG3	6:2G:137:GLU:HG3	1.92	0.51
1:2A:1155:A:OP1	16:2U:55:ARG:HD2	2.10	0.51
18:2W:86:LEU:N	18:2W:94:ASP:O	2.40	0.51
2:1B:9:G:O6	62:1B:3101:HOH:O	2.17	0.51
3:1D:180:GLY:HA3	3:1D:275:LYS:HB2	1.93	0.51
1:1A:999:G:H5''	12:1Q:13:GLN:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2557:G:H2'	1:2A:2558:C:C6	2.46	0.51
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.31	0.51
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.46	0.51
2:2B:18:G:H2'	2:2B:19:G:C8	2.46	0.51
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.25	0.51
8:2I:123:LEU:HA	8:2I:144:VAL:HG23	1.91	0.51
1:1A:603:C:H1'	62:1A:5102:HOH:O	2.11	0.51
1:1A:927:G:N2	1:1A:944:C:N3	2.59	0.51
1:1A:909:G:O2'	2:1B:78:A:N3	2.44	0.51
1:1A:831:A:N6	3:1D:229:VAL:HG11	2.26	0.51
3:1D:237:GLU:OE2	62:1D:401:HOH:O	2.19	0.51
26:24:55:ARG:O	26:24:56:VAL:HB	2.10	0.51
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.11	0.51
1:2A:2695:C:H2'	1:2A:2696:U:H6	1.76	0.51
1:2A:557:U:O2	9:2N:45:ASN:HB2	2.11	0.51
5:1F:18:ARG:HG2	5:1F:19:GLU:H	1.76	0.50
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.45	0.50
1:2A:191:A:H2'	1:2A:192:C:C6	2.46	0.50
1:2A:800:A:OP1	1:2A:800:A:H8	1.94	0.50
1:2A:2733:A:N1	4:2E:203:LYS:HA	2.26	0.50
6:2G:64:THR:HG22	6:2G:94:LEU:HD11	1.92	0.50
17:2V:80:GLN:HA	17:2V:82:ARG:NH1	2.26	0.50
1:1A:1305:G:H22	1:1A:1331:G:H1'	40.52	0.50
21:1Z:5:LEU:HD11	21:1Z:44:PHE:HA	1.93	0.50
1:2A:1308:A:H2'	1:2A:1309:G:O4'	2.11	0.50
1:2A:1360:A:OP1	1:2A:1360:A:H8	5.02	0.50
1:2A:2359:C:H2'	1:2A:2360:A:O4'	2.12	0.50
3:2D:3:VAL:HG21	3:2D:203:ASN:HB2	1.93	0.50
5:2F:11:VAL:HB	5:2F:18:ARG:HB3	1.92	0.50
10:2O:64:ARG:NH1	15:2T:70:VAL:HG21	2.22	0.50
1:1A:1014:U:H2'	1:1A:1015:C:C6	2.46	0.50
1:1A:1223:C:H2'	1:1A:1224:C:C6	2.46	0.50
1:1A:1515:C:H2'	1:1A:1516:A:C8	2.45	0.50
1:1A:572:A:N6	17:1V:19:LYS:H	2.08	0.50
1:1A:609:A:N1	1:1A:856:G:O2'	2.35	0.50
1:1A:923:C:H2'	1:1A:924:U:O4'	2.11	0.50
4:1E:14:ILE:HG13	4:1E:21:VAL:HG13	1.92	0.50
6:1G:64:THR:HB	6:1G:94:LEU:HD21	1.93	0.50
1:1A:2479:C:H4'	12:1Q:123:HIS:CD2	2.46	0.50
1:2A:1007:C:N3	1:2A:1022:G:C6	16.79	0.50
1:2A:400:G:O6	62:2A:3796:HOH:O	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:576:U:H2'	1:2A:577:G:C8	2.46	0.50
13:2R:33:ARG:HH21	13:2R:113:LEU:HD22	1.77	0.50
15:2T:92:GLY:O	15:2T:120:ARG:NH2	2.44	0.50
1:1A:2340:A:H2'	1:1A:2341:G:C8	2.47	0.50
1:1A:387:G:H2'	1:1A:388:A:H8	1.76	0.50
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.93	0.50
1:1A:721:G:H1'	5:1F:74:ARG:HD3	1.92	0.50
6:1G:115:ARG:HB3	6:1G:136:ARG:NH2	2.27	0.50
1:1A:2885:C:OP1	15:1T:3:ARG:NH1	2.42	0.50
1:2A:1364:G:P	23:21:3:LYS:HG3	2.51	0.50
4:2E:8:LYS:O	4:2E:193:GLY:N	2.38	0.50
19:2X:36:LYS:HG2	19:2X:54:VAL:HB	1.93	0.50
20:2Y:86:ARG:HD2	20:2Y:100:ALA:HA	1.94	0.50
23:11:77:ALA:HB1	23:11:82:LEU:HD11	1.94	0.50
1:1A:1410:G:OP2	23:11:3:LYS:HG3	2.12	0.50
1:1A:2158:C:N3	1:1A:2177:G:N2	2.59	0.50
1:1A:236:G:H4'	1:1A:413:G:C5	2.46	0.50
1:1A:305:G:H1'	1:1A:384:G:N2	2.26	0.50
1:2A:2507:C:H2'	1:2A:2508:G:O4'	2.11	0.50
1:2A:833:U:O2	11:2P:55:ARG:NH2	2.44	0.50
2:2B:104:U:O2'	21:2Z:72:ARG:HG2	2.12	0.50
1:1A:1159:U:H2'	1:1A:1160:G:C8	2.46	0.50
1:1A:1864:U:O2'	1:1A:1991:A:N1	2.31	0.50
1:1A:932:C:H3'	1:1A:933:C:C4'	2.42	0.50
1:1A:1845:G:H4'	3:1D:51:VAL:HG21	1.93	0.50
3:1D:76:PRO:HB2	3:1D:116:GLN:HE21	1.77	0.50
5:1F:195:ASP:CB	5:1F:198:ALA:H	2.25	0.50
11:1P:101:VAL:HG21	11:1P:108:LYS:HG2	1.93	0.50
1:2A:1713:U:H2'	1:2A:1714:G:H8	1.76	0.50
1:2A:2129:C:H42	1:2A:2159:G:H1	1.57	0.50
1:2A:2721:A:OP1	62:2A:3794:HOH:O	2.19	0.50
3:2D:77:ALA:HB2	3:2D:97:TYR:CD1	2.46	0.50
10:2O:29:ASN:OD1	10:2O:29:ASN:N	2.44	0.50
19:2X:11:PRO:HD3	24:22:37:PHE:CD1	2.47	0.50
20:2Y:86:ARG:HB2	20:2Y:98:VAL:HG23	1.93	0.50
21:2Z:24:LEU:HD12	21:2Z:25:PRO:HD2	1.92	0.50
1:1A:1140:U:H3	1:1A:1142:A:H3'	1.75	0.50
1:1A:1115:A:H1'	1:1A:1142:A:H4'	1.92	0.50
1:1A:847:A:OP1	1:1A:847:A:H8	1.95	0.50
1:2A:2116:G:O2'	1:2A:2117:A:N3	2.44	0.50
1:2A:2126:A:H4'	1:2A:2127:G:OP1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2875:C:O2'	15:2T:2:ASN:OD1	2.20	0.50
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.93	0.50
1:1A:1360:C:OP1	62:1A:4154:HOH:O	2.19	0.50
1:1A:481:C:N3	1:1A:499:G:H5'	2.27	0.50
5:1F:184:TYR:O	5:1F:188:ARG:HG3	2.12	0.50
1:2A:2167:U:H2'	1:2A:2168:G:N2	2.27	0.50
1:2A:2286:A:H4'	1:2A:2287:A:O4'	2.12	0.50
1:2A:2532:G:C6	1:2A:2533:A:C6	3.00	0.50
1:2A:652(C):G:H22	1:2A:653:A:H1'	1.76	0.50
8:2I:2:LYS:HG2	8:2I:20:ASP:OD1	2.12	0.50
21:2Z:138:GLU:H	21:2Z:156:LYS:NZ	2.08	0.50
8:1I:123:LEU:HA	8:1I:144:VAL:HG23	1.94	0.50
2:1B:9:G:OP1	14:1S:15:ARG:HD3	2.12	0.50
1:2A:1166:C:H2'	1:2A:1167:U:C6	2.46	0.50
6:2G:32:PRO:HB3	6:2G:163:ALA:HB2	1.94	0.50
1:1A:1324:A:OP1	13:1R:36:THR:HG23	2.12	0.49
1:1A:2156:A:OP2	1:1A:2179:G:N2	2.45	0.49
1:1A:2584:A:N7	4:1E:144:ARG:HD2	2.27	0.49
3:1D:132:PRO:HG2	3:1D:135:PHE:CD2	2.46	0.49
1:2A:2532:G:H2'	1:2A:2533:A:C8	2.47	0.49
1:2A:601:C:O2'	1:2A:605:C:H5''	2.12	0.49
30:18:26:LYS:HG2	30:18:46:ARG:O	2.12	0.49
17:1V:60:GLU:HB2	17:1V:97:LYS:HD3	1.94	0.49
19:2X:46:ALA:O	24:22:30:ARG:NH2	2.46	0.49
26:24:14:ILE:HB	26:24:22:ILE:HB	1.94	0.49
1:2A:1015:G:H2'	1:2A:1016:G:C8	2.46	0.49
1:2A:1286:A:H2'	1:2A:1287:A:H4'	6.59	0.49
1:2A:2312:U:H5'	6:2G:88:ILE:HD11	1.94	0.49
1:2A:2377:A:H2'	1:2A:2378:A:C8	2.47	0.49
1:2A:2864:G:OP1	15:2T:119:LYS:HD2	2.12	0.49
1:1A:1239:A:H62	1:1A:1299:A:H62	20.82	0.49
1:1A:2034:G:OP1	18:1W:11:ARG:NH2	2.45	0.49
1:1A:320:C:O3'	20:1Y:95:LYS:NZ	2.40	0.49
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.94	0.49
1:2A:1442:G:N3	1:2A:1442:G:H2'	3.05	0.49
1:2A:2344:U:OP1	28:26:37:ARG:HD3	2.12	0.49
1:2A:2478:A:C2	1:2A:2529:G:H2'	2.47	0.49
1:2A:597:U:H2'	1:2A:598:G:C8	2.47	0.49
20:2Y:98:VAL:HG12	20:2Y:105:ALA:HA	1.94	0.49
30:18:31:HIS:CE1	30:18:32:LEU:HD22	2.48	0.49
1:1A:2183:C:O2'	1:1A:2184:G:H5''	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2549:U:H2'	1:1A:2550:C:C6	2.48	0.49
1:1A:27:G:N2	1:1A:537:G:H1'	2.27	0.49
1:1A:572:A:H61	17:1V:19:LYS:N	2.11	0.49
1:1A:889:G:H2'	1:1A:890:G:O4'	2.12	0.49
8:1I:93:THR:HG22	8:1I:119:PRO:HB3	1.95	0.49
12:1Q:81:VAL:HB	22:10:7:LEU:HD21	1.95	0.49
1:2A:108:U:H2'	1:2A:109:G:C8	2.47	0.49
1:2A:1178:C:O2	1:2A:1178:C:H2'	2.12	0.49
1:2A:2156:G:O5'	1:2A:2156:G:H8	1.95	0.49
1:2A:2379:G:O2'	14:2S:17:ARG:NH2	2.45	0.49
1:2A:579:G:H2'	1:2A:580:C:C6	2.48	0.49
17:2V:80:GLN:HA	17:2V:82:ARG:HH12	1.76	0.49
20:2Y:56:PRO:C	20:2Y:58:GLY:H	2.15	0.49
2:1B:92:C:OP1	21:1Z:79:ARG:NH1	2.45	0.49
4:1E:175:VAL:O	4:1E:177:PRO:HD3	2.12	0.49
10:1O:104:ARG:CZ	15:1T:34:VAL:HG21	2.42	0.49
23:21:40:ARG:NH2	23:21:42:GLN:HG2	2.28	0.49
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.12	0.49
15:2T:31:SER:HB2	15:2T:85:LYS:HG2	1.93	0.49
16:2U:102:GLU:HG3	17:2V:2:PHE:CZ	2.47	0.49
1:1A:347:G:C8	5:1F:171:PRO:HG3	2.47	0.49
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.10	0.49
16:1U:104:GLN:HE21	16:1U:105:VAL:HG23	1.77	0.49
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.12	0.49
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.12	0.49
1:2A:2392:A:OP2	30:28:31:HIS:NE2	2.46	0.49
1:2A:887:A:H4'	1:2A:888:C:C5	2.48	0.49
24:12:22:GLU:HG3	24:12:64:LEU:HD11	1.94	0.49
1:1A:1900:G:H2'	1:1A:1901:C:C6	2.48	0.49
1:1A:2541:G:N7	31:19:31:LYS:NZ	2.58	0.49
1:2A:1291:C:H2'	1:2A:1292:U:C6	2.48	0.49
11:2P:19:VAL:HG12	11:2P:27:HIS:HB3	1.94	0.49
17:2V:61:VAL:HA	17:2V:94:LEU:HD23	1.95	0.49
25:13:16:PRO:HB2	25:13:18:ASP:OD1	2.12	0.49
26:14:40:HIS:O	26:14:44:THR:HG22	2.13	0.49
27:15:8:LYS:O	27:15:9:LYS:HD2	2.13	0.49
1:1A:174:U:H2'	1:1A:175:G:H8	1.76	0.49
1:1A:2149:G:N2	1:1A:2195:A:O2'	2.46	0.49
1:1A:383:A:C5	1:1A:384:G:H1'	3.28	0.49
1:1A:831:A:C6	3:1D:229:VAL:HG11	2.48	0.49
1:1A:1847:G:H3'	3:1D:62:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:16:ARG:HH21	15:1T:19:LEU:HD21	1.78	0.49
1:2A:1291:C:H2'	1:2A:1292:U:H6	1.77	0.49
1:2A:2080:G:OP1	23:21:35:THR:OG1	2.28	0.49
1:2A:527:C:H4'	1:2A:528:A:H5'	1.95	0.49
3:2D:26:LYS:HB3	3:2D:83:GLU:HG2	1.94	0.49
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.13	0.49
26:14:26:SER:OG	26:14:27:THR:N	2.46	0.49
30:18:26:LYS:HD2	30:18:48:PHE:CD2	2.48	0.49
1:1A:1117:G:O2'	1:1A:1135:G:H2'	2.12	0.49
1:1A:1284:G:OP2	62:1A:4190:HOH:O	2.20	0.49
1:1A:167:G:H2'	1:1A:168:G:C8	3.33	0.49
1:1A:2178:G:H2'	1:1A:2179:G:N3	2.28	0.49
1:1A:764:G:H2'	1:1A:765:A:O4'	2.13	0.49
21:1Z:101:PRO:HG2	21:1Z:135:GLU:O	2.12	0.49
1:2A:1800:C:P	3:2D:183:ARG:HH12	2.35	0.49
27:15:16:ARG:NH1	27:15:17:ASP:OD1	2.45	0.49
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.47	0.49
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.47	0.49
12:1Q:20:ALA:HB2	21:1Z:79:ARG:HG3	1.93	0.49
15:1T:56:GLY:O	15:1T:59:THR:HG22	2.12	0.49
16:1U:27:LEU:HB3	16:1U:31:SER:HB3	1.95	0.49
1:2A:116:C:H2'	1:2A:117:G:O4'	2.13	0.49
1:2A:1384:A:N3	1:2A:1405:U:H1'	2.28	0.49
1:2A:2127:G:H2'	1:2A:2128:C:C6	2.47	0.49
1:2A:247:G:H4'	1:2A:386:G:C5	2.48	0.49
1:2A:797:C:H2'	1:2A:798:G:O4'	2.12	0.49
1:2A:868:U:C4	1:2A:869:G:N7	2.81	0.49
12:2Q:45:GLN:N	12:2Q:45:GLN:OE1	2.45	0.49
22:10:43:THR:HG23	22:10:43:THR:O	2.12	0.48
1:1A:1110:C:H2'	1:1A:1111:U:H5'	1.95	0.48
1:1A:1904:C:H2'	1:1A:1905:G:O4'	2.13	0.48
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.52	0.48
15:1T:24:PRO:HD3	15:1T:52:ILE:HD12	1.95	0.48
18:1W:46:PHE:O	18:1W:50:VAL:HG23	2.13	0.48
20:1Y:97:ARG:HH11	20:1Y:107:ASP:C	2.17	0.48
1:2A:2119:A:O2'	1:2A:2120:G:H5''	2.13	0.48
4:2E:12:THR:HG22	4:2E:13:ARG:H	1.78	0.48
1:1A:1359:U:H5''	62:1A:4245:HOH:O	2.13	0.48
14:2S:64:GLU:HB3	26:24:59:PHE:CD2	86.78	0.48
1:2A:521:G:H2'	1:2A:522:G:C8	2.48	0.48
1:2A:629:G:H2'	1:2A:630:G:O4'	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:975(A):G:H1'	1:2A:990:A:C2	2.48	0.48
17:2V:16:PRO:HD3	17:2V:99:ILE:HD11	1.95	0.48
1:1A:1004:A:C6	1:1A:1037:C:N3	54.89	0.48
1:1A:223:C:H2'	1:1A:224:U:C6	2.49	0.48
1:1A:637:U:H5'	1:1A:640:A:N6	2.29	0.48
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.47	0.48
1:2A:2316:C:H2'	1:2A:2317:C:C6	2.48	0.48
2:2B:72:G:O2'	2:2B:105:A:N6	2.46	0.48
2:2B:89:G:OP2	2:2B:89:G:H8	1.97	0.48
5:2F:125:LEU:HD21	5:2F:199:TRP:CD2	2.48	0.48
7:2H:4:ILE:O	7:2H:69:ARG:HD2	2.14	0.48
1:1A:2348:A:H61	22:10:43:THR:CG2	2.27	0.48
1:1A:1435:G:H2'	1:1A:1436:U:C6	2.97	0.48
1:1A:2117:C:H2'	1:1A:2118:U:O4'	2.14	0.48
1:1A:2193:A:O2'	1:1A:2194:U:H5''	2.14	0.48
1:2A:1422:G:O3'	10:2O:49:ARG:NH2	99.17	0.48
1:2A:2292:C:H4'	1:2A:2375:G:H4'	1.96	0.48
12:2Q:43:THR:HG22	12:2Q:94:VAL:HG12	1.95	0.48
23:11:60:PHE:HE1	23:11:91:LYS:HG3	1.78	0.48
1:1A:1546:G:O2'	3:1D:100:GLY:O	2.26	0.48
15:1T:120:ARG:HA	15:1T:123:GLN:HG2	1.96	0.48
20:1Y:98:VAL:HG12	20:1Y:105:ALA:HA	1.95	0.48
1:2A:1010:A:N3	1:2A:1153:C:H1'	2.28	0.48
1:2A:1022:G:N2	1:2A:1023:U:O4	2.45	0.48
1:2A:1159:U:H2'	1:2A:1160:G:H8	1.77	0.48
1:2A:1501:C:H2'	1:2A:1502:C:H6	1.78	0.48
1:2A:1993:U:OP2	62:2A:3797:HOH:O	2.19	0.48
1:2A:2073:C:HO2'	1:2A:2598:A:HO2'	1.58	0.48
1:2A:81:G:H2'	1:2A:82:G:O4'	2.14	0.48
11:2P:128:HIS:NE2	11:2P:148:LEU:HD11	2.29	0.48
27:15:16:ARG:HG3	27:15:17:ASP:N	2.28	0.48
1:1A:1314:A:H2'	1:1A:1315:A:O4'	2.13	0.48
1:1A:1921:G:H2'	1:1A:1921:G:N3	2.27	0.48
1:1A:656:A:OP1	11:1P:65:ARG:NE	2.46	0.48
17:1V:80:GLN:HA	17:1V:82:ARG:HH12	1.78	0.48
24:22:21:LEU:HB2	24:22:64:LEU:HD12	1.94	0.48
1:2A:1501:C:H2'	1:2A:1502:C:C6	2.49	0.48
1:2A:2314:C:H2'	1:2A:2315:G:C8	2.48	0.48
6:2G:113:ARG:HD3	6:2G:140:ILE:O	2.14	0.48
14:2S:28:VAL:HG13	14:2S:35:ILE:HD11	1.96	0.48
14:2S:25:ARG:CG	14:2S:40:ILE:HB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2U:74:LEU:HD13	16:2U:79:PHE:HB2	1.96	0.48
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.46	0.48
1:1A:776:G:C6	3:1D:208:LYS:HB2	2.49	0.48
1:1A:1699:A:N6	13:1R:11:ASN:OD1	2.46	0.48
23:21:64:ALA:HA	23:21:67:ILE:HG13	1.94	0.48
1:2A:2526:G:H5'	1:2A:2742:C:O2'	2.14	0.48
1:2A:375:C:H2'	1:2A:376:C:C6	2.49	0.48
1:2A:686:G:N2	1:2A:788:A:H61	2.12	0.48
2:2B:119:G:H2'	2:2B:120:A:C8	2.48	0.48
1:2A:2313:C:C1'	6:2G:40:ASN:HD22	2.27	0.48
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.13	0.48
25:13:5:LYS:HG3	25:13:36:VAL:HG22	1.96	0.48
1:1A:1108:G:H5''	1:1A:1116:A:O2'	2.13	0.48
1:1A:1469:G:H2'	1:1A:1470:G:C8	2.76	0.48
13:1R:18:LEU:HD21	13:1R:22:ARG:NH1	2.29	0.48
30:28:14:VAL:HG22	30:28:24:ALA:HB2	1.96	0.48
1:2A:2659:G:N2	1:2A:2662:A:OP2	2.47	0.48
1:2A:322:A:OP1	5:2F:168:ARG:HD2	2.14	0.48
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	1.96	0.48
24:12:35:LEU:HD12	24:12:53:LEU:HD12	1.96	0.48
1:1A:1055:A:OP2	62:1A:4120:HOH:O	2.19	0.48
1:1A:327:U:H2'	1:1A:328:G:C8	2.49	0.48
1:1A:569:G:N2	1:1A:572:A:OP1	2.47	0.48
1:1A:931:C:H2'	1:1A:932:C:H4'	1.95	0.48
5:1F:24:LEU:HD23	5:1F:115:ALA:HA	1.95	0.48
5:1F:116:ASP:OD2	5:1F:117:ARG:NH1	2.47	0.48
7:1H:87:LEU:HD23	7:1H:164:TYR:HA	1.96	0.48
18:1W:18:ARG:NH2	18:1W:76:VAL:O	2.46	0.48
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.95	0.48
24:22:10:LEU:HB3	24:22:14:ARG:NH1	2.28	0.48
1:2A:1786:A:H1'	1:2A:1938:A:H61	1.77	0.48
1:2A:2025:C:H2'	1:2A:2026:C:C6	2.48	0.48
1:2A:2075:U:OP2	1:2A:2238:G:O2'	2.28	0.48
1:1A:1478:C:H2'	1:1A:1479:U:O4'	2.14	0.48
1:1A:794:U:O2	1:1A:2036:A:H1'	2.13	0.48
1:1A:2045:G:H5'	1:1A:2629:C:H4'	1.96	0.48
7:1H:109:PHE:O	62:1H:5001:HOH:O	2.20	0.48
10:1O:80:ASP:OD2	15:1T:64:ARG:NH2	2.46	0.48
25:23:26:LEU:O	25:23:35:ARG:NE	2.47	0.48
1:2A:1434:A:N6	1:2A:1558:A:H62	2.11	0.48
1:2A:1363:C:O2'	1:2A:1809:A:N3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1919:A:H3'	1:2A:1920:4OC:H6	1.96	0.48
1:2A:2335:A:C8	1:2A:2337:G:C5	3.02	0.48
6:2G:122:PRO:HB3	6:2G:170:ARG:NH1	2.29	0.48
2:2B:42:C:O2'	6:2G:67:LYS:O	2.22	0.48
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.60	0.48
12:2Q:111:GLU:OE1	12:2Q:133:ARG:NH2	2.46	0.48
1:1A:265:U:H2'	1:1A:266:C:C6	2.50	0.47
1:1A:858:U:H2'	11:1P:21:ARG:HA	1.96	0.47
3:1D:152:GLY:O	3:1D:154:LYS:HG2	2.14	0.47
4:1E:190:GLY:HA3	62:1E:414:HOH:O	2.14	0.47
1:2A:1019:U:OP1	1:2A:1035:U:O2'	2.26	0.47
1:2A:1186:G:H2'	1:2A:1187:G:O4'	2.14	0.47
1:2A:2337:G:H2'	1:2A:2338:G:H8	1.78	0.47
6:2G:115:ARG:H	6:2G:136:ARG:HH22	1.62	0.47
1:2A:84:A:H5'	20:2Y:8:LYS:HG2	1.96	0.47
22:10:10:THR:HG22	22:10:12:ASN:N	2.16	0.47
1:1A:1654:A:H1'	1:1A:1656:A:OP2	2.14	0.47
1:1A:1807:G:OP2	62:1A:4188:HOH:O	2.20	0.47
1:1A:2145:G:H1	1:1A:2197:C:H42	1.61	0.47
1:1A:2175:G:H2'	1:1A:2176:G:C8	2.49	0.47
1:1A:2658:C:H2'	1:1A:2659:U:O4'	2.14	0.47
1:1A:646:A:OP2	11:1P:108:LYS:NZ	2.47	0.47
1:1A:831:A:O4'	3:1D:227:ASN:ND2	2.48	0.47
3:1D:132:PRO:HG2	3:1D:135:PHE:HD2	1.78	0.47
1:1A:2346:G:N2	14:1S:16:ASN:OD1	2.40	0.47
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.49	0.47
1:2A:2784:C:H2'	1:2A:2785:C:C6	2.48	0.47
1:2A:2886:G:H2'	1:2A:2887:U:C6	2.49	0.47
1:2A:500:G:N2	1:2A:502:A:H3'	2.29	0.47
3:2D:274:ARG:N	62:2D:403:HOH:O	2.46	0.47
26:14:54:GLY:O	26:14:56:VAL:HA	2.14	0.47
30:28:26:LYS:HD2	30:28:48:PHE:CD2	2.50	0.47
1:2A:1836:C:H2'	1:2A:1837:C:H6	1.79	0.47
1:2A:2206:G:H3'	1:2A:2207:G:N7	2.28	0.47
1:2A:380:U:H4'	23:21:16:ASN:O	2.14	0.47
1:2A:518:G:H4'	18:2W:18:ARG:NE	2.30	0.47
1:2A:657:U:H2'	1:2A:658:C:C6	2.49	0.47
1:2A:813:U:H2'	1:2A:814:C:C6	2.49	0.47
1:2A:880:G:N2	1:2A:898:C:O2	2.47	0.47
1:2A:990:A:H1'	1:2A:1156:A:N3	2.29	0.47
12:2Q:35:VAL:HG13	12:2Q:130:LYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2T:29:ARG:HB3	15:2T:87:ASP:HB2	1.95	0.47
1:1A:2204:G:H2'	1:1A:2205:C:C6	2.50	0.47
1:1A:280:C:H2'	1:1A:281:G:C8	2.50	0.47
1:2A:2125:G:H21	1:2A:2173:A:H62	1.61	0.47
10:2O:7:TYR:CE1	10:2O:44:LYS:HG3	2.49	0.47
17:2V:14:VAL:HB	17:2V:96:ILE:HG13	1.96	0.47
1:1A:2190:G:H8	1:1A:2192:A:N7	2.12	0.47
1:1A:2486:C:H5''	1:1A:2487:C:OP2	2.15	0.47
1:2A:1529:G:N2	1:2A:1540:U:O2	2.42	0.47
1:2A:1971:A:C4	3:2D:241:PRO:HD3	2.50	0.47
1:2A:2127:G:O6	1:2A:2161:C:C4	2.68	0.47
1:2A:795:C:H2'	1:2A:796:C:C6	2.49	0.47
5:2F:183:VAL:O	5:2F:187:VAL:HG23	2.14	0.47
1:1A:1027:A:OP1	62:1A:4192:HOH:O	2.20	0.47
1:1A:223:C:H2'	1:1A:224:U:H6	1.78	0.47
1:1A:1834:A:H4'	3:1D:259:THR:HG23	1.96	0.47
8:1I:130:TYR:CE2	8:1I:132:PRO:HB3	2.49	0.47
1:1A:1700:G:H3'	13:1R:2:ARG:HD3	1.97	0.47
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.20	0.47
1:2A:635:C:H2'	1:2A:636:G:O4'	2.14	0.47
2:2B:33:G:C6	2:2B:34:U:C4	3.03	0.47
8:2I:5:LEU:HD23	8:2I:9:LEU:HD13	1.96	0.47
15:2T:26:ASP:O	15:2T:49:VAL:HG22	2.14	0.47
30:18:31:HIS:ND1	30:18:32:LEU:HD13	2.30	0.47
31:19:25:VAL:HB	31:19:34:GLN:HB2	1.97	0.47
1:1A:1733:C:H2'	1:1A:1734:G:O4'	2.15	0.47
1:1A:2145:G:H2'	1:1A:2146:G:H8	1.78	0.47
1:1A:2617:PSU:OP2	62:1A:4189:HOH:O	2.20	0.47
1:1A:2672:A:N7	7:1H:175:LYS:NZ	2.62	0.47
19:1X:95:LEU:HA	19:1X:95:LEU:HD23	1.69	0.47
1:2A:2366:A:H2'	1:2A:2367:G:O4'	2.15	0.47
1:2A:1999:C:H5''	1:2A:2723:C:O2'	2.15	0.47
1:2A:959:A:N3	1:2A:2457:U:O2'	2.43	0.47
14:2S:94:TYR:CZ	14:2S:99:LYS:HG3	2.49	0.47
1:1A:1375:U:H3'	1:1A:1376:C:H6	1.80	0.47
1:1A:1425:A:H4'	1:1A:1426:G:OP2	2.14	0.47
1:1A:2053:A:C6	1:1A:2510:C:H1'	2.50	0.47
1:1A:2550:C:H2'	1:1A:2551:C:H6	1.78	0.47
1:1A:342:C:O2	1:1A:347:G:N2	7.67	0.47
1:1A:407:U:H2'	1:1A:408:G:C8	2.50	0.47
6:1G:40:ASN:HB3	6:1G:156:ASP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:103:ARG:HG3	8:1I:104:GLN:H	1.79	0.47
1:1A:1423:G:H5'	10:1O:49:ARG:NH2	95.23	0.47
25:23:15:TYR:O	25:23:20:LYS:HE3	2.14	0.47
1:2A:1265:A:OP2	62:2A:3758:HOH:O	2.20	0.47
1:2A:236:C:H2'	1:2A:237:C:C6	2.50	0.47
1:2A:2893:G:H5''	1:2A:2894:G:O4'	2.15	0.47
1:2A:625:G:H2'	1:2A:626:U:C6	3.36	0.47
16:2U:88:ILE:HG22	16:2U:90:VAL:HG23	1.97	0.47
23:11:51:VAL:HG11	23:11:74:VAL:HG21	1.97	0.47
1:1A:1403:U:H2'	1:1A:1404:G:O4'	2.15	0.47
1:1A:217:A:H8	1:1A:218:A:H5'	1.79	0.47
1:1A:2143:G:N2	1:1A:2199:C:N3	2.52	0.47
1:1A:384:G:H2'	1:1A:385:G:C8	2.49	0.47
1:1A:1696:G:O2'	13:1R:107:ASP:OD2	2.31	0.47
20:1Y:86:ARG:HG3	20:1Y:100:ALA:HB2	1.95	0.47
1:2A:2376:A:H2'	1:2A:2377:A:O4'	2.14	0.47
1:2A:484:C:H2'	1:2A:485:C:C6	2.50	0.47
3:2D:132:PRO:HA	3:2D:190:TYR:HA	1.97	0.47
7:2H:164:TYR:HB2	7:2H:167:GLU:HB2	1.95	0.47
21:2Z:9:TYR:OH	21:2Z:61:LEU:HD23	2.15	0.47
1:1A:1375:U:H5''	1:1A:1376:C:H5	1.80	0.47
1:1A:1631:C:O2'	1:1A:1632:A:O5'	2.23	0.47
1:1A:2508:C:OP2	12:1Q:82:ARG:HD3	2.15	0.47
1:1A:282:G:H2'	1:1A:283:G:O4'	2.15	0.47
1:1A:2880:C:H2'	1:1A:2881:C:O4'	2.15	0.47
1:1A:895:G:H2'	1:1A:896:A:C8	2.50	0.47
1:1A:944:C:N4	1:1A:945:A:H62	2.13	0.47
11:1P:112:LEU:HD13	11:1P:114:ILE:HD11	1.97	0.47
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.50	0.47
1:2A:484:C:H2'	1:2A:485:C:H6	1.79	0.47
1:2A:495:G:N3	18:2W:61:ASN:ND2	2.63	0.47
1:2A:27:G:N2	1:2A:512:G:H1'	2.30	0.47
4:2E:48:GLN:NE2	4:2E:78:LEU:HD23	2.29	0.47
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.97	0.47
6:2G:114:ILE:HB	6:2G:117:PHE:HB2	1.97	0.47
1:2A:811:U:H2'	11:2P:21:ARG:HA	1.97	0.47
21:2Z:5:LEU:HD12	21:2Z:47:VAL:HG21	1.97	0.47
20:1Y:28:LYS:NZ	20:1Y:64:GLU:OE1	2.33	0.47
6:2G:7:LEU:HD23	6:2G:100:TRP:HE3	1.80	0.47
3:1D:159:ALA:HB1	3:1D:198:ASN:O	2.16	0.46
7:1H:40:GLU:CD	7:1H:60:ARG:HH12	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.50	0.46
11:1P:49:ARG:HG2	30:18:60:LEU:HD12	1.98	0.46
20:1Y:7:VAL:HG21	20:1Y:72:VAL:HG12	1.96	0.46
1:2A:102:G:OP1	24:22:7:ARG:NH2	2.48	0.46
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.51	0.46
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.79	0.46
1:2A:2316:C:H2'	1:2A:2317:C:H6	1.80	0.46
1:2A:514:A:N3	1:2A:581:C:O2'	2.37	0.46
6:2G:17:PRO:HA	6:2G:20:ILE:HD12	1.97	0.46
1:1A:600:G:O2'	1:1A:1300:A:OP1	2.31	0.46
1:1A:2146:G:H2'	1:1A:2147:G:O4'	2.16	0.46
1:1A:2177:G:H5'	1:1A:2178:G:OP2	2.15	0.46
1:1A:2430:A:OP2	30:18:29:LYS:NZ	2.32	0.46
1:1A:2490:A:OP2	31:19:2:LYS:NZ	2.28	0.46
1:1A:342:C:N3	1:1A:347:G:N1	6.49	0.46
4:1E:121:ASN:ND2	62:1E:404:HOH:O	2.42	0.46
4:1E:3:GLY:HA2	4:1E:198:VAL:O	2.15	0.46
6:1G:11:TYR:HA	6:1G:15:VAL:HB	1.96	0.46
9:1N:42:TRP:CH2	9:1N:44:PRO:HB3	2.50	0.46
11:1P:27:HIS:HB2	62:1P:3111:HOH:O	2.14	0.46
12:1Q:35:VAL:HA	12:1Q:101:ARG:O	2.15	0.46
14:1S:20:ARG:NH2	22:10:51:VAL:O	2.48	0.46
29:27:24:THR:O	29:27:28:ARG:HG3	2.16	0.46
1:2A:1328:G:H2'	1:2A:1330:C:C4	2.50	0.46
1:2A:142(A):C:H2'	1:2A:143:G:C8	2.50	0.46
1:2A:277:C:H4'	1:2A:278:A:C8	2.46	0.46
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.15	0.46
1:1A:1587:U:H2'	1:1A:1588:G:O4'	2.16	0.46
1:1A:166:G:H2'	1:1A:167:G:C8	3.66	0.46
1:1A:24:G:H2'	1:1A:25:U:O4'	2.16	0.46
1:1A:83:A:H5''	20:1Y:8:LYS:HE3	1.96	0.46
5:1F:195:ASP:HB3	5:1F:198:ALA:H	1.80	0.46
5:1F:89:VAL:O	62:1F:401:HOH:O	2.21	0.46
7:1H:4:ILE:O	7:1H:69:ARG:HD2	2.15	0.46
9:1N:1:MET:HE3	16:1U:93:LYS:HE3	1.96	0.46
10:1O:104:ARG:NH1	10:1O:122:LEU:OXT	2.48	0.46
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.33	0.46
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.62	0.46
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.16	0.46
1:2A:2769:C:H2'	1:2A:2770:G:O4'	2.15	0.46
1:2A:581:C:OP1	16:2U:33:ARG:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:724:U:H2'	1:2A:725:G:O4'	2.15	0.46
10:2O:102:VAL:HB	10:2O:106:LEU:HD12	1.97	0.46
12:2Q:32:TYR:HE1	12:2Q:133:ARG:HE	1.63	0.46
14:2S:15:ARG:O	14:2S:19:LYS:HG3	2.15	0.46
16:2U:102:GLU:OE1	16:2U:104:GLN:NE2	2.37	0.46
1:1A:602:G:O2'	1:1A:2041:A:OP1	2.30	0.46
1:1A:2203:G:O2'	1:1A:2204:G:OP1	2.32	0.46
1:1A:957:A:H2'	12:1Q:9:TYR:OH	2.16	0.46
1:1A:1464:G:OP2	15:1T:111:ARG:NH2	103.68	0.46
25:23:5:LYS:NZ	25:23:34:GLU:OE2	2.49	0.46
1:2A:137:C:H42	1:2A:143:G:H1	1.64	0.46
1:2A:1491:G:O4'	3:2D:99:ASP:HB3	2.15	0.46
16:2U:34:LYS:HA	16:2U:34:LYS:HD3	1.70	0.46
26:14:20:ASN:OD1	26:14:21:VAL:N	2.48	0.46
1:1A:449:A:H2'	1:1A:450:A:C8	2.50	0.46
1:1A:469:A:N7	5:1F:45:ARG:HG2	2.31	0.46
1:1A:645:G:H5'	1:1A:645:G:N3	2.30	0.46
1:1A:8:A:H2'	1:1A:9:U:C6	2.51	0.46
1:1A:662:A:H2'	11:1P:117:GLU:OE1	2.15	0.46
12:1Q:43:THR:HG22	12:1Q:94:VAL:HG12	1.98	0.46
14:1S:41:ASP:O	14:1S:45:GLY:N	2.49	0.46
16:1U:108:GLU:O	16:1U:112:ARG:HG2	2.15	0.46
25:23:7:LYS:HB2	25:23:34:GLU:HG2	1.96	0.46
13:2R:88:ARG:NH2	13:2R:89:ASP:OD1	2.49	0.46
15:2T:22:PHE:HA	15:2T:91:ARG:HH12	1.81	0.46
1:2A:64:A:O3'	19:2X:71:GLY:HA3	2.16	0.46
1:1A:1782:C:O2'	1:1A:2871:G:O2'	2.26	0.46
1:1A:1857:G:O2'	3:1D:242:ARG:NH2	2.49	0.46
1:1A:2830:A:OP2	13:1R:2:ARG:NH2	2.48	0.46
7:1H:3:ARG:HH11	7:1H:4:ILE:H	1.63	0.46
21:1Z:69:THR:HG22	21:1Z:90:VAL:HA	1.97	0.46
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.30	0.46
1:2A:1686:C:H2'	1:2A:1687:G:O4'	2.15	0.46
1:2A:171:G:H2'	1:2A:172:C:C6	2.50	0.46
1:2A:1848:A:C4	1:2A:1849:G:C8	3.04	0.46
1:2A:2398:U:H2'	1:2A:2399:G:H8	1.79	0.46
8:2I:14:ASP:OD1	8:2I:15:VAL:N	2.46	0.46
14:2S:85:VAL:HG11	14:2S:110:LEU:HD23	1.96	0.46
1:1A:737:G:H2'	1:1A:738:C:C6	2.51	0.46
1:1A:1857:G:H4'	3:1D:242:ARG:CZ	2.45	0.46
11:1P:2:LYS:HG2	11:1P:3:LEU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1913:A:H4'	1:2A:1914:C:O5'	2.16	0.46
1:2A:1662:C:O2'	1:2A:2687:U:OP1	2.31	0.46
1:2A:80:G:N1	1:2A:90:U:O2	27.48	0.46
62:2A:3981:HOH:O	5:2F:68:LYS:HE2	2.14	0.46
23:11:3:LYS:HB2	23:11:61:ARG:HH22	1.79	0.46
23:11:78:LYS:HA	23:11:78:LYS:HD3	1.79	0.46
1:1A:1189:A:OP1	9:1N:25:ARG:NH2	2.49	0.46
1:1A:1974:A:C6	1:1A:1975:A:N1	2.84	0.46
1:1A:2142:G:C2'	1:1A:2143:G:H5'	2.45	0.46
1:1A:2353:G:N7	62:1A:4300:HOH:O	2.36	0.46
1:1A:27:G:C2	1:1A:537:G:N3	2.83	0.46
4:1E:2:LYS:HB2	4:1E:95:ILE:HD12	1.98	0.46
6:1G:124:SER:HB2	6:1G:131:TYR:CE1	2.51	0.46
26:24:40:HIS:HB3	26:24:43:TYR:HD2	1.81	0.46
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.16	0.46
1:2A:1423:G:H5'	10:2O:49:ARG:NH2	97.44	0.46
1:2A:1942:5MC:HM53	1:2A:1943:U:C2	2.51	0.46
1:2A:271(U):G:H2'	1:2A:271(V):G:H8	1.80	0.46
1:2A:557:U:H2'	1:2A:558:G:H8	1.80	0.46
1:2A:760:G:H2'	1:2A:761:A:O4'	2.15	0.46
9:2N:123:TYR:HH	9:2N:130:HIS:CD2	2.33	0.46
19:2X:35:THR:HG23	19:2X:38:GLU:H	1.81	0.46
1:1A:1793:A:H2'	62:1A:5449:HOH:O	2.16	0.46
1:1A:2190:G:C8	1:1A:2192:A:N7	2.84	0.46
1:1A:297:C:H2'	1:1A:298:G:C8	2.51	0.46
1:1A:624:C:O2'	1:1A:628:C:OP1	2.29	0.46
7:1H:19:VAL:HG22	7:1H:24:VAL:HG12	1.97	0.46
5:1F:34:TRP:CH2	11:1P:8:PRO:HB3	2.51	0.46
24:22:1:MET:SD	24:22:56:GLN:NE2	2.89	0.46
1:2A:1589:C:H2'	1:2A:1590:U:C6	2.51	0.46
1:2A:2250:G:OP1	12:2Q:85:LYS:NZ	2.47	0.46
1:2A:2512:C:H2'	1:2A:2513:G:O4'	2.16	0.46
1:2A:647:G:O5'	1:2A:647:G:H8	1.99	0.46
5:2F:40:GLN:OE1	5:2F:184:TYR:HB2	2.16	0.46
24:12:54:LYS:HB3	24:12:54:LYS:HE2	1.79	0.46
30:18:63:PRO:HG2	30:18:64:TYR:CD2	2.51	0.46
1:1A:1997:G:H2'	1:1A:1998:U:O4'	2.16	0.46
1:1A:2139:A:O2'	1:1A:2140:U:H5''	2.16	0.46
1:1A:2596:U:H2'	1:1A:2597:U:C6	2.51	0.46
1:1A:940:C:H2'	1:1A:941:U:O4'	2.16	0.46
1:1A:2691:A:H5'	4:1E:165:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:27:LYS:HE3	7:1H:32:GLU:OE1	2.16	0.46
1:1A:956:A:H62	12:1Q:12:GLN:HA	1.81	0.46
13:1R:33:ARG:HG2	13:1R:115:GLU:CB	2.46	0.46
1:2A:1028:A:H2	1:2A:2486:G:N3	2.14	0.46
1:2A:1169:G:H1	1:2A:1180:C:H42	1.63	0.46
7:2H:87:LEU:HD23	7:2H:164:TYR:HA	1.97	0.46
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.50	0.46
1:1A:1525:G:H2'	1:1A:1526:G:H8	1.81	0.45
1:1A:174:U:H4'	1:1A:207:A:H4'	1.97	0.45
1:1A:2802:C:H1'	1:1A:2901:A:H2	1.81	0.45
1:1A:599:U:H2'	1:1A:600:G:C8	2.52	0.45
1:1A:905:U:O2	1:1A:2280:A:H2'	2.16	0.45
9:1N:45:ASN:OD1	9:1N:46:VAL:HG23	2.16	0.45
12:1Q:34:LEU:HB2	12:1Q:118:LEU:HD22	1.98	0.45
1:1A:2697:G:P	15:1T:51:ARG:HH12	2.39	0.45
1:2A:1027:A:H2	1:2A:2487:G:HO2'	1.62	0.45
1:2A:1821:A:H2'	1:2A:1822:G:C8	2.51	0.45
1:2A:2127:G:H2'	1:2A:2128:C:H6	1.81	0.45
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.51	0.45
1:2A:2698:U:H2'	1:2A:2699:C:C6	2.51	0.45
1:2A:29:U:H2'	1:2A:30:G:C8	2.51	0.45
1:2A:444:C:H4'	5:2F:49:ALA:HB2	1.98	0.45
5:2F:116:ASP:OD1	5:2F:119:ARG:NH2	2.50	0.45
8:2I:86:THR:HG22	8:2I:122:GLU:OE1	2.16	0.45
18:2W:45:TYR:CZ	18:2W:49:LYS:HE2	2.50	0.45
1:1A:1639:G:H2'	1:1A:1640:G:H8	1.77	0.45
1:1A:1830:G:N7	3:1D:179:SER:OG	2.42	0.45
1:1A:215:G:H21	1:1A:217:A:H62	1.63	0.45
1:1A:273:G:H21	8:1I:50:ARG:HH12	1.64	0.45
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.15	0.45
9:1N:67:LEU:HD23	9:1N:87:LEU:HD22	1.98	0.45
1:2A:1182:A:H2'	1:2A:1183:G:C8	2.50	0.45
1:2A:1540:U:H2'	1:2A:1541:G:O4'	2.16	0.45
1:2A:1616:A:O2'	62:2A:3800:HOH:O	2.21	0.45
1:2A:2102:U:H3	1:2A:2187:G:H1	1.65	0.45
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.52	0.45
1:2A:524:U:H2'	1:2A:525:U:C6	2.52	0.45
1:2A:829:A:N7	1:2A:2247:A:O2'	2.48	0.45
2:2B:55:U:H2'	2:2B:56:G:O4'	2.16	0.45
6:2G:15:VAL:HG21	6:2G:176:LEU:HD23	1.98	0.45
14:2S:48:LEU:HD23	14:2S:82:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:2V:52:VAL:HG23	17:2V:55:ALA:HB3	1.96	0.45
23:11:13:ILE:HD11	23:11:42:GLN:OE1	2.16	0.45
23:11:53:VAL:HG22	23:11:74:VAL:HG13	1.98	0.45
26:14:49:PHE:HD1	26:14:49:PHE:HA	1.71	0.45
1:1A:1053:C:H5''	9:1N:35:ARG:HH11	1.82	0.45
1:1A:1529:G:H4'	1:1A:1530:G:OP2	4.37	0.45
1:1A:2389:A:H2'	1:1A:2390:A:C8	2.51	0.45
1:1A:843:C:H2'	1:1A:844:C:C6	2.52	0.45
1:1A:2697:G:H5'	10:1O:68:GLU:OE2	2.16	0.45
14:1S:99:LYS:HE2	14:1S:103:GLU:OE2	2.16	0.45
19:1X:40:LYS:HG3	19:1X:51:VAL:HB	1.97	0.45
1:2A:1416:G:O2'	1:2A:1417:C:OP2	2.25	0.45
1:2A:1422:G:C1'	1:2A:1495:A:H61	2.29	0.45
1:2A:1656:C:H2'	1:2A:1657:C:C6	2.52	0.45
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.51	0.45
1:2A:2558:C:H2'	1:2A:2559:C:O4'	2.17	0.45
1:2A:2564:A:OP1	1:2A:2648:C:O2'	2.24	0.45
1:2A:26:G:H1'	1:2A:515:A:H61	1.80	0.45
1:2A:764:A:H5'	3:2D:210:GLY:CA	2.47	0.45
1:2A:942:G:OP2	11:2P:39:LYS:NZ	2.48	0.45
4:2E:7:VAL:HG12	4:2E:27:LEU:HB3	1.97	0.45
12:2Q:137:TYR:CE1	21:2Z:83:PRO:HG3	2.51	0.45
26:14:64:GLY:C	26:14:66:SER:H	2.20	0.45
29:17:34:ARG:NH1	29:17:39:ARG:HG2	2.31	0.45
1:1A:1059:C:OP2	62:1A:4195:HOH:O	2.21	0.45
1:1A:1269:G:N2	1:1A:1272:A:OP2	2.40	0.45
1:1A:141:C:H2'	1:1A:142:G:O4'	2.17	0.45
1:1A:1627:A:H5'	1:1A:1628:G:OP2	2.17	0.45
2:1B:95:C:H2'	2:1B:96:U:C6	2.51	0.45
9:1N:108:PRO:O	9:1N:113:GLY:HA3	2.17	0.45
14:1S:84:GLN:HA	14:1S:111:GLU:HB2	1.98	0.45
23:21:83:GLU:N	23:21:83:GLU:OE1	2.50	0.45
1:2A:78:A:H2'	1:2A:79:G:H8	1.81	0.45
3:2D:96:HIS:CD2	3:2D:102:LYS:HG2	2.52	0.45
13:2R:36:THR:HG22	13:2R:37:THR:N	2.32	0.45
14:2S:88:ASP:OD1	14:2S:90:GLY:N	2.48	0.45
21:2Z:126:VAL:HG11	21:2Z:161:VAL:HG23	1.98	0.45
1:1A:1312:G:O5'	18:1W:15:ARG:NH2	2.49	0.45
1:1A:1323:G:H2'	1:1A:1324:A:C8	3.14	0.45
1:1A:2710:U:H2'	1:1A:2711:C:C6	2.51	0.45
1:1A:831:A:OP1	1:1A:2600:G:H5''	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:7:LEU:HD23	6:1G:100:TRP:CE3	2.51	0.45
9:1N:96:GLU:H	9:1N:96:GLU:CD	2.19	0.45
11:1P:59:LEU:HD23	30:18:13:ARG:HD2	1.98	0.45
1:2A:2141:G:O6	1:2A:2150:U:O2	2.34	0.45
1:2A:2888:C:H2'	1:2A:2889:C:H6	1.82	0.45
1:2A:686:G:H21	1:2A:788:A:H61	1.64	0.45
1:2A:817:C:H2'	1:2A:818:G:O4'	2.17	0.45
14:2S:67:ARG:NH2	14:2S:103:GLU:OE1	2.47	0.45
30:18:23:VAL:HG22	30:18:47:LYS:HB3	1.98	0.45
1:1A:1117:G:N3	1:1A:1135:G:O2'	2.50	0.45
1:1A:1423:G:H5'	10:1O:49:ARG:HH22	94.49	0.45
1:1A:2145:G:H2'	1:1A:2146:G:C8	2.52	0.45
1:1A:2504:U:H2'	1:1A:2505:U:C6	2.52	0.45
1:1A:265:U:H2'	1:1A:266:C:H6	1.82	0.45
9:1N:14:VAL:HG22	9:1N:138:LEU:HG	1.99	0.45
12:1Q:32:TYR:HE1	12:1Q:133:ARG:HE	1.65	0.45
15:1T:112:ARG:HG3	15:1T:115:ARG:HH21	1.82	0.45
2:2B:43:C:OP1	26:24:6:HIS:NE2	2.50	0.45
1:2A:1371:G:H2'	1:2A:1372:U:H5	1.82	0.45
1:2A:1508:A:H4'	1:2A:1509(A):A:C5	2.52	0.45
1:2A:1592:C:H2'	1:2A:1593:G:H8	1.82	0.45
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.16	0.45
1:2A:2334:G:O6	22:20:74:ARG:NH1	2.32	0.45
1:2A:2842:G:H1	1:2A:2875:C:H42	1.65	0.45
15:2T:90:GLN:OE1	15:2T:121:ILE:HD11	2.15	0.45
16:2U:24:TYR:HB2	16:2U:29:SER:HB3	1.98	0.45
21:2Z:149:SER:OG	21:2Z:172:ALA:O	2.21	0.45
25:13:7:LYS:HA	25:13:33:GLN:O	2.16	0.45
1:1A:1100:A:C6	1:1A:1101:G:C6	3.05	0.45
1:1A:1093:G:C2'	1:1A:1156:G:H22	2.27	0.45
1:1A:1971:G:C6	1:1A:1972:G:C6	3.05	0.45
1:1A:2129:C:N3	1:1A:2204:G:N2	2.62	0.45
1:1A:2279:A:H5''	1:1A:2280:A:H5'	1.98	0.45
1:1A:636:G:N2	1:1A:640:A:O2'	2.49	0.45
1:1A:807:G:H2'	1:1A:808:A:O4'	2.17	0.45
15:1T:127:ALA:O	15:1T:128:GLU:HG2	2.16	0.45
16:1U:97:ASP:OD1	16:1U:101:ARG:NH1	2.50	0.45
26:24:64:GLY:C	26:24:66:SER:H	2.20	0.45
29:27:12:ARG:NH2	29:27:44:PRO:HB3	2.32	0.45
1:2A:1006:C:H2'	1:2A:1007:C:C6	3.65	0.45
1:2A:1321:A:H2'	1:2A:1322:A:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1515:G:H2'	1:2A:1516:C:C6	2.52	0.45
1:2A:1914:C:H2'	1:2A:1915:5MU:O4'	2.17	0.45
1:2A:2191:G:C2	1:2A:2192:G:H1'	2.52	0.45
1:2A:2554:U:H2'	1:2A:2555:U:C6	2.51	0.45
1:2A:271(O):C:H2'	1:2A:271(P):C:C6	2.52	0.45
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.51	0.45
7:2H:25:LYS:HB3	7:2H:27:LYS:NZ	2.28	0.45
7:2H:45:VAL:HG12	7:2H:50:VAL:HG22	1.99	0.45
15:2T:94:ALA:HB1	15:2T:99:LEU:HD21	1.98	0.45
18:2W:18:ARG:NH2	18:2W:76:VAL:O	2.49	0.45
1:1A:1410:G:P	23:11:3:LYS:HG3	2.57	0.45
1:1A:830:A:H1'	1:1A:1810:U:O4'	2.17	0.45
3:1D:72:LYS:HB3	3:1D:75:ILE:HD12	1.98	0.45
10:1O:7:TYR:HE1	10:1O:20:MET:HB2	1.82	0.45
11:1P:52:GLU:HG2	30:18:57:ARG:HH22	1.81	0.45
14:1S:105:ALA:O	14:1S:110:LEU:HB2	2.17	0.45
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.51	0.45
1:2A:1683:C:H2'	1:2A:1684:C:C6	2.52	0.45
1:2A:171:G:H2'	1:2A:172:C:H6	1.82	0.45
1:2A:2155:G:H5'	1:2A:2155:G:H8	1.82	0.45
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.81	0.45
1:2A:2801(A):A:N3	1:2A:2895:U:O2'	2.40	0.45
1:2A:531:C:H4'	1:2A:532:A:H5''	1.97	0.45
1:2A:588:U:H2'	1:2A:589:C:C6	2.51	0.45
1:2A:848:G:H2'	1:2A:849:A:C8	2.51	0.45
1:1A:1572:G:C6	1:1A:1573:G:C2	3.05	0.45
1:1A:784:C:H4'	1:1A:1868:C:OP1	59.46	0.45
1:1A:2735:G:OP2	62:1A:4196:HOH:O	2.21	0.45
1:1A:364:A:H2'	1:1A:365:G:O4'	2.17	0.45
2:1B:55:U:H2'	2:1B:56:G:O4'	2.16	0.45
21:1Z:128:VAL:HG23	21:1Z:160:GLY:O	2.16	0.45
1:2A:2471:C:H2'	1:2A:2472:G:O4'	2.17	0.45
1:2A:27:G:O2'	1:2A:28:A:OP2	2.27	0.45
2:2B:78:A:H2'	2:2B:79:C:O4'	2.17	0.45
1:2A:2572:A:N7	4:2E:144:ARG:HD2	2.32	0.45
8:2I:77:LEU:HD11	8:2I:101:LEU:HB2	1.98	0.45
11:2P:99:LEU:HA	11:2P:102:ARG:HE	1.81	0.45
1:2A:910:A:C5	12:2Q:13:GLN:HG3	2.52	0.45
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.99	0.45
1:1A:2623:U:C4	27:15:3:LYS:HG2	2.52	0.45
1:1A:1074:A:N6	1:1A:1171:G:H2'	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1653:C:H4'	1:1A:1654:A:O5'	2.16	0.45
1:1A:237:G:OP1	62:1A:4197:HOH:O	2.21	0.45
2:1B:1:U:H2'	2:1B:2:C:C6	2.51	0.45
9:1N:121:LYS:HG2	9:1N:130:HIS:NE2	2.32	0.45
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.17	0.45
1:2A:1899:G:N3	1:2A:1899:G:H2'	2.32	0.45
1:2A:848:G:N2	1:2A:933:A:H1'	2.32	0.45
6:2G:18:GLU:HA	6:2G:21:ARG:HG2	1.99	0.45
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	1.99	0.45
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.17	0.45
8:1I:38:LEU:HD13	23:11:75:GLU:OE1	2.18	0.44
1:1A:1057:G:OP1	16:1U:77:SER:OG	2.29	0.44
13:1R:103:ARG:HD3	13:1R:108:GLY:O	2.17	0.44
1:2A:857:C:H1'	22:20:26:TYR:HE1	1.82	0.44
1:2A:1184:G:H5'	25:23:29:ARG:NH2	2.32	0.44
26:24:40:HIS:HB3	26:24:43:TYR:CD2	2.52	0.44
1:2A:1022:G:N2	1:2A:1142(A):A:H2	2.03	0.44
1:2A:1200:C:H2'	1:2A:1201:C:C6	2.52	0.44
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.52	0.44
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.18	0.44
1:2A:2126:A:N6	1:2A:2163:C:H5'	2.32	0.44
1:2A:355:G:H2'	1:2A:356:G:C8	2.52	0.44
1:2A:918:A:C5	1:2A:919:G:H1'	2.52	0.44
1:2A:924:C:H2'	1:2A:925:C:C6	2.52	0.44
3:2D:20:ASP:OD1	3:2D:21:PHE:N	2.50	0.44
20:2Y:1:MET:HG2	20:2Y:2:ARG:H	1.82	0.44
1:1A:1569:U:H2'	1:1A:1570:G:C8	2.51	0.44
1:1A:185:A:N3	1:1A:185:A:H2'	2.32	0.44
1:1A:390:G:H2'	1:1A:391:G:C8	2.52	0.44
6:1G:43:LEU:HA	6:1G:45:GLU:OE1	2.16	0.44
1:1A:1051:C:O2'	9:1N:28:THR:HG21	2.17	0.44
9:1N:63:THR:OG1	9:1N:66:LYS:NZ	2.51	0.44
23:21:59:THR:O	23:21:91:LYS:NZ	2.40	0.44
1:2A:330:A:H2	1:2A:1210:A:O2'	2.00	0.44
2:2B:55:U:H1'	6:2G:29:TRP:HE1	1.82	0.44
13:2R:24:GLN:NE2	13:2R:36:THR:HG21	2.31	0.44
1:1A:2198:A:H2'	1:1A:2199:C:C6	2.52	0.44
1:1A:2623:U:H5'	1:1A:2623:U:H6	1.83	0.44
1:1A:2797:C:H1'	4:1E:37:ARG:NH1	2.29	0.44
4:1E:192:ASN:HB3	15:1T:3:ARG:NH2	2.32	0.44
1:1A:469:A:N6	5:1F:41:LEU:O	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1R:63:ARG:O	13:1R:67:LEU:HB2	2.17	0.44
13:1R:56:LYS:NZ	13:1R:90:ARG:O	2.51	0.44
15:1T:117:ASP:O	15:1T:121:ILE:HG13	2.17	0.44
16:1U:17:ILE:HD13	16:1U:17:ILE:HA	1.79	0.44
22:20:10:THR:HG22	22:20:11:ARG:N	2.33	0.44
11:2P:49:ARG:NH1	30:28:61:LEU:HD23	2.31	0.44
1:2A:1709:U:H2'	1:2A:1710:C:C6	2.53	0.44
1:2A:1709:U:H2'	1:2A:1710:C:H6	1.82	0.44
1:2A:652(A):A:C3'	1:2A:652(B):A:H5'	2.47	0.44
1:2A:711:G:H1	1:2A:720:C:H42	1.66	0.44
3:2D:242:ARG:HH11	3:2D:242:ARG:HG3	1.83	0.44
1:1A:1045:U:OP2	62:1A:4198:HOH:O	2.21	0.44
1:1A:1139:G:H3'	1:1A:1140:U:C5'	2.45	0.44
3:1D:108:PRO:HG2	3:1D:111:LEU:HG	1.98	0.44
11:1P:95:VAL:HG13	11:1P:125:VAL:HA	1.98	0.44
11:1P:63:PRO:HD3	30:18:27:THR:HG22	2.00	0.44
22:20:69:PHE:CE1	22:20:79:VAL:HG22	2.52	0.44
1:2A:1263:U:H1'	27:25:10:LYS:HG3	1.98	0.44
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.46	0.44
1:2A:58:G:O2'	1:2A:73:A:N1	2.47	0.44
3:2D:242:ARG:HD3	3:2D:246:PRO:HG3	1.99	0.44
6:2G:170:ARG:HH22	6:2G:180:PHE:HB2	1.82	0.44
1:2A:2378:A:H4'	14:2S:23:ARG:NH1	2.33	0.44
14:2S:9:ARG:O	14:2S:13:ARG:HG3	2.17	0.44
24:12:10:LEU:HB3	24:12:14:ARG:NH1	2.33	0.44
1:1A:1122:C:H4'	1:1A:1123:A:OP1	2.16	0.44
1:1A:1239:A:H62	1:1A:1299:A:N6	21.55	0.44
1:1A:1699:A:O2'	1:1A:1700:G:H5'	2.18	0.44
1:1A:2362:C:OP2	62:1A:4193:HOH:O	2.21	0.44
1:1A:327:U:H2'	1:1A:328:G:H8	1.82	0.44
3:1D:5:LYS:HG2	3:1D:17:THR:HG22	1.98	0.44
6:1G:136:ARG:HG3	6:1G:137:GLU:HG3	1.99	0.44
20:1Y:11:ASP:OD2	20:1Y:97:ARG:NH2	2.48	0.44
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.17	0.44
30:28:23:VAL:HG22	30:28:47:LYS:HB3	2.00	0.44
1:2A:140:G:N2	1:2A:1596:A:H4'	2.32	0.44
1:2A:1826:G:H4'	3:2D:242:ARG:CZ	2.47	0.44
1:2A:2478:A:O2'	1:2A:2536:G:N2	2.48	0.44
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.18	0.44
1:2A:624:C:H2'	1:2A:625:G:H8	2.46	0.44
11:2P:94:GLU:OE2	11:2P:124:LYS:NZ	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2283:G:OP1	22:10:18:ALA:HB1	2.17	0.44
1:1A:1117:G:H3'	1:1A:1117:G:OP1	2.17	0.44
11:1P:47:ASP:CG	11:1P:49:ARG:HH21	2.20	0.44
18:1W:66:GLU:HA	18:1W:69:LEU:HD12	1.99	0.44
27:25:25:LEU:HD23	27:25:25:LEU:HA	1.85	0.44
1:2A:307:G:N2	1:2A:310:A:O5'	2.47	0.44
2:2B:25:A:H2'	2:2B:26:A:O4'	2.17	0.44
2:2B:94:C:H2'	2:2B:95:C:C6	2.50	0.44
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.98	0.44
18:2W:82:LEU:HD22	18:2W:84:ARG:HH22	1.82	0.44
28:16:39:TYR:HB2	28:16:46:HIS:CE1	2.53	0.44
1:1A:1821:C:O2'	3:1D:209:ALA:HB2	2.16	0.44
1:1A:986:A:H2'	1:1A:987:G:O4'	2.46	0.44
16:1U:32:PHE:CZ	16:1U:36:ARG:HD2	2.52	0.44
1:2A:2166:G:H2'	1:2A:2167:U:C6	2.52	0.44
1:2A:2680:C:H1'	4:2E:187:ALA:HB1	1.99	0.44
1:2A:2793:G:H1	1:2A:2803:C:N4	2.09	0.44
5:2F:181:LEU:HD11	5:2F:186:ILE:HD11	2.00	0.44
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.83	0.44
18:2W:13:SER:O	18:2W:17:VAL:HG23	2.18	0.44
1:1A:2831:A:OP2	62:1A:4143:HOH:O	2.21	0.44
1:1A:661:G:OP1	11:1P:132:LYS:NZ	2.39	0.44
7:1H:154:PRO:HB3	7:1H:163:TYR:CE1	2.53	0.44
15:1T:102:ILE:HA	15:1T:105:LEU:HG	2.00	0.44
17:1V:80:GLN:HA	17:1V:82:ARG:NH1	2.32	0.44
1:2A:322:A:H5'	1:2A:340:A:H1'	1.99	0.44
1:2A:434:U:H2'	1:2A:435:C:C6	6.54	0.44
11:2P:96:THR:H	11:2P:99:LEU:HD21	1.82	0.44
12:2Q:39:PRO:HB3	12:2Q:99:PRO:HD3	1.99	0.44
18:2W:11:ARG:HA	18:2W:100:THR:HG22	1.99	0.44
1:1A:1320:A:N3	1:1A:1343:C:H1'	2.32	0.44
1:1A:1346:U:H4'	1:1A:1347:A:H5'	1.99	0.44
11:1P:36:LYS:HA	11:1P:41:ARG:HH12	1.83	0.44
16:1U:47:TYR:HA	16:1U:50:ARG:NH2	2.32	0.44
24:22:53:LEU:HA	24:22:53:LEU:HD23	1.84	0.44
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.52	0.44
1:2A:2096:U:H3	1:2A:2193:G:H1	1.65	0.44
1:2A:2590:A:O3'	3:2D:239:ARG:NH2	2.51	0.44
1:2A:900:A:HO2'	1:2A:901:A:P	2.40	0.44
10:2O:15:GLY:O	10:2O:47:ILE:HG12	2.18	0.44
1:1A:1068:G:C5	1:1A:1185:C:C4	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1945:U:H2'	1:1A:1946:C:C6	2.53	0.43
1:1A:1314:A:C2	1:1A:2035:A:C4	3.06	0.43
1:1A:2142:G:H2'	1:1A:2143:G:H5'	2.00	0.43
1:1A:602:G:H2'	1:1A:603:C:C6	2.53	0.43
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.53	0.43
3:1D:183:ARG:HG3	3:1D:184:LYS:N	2.32	0.43
8:1I:79:ILE:HG22	8:1I:81:VAL:HG13	2.00	0.43
12:1Q:30:GLY:HA2	12:1Q:107:ALA:HB2	1.99	0.43
1:2A:1484:G:N2	1:2A:1506:C:H1'	2.34	0.43
1:2A:1549:C:H2'	1:2A:1550:C:C6	2.53	0.43
1:2A:1647:G:H3'	1:2A:1647:G:OP2	2.17	0.43
1:2A:2126:A:C2	1:2A:2127:G:H1'	2.53	0.43
1:2A:2152:G:H8	1:2A:2152:G:O5'	2.00	0.43
1:2A:2327:A:H2'	1:2A:2328:A:H8	1.83	0.43
1:2A:2881:C:H2'	1:2A:2882:A:O4'	2.18	0.43
1:2A:588:U:H1'	5:2F:90:PHE:CG	2.53	0.43
1:2A:594:U:H2'	1:2A:595:C:C6	2.53	0.43
1:2A:774:A:N3	1:2A:774:A:H2'	2.33	0.43
1:2A:981:A:N1	1:2A:2027:G:O2'	2.46	0.43
21:2Z:121:HIS:N	21:2Z:172:ALA:HB2	2.32	0.43
24:12:25:VAL:HG13	24:12:57:ILE:HG23	1.99	0.43
1:1A:2825:C:C5'	27:15:29:THR:HG21	2.48	0.43
28:16:13:CYS:SG	28:16:47:THR:HG21	2.58	0.43
1:1A:1246:C:H2'	1:1A:1247:C:C6	2.53	0.43
1:1A:1765:U:H2'	1:1A:1766:G:O4'	2.18	0.43
1:1A:2141:A:C5	1:1A:2192:A:C2	3.06	0.43
1:1A:2622:C:H1'	62:1A:4329:HOH:O	2.18	0.43
1:1A:2705:A:H2'	1:1A:2706:G:H8	1.82	0.43
7:1H:75:ALA:O	7:1H:79:VAL:HG22	2.18	0.43
16:1U:46:ALA:O	16:1U:50:ARG:HG3	2.18	0.43
1:2A:1341:U:H3'	1:2A:1397:U:O2	2.18	0.43
2:2B:100:A:H3'	2:2B:101:G:H8	1.83	0.43
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	1.99	0.43
1:2A:443:A:N7	5:2F:45:ARG:HG2	2.33	0.43
6:2G:135:LEU:O	6:2G:154:GLY:HA3	2.18	0.43
1:1A:1071:G:C4	1:1A:1180:C:H1'	2.53	0.43
1:1A:153:C:N4	1:1A:168:G:H1	25.16	0.43
1:1A:2021:C:H4'	1:1A:2736:C:O2	2.18	0.43
1:1A:2077:C:OP1	27:15:8:LYS:NZ	2.51	0.43
1:1A:2204:G:O2'	1:1A:2205:C:O4'	2.28	0.43
4:1E:12:THR:HG22	4:1E:13:ARG:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:26:TYR:O	12:1Q:67:ARG:NH1	2.46	0.43
26:24:40:HIS:O	26:24:44:THR:HG22	2.18	0.43
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.33	0.43
1:2A:2841:C:H2'	1:2A:2842:G:C8	2.53	0.43
1:2A:513:A:H2	1:2A:582:G:H4'	1.82	0.43
3:2D:159:ALA:HB1	3:2D:198:ASN:O	2.19	0.43
9:2N:4:TYR:HB2	16:2U:101:ARG:NH1	2.33	0.43
15:2T:2:ASN:O	15:2T:6:LEU:HD13	2.18	0.43
21:2Z:40:ASP:OD2	21:2Z:42:VAL:HG22	2.18	0.43
24:12:32:LEU:O	24:12:36:ARG:HG3	2.19	0.43
1:1A:2040:G:H2'	1:1A:2041:A:O4'	2.18	0.43
1:1A:2125:C:O2	1:1A:2209:G:N2	2.52	0.43
6:1G:7:LEU:HD23	6:1G:100:TRP:HE3	1.83	0.43
1:2A:1002:G:N3	1:2A:1003:G:C8	4.02	0.43
1:2A:1184:G:H3'	1:2A:1184:G:OP1	4.81	0.43
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.33	0.43
1:2A:2726:U:O2'	1:2A:2727:G:H8	2.00	0.43
1:2A:721:C:H2'	1:2A:722:A:C8	2.54	0.43
1:2A:877:U:O2'	1:2A:900:A:N6	2.52	0.43
5:2F:120:GLU:HB2	5:2F:122:LYS:HG2	2.00	0.43
7:2H:125:VAL:HG12	7:2H:131:VAL:HG22	1.99	0.43
14:2S:28:VAL:HG11	14:2S:98:VAL:HG13	2.00	0.43
20:2Y:77:PRO:HD2	20:2Y:106:LEU:HD23	2.00	0.43
1:1A:2045:G:H4'	1:1A:2629:C:O3'	2.19	0.43
1:1A:2357:G:N3	1:1A:2393:C:H2'	2.34	0.43
1:1A:2592:U:OP1	62:1A:4199:HOH:O	2.21	0.43
2:1B:11:C:OP2	2:1B:12:C:N4	2.41	0.43
1:1A:1830:G:O2'	3:1D:181:GLU:OE2	2.26	0.43
16:1U:83:LEU:HD12	16:1U:113:ALA:HB2	2.00	0.43
25:23:6:VAL:O	25:23:34:GLU:HA	2.19	0.43
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.54	0.43
1:2A:570:G:H2'	1:2A:2030:A:C5	2.53	0.43
1:2A:27:G:HO2'	1:2A:28:A:P	2.40	0.43
1:2A:2888:C:H2'	1:2A:2889:C:C6	2.53	0.43
2:2B:50:G:OP1	14:2S:63:THR:N	2.50	0.43
6:2G:115:ARG:HB3	6:2G:136:ARG:HH21	1.84	0.43
2:2B:50:G:OP2	14:2S:62:LYS:HB2	2.19	0.43
19:2X:27:THR:HA	19:2X:79:ALA:O	2.19	0.43
1:1A:1117:G:H1'	1:1A:1135:G:H2'	1.99	0.43
1:1A:1217:G:H3'	1:1A:1218:G:H5'	2.01	0.43
1:1A:134:G:O6	62:1A:4191:HOH:O	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2327:G:H2'	1:1A:2328:C:C6	2.53	0.43
1:1A:471:C:N4	1:1A:472:G:C6	2.87	0.43
11:1P:128:HIS:NE2	11:1P:148:LEU:HD11	2.33	0.43
23:21:81:LYS:HB3	23:21:81:LYS:HE2	1.68	0.43
26:24:8:LYS:HE3	26:24:10:VAL:HG12	2.01	0.43
1:2A:1598:C:H2'	1:2A:1599:C:H6	1.83	0.43
1:2A:2111:C:OP2	1:2A:2111:C:H6	2.02	0.43
1:2A:2734:A:H2'	1:2A:2735:G:O4'	2.18	0.43
1:2A:2869:G:C2	1:2A:2870:C:C2	3.06	0.43
1:2A:479:A:N3	1:2A:481:G:H5''	2.33	0.43
6:2G:115:ARG:H	6:2G:136:ARG:NH2	2.16	0.43
14:2S:99:LYS:HE2	14:2S:103:GLU:OE2	2.19	0.43
30:18:30:ARG:HA	30:18:30:ARG:HD3	1.77	0.43
1:1A:1463:C:H2'	1:1A:1464:G:O4'	2.19	0.43
1:1A:1472:G:O2'	1:1A:1619:A:N6	2.45	0.43
1:1A:1847:G:O2'	1:1A:1848:G:OP2	2.34	0.43
1:1A:2661:U:H2'	1:1A:2662:U:C6	2.53	0.43
3:1D:242:ARG:HD3	3:1D:246:PRO:HG3	2.00	0.43
12:1Q:135:ASP:O	12:1Q:139:GLU:HG3	2.18	0.43
14:1S:15:ARG:O	14:1S:19:LYS:HG3	2.18	0.43
20:1Y:37:VAL:HG21	20:1Y:72:VAL:HG21	2.01	0.43
1:2A:1022:G:N2	1:2A:1142(A):A:C2	2.83	0.43
1:2A:1252:G:C2	1:2A:1253:A:C2	3.07	0.43
1:2A:1742:G:H2'	1:2A:1743:C:O4'	2.17	0.43
1:2A:1792:G:O2'	1:2A:1830:C:OP1	2.35	0.43
1:2A:2103:C:C2'	1:2A:2104:G:H5'	2.49	0.43
1:2A:2335:A:O2'	1:2A:2336:A:OP2	2.36	0.43
1:2A:918:A:O2'	2:2B:97:G:N2	2.47	0.43
6:2G:115:ARG:HB3	6:2G:136:ARG:NH2	2.34	0.43
7:2H:117:PRO:HG3	7:2H:123:PHE:CD2	2.54	0.43
11:2P:45:LEU:HD23	11:2P:46:LYS:O	2.19	0.43
13:2R:33:ARG:HG2	13:2R:115:GLU:HB3	2.01	0.43
31:19:32:HIS:O	31:19:34:GLN:HG3	2.19	0.43
1:1A:2311:G:H2'	1:1A:2312:G:C8	2.50	0.43
1:1A:26:G:C6	1:1A:27:G:N1	2.87	0.43
1:1A:2829:G:H2'	1:1A:2831:A:N7	2.34	0.43
1:1A:419:C:OP1	62:1A:4180:HOH:O	2.21	0.43
12:1Q:8:LYS:HG2	12:1Q:9:TYR:CE2	2.53	0.43
1:1A:582:G:H22	16:1U:49:HIS:CE1	2.36	0.43
20:1Y:7:VAL:HG21	20:1Y:72:VAL:CG1	2.49	0.43
29:27:20:ALA:N	62:27:102:HOH:O	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:150:C:H2'	1:2A:151:C:C6	2.54	0.43
1:2A:1848:A:H2'	1:2A:1849:G:H8	1.84	0.43
1:2A:2037:G:H2'	1:2A:2038:G:C8	2.54	0.43
1:2A:2275:C:H6	1:2A:2275:C:H5'	1.84	0.43
1:2A:2419:U:H2'	1:2A:2420:C:C6	2.54	0.43
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.81	0.43
1:2A:392:C:H5''	1:2A:409:C:H5''	2.01	0.43
1:2A:870:A:C2	1:2A:908:C:C2	3.07	0.43
6:2G:43:LEU:HB3	6:2G:44:GLY:H	1.73	0.43
14:2S:15:ARG:HB3	14:2S:19:LYS:HZ2	1.83	0.43
15:2T:64:ARG:HG3	15:2T:73:GLU:HG2	2.01	0.43
1:1A:1102:G:H2'	1:1A:1149:A:H61	1.83	0.43
1:1A:2698:G:OP2	62:1A:4200:HOH:O	2.21	0.43
1:1A:34:C:H5''	1:1A:35:G:OP2	2.18	0.43
1:1A:821:A:H2'	1:1A:821:A:N3	2.33	0.43
7:1H:54:ARG:NH2	7:1H:57:ASP:OD1	2.43	0.43
12:1Q:111:GLU:OE1	12:1Q:133:ARG:NH2	2.51	0.43
26:24:57:GLU:CB	26:24:58:ARG:HD2	2.49	0.43
30:28:62:LEU:HB3	30:28:65:GLU:CG	2.48	0.43
1:2A:2020:A:O2'	1:2A:2021:C:H5'	2.19	0.43
1:2A:2106:G:H2'	1:2A:2107:C:O4'	2.18	0.43
1:2A:2127:G:O6	1:2A:2161:C:N3	2.52	0.43
1:2A:2600:A:H2'	1:2A:2601:C:C6	2.53	0.43
1:2A:586:A:N1	1:2A:809:G:O2'	2.40	0.43
1:2A:903:C:H2'	1:2A:904:C:C6	2.53	0.43
2:2B:11:C:H3'	2:2B:12:C:H6	1.84	0.43
3:2D:145:VAL:HB	3:2D:155:LEU:HB2	2.01	0.43
8:2I:106:GLY:O	8:2I:107:VAL:HG23	2.19	0.43
9:2N:42:TRP:CH2	9:2N:44:PRO:HB3	2.54	0.43
1:1A:1136:U:C4	1:1A:1148:C:O2	2.72	0.43
1:1A:1402:G:N7	62:1A:4295:HOH:O	2.35	0.43
1:1A:1423:G:H2'	62:1A:5137:HOH:O	2.18	0.43
1:1A:1431:G:O2'	1:1A:1442:U:O2	2.29	0.43
1:1A:1517:G:H5''	1:1A:1518:A:OP1	2.19	0.43
1:1A:2828:G:O2'	1:1A:2829:G:H5'	2.19	0.43
1:1A:589:U:OP1	11:1P:29:LYS:NZ	2.41	0.43
1:1A:633:G:H2'	1:1A:634:C:C6	2.54	0.43
1:1A:2761:A:H5'	7:1H:4:ILE:HD12	2.00	0.43
13:1R:26:LYS:HE2	13:1R:70:LEU:O	2.19	0.43
24:22:63:VAL:HA	24:22:66:GLU:OE1	2.19	0.43
29:27:9:ARG:HH21	29:27:47:ARG:HD3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:28:30:ARG:HA	30:28:30:ARG:HD3	1.78	0.43
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.19	0.43
1:2A:2153:G:C2	1:2A:2154:G:C5	3.07	0.43
1:2A:2284:C:P	28:26:6:ARG:HG3	2.59	0.43
1:2A:2784:C:H2'	1:2A:2785:C:H6	1.82	0.43
1:2A:362:U:O2'	1:2A:363:G:H5'	2.19	0.43
2:2B:75:G:H5'	2:2B:76:G:OP2	2.19	0.43
1:2A:773:U:O2'	3:2D:48:ARG:HD3	2.19	0.43
1:1A:1115:A:O2'	1:1A:1119:A:OP1	2.21	0.42
1:1A:1195:G:H2'	1:1A:1196:C:C6	2.54	0.42
1:1A:1411:A:O2'	23:11:11:ARG:NH1	2.52	0.42
1:1A:1453:C:H6	1:1A:1453:C:O5'	2.02	0.42
1:1A:1848:G:OP1	3:1D:88:ARG:NH2	2.50	0.42
1:1A:2182:G:C6	1:1A:2183:C:N4	2.87	0.42
1:1A:2579:G:H2'	1:1A:2580:C:C6	2.54	0.42
1:1A:861:C:H2'	1:1A:862:C:H6	1.83	0.42
1:1A:346:A:OP2	5:1F:169:ASN:HB2	2.18	0.42
7:1H:40:GLU:OE1	7:1H:60:ARG:NH1	2.52	0.42
8:1I:2:LYS:HG2	8:1I:20:ASP:OD1	2.19	0.42
11:1P:95:VAL:HA	11:1P:99:LEU:HD21	2.01	0.42
10:1O:79:PHE:CD1	15:1T:72:VAL:HG22	2.54	0.42
21:1Z:45:ASP:O	21:1Z:49:ARG:HG2	2.18	0.42
1:2A:1422:G:H1'	1:2A:1495:A:H61	1.84	0.42
1:2A:902:C:H2'	1:2A:903:C:C6	2.54	0.42
2:2B:39:A:C6	2:2B:44:G:C6	3.07	0.42
9:2N:29:LYS:HD2	9:2N:140:VAL:HB	2.01	0.42
1:1A:155:C:O2	1:1A:166:G:N2	21.57	0.42
1:1A:1584:G:H2'	1:1A:1585:G:C8	2.50	0.42
1:1A:2023:A:H2'	1:1A:2024:G:C8	2.54	0.42
1:1A:2343:G:O2'	22:10:43:THR:HG22	2.19	0.42
1:1A:701:A:H2	1:1A:702:A:C2	2.37	0.42
1:1A:762:G:H2'	1:1A:763:A:O4'	2.19	0.42
1:1A:932:C:N4	1:1A:933:C:O2	2.52	0.42
8:1I:106:GLY:O	8:1I:107:VAL:HG23	2.19	0.42
12:1Q:112:GLU:HG3	12:1Q:113:GLN:N	2.34	0.42
16:1U:86:ALA:HB2	16:1U:116:ALA:HB2	2.00	0.42
1:2A:643:A:C8	28:26:44:ARG:NH1	2.87	0.42
1:2A:150:C:H2'	1:2A:151:C:H6	1.84	0.42
1:2A:1306:C:C2	1:2A:1623:G:C2	3.07	0.42
1:2A:184:C:H2'	1:2A:185:U:C6	2.54	0.42
1:2A:37:C:H4'	1:2A:451:C:OP1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:7:G:H2'	1:2A:8:A:H8	1.82	0.42
2:2B:17:C:H2'	2:2B:18:G:O4'	2.19	0.42
6:2G:101:ILE:HG22	6:2G:105:LYS:HE2	2.00	0.42
6:2G:11:TYR:HA	6:2G:15:VAL:HB	2.01	0.42
10:2O:98:VAL:HG23	10:2O:118:ALA:HA	2.01	0.42
1:1A:2407:C:O2'	23:11:30:VAL:HG22	2.20	0.42
1:1A:93:G:N2	24:12:47:ASN:OD1	2.47	0.42
62:1A:4704:HOH:O	30:18:42:ARG:HD2	2.18	0.42
1:1A:2088:C:H5''	62:1A:5169:HOH:O	2.17	0.42
1:1A:2569:G:H2'	1:1A:2570:C:C6	2.54	0.42
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	2.00	0.42
16:1U:34:LYS:HD3	16:1U:34:LYS:HA	1.69	0.42
23:21:67:ILE:N	23:21:68:PRO:HD2	2.34	0.42
26:24:5:ILE:HG13	26:24:6:HIS:CD2	2.54	0.42
1:2A:2126:A:N6	1:2A:2162:G:O2'	2.52	0.42
1:2A:2320:A:H2'	1:2A:2320:A:N3	2.33	0.42
1:2A:571:A:H1'	1:2A:573:G:H5''	2.02	0.42
1:2A:612:C:O2	1:2A:629:G:N2	50.61	0.42
1:2A:952:G:C6	1:2A:966:G:C6	3.08	0.42
4:2E:60:ASN:O	4:2E:64:LYS:HB2	2.20	0.42
14:2S:24:LEU:O	14:2S:86:ALA:N	2.50	0.42
21:2Z:145:GLU:H	21:2Z:148:ASP:HB2	1.85	0.42
24:12:1:MET:SD	24:12:56:GLN:NE2	2.92	0.42
1:1A:1576:G:H2'	1:1A:1577:C:O4'	2.19	0.42
1:1A:2078:G:N3	1:1A:2078:G:H2'	2.35	0.42
1:1A:215:G:N2	1:1A:217:A:H62	2.18	0.42
1:1A:207:A:C2	1:1A:224:U:H4'	2.53	0.42
1:1A:2482:G:O6	1:1A:2488:A:O2'	2.30	0.42
1:1A:2545:A:H2'	1:1A:2546:A:O4'	2.19	0.42
1:1A:2867:G:N2	1:1A:2870:A:OP2	2.44	0.42
1:1A:354:A:HO2'	1:1A:355:A:H8	1.66	0.42
8:1I:72:LEU:O	8:1I:74:ASN:N	2.48	0.42
1:1A:953:U:H4'	12:1Q:101:ARG:HH22	1.84	0.42
17:1V:34:GLU:HB3	17:1V:56:SER:HB2	2.02	0.42
21:1Z:152:ALA:HB1	21:1Z:163:LEU:HD21	2.00	0.42
1:2A:1484:G:H2'	1:2A:1485:G:H8	1.84	0.42
1:2A:184:C:H2'	1:2A:185:U:H6	1.84	0.42
1:2A:271(P):C:H2'	1:2A:271(Q):G:O4'	2.18	0.42
1:2A:493:G:H2'	1:2A:494:G:O4'	2.19	0.42
10:2O:80:ASP:OD2	15:2T:64:ARG:NH2	2.53	0.42
11:2P:95:VAL:HA	11:2P:99:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:12:GLN:HG3	12:2Q:72:LYS:HZ2	1.84	0.42
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	2.01	0.42
26:14:62:ARG:HD3	26:14:62:ARG:HA	1.69	0.42
1:1A:1073:A:C2	1:1A:2500:A:H5'	2.55	0.42
1:1A:1452:U:H2'	1:1A:1453:C:H6	1.85	0.42
1:1A:1469:G:H2'	1:1A:1470:G:H8	1.98	0.42
1:1A:2161:C:C2	1:1A:2175:G:N2	2.88	0.42
1:1A:2205:C:O2'	1:1A:2206:G:OP1	2.36	0.42
1:1A:559:U:H2'	1:1A:560:C:C6	2.54	0.42
4:1E:162:ALA:HB3	62:1E:407:HOH:O	2.20	0.42
5:1F:72:ARG:HE	5:1F:72:ARG:HB3	1.65	0.42
11:1P:2:LYS:HG2	11:1P:3:LEU:N	2.34	0.42
1:2A:1157:G:C6	1:2A:1158:C:C4	3.07	0.42
1:2A:1378:A:O2'	1:2A:1379:A:H5''	2.20	0.42
1:2A:2109:U:O2'	1:2A:2110:G:H5'	2.19	0.42
1:2A:2124:G:C5	1:2A:2125:G:H1'	2.55	0.42
1:2A:2307:G:OP1	1:2A:2307:G:H8	2.03	0.42
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	2.00	0.42
13:2R:98:LEU:HB2	13:2R:113:LEU:HD11	2.01	0.42
1:1A:1093:G:H2'	1:1A:1156:G:N2	2.27	0.42
1:1A:1769:G:H2'	1:1A:1770:A:H8	1.83	0.42
1:1A:1820:A:H2'	1:1A:1821:C:O4'	2.20	0.42
1:1A:2249:G:H5''	1:1A:2250:G:OP1	2.20	0.42
1:1A:2859:U:O4	15:1T:23:ARG:NH1	2.34	0.42
1:1A:753:A:OP1	3:1D:7:LYS:HE3	2.19	0.42
1:1A:2584:A:C8	4:1E:144:ARG:HD2	2.53	0.42
6:1G:73:ALA:HB3	6:1G:85:GLY:H	1.85	0.42
7:1H:3:ARG:HD2	7:1H:3:ARG:HA	1.73	0.42
11:1P:81:GLN:OE1	11:1P:107:LYS:N	2.46	0.42
25:23:18:ASP:OD1	25:23:19:GLN:HG3	2.19	0.42
26:24:48:ARG:HA	26:24:48:ARG:HD3	1.70	0.42
30:28:63:PRO:HG2	30:28:64:TYR:CE2	2.55	0.42
1:2A:1027:A:C2	1:2A:2488:A:H5'	2.54	0.42
1:2A:11:G:H2'	1:2A:12:U:H5'	2.01	0.42
1:2A:320:A:H4'	1:2A:322:A:N7	2.34	0.42
1:2A:566:U:H2'	1:2A:567:A:O4'	2.20	0.42
1:2A:1803:A:H4'	3:2D:259:THR:HG23	2.01	0.42
10:2O:7:TYR:HD1	10:2O:7:TYR:HA	1.74	0.42
16:2U:108:GLU:O	16:2U:112:ARG:HG2	2.20	0.42
20:2Y:9:LYS:HD2	20:2Y:28:LYS:O	2.20	0.42
1:1A:1004:A:H5'	1:1A:1024:G:O6	28.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:505:A:N3	1:1A:507:G:H5''	2.34	0.42
14:1S:43:GLU:OE1	14:1S:43:GLU:N	4.46	0.42
1:2A:1376:C:H2'	1:2A:1377:G:O4'	2.20	0.42
1:2A:1503:U:H2'	1:2A:1504:C:C6	2.55	0.42
1:2A:1529:G:C6	1:2A:1530:C:N4	2.88	0.42
1:2A:2140:C:H2'	1:2A:2141:G:H5'	2.01	0.42
1:2A:2317:C:N4	1:2A:2318:G:O6	2.52	0.42
1:2A:2571:C:H5''	1:2A:2572:A:H5''	2.02	0.42
1:2A:288:C:H2'	1:2A:289:A:H8	1.81	0.42
1:2A:296:C:H2'	1:2A:297:C:C6	2.55	0.42
1:2A:910:A:N1	1:2A:2277:G:H1'	2.35	0.42
2:2B:30:C:OP2	14:2S:32:LEU:HD11	2.19	0.42
3:2D:175:LEU:HD12	3:2D:185:VAL:HG21	2.02	0.42
6:2G:16:ARG:CZ	6:2G:31:VAL:HG11	2.50	0.42
17:2V:10:LYS:HB2	17:2V:10:LYS:HE2	1.91	0.42
23:11:2:SER:HB3	23:11:46:LEU:HD12	2.01	0.42
1:1A:1090:G:H5'	1:1A:1091:A:OP2	2.20	0.42
1:1A:2830:A:C5	13:1R:4:LEU:HD11	2.55	0.42
1:1A:365:G:N7	62:1A:4305:HOH:O	2.36	0.42
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	2.01	0.42
10:1O:24:VAL:HA	10:1O:39:ILE:HG22	2.01	0.42
25:23:23:LEU:HD12	25:23:50:VAL:HG11	2.00	0.42
1:2A:118:A:C8	1:2A:119:A:C8	3.08	0.42
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.84	0.42
1:2A:2168:G:H8	1:2A:2170:A:N7	2.18	0.42
1:2A:258:G:H1	1:2A:268:C:H42	33.54	0.42
1:2A:675:A:H2'	1:2A:676:A:O4'	2.47	0.42
4:2E:14:ILE:HG13	4:2E:21:VAL:HG13	2.02	0.42
5:2F:33:LEU:HD11	5:2F:112:MET:HB2	2.02	0.42
9:2N:110:GLY:O	9:2N:114:ARG:HG3	2.20	0.42
12:2Q:66:ILE:HG12	12:2Q:104:PHE:CD1	2.55	0.42
1:2A:747:U:O2'	18:2W:92:ARG:NH1	2.53	0.42
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.54	0.42
1:1A:1085:G:O2'	1:1A:1086:C:H5'	2.20	0.42
1:1A:1375:U:H5''	1:1A:1376:C:C5	2.54	0.42
1:1A:138:G:N3	62:1A:4151:HOH:O	2.52	0.42
1:1A:1566:U:H2'	1:1A:1567:G:O4'	2.20	0.42
1:1A:2168:C:H4'	1:1A:2169:G:C4	2.55	0.42
1:1A:2658:C:OP2	1:1A:2745:G:O2'	2.34	0.42
1:1A:738:C:H2'	1:1A:739:C:C6	2.74	0.42
6:1G:135:LEU:HB2	6:1G:155:MET:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:35:VAL:HG13	12:1Q:130:LYS:HB3	2.01	0.42
12:1Q:41:TRP:HB3	12:1Q:94:VAL:HG21	2.02	0.42
13:1R:45:ARG:HE	13:1R:45:ARG:HB2	1.65	0.42
23:21:3:LYS:HB3	23:21:4:VAL:H	1.63	0.42
28:26:34:LEU:HB2	28:26:51:GLU:HB2	2.02	0.42
1:2A:1447:G:H2'	1:2A:1448:G:O4'	2.20	0.42
1:2A:1388:G:H4'	1:2A:1525:G:O2'	2.20	0.42
1:2A:1548:C:H2'	1:2A:1549:C:H6	1.85	0.42
1:2A:1857:G:C6	1:2A:1858:G:N1	2.88	0.42
1:2A:2164:C:H5''	1:2A:2165:G:OP2	2.20	0.42
1:2A:533:G:H2'	1:2A:534:U:O4'	2.19	0.42
1:2A:559:G:H22	16:2U:49:HIS:CE1	2.38	0.42
1:2A:55:G:H2'	1:2A:56:A:H8	1.85	0.42
21:2Z:5:LEU:O	21:2Z:59:LEU:HA	2.20	0.42
1:1A:234:G:O5'	11:1P:73:GLY:HA2	2.19	0.42
11:1P:124:LYS:HA	11:1P:144:GLU:HB3	2.02	0.42
18:1W:68:ARG:HH11	18:1W:111:HIS:HA	1.85	0.42
25:23:46:ASN:O	25:23:50:VAL:HG22	2.20	0.42
30:28:31:HIS:ND1	30:28:32:LEU:HD13	2.35	0.42
1:2A:1179:C:H2'	1:2A:1180:C:C6	2.54	0.42
1:2A:1828:G:H8	1:2A:1828:G:OP2	2.03	0.42
1:2A:1952:A:N3	10:2O:22:ILE:HD12	2.35	0.42
1:2A:2133:G:O2'	1:2A:2157:G:N2	2.53	0.42
2:2B:42:C:O2'	6:2G:66:GLN:HG2	2.20	0.42
9:2N:42:TRP:HA	9:2N:48:MET:SD	2.60	0.42
16:2U:39:LEU:HA	16:2U:42:ALA:HB3	2.01	0.42
2:1B:1:U:HO2'	2:1B:2:C:P	2.42	0.41
4:1E:120:TRP:CD1	4:1E:155:LYS:HB3	2.55	0.41
17:1V:85:LYS:HB2	17:1V:85:LYS:HE2	1.81	0.41
1:2A:1360:A:H2'	1:2A:1361:G:C8	3.89	0.41
1:2A:1508:A:H5'	1:2A:1509(A):A:C8	2.55	0.41
1:2A:250:G:C6	1:2A:251:A:C6	3.07	0.41
1:2A:2619:C:H2'	1:2A:2620:C:H6	1.85	0.41
1:2A:2817:G:O2'	1:2A:2836:U:O2	2.29	0.41
1:2A:746:A:H2'	1:2A:2612:C:H5''	2.02	0.41
7:2H:84:SER:HA	7:2H:133:VAL:O	2.19	0.41
10:2O:2:ILE:O	10:2O:33:ALA:N	2.40	0.41
12:2Q:87:LYS:HE3	12:2Q:87:LYS:HB2	4.49	0.41
1:1A:1410:G:N7	23:11:3:LYS:HD2	2.35	0.41
1:1A:1540:A:H2	1:1A:1626:A:H1'	1.85	0.41
1:1A:1715:A:H4'	1:1A:1716:A:O5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2136:A:N6	1:1A:2141:A:H62	2.19	0.41
1:1A:2156:A:N3	1:1A:2181:G:O2'	2.38	0.41
1:1A:2444:A:H2'	1:1A:2445:A:C8	2.55	0.41
1:1A:313:A:H2'	1:1A:314:G:O4'	2.20	0.41
1:1A:402:C:H2'	1:1A:403:C:C6	2.56	0.41
1:1A:861:C:H2'	1:1A:862:C:C6	2.56	0.41
2:1B:45:A:O4'	6:1G:95:ARG:NH1	2.53	0.41
4:1E:33:VAL:HG12	4:1E:89:ASP:O	2.19	0.41
1:1A:1207:C:O2'	17:1V:8:GLY:HA2	2.20	0.41
1:2A:2390:U:P	30:28:35:GLN:HE22	2.43	0.41
1:2A:1523:U:H2'	1:2A:1524:G:C8	2.55	0.41
1:2A:1530:C:H42	1:2A:1539:G:H1	1.66	0.41
1:2A:1581:G:C6	1:2A:1582:C:C4	3.08	0.41
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.21	0.41
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.55	0.41
1:2A:2787:C:H2'	1:2A:2788:C:H6	1.85	0.41
1:2A:2886:G:H2'	1:2A:2887:U:H6	1.84	0.41
1:2A:825:C:H4'	1:2A:2428:G:N7	2.35	0.41
1:2A:93:G:H2'	1:2A:94:C:C6	2.55	0.41
7:2H:89:ILE:HD11	7:2H:131:VAL:HG23	2.02	0.41
7:2H:152:ARG:HG3	7:2H:161:GLY:HA2	2.02	0.41
16:2U:47:TYR:HA	16:2U:50:ARG:NH2	2.35	0.41
1:2A:84:A:H5''	20:2Y:8:LYS:HE3	2.01	0.41
1:1A:1091:A:O2'	1:1A:1093:G:C5	2.71	0.41
1:1A:1292:A:O2'	62:1A:4158:HOH:O	2.08	0.41
1:1A:580:U:H2'	1:1A:581:G:O4'	2.68	0.41
4:1E:194:GLY:HA3	62:1E:414:HOH:O	2.20	0.41
15:1T:31:SER:HB2	15:1T:85:LYS:HG2	2.02	0.41
21:1Z:126:VAL:HG12	21:1Z:128:VAL:HB	2.02	0.41
21:1Z:30:ASN:HA	21:1Z:89:PHE:HE1	1.85	0.41
1:2A:1362:C:H2'	1:2A:1363:C:H5''	3.97	0.41
1:2A:530:G:C5	1:2A:2022:U:H5''	2.55	0.41
1:2A:2095:C:C4	1:2A:2096:U:C4	3.09	0.41
1:2A:2136:C:HO2'	1:2A:2137:C:H6	1.65	0.41
1:2A:2182:G:H2'	1:2A:2183:C:C6	2.55	0.41
1:2A:2340:G:H2'	1:2A:2341:G:H8	1.85	0.41
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.19	0.41
4:2E:5:LEU:HD12	4:2E:51:PHE:HB2	2.02	0.41
30:18:62:LEU:HB3	30:18:65:GLU:HG3	2.01	0.41
1:1A:1099:C:N4	1:1A:1152:G:N1	2.38	0.41
1:1A:1508:G:H2'	1:1A:1509:C:H6	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2118:U:H3	1:1A:2215:G:H1	1.69	0.41
1:1A:94:G:H4'	24:12:45:SER:O	2.20	0.41
7:1H:88:LEU:HD23	7:1H:130:ARG:HG3	2.01	0.41
7:1H:8:PRO:O	7:1H:10:PRO:HD3	2.21	0.41
1:1A:604:C:OP1	16:1U:33:ARG:HG2	2.20	0.41
16:1U:58:ARG:HA	16:1U:61:TRP:CE3	2.55	0.41
19:2X:60:ARG:HH22	29:27:47:ARG:HH22	1.66	0.41
1:2A:2741:A:H2'	1:2A:2742:C:O4'	2.20	0.41
1:2A:2828:C:H2'	1:2A:2829:C:C6	2.56	0.41
1:2A:291:C:O2	1:2A:309:G:N2	48.55	0.41
7:2H:149:ARG:HA	7:2H:162:ILE:HG21	2.03	0.41
7:2H:86:GLU:OE2	7:2H:130:ARG:HD2	2.20	0.41
8:2I:93:THR:H	8:2I:96:ASP:HB2	1.86	0.41
11:2P:59:LEU:HD23	30:28:13:ARG:HD2	2.02	0.41
1:2A:2294:C:P	14:2S:89:ARG:HH22	2.43	0.41
16:2U:36:ARG:HH21	16:2U:40:PHE:HZ	1.69	0.41
22:10:70:GLN:OE1	22:10:80:HIS:NE2	2.53	0.41
26:14:16:CYS:SG	26:14:17:GLY:N	2.94	0.41
1:1A:1650:C:H5''	62:1A:4957:HOH:O	2.20	0.41
1:1A:2603:C:H2'	1:1A:2604:G:H8	1.84	0.41
4:1E:144:ARG:HB3	4:1E:145:LYS:H	1.53	0.41
5:1F:70:THR:HG23	62:1F:402:HOH:O	2.19	0.41
10:1O:2:ILE:HG23	10:1O:6:THR:HG21	2.02	0.41
17:1V:95:LEU:HD22	17:1V:97:LYS:HD2	2.03	0.41
21:1Z:9:TYR:OH	21:1Z:61:LEU:HD23	2.21	0.41
30:28:63:PRO:HG2	30:28:64:TYR:CD2	2.56	0.41
1:2A:1218:C:H42	1:2A:1231:G:H1	1.69	0.41
1:2A:1783:A:H5'	1:2A:2608:G:H4'	2.03	0.41
1:2A:2410:G:C2	1:2A:2411:A:H1'	2.56	0.41
1:2A:1669:A:O3'	1:2A:2549:G:H5''	2.21	0.41
1:2A:2623:G:OP1	1:2A:2826:A:O2'	2.27	0.41
4:2E:112:GLY:O	4:2E:159:HIS:HA	2.21	0.41
7:2H:8:PRO:O	7:2H:10:PRO:HD3	2.21	0.41
16:2U:106:PHE:O	16:2U:110:VAL:HG23	2.20	0.41
19:2X:3:THR:HG21	24:22:29:LYS:HD3	2.01	0.41
20:2Y:28:LYS:HD2	20:2Y:40:GLU:OE1	2.20	0.41
1:1A:1108:G:H1'	1:1A:1134:A:C8	2.55	0.41
1:1A:1527:G:C6	1:1A:1528:U:N3	2.88	0.41
1:1A:1897:C:H2'	1:1A:1898:A:O4'	2.20	0.41
1:1A:2366:G:H2'	1:1A:2367:C:H6	1.86	0.41
8:1I:2:LYS:HA	8:1I:19:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1001:G:OP2	12:1Q:14:ARG:NH2	2.54	0.41
14:1S:32:LEU:HA	14:1S:32:LEU:HD23	1.91	0.41
15:1T:127:ALA:C	15:1T:129:ARG:H	2.23	0.41
27:25:52:TYR:HB3	27:25:57:VAL:HG21	2.02	0.41
1:2A:2061:G:H5'	1:2A:2503:2MA:C2	2.50	0.41
1:2A:458:G:O2'	1:2A:469:G:O6	2.23	0.41
1:2A:794:G:H2'	1:2A:795:C:C6	2.55	0.41
3:2D:213:ARG:HD2	3:2D:217:ARG:O	2.21	0.41
4:2E:27:LEU:HD12	15:2T:6:LEU:CD2	2.50	0.41
7:2H:3:ARG:HG2	7:2H:6:ARG:HH11	1.85	0.41
21:2Z:36:LYS:HB2	21:2Z:36:LYS:HE3	1.89	0.41
1:1A:1550:C:H2'	1:1A:1551:C:H6	1.86	0.41
1:1A:173:C:H2'	1:1A:174:U:C6	2.55	0.41
1:1A:1846:A:OP1	1:1A:1846:A:H8	2.04	0.41
1:1A:2484:G:H2'	1:1A:2487:C:H42	1.86	0.41
1:1A:2518:U:C2	1:1A:2597:U:O4	2.74	0.41
1:1A:271:U:H1'	8:1I:50:ARG:CZ	2.51	0.41
4:1E:49:LEU:N	4:1E:79:ARG:O	2.50	0.41
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	2.02	0.41
15:1T:117:ASP:OD2	15:1T:120:ARG:NE	2.36	0.41
21:1Z:120:ILE:O	21:1Z:121:HIS:ND1	2.53	0.41
29:27:26:GLY:O	29:27:30:VAL:HG23	2.21	0.41
1:2A:1459:G:H2'	1:2A:1461:G:OP2	2.20	0.41
1:2A:1478:G:HO2'	1:2A:1558:A:H2	1.68	0.41
1:2A:680:G:H2'	1:2A:681:G:C8	2.55	0.41
1:2A:958:U:OP2	12:2Q:14:ARG:NH1	2.53	0.41
11:2P:112:LEU:HD23	11:2P:112:LEU:HA	1.86	0.41
11:2P:89:ALA:O	11:2P:121:LYS:NZ	2.40	0.41
16:2U:8:VAL:HG23	16:2U:11:ARG:NH2	2.35	0.41
1:1A:1255:A:C6	1:1A:1283:A:C5	3.08	0.41
1:1A:759:G:C6	1:1A:760:G:C5	3.09	0.41
5:1F:12:LEU:HB2	5:1F:124:LEU:HD11	2.02	0.41
1:1A:878:G:O2'	11:1P:38:GLN:HB2	2.21	0.41
14:1S:49:VAL:HG22	14:1S:73:LEU:HD12	2.02	0.41
17:1V:71:LEU:HD23	17:1V:71:LEU:HA	1.90	0.41
25:23:6:VAL:HG12	25:23:28:LEU:HD11	2.03	0.41
1:2A:137:C:O2	1:2A:226:G:N2	89.66	0.41
1:2A:1639:U:O2'	1:2A:1640:C:H5'	2.20	0.41
1:2A:2872:G:O2'	1:2A:2873:A:H5'	2.20	0.41
1:2A:768:G:C4	1:2A:769:G:C8	3.09	0.41
1:2A:799:G:C6	1:2A:800:A:C6	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:4:ILE:HG22	4:2E:96:PHE:HE2	1.86	0.41
1:2A:2685:G:P	15:2T:51:ARG:HH12	2.43	0.41
21:2Z:89:PHE:HE2	21:2Z:96:VAL:HG21	1.85	0.41
27:15:49:CYS:SG	27:15:51:TYR:HB2	2.61	0.41
1:1A:1121:C:H2'	1:1A:1122:C:H5'	2.02	0.41
1:1A:1526:G:H1'	1:1A:1605:A:OP1	2.20	0.41
1:1A:93:G:H2'	1:1A:94:G:O4'	2.21	0.41
3:1D:68:LYS:O	3:1D:69:ARG:HB2	2.21	0.41
6:1G:77:ILE:N	6:1G:82:LEU:O	2.48	0.41
8:1I:61:ARG:HA	8:1I:61:ARG:HD3	1.84	0.41
13:1R:38:VAL:HG12	13:1R:42:LYS:HE3	2.02	0.41
21:1Z:135:GLU:HG3	21:1Z:136:PHE:H	1.85	0.41
1:2A:127:A:H5''	1:2A:128:C:O4'	2.20	0.41
1:2A:1721:G:H3'	1:2A:1722:A:H5''	2.02	0.41
1:2A:189:G:H2'	1:2A:205:G:N2	2.36	0.41
1:2A:261:G:O2'	1:2A:610:G:O2'	2.28	0.41
1:2A:263:C:H2'	1:2A:264:C:O4'	2.21	0.41
2:2B:1:U:H2'	2:2B:2:C:C6	2.56	0.41
3:2D:233:HIS:HA	62:2D:405:HOH:O	2.19	0.41
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	2.03	0.41
19:2X:11:PRO:HG2	19:2X:13:LEU:HD21	2.03	0.41
24:12:63:VAL:O	24:12:67:LYS:HG2	2.21	0.41
24:12:9:GLN:HE22	24:12:56:GLN:HB3	1.86	0.41
1:1A:1143:U:O2	1:1A:1143:U:H2'	2.21	0.41
1:1A:115:G:H4'	1:1A:116:A:O5'	4.97	0.41
1:1A:1719:C:C2	1:1A:2594:G:H5'	2.56	0.41
1:1A:2219:U:H1'	1:1A:2220:A:C8	2.56	0.41
1:1A:39:C:H2'	1:1A:40:C:C6	2.55	0.41
1:1A:558:G:H8	1:1A:558:G:O5'	3.82	0.41
5:1F:108:LYS:HG2	5:1F:112:MET:HE2	2.03	0.41
5:1F:181:LEU:HA	5:1F:181:LEU:HD12	1.79	0.41
10:1O:66:LYS:HA	10:1O:79:PHE:O	2.21	0.41
11:1P:135:LEU:HA	11:1P:135:LEU:HD23	1.91	0.41
11:1P:41:ARG:HD3	11:1P:41:ARG:HH11	1.72	0.41
21:1Z:48:PHE:CE1	21:1Z:71:VAL:HG11	2.55	0.41
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.69	0.41
1:2A:1263:U:C4	1:2A:1264:G:C6	3.08	0.41
1:2A:1371:G:H2'	1:2A:1372:U:C5	2.56	0.41
1:2A:1434:A:H2'	1:2A:1435:G:O4'	2.61	0.41
1:2A:1547:C:H2'	1:2A:1548:C:C6	2.56	0.41
1:2A:2134:A:O2'	1:2A:2135:A:OP1	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2138:C:H2'	1:2A:2139:C:H5''	2.03	0.41
1:2A:2160:G:H2'	1:2A:2161:C:O4'	2.20	0.41
1:2A:2543:G:H2'	1:2A:2544:G:O4'	2.21	0.41
1:2A:2576:G:OP1	62:2A:3803:HOH:O	2.22	0.41
1:2A:2689:U:H4'	1:2A:2690:C:H5'	2.03	0.41
1:2A:506:G:O3'	1:2A:507:A:H8	2.03	0.41
1:2A:948:G:H21	1:2A:985:C:P	2.44	0.41
5:2F:176:LEU:HD23	5:2F:176:LEU:HA	1.96	0.41
5:2F:197:ASP:O	5:2F:200:GLU:HB3	2.21	0.41
5:2F:9:ILE:HG21	5:2F:125:LEU:HD13	2.02	0.41
6:2G:41:GLN:NE2	6:2G:153:ARG:HB2	2.36	0.41
15:2T:24:PRO:HA	15:2T:49:VAL:HG23	2.02	0.41
17:2V:33:VAL:O	17:2V:58:VAL:HA	2.21	0.41
25:13:31:LEU:HD23	25:13:31:LEU:HA	1.69	0.41
1:1A:1335:C:H2'	1:1A:1336:C:C6	2.56	0.41
1:1A:2255:U:H2'	1:1A:2256:U:C6	2.56	0.41
1:1A:806:G:OP1	62:1A:4202:HOH:O	2.22	0.41
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	2.02	0.41
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.36	0.41
1:2A:77:C:H5'	24:22:59:ARG:HG2	2.03	0.41
1:2A:1856:G:H2'	1:2A:1857:G:O4'	2.20	0.41
1:2A:2412:A:N6	1:2A:2413:G:C2	2.89	0.41
1:2A:321:G:OP1	5:2F:135:LYS:NZ	2.51	0.41
1:2A:817:C:O2'	1:2A:839:U:OP1	2.31	0.41
4:2E:144:ARG:HB3	4:2E:145:LYS:H	1.49	0.41
5:2F:53:THR:HG22	5:2F:56:GLU:CD	2.41	0.41
1:2A:2198:A:O5'	8:2I:33:ARG:NH2	2.54	0.41
21:2Z:70:LEU:HA	21:2Z:70:LEU:HD23	1.90	0.41
1:1A:1111:U:C5	1:1A:1112:U:C4	3.09	0.40
1:1A:2225:U:O4'	3:1D:151:LYS:HE2	2.22	0.40
1:1A:2372:A:H2'	1:1A:2373:A:O4'	2.20	0.40
1:1A:2612:A:H62	3:1D:237:GLU:HB3	1.87	0.40
1:1A:2697:G:OP2	15:1T:51:ARG:NH1	2.53	0.40
1:1A:2736:C:OP1	13:1R:3:HIS:ND1	2.34	0.40
1:1A:211:A:H5''	1:1A:448:U:OP1	2.21	0.40
1:1A:624:C:H2'	1:1A:625:G:C8	3.57	0.40
1:1A:77:A:C2	1:1A:107:G:C2	3.09	0.40
1:1A:811:A:OP1	3:1D:208:LYS:NZ	2.53	0.40
3:1D:232:PRO:HB3	3:1D:244:ARG:CZ	2.50	0.40
1:1A:2524:C:H4'	4:1E:122:PHE:CE2	2.56	0.40
7:1H:117:PRO:HG3	7:1H:123:PHE:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:104:PHE:HE2	12:1Q:125:LEU:HD11	1.85	0.40
15:1T:65:LYS:HG2	15:1T:66:VAL:N	2.36	0.40
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.56	0.40
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.56	0.40
1:2A:1003:G:N2	1:2A:1153:C:C2	2.89	0.40
1:2A:1022:G:OP1	1:2A:1022:G:H4'	3.45	0.40
1:2A:1908:C:H2'	1:2A:1909:C:H6	1.85	0.40
1:2A:923:C:H2'	1:2A:924:C:C6	2.56	0.40
2:2B:74:U:O5'	2:2B:74:U:H6	2.03	0.40
6:2G:106:LEU:O	6:2G:110:ALA:HB3	2.20	0.40
10:2O:53:LYS:N	10:2O:56:ASP:OD2	2.35	0.40
11:2P:101:VAL:HG23	11:2P:106:LEU:O	2.20	0.40
11:2P:127:ALA:HB3	11:2P:130:PHE:CE2	2.56	0.40
22:10:27:GLU:HB2	22:10:69:PHE:HD2	1.86	0.40
30:18:26:LYS:HB2	30:18:44:LYS:O	2.21	0.40
1:1A:121:G:H2'	1:1A:122:G:C8	2.56	0.40
1:1A:1857:G:H4'	3:1D:242:ARG:NH2	2.37	0.40
1:1A:1859:G:H4'	1:1A:1860:A:OP1	2.22	0.40
1:1A:2141:A:O2'	1:1A:2142:G:H5'	2.22	0.40
6:1G:131:TYR:HE2	6:1G:133:LEU:HD23	1.86	0.40
18:1W:7:ALA:HB2	18:1W:50:VAL:HG22	2.04	0.40
21:1Z:89:PHE:HE2	21:1Z:96:VAL:HG21	1.85	0.40
1:2A:1314:C:OP1	62:2A:3778:HOH:O	2.22	0.40
1:2A:1579:A:C6	1:2A:1580:A:C6	3.09	0.40
1:2A:854:G:H2'	1:2A:855:G:C8	2.55	0.40
1:2A:901:A:H2'	1:2A:902:C:C6	2.56	0.40
11:2P:93:GLY:N	11:2P:123:LEU:HD22	2.33	0.40
11:2P:82:GLY:HA3	11:2P:115:LEU:HD11	2.03	0.40
12:2Q:33:GLY:O	12:2Q:118:LEU:HD13	2.20	0.40
1:1A:1067:A:H61	1:1A:1188:A:H61	1.69	0.40
1:1A:1400:A:O3'	3:1D:38:LYS:HE3	2.21	0.40
1:1A:2178:G:H8	1:1A:2178:G:O5'	2.04	0.40
2:1B:12:C:O5'	2:1B:12:C:H6	2.04	0.40
2:1B:87:G:N2	2:1B:89:G:H3'	2.35	0.40
5:1F:150:GLY:HA2	5:1F:172:TRP:CD2	2.56	0.40
6:1G:43:LEU:HB3	6:1G:44:GLY:H	1.70	0.40
7:1H:105:LEU:HB3	7:1H:107:VAL:HG13	2.03	0.40
1:1A:1201:A:OP1	16:1U:55:ARG:HD2	2.21	0.40
19:1X:47:PHE:O	19:1X:49:VAL:HG13	2.21	0.40
1:2A:1354:A:H3'	1:2A:1355:G:H8	1.87	0.40
1:2A:2129:C:N3	1:2A:2159:G:N2	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2531:A:H61	1:2A:2662:A:N6	2.15	0.40
1:2A:49:A:H4'	1:2A:50:U:H5'	2.04	0.40
1:2A:652(A):A:H2'	1:2A:652(A):A:N3	2.35	0.40
1:2A:801:G:OP2	5:2F:55:GLY:HA2	2.21	0.40
2:2B:32:C:C2	2:2B:51:G:C2	3.09	0.40
13:2R:63:ARG:HG2	13:2R:80:PHE:CE2	2.57	0.40
14:2S:26:LEU:HD22	14:2S:87:PHE:CD1	2.55	0.40
27:15:8:LYS:HA	27:15:8:LYS:HD2	1.95	0.40
1:1A:107:G:H2'	1:1A:108:G:O4'	2.21	0.40
1:1A:1216:G:C2	1:1A:1217:G:H1'	2.56	0.40
1:1A:1465:A:C8	1:1A:1467:G:C6	3.10	0.40
1:1A:1845:G:C6	1:1A:1846:A:C6	3.09	0.40
1:1A:2054:G:H4'	62:1A:5358:HOH:O	2.21	0.40
1:1A:2291:G:O6	22:10:14:ARG:HG3	2.21	0.40
1:1A:839:G:H5''	1:1A:840:A:H5'	2.03	0.40
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	2.04	0.40
3:1D:5:LYS:HB3	3:1D:5:LYS:HE3	1.87	0.40
20:1Y:13:VAL:HB	20:1Y:72:VAL:HG13	2.03	0.40
21:1Z:105:VAL:O	21:1Z:141:VAL:HG22	2.22	0.40
1:2A:2466:C:OP1	31:29:4:ARG:HB2	2.21	0.40
1:2A:1011:G:C2	1:2A:1013:C:C2	3.10	0.40
1:2A:2032:G:H1'	4:2E:145:LYS:HD3	2.02	0.40
1:2A:2070:G:H2'	1:2A:2071:A:O4'	2.22	0.40
1:2A:298:G:H5''	1:2A:299:A:OP1	2.21	0.40
1:2A:827:U:C2	1:2A:874:G:N2	70.51	0.40
2:2B:119:G:C6	2:2B:120:A:C6	3.10	0.40
6:2G:96:ARG:H	6:2G:99:MET:HE2	1.86	0.40
7:2H:98:LEU:HB2	7:2H:125:VAL:HG22	2.03	0.40
10:2O:76:ALA:O	15:2T:74:ARG:HG3	2.22	0.40
29:17:47:ARG:HE	29:17:47:ARG:HB3	1.43	0.40
1:1A:1102:G:H21	1:1A:1149:A:H62	1.68	0.40
1:1A:2094:G:H2'	1:1A:2095:C:O4'	2.21	0.40
8:1I:72:LEU:C	8:1I:74:ASN:N	2.72	0.40
10:1O:70:LYS:HE2	10:1O:70:LYS:HB3	1.96	0.40
11:1P:93:GLY:H	11:1P:123:LEU:HD22	1.87	0.40
12:1Q:56:ARG:HD2	12:1Q:56:ARG:HA	1.92	0.40
15:1T:28:VAL:HG13	15:1T:86:ILE:HG23	2.04	0.40
15:1T:26:ASP:O	15:1T:49:VAL:HG22	2.21	0.40
16:1U:33:ARG:H	16:1U:33:ARG:HG2	1.57	0.40
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.56	0.40
25:23:8:LEU:HA	25:23:8:LEU:HD23	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1011:G:H1'	1:2A:1013:C:O4'	2.22	0.40
1:2A:1262:A:H2	27:25:10:LYS:HD2	1.86	0.40
1:2A:176:G:O2'	1:2A:177:G:H5'	2.22	0.40
1:2A:1813:G:H1'	3:2D:50:THR:OG1	2.21	0.40
1:2A:2315:G:H2'	1:2A:2316:C:H6	1.84	0.40
1:2A:2756:U:H4'	1:2A:2757:A:OP1	2.20	0.40
1:2A:321:G:O2'	1:2A:340:A:N3	2.50	0.40
1:2A:391:G:C2	1:2A:411:G:C5	3.09	0.40
1:2A:709:U:H2'	1:2A:710:G:H8	1.85	0.40
1:2A:836:G:C5	1:2A:837:C:C4	3.09	0.40
1:2A:857:C:H1'	22:20:26:TYR:CE1	2.56	0.40
2:2B:3:C:H2'	2:2B:4:C:H6	1.87	0.40
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	2.03	0.40
14:2S:106:ARG:NE	14:2S:112:PHE:OXT	2.51	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%)	258 (94%)	13 (5%)	2 (1%)	22	43
3	2D	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	34	57
4	1E	202/206 (98%)	190 (94%)	10 (5%)	2 (1%)	15	32
4	2E	202/206 (98%)	191 (95%)	9 (4%)	2 (1%)	15	32
5	1F	201/210 (96%)	198 (98%)	2 (1%)	1 (0%)	29	52
5	2F	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	15	32
6	1G	179/182 (98%)	164 (92%)	13 (7%)	2 (1%)	14	30
6	2G	179/182 (98%)	172 (96%)	7 (4%)	0	100	100
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	25	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	2H	172/180 (96%)	162 (94%)	7 (4%)	3 (2%)	9	18
8	1I	144/148 (97%)	126 (88%)	13 (9%)	5 (4%)	3	5
8	2I	144/148 (97%)	126 (88%)	16 (11%)	2 (1%)	11	22
9	1N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
9	2N	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	22	43
11	2P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	22	43
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
12	2Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
13	1R	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
13	2R	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
15	1T	129/146 (88%)	125 (97%)	2 (2%)	2 (2%)	9	19
15	2T	129/146 (88%)	122 (95%)	6 (5%)	1 (1%)	19	39
16	1U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
16	2U	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
17	1V	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
17	2V	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
19	2X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	14	30
20	1Y	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
20	2Y	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
21	1Z	148/206 (72%)	131 (88%)	14 (10%)	3 (2%)	7	14
21	2Z	156/206 (76%)	136 (87%)	17 (11%)	3 (2%)	8	15
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	79 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	30
23	21	95/98 (97%)	94 (99%)	0	1 (1%)	14	30
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	68 (100%)	0	0	100	100
25	13	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	52 (78%)	11 (16%)	4 (6%)	1	1
26	24	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	1
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%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	203 (89%)	21 (9%)	5 (2%)	6	12
33	2b	229/256 (90%)	202 (88%)	21 (9%)	6 (3%)	5	9
34	1c	204/239 (85%)	196 (96%)	7 (3%)	1 (0%)	29	52
34	2c	204/239 (85%)	192 (94%)	11 (5%)	1 (0%)	29	52
35	1d	206/209 (99%)	196 (95%)	8 (4%)	2 (1%)	15	32
35	2d	206/209 (99%)	195 (95%)	8 (4%)	3 (2%)	10	21
36	1e	146/162 (90%)	138 (94%)	6 (4%)	2 (1%)	11	22
36	2e	146/162 (90%)	138 (94%)	6 (4%)	2 (1%)	11	22
37	1f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	2f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
38	1g	153/156 (98%)	140 (92%)	11 (7%)	2 (1%)	12	24
38	2g	153/156 (98%)	143 (94%)	7 (5%)	3 (2%)	7	14
39	1h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	2h	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
40	1i	125/128 (98%)	111 (89%)	12 (10%)	2 (2%)	9	19
40	2i	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	19	39
41	1j	95/105 (90%)	86 (90%)	8 (8%)	1 (1%)	14	30
41	2j	94/105 (90%)	81 (86%)	12 (13%)	1 (1%)	14	30
42	1k	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	8	16
42	2k	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	8	16
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	110 (92%)	9 (8%)	0	100	100
44	1m	121/126 (96%)	112 (93%)	9 (7%)	0	100	100
44	2m	120/126 (95%)	110 (92%)	10 (8%)	0	100	100
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	56 (97%)	0	2 (3%)	3	5
46	1o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
46	2o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
47	1p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	12	24
47	2p	80/88 (91%)	75 (94%)	4 (5%)	1 (1%)	12	24
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
48	2q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
49	1r	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
50	2s	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
51	1t	94/106 (89%)	86 (92%)	7 (7%)	1 (1%)	14	30
51	2t	94/106 (89%)	86 (92%)	7 (7%)	1 (1%)	14	30
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
All	All	11370/12128 (94%)	10678 (94%)	605 (5%)	87 (1%)	19	39

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA

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Mol	Chain	Res	Type
8	1I	117	GLU
21	1Z	152	ALA
23	11	3	LYS
26	14	55	ARG
33	1b	22	LYS
35	1d	168	ARG
40	1i	54	ASP
5	2F	130	ALA
8	2I	107	VAL
21	2Z	152	ALA
26	24	56	VAL
33	2b	10	LEU
33	2b	22	LYS
35	2d	168	ARG
40	2i	54	ASP
4	1E	71	GLY
26	14	65	ASP
36	1e	85	GLY
41	1j	29	ARG
42	1k	49	GLY
4	2E	71	GLY
7	2H	47	GLU
23	21	3	LYS
26	24	65	ASP
33	2b	123	ALA
35	2d	173	TRP
36	2e	85	GLY
38	2g	52	GLU
3	1D	3	VAL
8	1I	42	SER
15	1T	127	ALA
26	14	64	GLY
33	1b	10	LEU
33	1b	17	PHE
40	1i	107	ARG
47	1p	53	VAL
11	2P	29	LYS
21	2Z	2	GLU
26	24	45	GLY
26	24	64	GLY
35	2d	3	ARG
36	2e	27	ARG

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Mol	Chain	Res	Type
42	2k	49	GLY
47	2p	53	VAL
3	1D	275	LYS
4	1E	52	LEU
6	1G	51	ARG
8	1I	105	HIS
8	1I	107	VAL
33	1b	126	GLU
35	1d	5	ILE
4	2E	52	LEU
19	2X	94	GLY
33	2b	124	SER
45	2n	3	ARG
15	1T	128	GLU
21	1Z	2	GLU
26	14	57	GLU
33	1b	20	GLU
34	1c	66	VAL
38	1g	81	GLY
3	2D	3	VAL
7	2H	92	ILE
21	2Z	172	ALA
33	2b	128	GLU
34	2c	66	VAL
38	2g	54	THR
51	2t	100	ILE
6	1G	42	GLY
8	1I	73	GLU
11	1P	29	LYS
38	1g	55	GLY
5	2F	89	VAL
8	2I	85	GLU
33	2b	20	GLU
41	2j	55	LYS
7	1H	92	ILE
36	1e	69	VAL
42	1k	105	VAL
51	1t	100	ILE
38	2g	81	GLY
21	1Z	134	PRO
45	2n	14	PRO
15	2T	37	GLY

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Mol	Chain	Res	Type
7	2H	126	PRO
42	2k	105	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	210 (98%)	5 (2%)	50	75
3	2D	215/218 (99%)	210 (98%)	5 (2%)	50	75
4	1E	164/166 (99%)	158 (96%)	6 (4%)	34	60
4	2E	164/166 (99%)	159 (97%)	5 (3%)	41	67
5	1F	160/166 (96%)	150 (94%)	10 (6%)	18	36
5	2F	159/166 (96%)	153 (96%)	6 (4%)	33	59
6	1G	144/156 (92%)	139 (96%)	5 (4%)	36	62
6	2G	143/156 (92%)	141 (99%)	2 (1%)	67	85
7	1H	144/148 (97%)	142 (99%)	2 (1%)	67	85
7	2H	144/148 (97%)	143 (99%)	1 (1%)	84	94
8	1I	113/124 (91%)	112 (99%)	1 (1%)	78	91
8	2I	105/124 (85%)	102 (97%)	3 (3%)	42	68
9	1N	118/119 (99%)	113 (96%)	5 (4%)	30	55
9	2N	118/119 (99%)	115 (98%)	3 (2%)	47	73
10	1O	100/100 (100%)	96 (96%)	4 (4%)	31	57
10	2O	100/100 (100%)	99 (99%)	1 (1%)	76	90
11	1P	115/116 (99%)	113 (98%)	2 (2%)	60	81
11	2P	115/116 (99%)	110 (96%)	5 (4%)	29	54
12	1Q	111/111 (100%)	106 (96%)	5 (4%)	27	52
12	2Q	111/111 (100%)	110 (99%)	1 (1%)	78	91
13	1R	101/101 (100%)	93 (92%)	8 (8%)	12	24
13	2R	101/101 (100%)	97 (96%)	4 (4%)	31	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	1S	86/88 (98%)	85 (99%)	1 (1%)	71	87
14	2S	85/88 (97%)	85 (100%)	0	100	100
15	1T	115/127 (91%)	114 (99%)	1 (1%)	78	91
15	2T	113/127 (89%)	112 (99%)	1 (1%)	78	91
16	1U	93/94 (99%)	87 (94%)	6 (6%)	17	34
16	2U	93/94 (99%)	92 (99%)	1 (1%)	73	88
17	1V	80/82 (98%)	76 (95%)	4 (5%)	24	47
17	2V	80/82 (98%)	79 (99%)	1 (1%)	69	86
18	1W	90/92 (98%)	85 (94%)	5 (6%)	21	42
18	2W	90/92 (98%)	90 (100%)	0	100	100
19	1X	77/78 (99%)	74 (96%)	3 (4%)	32	58
19	2X	77/78 (99%)	77 (100%)	0	100	100
20	1Y	85/91 (93%)	84 (99%)	1 (1%)	71	87
20	2Y	85/91 (93%)	84 (99%)	1 (1%)	71	87
21	1Z	135/179 (75%)	134 (99%)	1 (1%)	84	94
21	2Z	137/179 (76%)	137 (100%)	0	100	100
22	10	65/67 (97%)	64 (98%)	1 (2%)	65	83
22	20	65/67 (97%)	65 (100%)	0	100	100
23	11	80/83 (96%)	77 (96%)	3 (4%)	33	59
23	21	80/83 (96%)	78 (98%)	2 (2%)	47	73
24	12	65/67 (97%)	65 (100%)	0	100	100
24	22	65/67 (97%)	65 (100%)	0	100	100
25	13	51/52 (98%)	48 (94%)	3 (6%)	19	39
25	23	50/52 (96%)	48 (96%)	2 (4%)	31	57
26	14	59/63 (94%)	56 (95%)	3 (5%)	24	46
26	24	53/63 (84%)	51 (96%)	2 (4%)	33	59
27	15	50/52 (96%)	49 (98%)	1 (2%)	55	78
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	39
28	16	51/52 (98%)	51 (100%)	0	100	100
28	26	50/52 (96%)	50 (100%)	0	100	100
29	17	41/42 (98%)	39 (95%)	2 (5%)	25	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	27	41/42 (98%)	39 (95%)	2 (5%)	25	48
30	18	54/55 (98%)	51 (94%)	3 (6%)	21	42
30	28	54/55 (98%)	54 (100%)	0	100	100
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	68
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	188 (98%)	4 (2%)	53	77
33	2b	187/220 (85%)	187 (100%)	0	100	100
34	1c	142/188 (76%)	141 (99%)	1 (1%)	84	94
34	2c	140/188 (74%)	138 (99%)	2 (1%)	67	85
35	1d	169/181 (93%)	167 (99%)	2 (1%)	71	87
35	2d	173/181 (96%)	172 (99%)	1 (1%)	86	95
36	1e	113/123 (92%)	109 (96%)	4 (4%)	36	62
36	2e	114/123 (93%)	112 (98%)	2 (2%)	59	80
37	1f	84/90 (93%)	83 (99%)	1 (1%)	71	87
37	2f	85/90 (94%)	84 (99%)	1 (1%)	71	87
38	1g	119/127 (94%)	118 (99%)	1 (1%)	81	92
38	2g	120/127 (94%)	118 (98%)	2 (2%)	60	81
39	1h	114/119 (96%)	113 (99%)	1 (1%)	78	91
39	2h	114/119 (96%)	113 (99%)	1 (1%)	78	91
40	1i	90/99 (91%)	86 (96%)	4 (4%)	28	53
40	2i	89/99 (90%)	84 (94%)	5 (6%)	21	42
41	1j	66/92 (72%)	63 (96%)	3 (4%)	27	52
41	2j	69/92 (75%)	67 (97%)	2 (3%)	42	68
42	1k	82/99 (83%)	81 (99%)	1 (1%)	71	87
42	2k	83/99 (84%)	81 (98%)	2 (2%)	49	74
43	1l	96/108 (89%)	94 (98%)	2 (2%)	53	77
43	2l	96/108 (89%)	95 (99%)	1 (1%)	76	90
44	1m	93/101 (92%)	93 (100%)	0	100	100
44	2m	92/101 (91%)	92 (100%)	0	100	100
45	1n	49/50 (98%)	48 (98%)	1 (2%)	55	78
45	2n	49/50 (98%)	48 (98%)	1 (2%)	55	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	1o	78/80 (98%)	78 (100%)	0	100	100
46	2o	78/80 (98%)	77 (99%)	1 (1%)	69	86
47	1p	69/74 (93%)	67 (97%)	2 (3%)	42	68
47	2p	68/74 (92%)	66 (97%)	2 (3%)	42	68
48	1q	94/97 (97%)	94 (100%)	0	100	100
48	2q	94/97 (97%)	94 (100%)	0	100	100
49	1r	59/77 (77%)	59 (100%)	0	100	100
49	2r	59/77 (77%)	59 (100%)	0	100	100
50	1s	69/80 (86%)	68 (99%)	1 (1%)	67	85
50	2s	67/80 (84%)	65 (97%)	2 (3%)	41	67
51	1t	70/82 (85%)	70 (100%)	0	100	100
51	2t	70/82 (85%)	69 (99%)	1 (1%)	67	85
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9304/10064 (92%)	9107 (98%)	197 (2%)	53	77

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	111	LEU
3	1D	176	ARG
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
4	1E	12	THR
4	1E	21	VAL
4	1E	73	GLU
4	1E	113	PHE
4	1E	116	VAL
4	1E	144	ARG
5	1F	46	ARG
5	1F	57	VAL
5	1F	70	THR
5	1F	88	VAL
5	1F	106	ARG
5	1F	132	VAL
5	1F	170	LEU

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Mol	Chain	Res	Type
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	5	VAL
6	1G	7	LEU
6	1G	43	LEU
6	1G	126	ASP
6	1G	139	LEU
7	1H	69	ARG
7	1H	71	LEU
8	1I	92	VAL
9	1N	1	MET
9	1N	14	VAL
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
10	1O	7	TYR
10	1O	24	VAL
10	1O	28	SER
10	1O	39	ILE
11	1P	95	VAL
11	1P	112	LEU
12	1Q	8	LYS
12	1Q	35	VAL
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	111	GLU
13	1R	6	SER
13	1R	18	LEU
13	1R	28	LEU
13	1R	29	LEU
13	1R	36	THR
13	1R	44	LEU
13	1R	96	ARG
13	1R	111	LEU
14	1S	27	SER
15	1T	59	THR
16	1U	8	VAL
16	1U	31	SER
16	1U	59	ARG
16	1U	60	LEU
16	1U	74	LEU

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Mol	Chain	Res	Type
16	1U	77	SER
17	1V	39	LEU
17	1V	61	VAL
17	1V	72	VAL
17	1V	73	SER
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	51	LEU
18	1W	107	LEU
19	1X	35	THR
19	1X	76	ARG
19	1X	95	LEU
20	1Y	72	VAL
21	1Z	5	LEU
22	10	39	ARG
23	11	30	VAL
23	11	59	THR
23	11	85	LEU
25	13	8	LEU
25	13	54	VAL
25	13	60	GLU
26	14	1	MET
26	14	49	PHE
26	14	56	VAL
27	15	29	THR
29	17	34	ARG
29	17	47	ARG
30	18	14	VAL
30	18	30	ARG
30	18	32	LEU
31	19	1	MET
33	1b	127	ILE
33	1b	142	LEU
33	1b	221	LEU
33	1b	229	VAL
34	1c	3	ASN
35	1d	135	LEU
35	1d	193	ASP
36	1e	5	ASP
36	1e	20	GLN
36	1e	34	VAL

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Mol	Chain	Res	Type
36	1e	51	VAL
37	1f	75	LEU
38	1g	104	LEU
39	1h	112	LEU
40	1i	50	LEU
40	1i	53	VAL
40	1i	103	THR
40	1i	128	ARG
41	1j	38	ILE
41	1j	67	THR
41	1j	92	THR
42	1k	41	THR
43	1l	83	VAL
43	1l	84	LEU
45	1n	33	VAL
47	1p	20	VAL
47	1p	67	THR
50	1s	78	ARG
3	2D	94	LEU
3	2D	173	VAL
3	2D	176	ARG
3	2D	229	VAL
3	2D	242	ARG
4	2E	34	VAL
4	2E	73	GLU
4	2E	116	VAL
4	2E	144	ARG
4	2E	181	LEU
5	2F	57	VAL
5	2F	70	THR
5	2F	74	ARG
5	2F	132	VAL
5	2F	158	THR
5	2F	183	VAL
6	2G	5	VAL
6	2G	7	LEU
7	2H	107	VAL
8	2I	92	VAL
8	2I	127	VAL
8	2I	144	VAL
9	2N	14	VAL
9	2N	58	ASP

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Mol	Chain	Res	Type
9	2N	120	LEU
10	2O	24	VAL
11	2P	45	LEU
11	2P	56	SER
11	2P	95	VAL
11	2P	106	LEU
11	2P	112	LEU
12	2Q	109	VAL
13	2R	28	LEU
13	2R	29	LEU
13	2R	65	LEU
13	2R	111	LEU
15	2T	28	VAL
16	2U	74	LEU
17	2V	61	VAL
20	2Y	72	VAL
23	21	4	VAL
23	21	85	LEU
25	23	8	LEU
25	23	54	VAL
26	24	26	SER
26	24	49	PHE
27	25	6	VAL
27	25	19	ARG
27	25	29	THR
29	27	34	ARG
29	27	43	THR
34	2c	3	ASN
34	2c	70	VAL
35	2d	135	LEU
36	2e	20	GLN
36	2e	51	VAL
37	2f	75	LEU
38	2g	75	VAL
38	2g	96	GLN
39	2h	127	LEU
40	2i	50	LEU
40	2i	53	VAL
40	2i	102	LEU
40	2i	124	GLN
40	2i	128	ARG
41	2j	67	THR

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Mol	Chain	Res	Type
41	2j	74	ILE
42	2k	48	ILE
42	2k	116	HIS
43	2l	122	THR
45	2n	33	VAL
46	2o	21	ASP
47	2p	20	VAL
47	2p	67	THR
50	2s	41	VAL
50	2s	78	ARG
51	2t	56	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
5	1F	8	GLN
6	1G	41	GLN
6	1G	79	ASN
12	1Q	12	GLN
12	1Q	123	HIS
13	1R	24	GLN
15	1T	58	ASN
19	1X	31	HIS
21	1Z	132	ASN
21	1Z	151	HIS
22	10	50	ASN
25	13	32	GLN
33	1b	40	HIS
33	1b	212	GLN
34	1c	6	HIS
34	1c	136	GLN
34	1c	139	GLN
34	1c	162	GLN
34	1c	176	HIS
34	1c	181	ASN
35	1d	161	ASN
36	1e	20	GLN
37	1f	100	ASN
38	1g	28	ASN
38	1g	64	GLN
38	1g	68	ASN

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Mol	Chain	Res	Type
38	1g	86	GLN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	58	HIS
40	1i	73	GLN
40	1i	124	GLN
41	1j	56	HIS
43	1l	99	HIS
48	1q	26	GLN
50	1s	23	ASN
50	1s	69	HIS
50	1s	83	HIS
3	2D	87	ASN
3	2D	116	GLN
5	2F	75	HIS
12	2Q	12	GLN
12	2Q	57	HIS
12	2Q	123	HIS
13	2R	24	GLN
16	2U	94	ASN
19	2X	31	HIS
21	2Z	32	HIS
21	2Z	151	HIS
24	22	65	ASN
33	2b	40	HIS
33	2b	78	GLN
33	2b	95	GLN
33	2b	212	GLN
34	2c	6	HIS
34	2c	102	ASN
34	2c	162	GLN
35	2d	77	ASN
35	2d	125	HIS
36	2e	20	GLN
37	2f	64	GLN
37	2f	73	ASN
37	2f	100	ASN
40	2i	3	GLN
40	2i	58	HIS
40	2i	73	GLN
40	2i	89	ASN

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Mol	Chain	Res	Type
40	2i	124	GLN
41	2j	56	HIS
43	2l	99	HIS
46	2o	62	GLN
48	2q	26	GLN
50	2s	23	ASN
50	2s	47	HIS
50	2s	69	HIS
50	2s	83	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2859/2915 (98%)	431 (15%)	33 (1%)
1	2A	2788/2915 (95%)	483 (17%)	26 (0%)
2	1B	120/121 (99%)	9 (7%)	1 (0%)
2	2B	118/121 (97%)	28 (23%)	0
32	1a	1494/1521 (98%)	248 (16%)	0
32	2a	1498/1521 (98%)	251 (16%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	2 (16%)	0
54	1w	70/76 (92%)	16 (22%)	0
54	2w	67/76 (88%)	20 (29%)	0
55	1x	75/77 (97%)	10 (13%)	0
55	2x	75/77 (97%)	8 (10%)	0
56	1y	71/76 (93%)	21 (29%)	0
56	2y	69/76 (90%)	20 (28%)	0
All	All	9328/9620 (96%)	1549 (16%)	60 (0%)

All (1549) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	36	G
1	1A	45	C
1	1A	57	G
1	1A	63	A
1	1A	70	A
1	1A	73	A
1	1A	74	G

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Mol	Chain	Res	Type
1	1A	83	A
1	1A	89	U
1	1A	90	A
1	1A	92	C
1	1A	94	G
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	138	G
1	1A	170	A
1	1A	185	A
1	1A	188	A
1	1A	194	G
1	1A	204	G
1	1A	205	A
1	1A	211	A
1	1A	218	A
1	1A	219	U
1	1A	222	A
1	1A	237	G
1	1A	255	G
1	1A	258	U
1	1A	271	U
1	1A	272	U
1	1A	273	G
1	1A	275	C
1	1A	279	G
1	1A	288	U
1	1A	289	G
1	1A	299	G
1	1A	303	C
1	1A	305	G
1	1A	307	A
1	1A	326	C
1	1A	335	A
1	1A	348	A
1	1A	353	G
1	1A	354	A
1	1A	376	G
1	1A	387	G
1	1A	389	G
1	1A	399	G

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Mol	Chain	Res	Type
1	1A	407	U
1	1A	413	G
1	1A	423	G
1	1A	432	U
1	1A	438	G
1	1A	439	A
1	1A	445	G
1	1A	455	A
1	1A	470	C
1	1A	474	U
1	1A	482	C
1	1A	483	A
1	1A	505	A
1	1A	507	G
1	1A	516	G
1	1A	529	U
1	1A	530	A
1	1A	534	C
1	1A	537	G
1	1A	553	A
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	609	A
1	1A	615	G
1	1A	617	U
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	633	G
1	1A	636	G
1	1A	639	G
1	1A	641	G
1	1A	642	G
1	1A	652	A
1	1A	662	A

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Mol	Chain	Res	Type
1	1A	670	C
1	1A	671	A
1	1A	697	C
1	1A	699	C
1	1A	733	G
1	1A	777	C
1	1A	787	U
1	1A	793	A
1	1A	794	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
1	1A	866	A
1	1A	874	U
1	1A	875	U
1	1A	877	G
1	1A	906	G
1	1A	913	A
1	1A	924	U
1	1A	926	G
1	1A	927	G
1	1A	931	C
1	1A	932	C
1	1A	933	C
1	1A	934	A
1	1A	935	C
1	1A	937	A
1	1A	941	U
1	1A	942	A
1	1A	943	C
1	1A	944	C
1	1A	945	A
1	1A	956	A
1	1A	972	A

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Mol	Chain	Res	Type
1	1A	977	G
1	1A	986	A
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	1029	A
1	1A	1042	A
1	1A	1058	U
1	1A	1059	C
1	1A	1068	G
1	1A	1071	G
1	1A	1072	U
1	1A	1079	U
1	1A	1084	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	1109	G
1	1A	1114	G
1	1A	1117	G
1	1A	1118	C
1	1A	1119	A
1	1A	1121	C
1	1A	1123	A
1	1A	1124	U
1	1A	1125	C
1	1A	1126	C
1	1A	1134	A
1	1A	1136	U
1	1A	1137	G
1	1A	1140	U
1	1A	1142	A
1	1A	1145	G
1	1A	1147	U

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Mol	Chain	Res	Type
1	1A	1148	C
1	1A	1155	C
1	1A	1156	G
1	1A	1157	A
1	1A	1158	G
1	1A	1176	U
1	1A	1180	C
1	1A	1181	G
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1222	A
1	1A	1223	C
1	1A	1255	A
1	1A	1256	U
1	1A	1265	A
1	1A	1277	G
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1319	U
1	1A	1322	A
1	1A	1346	U
1	1A	1347	A
1	1A	1364	C
1	1A	1366	C
1	1A	1375	U
1	1A	1380	G
1	1A	1391	C
1	1A	1394	G
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1416	C
1	1A	1430	A
1	1A	1431	G
1	1A	1462	G
1	1A	1463	C

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Mol	Chain	Res	Type
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1483	C
1	1A	1491	A
1	1A	1497	G
1	1A	1502	G
1	1A	1506	G
1	1A	1513	G
1	1A	1514	C
1	1A	1518	A
1	1A	1529	G
1	1A	1539	C
1	1A	1555	C
1	1A	1556	A
1	1A	1590	C
1	1A	1601	A
1	1A	1605	A
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1626	A
1	1A	1627	A
1	1A	1628	G
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1656	A
1	1A	1695	C
1	1A	1701	A
1	1A	1721	G
1	1A	1747	A
1	1A	1750	G
1	1A	1767	A
1	1A	1776	G
1	1A	1781	G
1	1A	1787	G
1	1A	1793	A
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1811	A

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Mol	Chain	Res	Type
1	1A	1813	C
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1847	G
1	1A	1859	G
1	1A	1870	G
1	1A	1878	A
1	1A	1890	A
1	1A	1899	A
1	1A	1922	A
1	1A	1928	G
1	1A	1935	A
1	1A	1951	G
1	1A	1952	G
1	1A	1960	A
1	1A	1977	U
1	1A	1982	A
1	1A	1985	U
1	1A	1987	C
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2014	G
1	1A	2015	U
1	1A	2019	G
1	1A	2045	G
1	1A	2053	A
1	1A	2055	A
1	1A	2065	C
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2091	G
1	1A	2115	G
1	1A	2118	U
1	1A	2121	U
1	1A	2123	G
1	1A	2124	U
1	1A	2134	G

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Mol	Chain	Res	Type
1	1A	2135	U
1	1A	2137	G
1	1A	2138	G
1	1A	2139	A
1	1A	2141	A
1	1A	2142	G
1	1A	2143	G
1	1A	2149	G
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	2160	C
1	1A	2162	C
1	1A	2164	C
1	1A	2166	U
1	1A	2168	C
1	1A	2173	G
1	1A	2175	G
1	1A	2177	G
1	1A	2180	A
1	1A	2181	G
1	1A	2188	G
1	1A	2193	A
1	1A	2194	U
1	1A	2195	A
1	1A	2204	G
1	1A	2206	G
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2237	A
1	1A	2250	G
1	1A	2251	G
1	1A	2281	A
1	1A	2287	C
1	1A	2295	C
1	1A	2299	A
1	1A	2300	A

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Mol	Chain	Res	Type
1	1A	2317	A
1	1A	2320	G
1	1A	2324	U
1	1A	2332	A
1	1A	2337	G
1	1A	2346	G
1	1A	2348	A
1	1A	2359	C
1	1A	2373	A
1	1A	2380	C
1	1A	2391	G
1	1A	2395	G
1	1A	2397	C
1	1A	2403	G
1	1A	2417	G
1	1A	2418	U
1	1A	2422	G
1	1A	2436	C
1	1A	2437	A
1	1A	2441	G
1	1A	2442	A
1	1A	2443	U
1	1A	2444	A
1	1A	2447	A
1	1A	2451	A
1	1A	2453	C
1	1A	2460	A
1	1A	2461	U
1	1A	2486	C
1	1A	2488	A
1	1A	2489	C
1	1A	2490	A
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	2541	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G

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Mol	Chain	Res	Type
1	1A	2581	G
1	1A	2584	A
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	2691	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
1	1A	2726	A
1	1A	2727	G
1	1A	2736	C
1	1A	2737	C
1	1A	2739	U
1	1A	2746	A
1	1A	2770	A
1	1A	2771	A
1	1A	2778	A
1	1A	2779	G
1	1A	2791	A
1	1A	2803	A
1	1A	2805	G
1	1A	2807	C
1	1A	2813	G
1	1A	2818	U
1	1A	2828	G
1	1A	2830	A
1	1A	2831	A
1	1A	2844	G
1	1A	2868	C
1	1A	2876	U
1	1A	2882	G
1	1A	2883	A
1	1A	2901	A

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Mol	Chain	Res	Type
1	1A	2903	G
1	1A	2904	U
2	1B	2	C
2	1B	12	C
2	1B	35	U
2	1B	45	A
2	1B	56	G
2	1B	73	A
2	1B	106	G
2	1B	110	G
2	1B	119	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	54	C
32	1a	61	G
32	1a	79	G
32	1a	91	C
32	1a	96	U
32	1a	99	U
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	146	G
32	1a	154	C
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	185	A
32	1a	189(A)	C
32	1a	189(B)	C
32	1a	189(J)	G
32	1a	195	A
32	1a	196	A

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Mol	Chain	Res	Type
32	1a	197	A
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	217	C
32	1a	247	G
32	1a	251	G
32	1a	262	A
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	321	A
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	344	A
32	1a	349	A
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	355	C
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	483	C
32	1a	485	G
32	1a	496	A

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Mol	Chain	Res	Type
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	531	U
32	1a	532	A
32	1a	533	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	592	G
32	1a	596	C
32	1a	619	U
32	1a	630	G
32	1a	650	G
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	671	G
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	702	A
32	1a	724	G
32	1a	731	G
32	1a	749	C
32	1a	753	A
32	1a	755	G
32	1a	774	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	802	A

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Mol	Chain	Res	Type
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	859	A
32	1a	870	U
32	1a	874	G
32	1a	897	C
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	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	1001(A)	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1016	A
32	1a	1020	U
32	1a	1021	G
32	1a	1022	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C

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Mol	Chain	Res	Type
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1037	C
32	1a	1039	C
32	1a	1044	A
32	1a	1054	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1104	G
32	1a	1124	G
32	1a	1125	U
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1157	A
32	1a	1159	U
32	1a	1160	G
32	1a	1161	C
32	1a	1181	G
32	1a	1183	A
32	1a	1184	G
32	1a	1186	G
32	1a	1192	C
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1204	A
32	1a	1212	U
32	1a	1213	A

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Mol	Chain	Res	Type
32	1a	1214	C
32	1a	1224	G
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1240	U
32	1a	1241	G
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1269	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1320	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1363	C
32	1a	1370	G
32	1a	1381	U
32	1a	1397	C
32	1a	1413	A
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1487	G
32	1a	1492	A
32	1a	1497	G
32	1a	1503	A

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Mol	Chain	Res	Type
32	1a	1504	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
53	1v	24	A
54	1w	2	C
54	1w	8	4SU
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	24	G
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	64	A
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	14	A
55	1x	19	G
55	1x	21	A
55	1x	47	U
55	1x	56	C
55	1x	59	A
55	1x	67	C
55	1x	68	C
55	1x	76	A
56	1y	3	C
56	1y	5	G
56	1y	9	A
56	1y	13	C
56	1y	19	G
56	1y	20	U
56	1y	21	A

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Mol	Chain	Res	Type
56	1y	24	G
56	1y	46	7MG
56	1y	47	U
56	1y	48	C
56	1y	52	G
56	1y	53	G
56	1y	54	5MU
56	1y	57	G
56	1y	59	U
56	1y	61	C
56	1y	65	G
56	1y	69	G
56	1y	70	G
56	1y	71	G
1	2A	11	G
1	2A	14	A
1	2A	15	G
1	2A	34	C
1	2A	36	G
1	2A	45	C
1	2A	50	U
1	2A	51	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	79	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	95	G
1	2A	98	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	120	U
1	2A	131	G
1	2A	150	C
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	199	A

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Mol	Chain	Res	Type
1	2A	205	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	266	G
1	2A	271(F)	C
1	2A	271(I)	G
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	271(P)	C
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	289	A
1	2A	303	U
1	2A	311	A
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	338	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(D)	G
1	2A	372	G
1	2A	380	U
1	2A	385	C
1	2A	386	G
1	2A	391	G
1	2A	396	G
1	2A	406	G
1	2A	407	G

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Mol	Chain	Res	Type
1	2A	411	G
1	2A	412	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	470	A
1	2A	481	G
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	527	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	551	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	583	G
1	2A	586	A
1	2A	588	U
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	653	A

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Mol	Chain	Res	Type
1	2A	669	G
1	2A	686	G
1	2A	709	U
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	764	A
1	2A	775	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	811	U
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	847	U
1	2A	848	G
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	874	G
1	2A	875	G
1	2A	877	U
1	2A	878	A
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	895	U
1	2A	896	A
1	2A	897	C
1	2A	900	A

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Mol	Chain	Res	Type
1	2A	901	A
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	957	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	993	G
1	2A	996	A
1	2A	1006	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
1	2A	1039	G
1	2A	1040	C
1	2A	1043	C
1	2A	1116	C
1	2A	1126	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1171	G
1	2A	1180	C
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1229	G
1	2A	1242	A

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Mol	Chain	Res	Type
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1289	C
1	2A	1298	C
1	2A	1300	U
1	2A	1301	A
1	2A	1313	U
1	2A	1314	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1373	A
1	2A	1378	A
1	2A	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1392	A
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C

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Mol	Chain	Res	Type
1	2A	1509(A)	A
1	2A	1530	C
1	2A	1531	C
1	2A	1533	G
1	2A	1537	G
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1582	C
1	2A	1583	A
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1618	A
1	2A	1648	C
1	2A	1649	G
1	2A	1653	G
1	2A	1654	A
1	2A	1674	G
1	2A	1693	U
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1714	G
1	2A	1721	G
1	2A	1722	A
1	2A	1741	A
1	2A	1743	C
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1769	G

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Mol	Chain	Res	Type
1	2A	1773	A
1	2A	1780	A
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1820	U
1	2A	1828	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1860	G
1	2A	1877	A
1	2A	1878	G
1	2A	1896	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	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1965	C
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G

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Mol	Chain	Res	Type
1	2A	2069	G
1	2A	2092	U
1	2A	2093	G
1	2A	2099	U
1	2A	2104	G
1	2A	2108	C
1	2A	2109	U
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2113	U
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	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	2139	C
1	2A	2142	C
1	2A	2144	U
1	2A	2145	C
1	2A	2146	C
1	2A	2148	G
1	2A	2149	G
1	2A	2150	U
1	2A	2152	G
1	2A	2154	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G

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Mol	Chain	Res	Type
1	2A	2160	G
1	2A	2163	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	2174	C
1	2A	2175	C
1	2A	2182	G
1	2A	2184	G
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	2219	G
1	2A	2225	A
1	2A	2239	G
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2305	A
1	2A	2308	G
1	2A	2311	A
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2338	G
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G

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Mol	Chain	Res	Type
1	2A	2370	G
1	2A	2377	A
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2406	U
1	2A	2424	C
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2460	U
1	2A	2474	C
1	2A	2476	A
1	2A	2478	A
1	2A	2491	U
1	2A	2492	U
1	2A	2494	G
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2518	A
1	2A	2520	C
1	2A	2554	U
1	2A	2562	U
1	2A	2566	A
1	2A	2567	G
1	2A	2574	G
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2623	G
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2689	U
1	2A	2690	C

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Mol	Chain	Res	Type
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2726	U
1	2A	2733	A
1	2A	2744	G
1	2A	2745	C
1	2A	2748	A
1	2A	2751	G
1	2A	2755	C
1	2A	2757	A
1	2A	2758	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
1	2A	2794	C
1	2A	2803	C
1	2A	2807	G
1	2A	2808	U
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2872	G
1	2A	2876	G
1	2A	2879	C
1	2A	2880	C
1	2A	2884	U
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	7	G
2	2B	8	U
2	2B	9	G
2	2B	13	A
2	2B	17	C
2	2B	19	G

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Mol	Chain	Res	Type
2	2B	24	G
2	2B	33	G
2	2B	34	U
2	2B	38	C
2	2B	42	C
2	2B	53	A
2	2B	56	G
2	2B	57	A
2	2B	65	C
2	2B	66	A
2	2B	67	G
2	2B	73	A
2	2B	75	G
2	2B	85	G
2	2B	88	C
2	2B	89	G
2	2B	91	C
2	2B	95	C
2	2B	106	G
2	2B	108	U
2	2B	110	G
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	30	U
32	2a	31	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	52	G
32	2a	58	C
32	2a	66	G
32	2a	73	G
32	2a	78	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C

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Mol	Chain	Res	Type
32	2a	131	C
32	2a	159	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(E)	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	217	C
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	300	A
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	344	A
32	2a	346	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	356	A
32	2a	367	U
32	2a	372	C
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	411	A
32	2a	412	A
32	2a	413	G
32	2a	424	G
32	2a	429	U
32	2a	430	A

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Mol	Chain	Res	Type
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	470	C
32	2a	477	A
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	508	C
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	512	U
32	2a	518	C
32	2a	528	C
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	630	G
32	2a	650	G
32	2a	653	A
32	2a	665	A
32	2a	673	G
32	2a	687	A
32	2a	688	G
32	2a	723	U
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	773	G
32	2a	774	G
32	2a	777	A

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Mol	Chain	Res	Type
32	2a	793	U
32	2a	794	A
32	2a	817	C
32	2a	819	A
32	2a	821	G
32	2a	828	A
32	2a	836	G
32	2a	840	C
32	2a	841	U
32	2a	859	A
32	2a	873	A
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	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	992	U
32	2a	993	G
32	2a	994	A
32	2a	997	U
32	2a	1000	U
32	2a	1001	A
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1008	C
32	2a	1011	G

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Mol	Chain	Res	Type
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1027	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1044	A
32	2a	1045	C
32	2a	1046	A
32	2a	1050	G
32	2a	1055	A
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1080	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1104	G
32	2a	1108	G
32	2a	1117	G
32	2a	1118	C
32	2a	1119	C
32	2a	1125	U
32	2a	1129	C
32	2a	1133	G
32	2a	1135	U
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1146	A
32	2a	1152	A
32	2a	1154	G

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Mol	Chain	Res	Type
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1169	A
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
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	1250	A
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1270	C
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1297	C
32	2a	1302	U
32	2a	1305	G
32	2a	1320	C
32	2a	1322	C
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1364	U
32	2a	1370	G
32	2a	1379	G
32	2a	1381	U
32	2a	1397	C
32	2a	1419	G
32	2a	1442	G

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Mol	Chain	Res	Type
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1446	U
32	2a	1452	C
32	2a	1456	G
32	2a	1487	G
32	2a	1492	A
32	2a	1494	G
32	2a	1497	G
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	1526	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	15	A
54	2w	3	C
54	2w	4	C
54	2w	8	4SU
54	2w	12	U
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	26	A
54	2w	29	G
54	2w	46	7MG
54	2w	47	U
54	2w	48	C
54	2w	49	C
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	71	G
54	2w	72	C
54	2w	73	A
54	2w	74	C

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Mol	Chain	Res	Type
55	2x	9	G
55	2x	14	A
55	2x	19	G
55	2x	21	A
55	2x	47	U
55	2x	48	C
55	2x	68	C
55	2x	76	A
56	2y	2	C
56	2y	13	C
56	2y	14	A
56	2y	15	G
56	2y	19	G
56	2y	24	G
56	2y	30	G
56	2y	46	7MG
56	2y	49	C
56	2y	52	G
56	2y	53	G
56	2y	55	PSU
56	2y	57	G
56	2y	58	A
56	2y	59	U
56	2y	60	U
56	2y	62	C
56	2y	65	G
56	2y	70	G
56	2y	73	A

All (60) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	115	G
1	1A	185	A
1	1A	204	G
1	1A	509	A
1	1A	793	A
1	1A	913	A
1	1A	941	U
1	1A	1019	G
1	1A	1065	U
1	1A	1067	A

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Mol	Chain	Res	Type
1	1A	1093	G
1	1A	1120	G
1	1A	1135	G
1	1A	1136	U
1	1A	1188	A
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A
1	1A	1321	A
1	1A	1466	U
1	1A	1700	G
1	1A	2014	G
1	1A	2148	A
1	1A	2156	A
1	1A	2179	G
1	1A	2192	A
1	1A	2203	G
1	1A	2205	C
1	1A	2418	U
1	1A	2701	U
1	1A	2769	U
2	1B	1	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	587	C
1	2A	752	A
1	2A	839	U
1	2A	856	C
1	2A	883	G
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1300	U
1	2A	1420	U
1	2A	1442	G

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Mol	Chain	Res	Type
1	2A	1493	C
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2134	A
1	2A	2689	U
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	PSU	2y	39	56	17,21,22	1.45	2 (11%)	20,30,33	3.29	6 (30%)
56	5MU	1y	54	56	15,22,23	1.10	1 (6%)	16,32,35	1.92	2 (12%)
54	F3N	1w	76	1,54	30,36,37	1.52	6 (20%)	29,51,54	1.33	1 (3%)
56	5MU	2y	54	56	15,22,23	1.07	1 (6%)	16,32,35	2.00	1 (6%)
54	7MG	2w	46	54	22,26,27	1.78	4 (18%)	28,39,42	2.77	10 (35%)
56	MIA	2y	37	56	18,24,32	1.14	2 (11%)	18,35,47	1.28	2 (11%)
32	5MC	2a	1400	32	15,22,23	1.36	1 (6%)	19,32,35	1.25	3 (15%)
1	2MA	1A	2515	1,57	17,25,26	1.34	2 (11%)	19,37,40	2.13	3 (15%)
54	PSU	1w	32	54,57	17,21,22	1.62	2 (11%)	20,30,33	3.14	6 (30%)
56	MIA	1y	37	56	18,24,32	1.16	2 (11%)	18,35,47	1.19	2 (11%)
54	PSU	2w	32	54	17,21,22	1.65	3 (17%)	20,30,33	3.21	6 (30%)
56	4SU	1y	8	56	14,21,22	1.37	1 (7%)	15,30,33	1.35	2 (13%)
1	5MC	2A	1962	1,57	15,22,23	1.27	1 (6%)	19,32,35	1.37	3 (15%)
1	OMG	1A	2263	1,55,57	18,26,27	1.22	2 (11%)	20,38,41	2.19	6 (30%)
1	5MU	2A	1915	1	15,22,23	1.05	1 (6%)	16,32,35	1.72	2 (12%)
56	7MG	2y	46	56	22,26,27	1.88	4 (18%)	28,39,42	3.01	12 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1A	1939	1	17,21,22	1.45	2 (11%)	20,30,33	3.12	5 (25%)
1	2MA	2A	2503	1,57	17,25,26	1.28	2 (11%)	19,37,40	1.89	3 (15%)
55	5MU	2x	54	55	15,22,23	1.10	2 (13%)	16,32,35	1.90	2 (12%)
1	4OC	2A	1920	1	15,22,24	0.70	0	17,31,35	1.30	1 (5%)
32	M2G	1a	966	32	20,27,28	1.33	3 (15%)	22,40,43	2.04	6 (27%)
43	0TD	1l	92	43	4,9,10	3.23	1 (25%)	3,11,13	7.00	1 (33%)
32	4OC	2a	1402	32,57	16,23,24	0.64	0	17,32,35	1.41	1 (5%)
1	PSU	2A	2605	1	17,21,22	1.68	3 (17%)	20,30,33	3.10	6 (30%)
32	5MC	1a	1400	32	15,22,23	1.35	1 (6%)	19,32,35	1.31	3 (15%)
55	5MC	2x	32	55	15,22,23	1.23	1 (6%)	19,32,35	1.38	4 (21%)
54	PSU	2w	39	54	17,21,22	1.54	3 (17%)	20,30,33	3.30	6 (30%)
32	7MG	1a	527	32	22,26,27	1.76	4 (18%)	28,39,42	2.86	9 (32%)
32	PSU	1a	516	32,57	17,21,22	1.47	3 (17%)	20,30,33	3.04	6 (30%)
56	PSU	1y	39	56	17,21,22	1.56	2 (11%)	20,30,33	2.80	5 (25%)
1	PSU	2A	1911	1	17,21,22	1.52	2 (11%)	20,30,33	3.19	6 (30%)
32	2MG	1a	1207	32	19,26,27	1.41	2 (10%)	21,38,41	2.44	7 (33%)
32	PSU	2a	516	32	17,21,22	1.63	3 (17%)	20,30,33	3.07	6 (30%)
1	5MU	1A	1937	1	15,22,23	1.12	1 (6%)	16,32,35	1.62	2 (12%)
54	4SU	2w	8	54	14,21,22	1.37	2 (14%)	15,30,33	1.39	2 (13%)
1	5MC	1A	1964	1,57	15,22,23	1.20	1 (6%)	19,32,35	1.41	3 (15%)
54	PSU	2w	55	54	17,21,22	1.45	2 (11%)	20,30,33	3.31	6 (30%)
56	4SU	2y	8	56	14,21,22	1.24	1 (7%)	15,30,33	1.36	2 (13%)
1	OMG	2A	2251	1,55	18,26,27	1.09	2 (11%)	20,38,41	1.96	5 (25%)
54	4SU	1w	8	54	14,21,22	1.37	2 (14%)	15,30,33	1.56	2 (13%)
54	5MU	2w	54	54	15,22,23	1.06	1 (6%)	16,32,35	1.88	2 (12%)
1	PSU	1A	2617	1	17,21,22	1.50	2 (11%)	20,30,33	3.40	6 (30%)
55	4SU	2x	8	55	14,21,22	1.34	2 (14%)	15,30,33	2.19	2 (13%)
32	M2G	2a	966	32	20,27,28	1.45	3 (15%)	22,40,43	2.15	5 (22%)
1	5MU	1A	1961	1,57	15,22,23	1.09	2 (13%)	16,32,35	1.78	2 (12%)
1	5MC	2A	1942	1	15,22,23	1.26	1 (6%)	19,32,35	1.38	3 (15%)
1	PSU	1A	1933	1	17,21,22	1.53	2 (11%)	20,30,33	3.07	6 (30%)
54	5MU	1w	54	54	15,22,23	1.05	1 (6%)	16,32,35	1.85	2 (12%)
55	5MC	1x	32	55	15,22,23	1.31	1 (6%)	19,32,35	1.49	4 (21%)
1	4OC	1A	1942	1,57	15,22,24	0.64	0	17,31,35	1.46	2 (11%)
32	UR3	2a	1498	32	14,22,23	0.75	1 (7%)	15,32,35	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	UR3	1a	1498	32	14,22,23	0.71	0	15,32,35	0.75	0
32	5MC	1a	967	32	15,22,23	1.38	1 (6%)	19,32,35	1.29	2 (10%)
1	2MU	1A	2564	1,57	14,22,24	0.93	1 (7%)	14,31,36	0.98	1 (7%)
55	PSU	2x	55	55	17,21,22	1.48	2 (11%)	20,30,33	3.17	5 (25%)
32	7MG	2a	527	32	22,26,27	1.76	4 (18%)	28,39,42	2.76	10 (35%)
32	5MC	1a	1407	32	15,22,23	1.34	1 (6%)	19,32,35	1.36	3 (15%)
32	2MG	2a	1207	32,57	19,26,27	1.24	2 (10%)	21,38,41	2.25	8 (38%)
1	2MU	2A	2552	1,57	14,22,24	0.89	0	14,31,36	0.75	1 (7%)
55	PSU	1x	55	55	17,21,22	1.67	3 (17%)	20,30,33	3.32	6 (30%)
54	F3N	2w	76	1,54	30,36,37	1.49	5 (16%)	29,51,54	1.23	1 (3%)
32	MA6	1a	1519	32	19,26,27	1.01	1 (5%)	18,38,41	1.63	3 (16%)
54	MIA	2w	37	54	20,27,32	1.88	3 (15%)	22,39,47	1.87	8 (36%)
54	7MG	1w	46	54	22,26,27	1.73	4 (18%)	28,39,42	2.75	8 (28%)
32	MA6	2a	1519	32	19,26,27	1.07	1 (5%)	18,38,41	1.65	3 (16%)
55	5MU	1x	54	55,57	15,22,23	1.09	2 (13%)	16,32,35	1.81	2 (12%)
1	5MC	1A	1984	1,57	15,22,23	1.25	1 (6%)	19,32,35	1.10	1 (5%)
54	PSU	1w	39	54	17,21,22	1.52	2 (11%)	20,30,33	3.07	6 (30%)
1	PSU	2A	1917	1	17,21,22	1.57	3 (17%)	20,30,33	3.05	6 (30%)
32	5MC	2a	1404	32	15,22,23	1.32	1 (6%)	19,32,35	1.25	3 (15%)
56	7MG	1y	46	56	22,26,27	1.86	4 (18%)	28,39,42	2.98	10 (35%)
56	PSU	2y	32	56	17,21,22	1.43	2 (11%)	20,30,33	3.20	5 (25%)
32	5MC	1a	1404	32	15,22,23	1.32	1 (6%)	19,32,35	1.33	3 (15%)
54	MIA	1w	37	54	24,31,32	2.23	3 (12%)	26,44,47	2.47	11 (42%)
32	4OC	1a	1402	32	16,23,24	0.68	0	17,32,35	1.50	1 (5%)
1	5MU	2A	1939	1	15,22,23	1.14	2 (13%)	16,32,35	1.81	2 (12%)
32	MA6	2a	1518	32	19,26,27	0.98	1 (5%)	18,38,41	1.64	5 (27%)
32	5MC	2a	967	32	15,22,23	1.33	1 (6%)	19,32,35	1.32	3 (15%)
56	PSU	2y	55	56	17,21,22	1.51	5 (29%)	20,30,33	3.13	6 (30%)
32	5MC	2a	1407	32	15,22,23	1.33	1 (6%)	19,32,35	1.53	4 (21%)
54	PSU	1w	55	54	17,21,22	1.45	2 (11%)	20,30,33	3.31	6 (30%)
56	PSU	1y	32	56	17,21,22	1.41	2 (11%)	20,30,33	3.22	7 (35%)
55	4SU	1x	8	55	14,21,22	1.34	2 (14%)	15,30,33	2.73	2 (13%)
43	0TD	2l	92	43	4,9,10	3.11	1 (25%)	3,11,13	5.61	1 (33%)
56	PSU	1y	55	56	17,21,22	1.41	2 (11%)	20,30,33	3.04	6 (30%)
32	MA6	1a	1518	32	19,26,27	0.99	1 (5%)	18,38,41	1.66	5 (27%)

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
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	2/5/25/26	0/2/2/2
54	F3N	1w	76	1,54	-	0/15/37/38	0/4/4/4
56	5MU	2y	54	56	-	3/5/25/26	0/2/2/2
54	7MG	2w	46	54	-	3/7/37/38	0/3/3/3
56	MIA	2y	37	56	-	3/3/25/34	0/3/3/3
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
1	2MA	1A	2515	1,57	-	2/3/25/26	0/3/3/3
54	PSU	1w	32	54,57	-	0/7/25/26	0/2/2/2
56	MIA	1y	37	56	-	2/3/25/34	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
56	4SU	1y	8	56	-	1/5/25/26	0/2/2/2
1	5MC	2A	1962	1,57	-	2/5/25/26	0/2/2/2
1	OMG	1A	2263	1,55,57	-	0/5/27/28	0/3/3/3
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
56	7MG	2y	46	56	-	3/7/37/38	0/3/3/3
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,57	-	2/3/25/26	0/3/3/3
55	5MU	2x	54	55	-	0/5/25/26	0/2/2/2
1	4OC	2A	1920	1	-	2/7/27/30	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
43	0TD	1l	92	43	-	1/3/12/14	-
32	4OC	2a	1402	32,57	-	1/9/29/30	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/5/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/5/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32	-	1/7/37/38	0/3/3/3
32	PSU	1a	516	32,57	-	0/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/5/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/5/25/26	0/2/2/2
1	5MC	1A	1964	1,57	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	1/5/25/26	0/2/2/2
1	OMG	2A	2251	1,55	-	0/5/27/28	0/3/3/3
54	4SU	1w	8	54	-	0/5/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/5/25/26	0/2/2/2
1	PSU	1A	2617	1	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/5/25/26	0/2/2/2
32	M2G	2a	966	32	-	1/7/29/30	0/3/3/3
1	5MU	1A	1961	1,57	-	0/5/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/5/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/5/25/26	0/2/2/2
1	4OC	1A	1942	1,57	-	1/7/27/30	0/2/2/2
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/5/25/26	0/2/2/2
1	2MU	1A	2564	1,57	-	0/7/27/28	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	32	-	1/7/37/38	0/3/3/3
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
32	2MG	2a	1207	32,57	-	0/5/27/28	0/3/3/3
1	2MU	2A	2552	1,57	-	0/7/27/28	0/2/2/2
55	PSU	1x	55	55	-	1/7/25/26	0/2/2/2
54	F3N	2w	76	1,54	-	4/15/37/38	0/4/4/4
32	MA6	1a	1519	32	-	4/7/29/30	0/3/3/3
54	MIA	2w	37	54	-	0/7/29/34	0/3/3/3
54	7MG	1w	46	54	-	2/7/37/38	0/3/3/3
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3
55	5MU	1x	54	55,57	-	0/5/25/26	0/2/2/2
1	5MC	1A	1984	1,57	-	2/5/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
56	7MG	1y	46	56	-	6/7/37/38	0/3/3/3
56	PSU	2y	32	56	-	2/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
54	MIA	1w	37	54	-	6/11/33/34	0/3/3/3
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
1	5MU	2A	1939	1	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	2a	1518	32	-	2/7/29/30	0/3/3/3
32	5MC	2a	967	32	-	1/5/25/26	0/2/2/2
56	PSU	2y	55	56	-	5/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	1/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/5/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/3/12/14	-
56	PSU	1y	55	56	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/7/29/30	0/3/3/3

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	37	MIA	C2-S10	-7.18	1.69	1.75
54	1w	37	MIA	C13-C14	7.18	1.53	1.32
54	1w	37	MIA	C2-S10	-6.73	1.70	1.75
43	1l	92	0TD	CB-SB	-6.21	1.69	1.84
43	2l	92	0TD	CB-SB	-5.94	1.69	1.84
54	1w	76	F3N	CB-CG	-5.32	1.38	1.51
1	2A	2605	PSU	C5-C1'	-5.11	1.47	1.52
56	2y	46	7MG	C6-C5	5.09	1.48	1.41
56	1y	46	7MG	C6-C5	5.03	1.48	1.41
32	1a	967	5MC	C5-C4	5.03	1.49	1.41
32	1a	1207	2MG	C6-C5	4.98	1.49	1.41
54	2w	46	7MG	C6-C5	4.96	1.48	1.41
56	2y	46	7MG	C5-C4	4.94	1.48	1.39
32	2a	527	7MG	C6-C5	4.87	1.48	1.41
56	1y	46	7MG	C5-C4	4.87	1.48	1.39
54	2w	76	F3N	CB-CG	-4.84	1.39	1.51
55	1x	55	PSU	C5-C1'	-4.82	1.48	1.52
32	2a	1400	5MC	C5-C4	4.82	1.48	1.41
54	2w	32	PSU	C5-C1'	-4.74	1.48	1.52
32	2a	516	PSU	C5-C1'	-4.73	1.48	1.52
32	1a	1400	5MC	C5-C4	4.73	1.48	1.41
32	2a	967	5MC	C5-C4	4.72	1.48	1.41
32	2a	1404	5MC	C5-C4	4.70	1.48	1.41
32	1a	1407	5MC	C5-C4	4.69	1.48	1.41
32	2a	1407	5MC	C5-C4	4.66	1.48	1.41
55	1x	32	5MC	C5-C4	4.65	1.48	1.41
32	1a	1404	5MC	C5-C4	4.63	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2515	2MA	C6-C5	4.58	1.48	1.41
32	2a	527	7MG	C5-C4	4.56	1.48	1.39
54	1w	32	PSU	C5-C1'	-4.55	1.48	1.52
32	1a	527	7MG	C5-C4	4.49	1.47	1.39
54	2w	46	7MG	C5-C4	4.47	1.47	1.39
1	2A	1942	5MC	C5-C4	4.47	1.48	1.41
1	2A	1962	5MC	C5-C4	4.45	1.48	1.41
54	1w	46	7MG	C6-C5	4.45	1.47	1.41
54	1w	46	7MG	C5-C4	4.44	1.47	1.39
1	1A	1984	5MC	C5-C4	4.39	1.48	1.41
55	2x	32	5MC	C5-C4	4.39	1.48	1.41
32	1a	527	7MG	C6-C5	4.36	1.47	1.41
56	1y	8	4SU	C4-S4	-4.31	1.59	1.67
1	1A	1964	5MC	C5-C4	4.30	1.48	1.41
54	1w	8	4SU	C4-S4	-4.21	1.59	1.67
1	2A	2503	2MA	C6-C5	4.20	1.47	1.41
54	2w	39	PSU	C5-C1'	-4.18	1.48	1.52
32	2a	1207	2MG	C6-C5	4.18	1.48	1.41
1	2A	1917	PSU	C5-C1'	-4.15	1.48	1.52
32	2a	966	M2G	C6-C5	4.12	1.48	1.41
55	2x	8	4SU	C4-S4	-4.10	1.60	1.67
54	2w	8	4SU	C4-S4	-4.06	1.60	1.67
54	1w	39	PSU	C5-C1'	-4.05	1.48	1.52
56	2y	8	4SU	C4-S4	-4.01	1.60	1.67
56	1y	32	PSU	C4-C5	4.00	1.50	1.41
56	1y	39	PSU	C5-C1'	-4.00	1.48	1.52
32	1a	527	7MG	C5-N7	-3.98	1.33	1.39
1	2A	1911	PSU	C5-C1'	-3.94	1.48	1.52
1	1A	2617	PSU	C5-C1'	-3.92	1.48	1.52
1	1A	2263	OMG	C6-C5	3.90	1.48	1.41
32	1a	966	M2G	C6-C5	3.80	1.47	1.41
54	2w	55	PSU	C4-C5	3.77	1.49	1.41
55	2x	55	PSU	C4-C5	3.75	1.49	1.41
1	1A	1933	PSU	C4-C5	3.75	1.49	1.41
32	2a	966	M2G	C2-N2	3.74	1.41	1.34
56	1y	39	PSU	C4-C5	3.73	1.49	1.41
56	1y	55	PSU	C5-C1'	-3.72	1.49	1.52
56	2y	39	PSU	C5-C1'	-3.66	1.49	1.52
55	1x	8	4SU	C4-S4	-3.65	1.60	1.67
56	2y	55	PSU	C4-C5	3.64	1.49	1.41
32	1a	516	PSU	C5-C1'	-3.62	1.49	1.52
1	1A	1933	PSU	C5-C1'	-3.61	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	1y	54	5MU	C4-C5	3.60	1.49	1.41
56	2y	32	PSU	C4-C5	3.56	1.49	1.41
54	1w	55	PSU	C5-C1'	-3.52	1.49	1.52
1	1A	1937	5MU	C4-C5	3.51	1.49	1.41
54	1w	39	PSU	C4-C5	3.47	1.48	1.41
1	1A	1939	PSU	C4-C5	3.47	1.48	1.41
1	2A	2251	OMG	C6-C5	3.44	1.47	1.41
54	2w	54	5MU	C4-C5	3.42	1.48	1.41
55	1x	55	PSU	C4-C5	3.42	1.48	1.41
54	1w	46	7MG	C5-N7	-3.42	1.34	1.39
54	1w	32	PSU	C4-C5	3.41	1.48	1.41
56	2y	39	PSU	C4-C5	3.39	1.48	1.41
55	2x	55	PSU	C5-C1'	-3.39	1.49	1.52
55	2x	54	5MU	C4-C5	3.38	1.48	1.41
54	2w	32	PSU	C4-C5	3.37	1.48	1.41
1	2A	1939	5MU	C4-C5	3.37	1.48	1.41
32	2a	527	7MG	C5-N7	-3.37	1.34	1.39
1	2A	1911	PSU	C4-C5	3.36	1.48	1.41
1	2A	1915	5MU	C4-C5	3.34	1.48	1.41
32	1a	516	PSU	C4-C5	3.33	1.48	1.41
1	1A	2617	PSU	C4-C5	3.33	1.48	1.41
56	2y	46	7MG	C5-N7	-3.31	1.34	1.39
1	1A	1939	PSU	C5-C1'	-3.31	1.49	1.52
54	2w	55	PSU	C5-C1'	-3.30	1.49	1.52
56	2y	54	5MU	C4-C5	3.28	1.48	1.41
56	2y	55	PSU	C5-C1'	-3.26	1.49	1.52
54	2w	76	F3N	C5-C4	-3.26	1.32	1.40
32	1a	966	M2G	C2-N2	3.26	1.40	1.34
54	2w	39	PSU	C4-C5	3.25	1.48	1.41
55	1x	54	5MU	C4-C5	3.25	1.48	1.41
32	2a	516	PSU	C4-C5	3.23	1.48	1.41
1	2A	1917	PSU	C4-C5	3.21	1.48	1.41
56	2y	32	PSU	C5-C1'	-3.20	1.49	1.52
54	2w	46	7MG	C5-N7	-3.20	1.34	1.39
54	1w	54	5MU	C4-C5	3.19	1.48	1.41
56	1y	46	7MG	C5-N7	-3.16	1.34	1.39
54	1w	55	PSU	C4-C5	3.15	1.48	1.41
1	2A	2605	PSU	C4-C5	3.13	1.48	1.41
55	1x	8	4SU	C2-N3	-3.10	1.32	1.38
1	1A	1961	5MU	C4-C5	3.09	1.48	1.41
54	2w	76	F3N	O4'-C1'	3.07	1.45	1.41
56	1y	55	PSU	C4-C5	3.06	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	76	F3N	O4'-C1'	2.90	1.45	1.41
56	1y	37	MIA	C2-N3	2.80	1.36	1.32
56	1y	37	MIA	C5-C4	2.78	1.48	1.40
56	2y	37	MIA	C2-N3	2.75	1.36	1.32
32	2a	1519	MA6	C5-C4	2.70	1.48	1.40
56	2y	37	MIA	C5-C4	2.69	1.48	1.40
32	2a	1518	MA6	C5-C4	2.63	1.47	1.40
56	1y	32	PSU	C5-C1'	-2.63	1.50	1.52
32	2a	966	M2G	C5-C4	2.62	1.47	1.40
54	2w	37	MIA	C5-C4	2.61	1.47	1.40
32	2a	1207	2MG	C5-C4	2.59	1.47	1.40
54	1w	37	MIA	C5-C4	2.58	1.47	1.40
54	1w	46	7MG	C4-N9	-2.57	1.33	1.38
32	1a	1207	2MG	C5-C4	2.57	1.47	1.40
54	2w	76	F3N	C6-C5	-2.54	1.33	1.43
54	1w	76	F3N	C6-C5	-2.53	1.33	1.43
32	1a	1518	MA6	C5-C4	2.51	1.47	1.40
54	1w	76	F3N	C2'-C3'	-2.49	1.49	1.53
54	2w	46	7MG	C4-N9	-2.47	1.33	1.38
32	1a	966	M2G	C5-C4	2.47	1.47	1.40
32	1a	1519	MA6	C5-C4	2.44	1.47	1.40
55	2x	8	4SU	C2-N3	-2.44	1.33	1.38
1	2A	2251	OMG	C5-C4	2.41	1.47	1.40
1	1A	1961	5MU	C2-N3	-2.39	1.33	1.38
54	1w	76	F3N	C5-C4	-2.38	1.34	1.40
1	1A	2263	OMG	C5-C4	2.35	1.47	1.40
1	2A	1917	PSU	C2-N3	-2.33	1.33	1.38
1	2A	2503	2MA	C5-C4	2.31	1.47	1.40
54	1w	76	F3N	C5-N7	-2.29	1.31	1.39
1	2A	1939	5MU	C2-N3	-2.27	1.33	1.38
56	2y	55	PSU	O4'-C1'	-2.18	1.41	1.44
32	2a	516	PSU	O4'-C1'	-2.17	1.41	1.44
32	2a	527	7MG	C4-N9	-2.16	1.34	1.38
56	1y	46	7MG	C4-N3	2.16	1.37	1.34
54	2w	8	4SU	C2-N3	-2.15	1.33	1.38
55	1x	54	5MU	C2-N3	-2.13	1.34	1.38
55	1x	55	PSU	O4'-C1'	-2.13	1.41	1.44
1	2A	2605	PSU	C2-N3	-2.12	1.34	1.38
56	2y	55	PSU	C2-N1	-2.11	1.34	1.38
1	1A	2564	2MU	C2-N3	-2.10	1.34	1.38
54	1w	8	4SU	C2-N3	-2.09	1.34	1.38
54	2w	76	F3N	C5-N7	-2.06	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	516	PSU	O4'-C1'	-2.05	1.41	1.44
54	2w	37	MIA	C6-N1	2.05	1.35	1.32
54	2w	39	PSU	O4'-C1'	-2.05	1.41	1.44
32	2a	1498	UR3	C4-N3	2.04	1.41	1.38
56	2y	46	7MG	C4-N3	2.03	1.36	1.34
32	1a	527	7MG	C4-N9	-2.03	1.34	1.38
55	2x	54	5MU	C2-N3	-2.03	1.34	1.38
54	2w	32	PSU	O4'-C1'	-2.03	1.41	1.44
56	2y	55	PSU	C2-N3	-2.01	1.34	1.38
1	1A	2515	2MA	C5-C4	2.01	1.46	1.40

All (354) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-12.02	78.21	101.85
56	1y	46	7MG	N3-C4-N9	9.87	139.59	126.91
1	1A	2617	PSU	N1-C2-N3	-9.66	120.75	128.43
32	1a	527	7MG	N3-C4-N9	9.63	139.28	126.91
43	2l	92	0TD	CSB-SB-CB	-9.60	82.97	101.85
56	2y	46	7MG	N3-C4-N9	9.56	139.19	126.91
32	2a	527	7MG	N3-C4-N9	9.24	138.78	126.91
55	1x	8	4SU	C2-N3-C4	9.20	128.49	115.15
56	2y	32	PSU	N1-C2-N3	-9.08	121.21	128.43
54	2w	39	PSU	N1-C2-N3	-9.05	121.24	128.43
54	2w	46	7MG	N3-C4-N9	9.00	138.47	126.91
54	1w	55	PSU	N1-C2-N3	-8.88	121.37	128.43
55	1x	55	PSU	N1-C2-N3	-8.87	121.38	128.43
54	1w	46	7MG	N3-C4-N9	8.84	138.26	126.91
56	2y	55	PSU	N1-C2-N3	-8.83	121.41	128.43
1	2A	1911	PSU	N1-C2-N3	-8.80	121.43	128.43
55	2x	55	PSU	N1-C2-N3	-8.74	121.48	128.43
56	2y	39	PSU	N1-C2-N3	-8.69	121.52	128.43
1	1A	1939	PSU	N1-C2-N3	-8.68	121.53	128.43
56	1y	32	PSU	N1-C2-N3	-8.59	121.60	128.43
54	2w	55	PSU	N1-C2-N3	-8.53	121.64	128.43
54	2w	32	PSU	N1-C2-N3	-8.50	121.67	128.43
54	1w	39	PSU	N1-C2-N3	-8.46	121.70	128.43
32	1a	516	PSU	N1-C2-N3	-8.46	121.70	128.43
56	1y	55	PSU	N1-C2-N3	-8.40	121.75	128.43
54	1w	32	PSU	N1-C2-N3	-8.29	121.84	128.43
32	2a	516	PSU	N1-C2-N3	-8.17	121.94	128.43
1	1A	1933	PSU	N1-C2-N3	-7.89	122.16	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2605	PSU	N1-C2-N3	-7.78	122.25	128.43
1	2A	1917	PSU	N1-C2-N3	-7.57	122.41	128.43
54	1w	37	MIA	C12-C13-C14	-7.53	112.48	127.14
54	1w	55	PSU	C4-N3-C2	7.44	121.42	115.14
54	2w	39	PSU	C4-N3-C2	7.42	121.41	115.14
56	2y	32	PSU	C4-N3-C2	7.40	121.39	115.14
1	1A	2617	PSU	C4-N3-C2	7.39	121.38	115.14
56	1y	39	PSU	N1-C2-N3	-7.35	122.59	128.43
55	1x	55	PSU	C4-N3-C2	7.32	121.32	115.14
55	2x	8	4SU	C2-N3-C4	7.30	125.73	115.15
56	2y	54	5MU	C4-N3-C2	7.26	121.27	115.14
54	2w	55	PSU	C4-N3-C2	7.24	121.25	115.14
56	1y	32	PSU	C4-N3-C2	7.19	121.21	115.14
55	2x	55	PSU	C4-N3-C2	7.13	121.16	115.14
54	1w	32	PSU	C4-N3-C2	6.99	121.04	115.14
56	1y	54	5MU	C4-N3-C2	6.94	121.00	115.14
56	2y	39	PSU	C4-N3-C2	6.92	120.99	115.14
1	1A	2515	2MA	C2-N3-C4	6.90	121.13	115.52
54	1w	54	5MU	C4-N3-C2	6.88	120.95	115.14
1	1A	1933	PSU	C4-N3-C2	6.88	120.95	115.14
54	2w	32	PSU	C4-N3-C2	6.85	120.92	115.14
55	2x	54	5MU	C4-N3-C2	6.83	120.91	115.14
32	1a	516	PSU	C4-N3-C2	6.83	120.91	115.14
1	2A	1911	PSU	C4-N3-C2	6.67	120.77	115.14
55	1x	54	5MU	C4-N3-C2	6.64	120.75	115.14
1	1A	1939	PSU	C4-N3-C2	6.58	120.70	115.14
32	2a	516	PSU	C4-N3-C2	6.53	120.66	115.14
54	2w	54	5MU	C4-N3-C2	6.46	120.60	115.14
56	2y	55	PSU	C4-N3-C2	6.44	120.58	115.14
1	2A	2605	PSU	C4-N3-C2	6.37	120.52	115.14
54	1w	39	PSU	C4-N3-C2	6.33	120.48	115.14
56	1y	55	PSU	C4-N3-C2	6.13	120.32	115.14
56	2y	46	7MG	C6-N1-C2	6.10	125.62	115.93
1	2A	1915	5MU	C4-N3-C2	6.09	120.28	115.14
1	2A	1917	PSU	C4-N3-C2	6.07	120.27	115.14
55	1x	55	PSU	C5-C4-N3	-5.94	117.70	125.36
1	1A	1961	5MU	C4-N3-C2	5.86	120.09	115.14
1	2A	1939	5MU	C4-N3-C2	5.83	120.06	115.14
1	1A	1937	5MU	C4-N3-C2	5.77	120.01	115.14
1	2A	2503	2MA	C2-N3-C4	5.75	120.19	115.52
54	2w	55	PSU	C5-C4-N3	-5.75	117.96	125.36
54	1w	32	PSU	C5-C4-N3	-5.74	117.96	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1933	PSU	C5-C4-N3	-5.72	117.99	125.36
54	1w	76	F3N	N3-C2-N1	-5.70	119.76	128.68
32	1a	527	7MG	C5-C4-N3	-5.65	117.27	126.49
54	2w	32	PSU	C5-C4-N3	-5.60	118.14	125.36
54	2w	46	7MG	N7-C8-N9	-5.57	95.42	103.38
32	2a	516	PSU	C5-C4-N3	-5.53	118.24	125.36
54	2w	39	PSU	C5-C4-N3	-5.45	118.34	125.36
56	1y	46	7MG	C6-N1-C2	5.42	124.54	115.93
54	1w	46	7MG	N7-C8-N9	-5.41	95.64	103.38
56	2y	32	PSU	C5-C4-N3	-5.41	118.39	125.36
55	2x	55	PSU	C5-C4-N3	-5.39	118.41	125.36
32	1a	1402	4OC	CM4-N4-C4	-5.38	118.34	122.97
54	2w	76	F3N	N3-C2-N1	-5.37	120.29	128.68
32	2a	527	7MG	C5-C4-N3	-5.36	117.74	126.49
56	1y	46	7MG	C5-C4-N3	-5.33	117.78	126.49
1	2A	2605	PSU	C5-C4-N3	-5.26	118.58	125.36
56	2y	39	PSU	C5-C4-N3	-5.25	118.60	125.36
56	1y	39	PSU	C5-C4-N3	-5.23	118.62	125.36
32	1a	516	PSU	C5-C4-N3	-5.23	118.62	125.36
54	1w	55	PSU	C5-C4-N3	-5.21	118.64	125.36
56	1y	32	PSU	C5-C4-N3	-5.20	118.66	125.36
32	2a	966	M2G	C6-N1-C2	5.19	122.36	116.18
56	2y	46	7MG	C5-C4-N3	-5.14	118.09	126.49
1	1A	2263	OMG	C2-N3-C4	5.14	121.23	115.36
1	1A	1939	PSU	C5-C4-N3	-5.14	118.74	125.36
1	2A	1917	PSU	C5-C4-N3	-5.14	118.74	125.36
32	2a	966	M2G	C2-N3-C4	5.13	121.11	115.28
54	1w	39	PSU	C5-C4-N3	-5.09	118.81	125.36
1	1A	2617	PSU	C5-C4-N3	-5.08	118.82	125.36
32	1a	527	7MG	C6-C5-C4	5.06	120.63	115.20
1	2A	1911	PSU	C5-C4-N3	-5.05	118.85	125.36
56	1y	39	PSU	C4-N3-C2	5.04	119.40	115.14
32	1a	1207	2MG	C2-N3-C4	5.02	120.98	115.28
1	2A	2605	PSU	C5-C6-N1	-5.02	118.27	124.44
56	1y	55	PSU	C5-C4-N3	-4.97	118.96	125.36
56	2y	55	PSU	C5-C4-N3	-4.96	118.97	125.36
54	1w	46	7MG	C6-N1-C2	4.94	123.77	115.93
32	2a	527	7MG	N7-C8-N9	-4.91	96.36	103.38
32	1a	966	M2G	C6-N1-C2	4.90	122.02	116.18
54	1w	8	4SU	C2-N3-C4	4.86	122.20	115.15
56	1y	46	7MG	N7-C8-N9	-4.85	96.44	103.38
54	2w	46	7MG	C6-N1-C2	4.82	123.60	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2y	46	7MG	N7-C8-N9	-4.80	96.51	103.38
1	2A	2503	2MA	C5-C6-N1	-4.79	118.04	123.06
54	1w	55	PSU	C5-C1'-C2'	-4.75	106.84	115.32
1	1A	2515	2MA	C5-C6-N1	-4.73	118.10	123.06
32	1a	1207	2MG	C5-C6-N1	-4.72	116.97	123.43
32	1a	527	7MG	N7-C8-N9	-4.69	96.66	103.38
1	2A	1917	PSU	C5-C6-N1	-4.69	118.68	124.44
56	2y	55	PSU	C6-N1-C2	4.68	123.08	115.36
32	1a	1207	2MG	C6-N1-C2	4.67	123.55	115.18
55	1x	8	4SU	C5-C4-N3	-4.66	117.59	123.83
54	2w	46	7MG	C5-C4-N3	-4.62	118.95	126.49
1	1A	1942	4OC	C2-N3-C4	4.60	121.00	116.34
32	2a	1207	2MG	C6-N1-C2	4.56	123.35	115.18
54	1w	46	7MG	C5-C4-N3	-4.55	119.06	126.49
32	2a	1207	2MG	C5-C6-N1	-4.52	117.25	123.43
56	2y	39	PSU	C5-C1'-C2'	-4.50	107.28	115.32
56	1y	39	PSU	C5-C6-N1	-4.47	118.94	124.44
1	1A	1939	PSU	C6-N1-C2	4.43	122.67	115.36
32	2a	527	7MG	C6-C5-C4	4.42	119.95	115.20
32	2a	516	PSU	C5-C6-N1	-4.42	119.01	124.44
1	2A	1920	4OC	C2-N3-C4	4.40	120.80	116.34
1	1A	1939	PSU	C5-C6-N1	-4.38	119.06	124.44
32	1a	966	M2G	C2-N3-C4	4.38	120.25	115.28
56	2y	55	PSU	C5-C6-N1	-4.38	119.06	124.44
1	2A	2251	OMG	C2-N3-C4	4.37	120.35	115.36
32	2a	1207	2MG	C2-N3-C4	4.35	120.21	115.28
32	2a	1402	4OC	CM4-N4-C4	-4.32	119.26	122.97
54	2w	32	PSU	C5-C6-N1	-4.31	119.14	124.44
1	1A	2617	PSU	C6-N1-C2	4.29	122.44	115.36
1	2A	1911	PSU	C6-N1-C2	4.29	122.43	115.36
56	1y	39	PSU	C6-N1-C2	4.27	122.41	115.36
54	1w	39	PSU	C6-N1-C2	4.23	122.34	115.36
54	2w	37	MIA	C2-N3-C4	4.22	121.14	115.32
54	1w	39	PSU	C5-C6-N1	-4.21	119.26	124.44
55	2x	55	PSU	C6-N1-C2	4.21	122.30	115.36
54	2w	39	PSU	C5-C6-N1	-4.20	119.28	124.44
54	1w	37	MIA	C15-C14-C13	-4.20	110.52	122.65
55	1x	55	PSU	C5-C6-N1	-4.19	119.28	124.44
32	1a	527	7MG	C6-N1-C2	4.19	122.59	115.93
32	2a	966	M2G	C5-C6-N1	-4.19	117.70	123.43
32	2a	527	7MG	C6-N1-C2	4.18	122.56	115.93
54	2w	32	PSU	C6-N1-C2	4.16	122.23	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	8	4SU	C2-N3-C4	4.15	121.16	115.15
1	2A	1911	PSU	C5-C6-N1	-4.14	119.36	124.44
56	2y	46	7MG	C5-C6-N1	-4.13	114.65	123.14
54	2w	39	PSU	C6-N1-C2	4.13	122.17	115.36
55	1x	55	PSU	C6-N1-C2	4.12	122.16	115.36
54	1w	32	PSU	C5-C6-N1	-4.11	119.38	124.44
56	1y	55	PSU	C6-N1-C2	4.11	122.14	115.36
56	1y	55	PSU	C5-C6-N1	-4.10	119.40	124.44
56	2y	39	PSU	C6-N1-C2	4.08	122.10	115.36
1	2A	1917	PSU	C6-N1-C2	4.08	122.10	115.36
56	2y	46	7MG	C6-C5-C4	4.08	119.58	115.20
56	2y	39	PSU	C5-C6-N1	-4.08	119.43	124.44
54	2w	55	PSU	C6-N1-C2	4.07	122.08	115.36
56	1y	46	7MG	C6-C5-C4	4.07	119.57	115.20
1	2A	1917	PSU	C5-C1'-C2'	-4.07	108.06	115.32
1	1A	2263	OMG	C6-N1-C2	4.07	122.39	115.93
1	2A	2605	PSU	C6-N1-C2	4.06	122.05	115.36
32	2a	516	PSU	C6-N1-C2	4.05	122.05	115.36
54	1w	37	MIA	C2-N3-C4	4.05	120.90	115.32
55	2x	55	PSU	C5-C6-N1	-4.04	119.47	124.44
32	1a	966	M2G	C5-C6-N1	-4.03	117.92	123.43
56	1y	8	4SU	C2-N3-C4	4.03	120.99	115.15
32	1a	1207	2MG	C6-C5-C4	-4.02	116.96	120.80
54	2w	55	PSU	C5-C1'-C2'	-4.02	108.15	115.32
56	2y	32	PSU	C6-N1-C2	4.01	121.98	115.36
56	1y	32	PSU	C6-N1-C2	4.00	121.96	115.36
54	1w	46	7MG	C6-C5-C4	3.98	119.47	115.20
54	1w	32	PSU	C6-N1-C2	3.98	121.92	115.36
32	2a	1519	MA6	C4-C5-N7	-3.96	105.27	109.40
54	2w	37	MIA	C5-C6-N1	-3.94	117.54	120.81
1	1A	2617	PSU	C5-C6-N1	-3.93	119.61	124.44
32	1a	516	PSU	C6-N1-C2	3.93	121.84	115.36
54	1w	46	7MG	C5-C6-N1	-3.92	115.08	123.14
54	2w	55	PSU	C5-C6-N1	-3.90	119.64	124.44
1	1A	2263	OMG	C5-C6-N1	-3.90	118.10	123.43
1	1A	1933	PSU	C6-N1-C2	3.88	121.76	115.36
1	1A	1933	PSU	C5-C6-N1	-3.84	119.72	124.44
32	1a	967	5MC	C2-N3-C4	3.83	120.64	116.02
32	2a	1207	2MG	C6-C5-C4	-3.83	117.14	120.80
1	2A	2251	OMG	C6-N1-C2	3.82	121.99	115.93
56	1y	46	7MG	C5-C6-N1	-3.77	115.39	123.14
54	1w	55	PSU	C6-N1-C2	3.76	121.56	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1939	5MU	C5-C6-N1	-3.75	118.15	122.19
32	1a	527	7MG	C5-C6-N1	-3.74	115.46	123.14
1	1A	2263	OMG	N3-C2-N1	-3.73	122.25	127.22
32	2a	1407	5MC	C2-N3-C4	3.73	120.52	116.02
32	1a	1207	2MG	C4-C5-N7	-3.72	105.52	109.40
54	1w	37	MIA	C16-C14-C13	-3.69	111.98	122.65
56	2y	8	4SU	C2-N3-C4	3.68	120.49	115.15
54	2w	46	7MG	C5-C6-N1	-3.68	115.59	123.14
32	1a	516	PSU	C5-C6-N1	-3.66	119.94	124.44
32	1a	1518	MA6	C4-C5-N7	-3.66	105.59	109.40
32	2a	1518	MA6	C9-N6-C6	-3.64	108.48	119.51
32	2a	527	7MG	C5-C6-N1	-3.64	115.65	123.14
1	1A	2617	PSU	C5-C1'-C2'	-3.63	108.84	115.32
55	2x	8	4SU	C5-C4-N3	-3.63	118.97	123.83
32	1a	1518	MA6	C9-N6-C6	-3.61	108.59	119.51
32	2a	1404	5MC	C2-N3-C4	3.60	120.36	116.02
32	1a	1519	MA6	N3-C2-N1	-3.59	123.06	128.68
1	2A	2251	OMG	C5-C6-N1	-3.59	118.52	123.43
56	1y	32	PSU	C5-C6-N1	-3.58	120.04	124.44
55	1x	32	5MC	C2-N3-C4	3.58	120.34	116.02
1	2A	1911	PSU	C5-C1'-C2'	-3.55	108.99	115.32
54	2w	46	7MG	C6-C5-C4	3.51	118.97	115.20
1	2A	2251	OMG	C6-C5-C4	-3.51	117.44	120.80
55	2x	32	5MC	C2-N3-C4	3.47	120.21	116.02
32	1a	1407	5MC	C2-N3-C4	3.47	120.20	116.02
56	2y	32	PSU	C5-C6-N1	-3.44	120.21	124.44
1	1A	1964	5MC	C2-N3-C4	3.41	120.14	116.02
1	2A	2605	PSU	C5-C1'-C2'	-3.40	109.25	115.32
32	1a	1519	MA6	C9-N6-C6	-3.38	109.28	119.51
32	1a	1400	5MC	C2-N3-C4	3.35	120.07	116.02
32	1a	1519	MA6	C4-C5-N7	-3.35	105.91	109.40
1	1A	1964	5MC	N4-C4-N3	3.32	121.72	117.03
54	1w	37	MIA	C12-N6-C6	-3.31	117.64	122.55
32	1a	966	M2G	C6-C5-C4	-3.29	117.65	120.80
54	2w	32	PSU	C5-C1'-C2'	-3.27	109.48	115.32
1	1A	2263	OMG	C6-C5-C4	-3.27	117.67	120.80
54	1w	37	MIA	C5-C6-N1	-3.23	118.13	120.81
1	1A	1984	5MC	C2-N3-C4	3.23	119.91	116.02
56	2y	37	MIA	N3-C2-N1	-3.23	123.64	128.68
32	2a	1518	MA6	C4-C5-N7	-3.19	106.07	109.40
1	2A	1942	5MC	C2-N3-C4	3.18	119.86	116.02
32	2a	1519	MA6	C9-N6-C6	-3.18	109.89	119.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1y	37	MIA	N3-C2-N1	-3.17	123.72	128.68
32	2a	1400	5MC	C2-N3-C4	3.14	119.81	116.02
1	2A	1962	5MC	C2-N3-C4	3.14	119.81	116.02
55	1x	55	PSU	C5-C1'-C2'	-3.13	109.73	115.32
32	2a	967	5MC	C2-N3-C4	3.12	119.79	116.02
54	1w	55	PSU	C5-C6-N1	-3.09	120.65	124.44
32	1a	1518	MA6	N3-C2-N1	-3.06	123.89	128.68
32	2a	966	M2G	C6-C5-C4	-3.04	117.89	120.80
54	2w	37	MIA	C11-S10-C2	-3.03	100.00	102.27
1	2A	2251	OMG	N3-C2-N1	-3.01	123.20	127.22
56	1y	32	PSU	O4'-C1'-C5	2.99	114.55	109.93
32	2a	1207	2MG	CM2-N2-C2	-2.98	119.99	123.59
32	2a	1519	MA6	N3-C2-N1	-2.97	124.03	128.68
32	2a	1518	MA6	N3-C2-N1	-2.93	124.10	128.68
32	1a	1404	5MC	C5-C6-N1	-2.92	119.04	122.19
32	1a	1404	5MC	C2-N3-C4	2.92	119.55	116.02
54	1w	8	4SU	C5-C4-N3	-2.90	119.95	123.83
54	1w	37	MIA	C2-N1-C6	2.89	122.36	117.19
1	1A	1961	5MU	C5-C6-N1	-2.87	119.10	122.19
54	2w	8	4SU	C5-C4-N3	-2.84	120.03	123.83
56	2y	8	4SU	C5-C4-N3	-2.84	120.03	123.83
54	2w	39	PSU	C5-C1'-C2'	-2.84	110.25	115.32
1	1A	2515	2MA	C4-C5-N7	-2.84	106.44	109.40
56	2y	37	MIA	C4-C5-N7	-2.83	106.45	109.40
1	2A	1962	5MC	N4-C4-N3	2.83	121.03	117.03
32	2a	1407	5MC	N4-C4-N3	2.83	121.03	117.03
54	2w	54	5MU	C5-C6-N1	-2.83	119.15	122.19
54	2w	46	7MG	C5-C4-N9	-2.77	102.56	106.44
1	1A	1933	PSU	C5-C1'-C2'	-2.77	110.38	115.32
54	2w	37	MIA	C2-N1-C6	2.76	122.12	117.19
55	1x	32	5MC	N4-C4-N3	2.74	120.90	117.03
1	2A	1962	5MC	C5-C6-N1	-2.74	119.25	122.19
1	2A	1942	5MC	N4-C4-N3	2.73	120.89	117.03
56	1y	46	7MG	C5-C4-N9	-2.72	102.62	106.44
54	1w	46	7MG	C5-C4-N9	-2.71	102.64	106.44
32	1a	1207	2MG	CM2-N2-C2	-2.71	120.33	123.59
32	2a	1407	5MC	C5-C6-N1	-2.70	119.29	122.19
32	1a	966	M2G	CM2-N2-C2	-2.69	118.72	121.29
55	1x	32	5MC	C5-C6-N1	-2.68	119.31	122.19
56	2y	46	7MG	C5-C4-N9	-2.67	102.70	106.44
54	2w	46	7MG	C8-N7-C5	2.66	115.86	108.94
54	2w	37	MIA	C4-C5-N7	-2.66	106.63	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1404	5MC	N4-C4-N3	2.65	120.78	117.03
55	2x	32	5MC	N4-C4-N3	2.64	120.76	117.03
32	1a	1407	5MC	N4-C4-N3	2.63	120.76	117.03
1	2A	1942	5MC	C5-C6-N1	-2.63	119.36	122.19
56	2y	46	7MG	N2-C2-N3	2.63	121.34	117.25
56	1y	55	PSU	C5-C1'-C2'	-2.60	110.67	115.32
32	2a	527	7MG	C8-N7-C5	2.60	115.70	108.94
32	1a	1400	5MC	C5-C6-N1	-2.59	119.40	122.19
56	2y	46	7MG	C8-N7-C5	2.59	115.67	108.94
32	2a	1400	5MC	N4-C4-N3	2.58	120.68	117.03
32	2a	1207	2MG	C4-C5-N7	-2.58	106.71	109.40
55	2x	54	5MU	C5-C6-N1	-2.57	119.43	122.19
56	1y	8	4SU	C5-C4-N3	-2.55	120.42	123.83
56	1y	46	7MG	C8-N7-C5	2.54	115.55	108.94
32	2a	1207	2MG	N2-C2-N3	2.54	119.40	116.96
54	1w	46	7MG	C8-N7-C5	2.53	115.52	108.94
32	2a	966	M2G	C4-C5-N7	-2.53	106.76	109.40
56	1y	32	PSU	C5-C1'-C2'	-2.52	110.82	115.32
54	2w	37	MIA	C12-N6-C6	-2.51	120.71	122.87
32	2a	967	5MC	N4-C4-N3	2.50	120.57	117.03
56	1y	37	MIA	C4-C5-N7	-2.50	106.80	109.40
32	2a	967	5MC	C5-C6-N1	-2.50	119.50	122.19
32	1a	527	7MG	C8-N7-C5	2.49	115.42	108.94
32	1a	1400	5MC	N4-C4-N3	2.48	120.53	117.03
54	1w	37	MIA	C4-C5-N7	-2.46	106.84	109.40
54	1w	37	MIA	N3-C2-N1	-2.41	122.55	126.98
54	1w	39	PSU	C5-C1'-C2'	-2.41	111.03	115.32
32	2a	1400	5MC	C5-C6-N1	-2.40	119.60	122.19
54	1w	32	PSU	C5-C1'-C2'	-2.40	111.04	115.32
56	1y	54	5MU	C5-C6-N1	-2.39	119.62	122.19
32	1a	966	M2G	C4-C5-N7	-2.33	106.97	109.40
1	2A	1915	5MU	C5-C6-N1	-2.32	119.69	122.19
32	2a	516	PSU	O4'-C1'-C2'	2.31	108.41	104.66
56	1y	46	7MG	C2-N3-C4	2.30	120.26	113.89
32	1a	1207	2MG	N3-C2-N1	-2.29	122.60	126.23
55	1x	32	5MC	CM5-C5-C4	-2.29	119.41	121.72
1	1A	2263	OMG	C4-C5-N7	-2.25	107.05	109.40
1	1A	1937	5MU	C5-C6-N1	-2.24	119.78	122.19
55	1x	54	5MU	C5-C6-N1	-2.23	119.79	122.19
54	2w	37	MIA	N3-C2-N1	-2.22	122.90	126.98
32	2a	1518	MA6	C10-N6-C9	-2.22	108.97	116.12
32	2a	1404	5MC	N4-C4-N3	2.20	120.14	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2y	46	7MG	C2-N3-C4	2.17	119.90	113.89
32	1a	1518	MA6	C10-N6-C6	-2.17	112.95	119.51
1	1A	1964	5MC	C5-C6-N1	-2.17	119.86	122.19
1	1A	2564	2MU	C5-C4-N3	-2.15	118.57	123.31
54	1w	37	MIA	C11-S10-C2	-2.15	100.66	102.27
54	1w	37	MIA	C16-C14-C15	-2.14	109.87	114.60
1	2A	2503	2MA	C4-C5-N7	-2.14	107.16	109.40
32	1a	527	7MG	C5-C4-N9	-2.14	103.44	106.44
55	2x	32	5MC	CM5-C5-C4	-2.14	119.56	121.72
32	2a	1518	MA6	C10-N6-C6	-2.13	113.05	119.51
32	2a	527	7MG	C5-C4-N9	-2.12	103.47	106.44
32	1a	1407	5MC	C5-C6-N1	-2.12	119.92	122.19
32	2a	1407	5MC	CM5-C5-C4	-2.11	119.58	121.72
54	2w	46	7MG	CM7-N7-C5	2.10	132.07	124.01
32	2a	1207	2MG	N3-C2-N1	-2.09	122.92	126.23
55	2x	32	5MC	C5-C6-N1	-2.09	119.94	122.19
56	2y	55	PSU	O4'-C1'-C2'	2.09	108.05	104.66
54	1w	54	5MU	C5-C6-N1	-2.09	119.94	122.19
56	2y	46	7MG	N1-C2-N3	-2.09	122.14	125.42
32	1a	967	5MC	N4-C4-N3	2.08	119.97	117.03
1	2A	2552	2MU	C5-C4-N3	-2.08	118.74	123.31
32	1a	527	7MG	C2-N3-C4	2.07	119.61	113.89
54	2w	37	MIA	N6-C6-N1	2.07	121.08	118.50
32	2a	527	7MG	CM7-N7-C5	2.06	131.93	124.01
32	2a	1404	5MC	C5-C6-N1	-2.05	119.98	122.19
56	1y	46	7MG	CM7-N7-C5	2.05	131.89	124.01
56	2y	46	7MG	CM7-N7-C5	2.05	131.88	124.01
1	1A	1942	4OC	N4-C4-N3	2.05	119.73	116.49
32	2a	527	7MG	C2-N3-C4	2.04	119.53	113.89
54	2w	46	7MG	C2-N3-C4	2.03	119.49	113.89
32	1a	1518	MA6	C10-N6-C9	-2.02	109.62	116.12
32	1a	516	PSU	O4'-C1'-C2'	2.00	107.91	104.66

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	1y	54	5MU	C3'-C4'-C5'-O5'
56	1y	54	5MU	O4'-C4'-C5'-O5'
56	2y	54	5MU	C2'-C1'-N1-C6
56	2y	37	MIA	C3'-C4'-C5'-O5'
32	2a	1400	5MC	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
32	2a	1400	5MC	C2'-C1'-N1-C6
56	1y	37	MIA	C3'-C4'-C5'-O5'
56	1y	8	4SU	C2'-C1'-N1-C6
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
1	2A	1920	4OC	C2'-C1'-N1-C6
32	2a	1402	4OC	C5-C4-N4-CM4
56	2y	8	4SU	C2'-C1'-N1-C6
1	1A	1942	4OC	C2'-C1'-N1-C6
54	2w	76	F3N	C-CA-CB-CG
32	1a	1519	MA6	C5-C6-N6-C10
54	1w	46	7MG	C4'-C5'-O5'-P
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10
1	1A	1984	5MC	O4'-C1'-N1-C6
1	1A	1984	5MC	C2'-C1'-N1-C6
56	1y	46	7MG	C4'-C5'-O5'-P
56	1y	46	7MG	C3'-C4'-C5'-O5'
54	1w	37	MIA	C5-C6-N6-C12
54	1w	37	MIA	N1-C2-S10-C11
54	1w	37	MIA	N3-C2-S10-C11
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16
32	2a	1518	MA6	C5-C6-N6-C10
56	2y	55	PSU	C2'-C1'-C5-C4
56	2y	55	PSU	C2'-C1'-C5-C6
43	2l	92	0TD	CG-CB-SB-CSB
32	1a	1518	MA6	C5-C6-N6-C10
32	1a	1519	MA6	O4'-C4'-C5'-O5'
56	2y	37	MIA	O4'-C4'-C5'-O5'
56	1y	37	MIA	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
54	1w	37	MIA	N1-C6-N6-C12
56	2y	54	5MU	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
56	1y	46	7MG	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C9
32	2a	1518	MA6	C5-C6-N6-C9
32	1a	1518	MA6	C5-C6-N6-C9
56	2y	54	5MU	O4'-C4'-C5'-O5'
56	2y	46	7MG	O4'-C1'-N9-C4
56	2y	32	PSU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
56	2y	46	7MG	C2'-C1'-N9-C8
56	1y	46	7MG	C2'-C1'-N9-C8
54	2w	46	7MG	C4'-C5'-O5'-P
54	2w	76	F3N	N-CA-CB-CG
55	1x	55	PSU	O4'-C4'-C5'-O5'
56	2y	46	7MG	O4'-C1'-N9-C8
1	2A	1920	4OC	C3'-C2'-O2'-CM2
54	1w	46	7MG	C2'-C1'-N9-C8
32	2a	1519	MA6	C4'-C5'-O5'-P
54	2w	76	F3N	C2'-C3'-N3'-C
56	2y	55	PSU	O4'-C1'-C5-C6
1	2A	2503	2MA	O4'-C4'-C5'-O5'
56	1y	46	7MG	C2'-C1'-N9-C4
56	2y	55	PSU	O4'-C1'-C5-C4
43	2l	92	0TD	CA-CB-SB-CSB
32	1a	527	7MG	C3'-C4'-C5'-O5'
56	1y	32	PSU	C2'-C1'-C5-C6
32	2a	967	5MC	O4'-C4'-C5'-O5'
56	1y	46	7MG	O4'-C1'-N9-C8
1	2A	2503	2MA	C4'-C5'-O5'-P
56	2y	32	PSU	C3'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
54	2w	46	7MG	C2'-C1'-N9-C8
1	1A	2515	2MA	O4'-C4'-C5'-O5'
56	2y	55	PSU	O4'-C4'-C5'-O5'
56	2y	37	MIA	C4'-C5'-O5'-P
1	1A	2515	2MA	C4'-C5'-O5'-P
32	2a	527	7MG	C4'-C5'-O5'-P
32	2a	966	M2G	N3-C2-N2-CM1
54	2w	46	7MG	C3'-C4'-C5'-O5'
54	2w	76	F3N	CA-CB-CG-CD1

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	2515	2MA	1	0
1	2A	1915	5MU	1	0
1	2A	2503	2MA	2	0
1	2A	1920	4OC	3	0
1	1A	2617	PSU	1	0
1	2A	1942	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	2564	2MU	1	0
1	2A	2552	2MU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2411 ligands modelled in this entry, 2407 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	AQJ	1A	3969	-	38,38,38	3.10	7 (18%)	44,56,56	1.54	8 (18%)
61	SF4	2d	501	35	0,12,12	0.00	-	-		
59	AQJ	2A	3677	-	38,38,38	3.14	7 (18%)	44,56,56	1.53	4 (9%)
61	SF4	1d	501	35	0,12,12	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	AQJ	1A	3969	-	-	14/54/70/70	0/1/2/2
61	SF4	2d	501	35	-	-	0/6/5/5
59	AQJ	2A	3677	-	-	5/54/70/70	0/1/2/2
61	SF4	1d	501	35	-	-	0/6/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1A	3969	AQJ	CBK-CAP	-9.82	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	2A	3677	AQJ	CBK-CAP	-9.67	1.39	1.51
59	2A	3677	AQJ	CBC-CAY	-9.28	1.39	1.52
59	1A	3969	AQJ	CBD-CAY	-8.55	1.39	1.52
59	1A	3969	AQJ	CBC-CAY	-7.66	1.42	1.52
59	2A	3677	AQJ	CBD-CAY	-7.66	1.40	1.52
59	2A	3677	AQJ	CBC-CAX	-7.64	1.37	1.51
59	1A	3969	AQJ	CBA-CAW	-7.49	1.38	1.51
59	2A	3677	AQJ	CBA-CAW	-6.62	1.39	1.51
59	1A	3969	AQJ	CBC-CAX	-5.44	1.41	1.51
59	1A	3969	AQJ	CBB-CBH	3.90	1.60	1.53
59	1A	3969	AQJ	CAO-CAP	3.31	1.39	1.32
59	2A	3677	AQJ	CAO-CAP	3.14	1.39	1.32
59	2A	3677	AQJ	OAV-CBF	2.07	1.47	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	2A	3677	AQJ	CBG-OAT-CAX	-4.78	109.67	118.18
59	1A	3969	AQJ	OAT-CAX-CBC	4.73	115.69	110.88
59	2A	3677	AQJ	OAT-CAX-CBC	4.06	115.01	110.88
59	2A	3677	AQJ	OAK-CAX-CBC	-3.64	119.99	124.77
59	1A	3969	AQJ	CBG-OAT-CAX	-3.57	111.83	118.18
59	1A	3969	AQJ	OAK-CAX-CBC	-3.14	120.64	124.77
59	2A	3677	AQJ	OAT-CBG-CAQ	3.12	113.34	107.40
59	1A	3969	AQJ	OAT-CBG-CAQ	3.04	113.18	107.40
59	1A	3969	AQJ	CAB-CAZ-CAS	-3.03	108.64	113.40
59	1A	3969	AQJ	CBF-CBE-CBI	2.24	112.86	109.19
59	1A	3969	AQJ	CAS-CBI-NBJ	-2.18	109.51	115.67
59	1A	3969	AQJ	CAP-CAO-CAW	-2.08	117.48	121.93

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1A	3969	AQJ	CAO-CAP-CBK-OAN
59	2A	3677	AQJ	CAO-CAP-CBK-OAN
59	1A	3969	AQJ	OAU-CBF-OAV-CBH
59	1A	3969	AQJ	CBA-CAR-CBB-CAD
59	1A	3969	AQJ	OAJ-CAW-CBA-CAC
59	1A	3969	AQJ	CAO-CAW-CBA-CAC
59	2A	3677	AQJ	CAS-CBI-NBJ-CAH
59	2A	3677	AQJ	CAO-CAP-CBK-CBG

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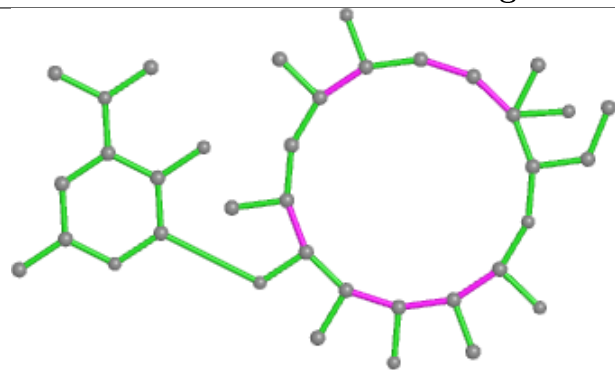
Mol	Chain	Res	Type	Atoms
59	2A	3677	AQJ	CAA-CAQ-CBG-OAT
59	1A	3969	AQJ	CAS-CBI-NBJ-CAH
59	1A	3969	AQJ	CBA-CAR-CBB-CBH
59	2A	3677	AQJ	CAA-CAQ-CBG-CBK
59	1A	3969	AQJ	CBB-CAR-CBA-CAC
59	1A	3969	AQJ	CBE-CBF-OAV-CBH
59	1A	3969	AQJ	CBB-CAR-CBA-CAW
59	1A	3969	AQJ	OAL-CAY-CBC-CAX
59	1A	3969	AQJ	CAA-CAQ-CBG-OAT
59	1A	3969	AQJ	CBD-CAY-CBC-CAX
59	1A	3969	AQJ	CAA-CAQ-CBG-CBK

There are no ring outliers.

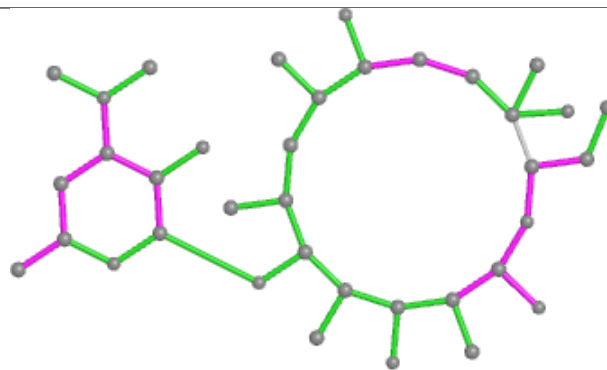
No monomer is involved in short contacts.

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

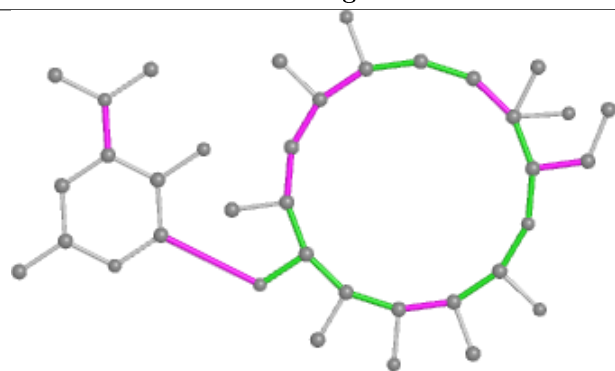
Ligand AQJ 1A 3969



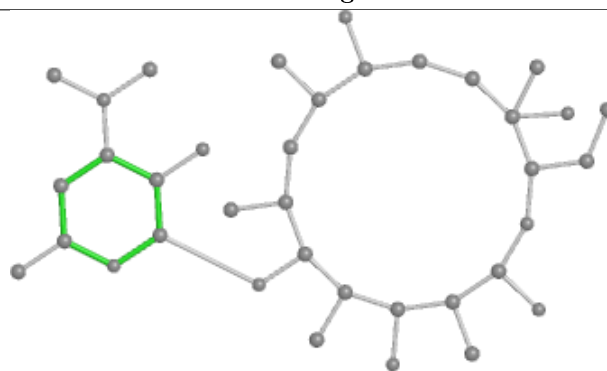
Bond lengths



Bond angles

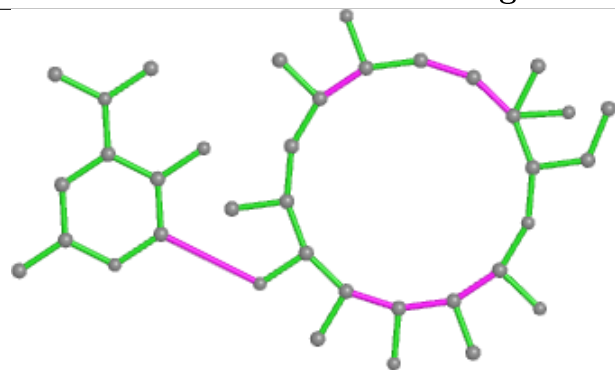


Torsions

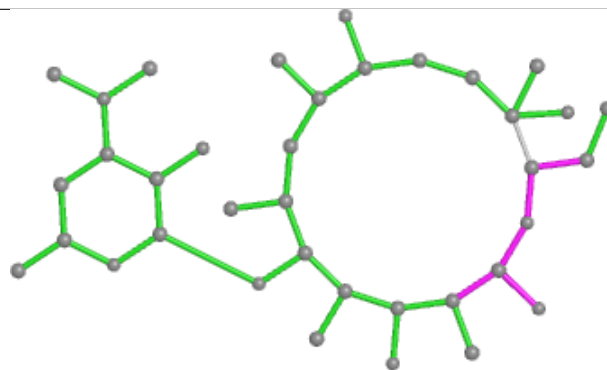


Rings

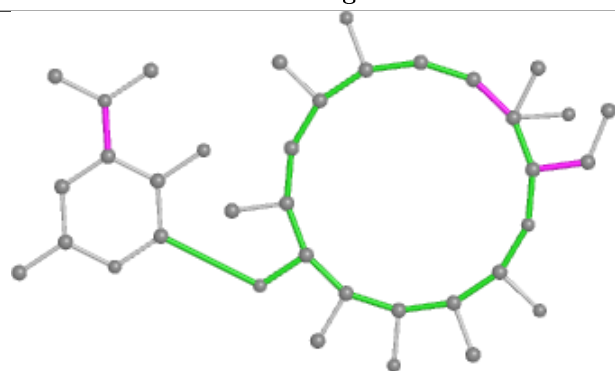
Ligand AQJ 2A 3677



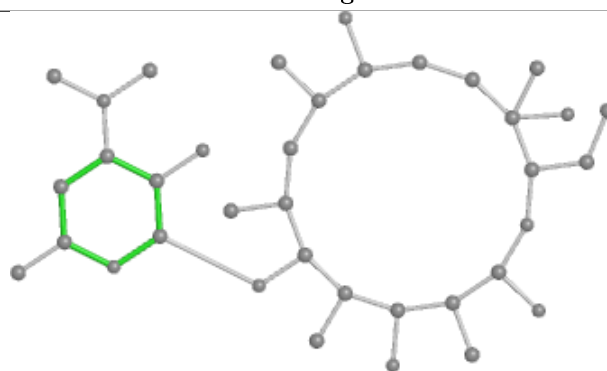
Bond lengths



Bond angles



Torsions



Rings

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%)	0.37	105 (3%) 41 34	13, 30, 84, 98	0
1	2A	2789/2915 (95%)	0.25	64 (2%) 60 54	27, 51, 81, 94	0
2	1B	120/121 (99%)	0.14	0 100 100	21, 40, 54, 78	0
2	2B	120/121 (99%)	0.37	5 (4%) 36 29	53, 71, 81, 88	0
3	1D	275/276 (99%)	0.40	1 (0%) 92 91	14, 34, 49, 66	0
3	2D	275/276 (99%)	0.50	3 (1%) 80 78	25, 47, 58, 76	0
4	1E	204/206 (99%)	0.34	0 100 100	12, 37, 53, 65	0
4	2E	204/206 (99%)	0.47	3 (1%) 73 70	30, 52, 66, 79	0
5	1F	203/210 (96%)	0.24	0 100 100	14, 38, 60, 72	0
5	2F	203/210 (96%)	0.41	1 (0%) 91 89	29, 61, 73, 80	0
6	1G	181/182 (99%)	0.17	1 (0%) 89 88	32, 50, 66, 77	0
6	2G	181/182 (99%)	1.30	44 (24%) 0 0	61, 73, 80, 85	0
7	1H	174/180 (96%)	0.20	0 100 100	32, 48, 60, 68	0
7	2H	174/180 (96%)	2.18	91 (52%) 0 0	57, 75, 82, 87	0
8	1I	146/148 (98%)	0.34	3 (2%) 63 58	39, 65, 74, 79	0
8	2I	146/148 (98%)	0.75	22 (15%) 2 1	49, 68, 78, 85	0
9	1N	140/140 (100%)	0.40	0 100 100	22, 35, 53, 59	0
9	2N	140/140 (100%)	0.78	8 (5%) 23 18	40, 58, 69, 73	0
10	1O	122/122 (100%)	0.29	1 (0%) 86 84	20, 37, 55, 62	0
10	2O	122/122 (100%)	0.48	2 (1%) 72 68	35, 51, 62, 69	0
11	1P	149/150 (99%)	0.32	1 (0%) 87 86	12, 40, 62, 73	0
11	2P	149/150 (99%)	0.68	4 (2%) 54 48	33, 61, 74, 82	0
12	1Q	141/141 (100%)	0.38	0 100 100	19, 36, 47, 69	0
12	2Q	141/141 (100%)	1.43	38 (26%) 0 0	37, 59, 70, 78	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.27	0 100 100	19, 31, 46, 56	0
13	2R	118/118 (100%)	0.39	2 (1%) 70 66	35, 48, 59, 65	0
14	1S	110/112 (98%)	0.32	0 100 100	30, 43, 53, 60	0
14	2S	110/112 (98%)	1.22	21 (19%) 1 0	57, 67, 76, 79	0
15	1T	131/146 (89%)	0.30	5 (3%) 40 33	28, 41, 63, 82	0
15	2T	131/146 (89%)	0.37	3 (2%) 60 54	45, 55, 69, 79	0
16	1U	116/118 (98%)	0.41	0 100 100	15, 26, 43, 63	0
16	2U	116/118 (98%)	0.47	1 (0%) 84 82	38, 54, 68, 75	0
17	1V	101/101 (100%)	0.20	0 100 100	18, 36, 50, 65	0
17	2V	101/101 (100%)	0.39	2 (1%) 65 60	42, 64, 73, 77	0
18	1W	112/113 (99%)	0.40	1 (0%) 84 82	20, 27, 46, 73	0
18	2W	112/113 (99%)	0.52	1 (0%) 84 82	34, 45, 60, 74	0
19	1X	95/96 (98%)	0.38	0 100 100	23, 33, 53, 60	0
19	2X	95/96 (98%)	0.47	2 (2%) 63 58	44, 54, 65, 74	0
20	1Y	107/110 (97%)	0.32	0 100 100	28, 42, 61, 72	0
20	2Y	107/110 (97%)	0.71	2 (1%) 66 62	51, 64, 74, 83	0
21	1Z	154/206 (74%)	0.40	5 (3%) 47 40	36, 54, 73, 95	0
21	2Z	160/206 (77%)	1.36	36 (22%) 0 0	61, 71, 82, 92	0
22	10	83/85 (97%)	0.35	0 100 100	22, 31, 41, 55	0
22	20	83/85 (97%)	1.01	9 (10%) 5 3	41, 55, 65, 71	0
23	11	97/98 (98%)	0.38	1 (1%) 82 80	21, 41, 62, 71	0
23	21	97/98 (98%)	0.47	2 (2%) 63 58	35, 52, 67, 72	0
24	12	70/72 (97%)	0.48	0 100 100	29, 43, 55, 59	0
24	22	70/72 (97%)	0.24	0 100 100	52, 64, 70, 75	0
25	13	59/60 (98%)	0.31	0 100 100	22, 32, 53, 68	0
25	23	59/60 (98%)	1.24	16 (27%) 0 0	49, 59, 71, 76	0
26	14	69/71 (97%)	0.37	4 (5%) 23 17	48, 63, 79, 86	0
26	24	69/71 (97%)	1.50	22 (31%) 0 0	66, 79, 87, 88	0
27	15	59/60 (98%)	0.42	1 (1%) 70 66	17, 28, 44, 56	0
27	25	59/60 (98%)	0.31	0 100 100	28, 46, 61, 66	0
28	16	53/54 (98%)	0.14	0 100 100	25, 38, 47, 57	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.67	3 (5%) 23 18	45, 55, 62, 67	0
29	17	48/49 (97%)	0.53	2 (4%) 36 29	15, 24, 52, 57	0
29	27	48/49 (97%)	0.58	2 (4%) 36 29	28, 40, 56, 63	0
30	18	64/65 (98%)	0.40	0 100 100	23, 28, 38, 49	0
30	28	64/65 (98%)	0.71	1 (1%) 72 68	39, 50, 58, 64	0
31	19	37/37 (100%)	0.39	0 100 100	22, 34, 50, 56	0
31	29	37/37 (100%)	1.66	12 (32%) 0 0	51, 59, 69, 74	0
32	1a	1488/1521 (97%)	0.22	37 (2%) 57 51	30, 56, 80, 95	0
32	2a	1491/1521 (98%)	0.28	68 (4%) 32 26	44, 67, 83, 96	0
33	1b	231/256 (90%)	0.28	6 (2%) 56 50	52, 67, 78, 85	0
33	2b	231/256 (90%)	1.13	41 (17%) 1 0	62, 76, 84, 91	0
34	1c	206/239 (86%)	0.44	9 (4%) 34 27	50, 60, 71, 84	0
34	2c	206/239 (86%)	1.35	58 (28%) 0 0	63, 74, 80, 87	0
35	1d	208/209 (99%)	0.62	7 (3%) 45 38	47, 60, 68, 79	0
35	2d	208/209 (99%)	0.77	14 (6%) 17 13	50, 61, 70, 83	0
36	1e	148/162 (91%)	0.42	2 (1%) 75 71	44, 56, 65, 73	0
36	2e	148/162 (91%)	0.89	15 (10%) 7 4	59, 69, 77, 82	0
37	1f	100/101 (99%)	0.36	6 (6%) 21 16	44, 55, 66, 71	0
37	2f	100/101 (99%)	0.11	0 100 100	55, 64, 72, 76	0
38	1g	155/156 (99%)	0.49	9 (5%) 23 17	49, 61, 72, 88	0
38	2g	155/156 (99%)	1.09	25 (16%) 1 1	63, 72, 80, 90	0
39	1h	137/138 (99%)	0.61	8 (5%) 23 17	49, 59, 68, 75	0
39	2h	137/138 (99%)	0.72	9 (6%) 18 13	58, 69, 76, 88	0
40	1i	127/128 (99%)	0.52	5 (3%) 39 32	40, 63, 74, 78	0
40	2i	127/128 (99%)	1.76	49 (38%) 0 0	63, 75, 81, 84	0
41	1j	97/105 (92%)	0.48	3 (3%) 49 42	46, 66, 77, 80	0
41	2j	96/105 (91%)	1.60	32 (33%) 0 0	67, 75, 82, 84	0
42	1k	114/129 (88%)	0.79	9 (7%) 12 9	35, 58, 70, 74	0
42	2k	114/129 (88%)	0.64	8 (7%) 16 12	53, 67, 74, 80	0
43	1l	121/132 (91%)	0.33	3 (2%) 57 51	39, 48, 62, 66	0
43	2l	121/132 (91%)	0.86	10 (8%) 11 8	46, 58, 67, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.41	4 (3%) 46 39	43, 60, 66, 73	0
44	2m	122/126 (96%)	1.45	34 (27%) 0 0	63, 73, 80, 84	0
45	1n	60/61 (98%)	0.86	4 (6%) 17 13	49, 56, 62, 66	0
45	2n	60/61 (98%)	3.17	41 (68%) 0 0	68, 74, 80, 81	0
46	1o	88/89 (98%)	0.38	0 100 100	42, 56, 68, 73	0
46	2o	88/89 (98%)	0.30	0 100 100	54, 64, 72, 78	0
47	1p	82/88 (93%)	1.12	13 (15%) 1 1	53, 63, 69, 76	0
47	2p	82/88 (93%)	0.69	4 (4%) 29 23	52, 61, 68, 71	0
48	1q	99/105 (94%)	0.90	10 (10%) 7 4	48, 59, 69, 72	0
48	2q	99/105 (94%)	1.09	19 (19%) 1 0	57, 66, 72, 76	0
49	1r	68/88 (77%)	0.32	2 (2%) 51 45	46, 57, 70, 72	0
49	2r	68/88 (77%)	0.44	2 (2%) 51 45	57, 66, 74, 77	0
50	1s	83/93 (89%)	0.37	3 (3%) 42 35	48, 60, 69, 73	0
50	2s	83/93 (89%)	1.55	28 (33%) 0 0	66, 75, 81, 88	0
51	1t	96/106 (90%)	1.29	23 (23%) 0 0	54, 62, 73, 80	0
51	2t	96/106 (90%)	0.94	9 (9%) 8 5	51, 61, 73, 77	0
52	1u	23/27 (85%)	0.97	2 (8%) 10 7	51, 58, 61, 65	0
52	2u	23/27 (85%)	3.44	18 (78%) 0 0	66, 74, 80, 84	0
53	1v	13/24 (54%)	1.46	3 (23%) 0 0	37, 50, 80, 82	0
53	2v	13/24 (54%)	2.49	8 (61%) 0 0	59, 68, 88, 89	0
54	1w	66/76 (86%)	0.34	4 (6%) 21 16	24, 65, 79, 91	0
54	2w	64/76 (84%)	1.15	14 (21%) 0 0	42, 76, 83, 86	0
55	1x	72/77 (93%)	0.23	1 (1%) 75 71	22, 55, 71, 82	0
55	2x	72/77 (93%)	0.69	3 (4%) 36 29	35, 69, 79, 85	0
56	1y	67/76 (88%)	2.51	43 (64%) 0 0	43, 85, 89, 93	0
56	2y	66/76 (86%)	2.47	38 (57%) 0 0	54, 88, 91, 93	0
All	All	20873/21748 (95%)	0.52	1316 (6%) 20 15	12, 56, 79, 98	0

All (1316) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
38	2g	82	GLY	9.6
56	1y	35	A	9.5

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Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	9.3
38	1g	82	GLY	9.3
44	2m	124	PRO	9.3
38	2g	80	VAL	9.2
45	2n	34	TYR	8.6
56	2y	34	G	8.6
21	2Z	155	LEU	7.6
40	2i	108	VAL	7.3
26	24	51	ASP	7.1
45	2n	39	LEU	7.0
41	2j	44	VAL	6.9
53	2v	14	A	6.8
34	2c	160	ALA	6.8
21	1Z	147	GLY	6.6
14	2S	32	LEU	6.5
26	24	49	PHE	6.5
1	1A	1141	A	6.5
32	2a	1257	U	6.4
40	2i	125	TYR	6.4
1	2A	885	C	6.4
45	2n	25	VAL	6.4
45	2n	42	ILE	6.4
1	1A	2162	C	6.3
33	2b	187	LEU	6.2
1	2A	1509	C	6.1
41	2j	47	PHE	6.1
33	2b	165	VAL	6.1
21	2Z	148	ASP	6.1
52	2u	17	THR	6.1
51	2t	9	ASN	6.1
38	2g	81	GLY	6.0
56	2y	36	A	6.0
44	2m	122	LYS	6.0
45	2n	44	LEU	6.0
32	2a	1030(B)	C	6.0
33	2b	81	VAL	5.9
7	2H	30	LYS	5.8
52	2u	24	ARG	5.8
53	1v	13	A	5.8
38	1g	79	ARG	5.8
44	2m	121	LYS	5.8
45	2n	10	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	2A	883	G	5.8
41	2j	67	THR	5.7
1	1A	2151	C	5.7
38	2g	155	ARG	5.7
45	2n	35	ARG	5.6
21	2Z	124	ILE	5.6
45	2n	41	ARG	5.6
21	2Z	141	VAL	5.6
50	2s	82	GLY	5.6
52	2u	9	ARG	5.5
41	2j	66	ARG	5.5
56	1y	23	A	5.5
1	2A	884	C	5.4
52	2u	6	ARG	5.4
56	1y	36	A	5.4
56	1y	5	G	5.4
34	2c	158	GLY	5.3
6	2G	140	ILE	5.3
32	2a	1036	G	5.3
7	2H	101	ARG	5.3
7	2H	72	ILE	5.3
7	2H	35	VAL	5.3
45	2n	51	GLY	5.3
40	2i	109	VAL	5.3
56	1y	34	G	5.3
34	2c	155	GLY	5.3
6	2G	41	GLN	5.2
56	2y	35	A	5.2
1	1A	2152	U	5.2
6	2G	29	TRP	5.1
34	2c	8	ILE	5.1
38	1g	156	TRP	5.1
1	1A	2155	G	5.1
52	2u	14	TRP	5.1
45	2n	36	PHE	5.1
56	2y	62	C	5.0
21	2Z	147	GLY	5.0
1	1A	2154	U	5.0
1	1A	2164	C	5.0
32	1a	1030(B)	C	5.0
1	1A	931	C	5.0
1	1A	2153	G	5.0

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Mol	Chain	Res	Type	RSRZ
25	23	51	ALA	4.9
32	1a	1531	A	4.9
32	2a	1007	C	4.9
40	2i	14	VAL	4.9
38	2g	83	ALA	4.9
45	2n	31	ARG	4.9
7	2H	97	ARG	4.9
1	1A	2179	G	4.9
45	2n	61	TRP	4.9
53	2v	12	A	4.8
40	2i	114	TYR	4.8
32	2a	1034	G	4.8
38	2g	154	TYR	4.8
52	2u	2	GLY	4.8
26	24	52	THR	4.8
40	2i	128	ARG	4.8
52	2u	22	ARG	4.8
7	2H	2	SER	4.8
56	1y	24	G	4.8
32	1a	1028	C	4.8
1	1A	2167	C	4.7
1	1A	2183	C	4.7
56	2y	1	G	4.7
31	29	13	LYS	4.7
6	2G	23	PHE	4.7
1	2A	2112	G	4.7
56	2y	65	G	4.7
1	1A	2181	G	4.6
32	2a	1001(A)	G	4.6
44	2m	60	VAL	4.6
34	2c	163	ALA	4.6
1	1A	2163	G	4.6
7	2H	14	GLY	4.6
38	1g	80	VAL	4.6
40	2i	76	ALA	4.6
33	2b	122	PHE	4.6
54	2w	73	A	4.6
26	24	54	GLY	4.6
1	2A	886	C	4.6
32	1a	1030(D)	A	4.6
12	2Q	1	MET	4.6
32	2a	1001	A	4.5

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Mol	Chain	Res	Type	RSRZ
14	2S	4	LEU	4.5
38	1g	83	ALA	4.5
34	2c	199	LYS	4.5
52	2u	10	ARG	4.5
1	1A	2176	G	4.5
7	2H	115	VAL	4.5
33	2b	232	PRO	4.5
7	2H	121	ILE	4.5
7	2H	19	VAL	4.5
32	1a	1257	U	4.4
32	2a	1532	U	4.4
1	2A	229	A	4.4
34	2c	94	LEU	4.4
40	2i	111	ARG	4.4
1	2A	2147	G	4.4
40	2i	75	ASP	4.4
41	2j	6	ILE	4.4
52	2u	13	ILE	4.4
32	2a	1286	A	4.4
1	1A	932	C	4.3
1	2A	2146	C	4.3
33	2b	93	VAL	4.3
1	2A	2167	U	4.3
56	1y	47	U	4.3
12	2Q	79	LEU	4.3
26	24	45	GLY	4.3
40	2i	115	GLY	4.3
45	2n	33	VAL	4.3
21	2Z	144	LEU	4.3
41	2j	65	LEU	4.3
56	1y	64	A	4.3
56	1y	14	A	4.3
31	29	37	GLY	4.3
1	2A	887	A	4.2
41	2j	62	HIS	4.2
36	2e	12	LEU	4.2
44	2m	66	LEU	4.2
32	1a	163	C	4.2
21	2Z	126	VAL	4.2
7	2H	123	PHE	4.2
1	2A	2116	G	4.2
41	2j	54	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
50	2s	49	ILE	4.2
1	2A	2133	G	4.1
44	2m	96	LEU	4.1
1	1A	2174	G	4.1
33	2b	70	PHE	4.1
34	2c	190	ARG	4.1
7	2H	71	LEU	4.1
21	2Z	137	ILE	4.1
33	2b	214	ILE	4.1
3	2D	2	ALA	4.1
34	2c	28	GLN	4.1
38	2g	85	TYR	4.1
45	2n	26	ARG	4.1
34	1c	81	GLY	4.1
45	2n	38	GLY	4.1
56	2y	52	G	4.1
56	2y	61	C	4.1
26	24	68	ARG	4.1
7	2H	94	TYR	4.1
51	2t	20	LEU	4.0
1	2A	896	A	4.0
40	2i	36	TYR	4.0
38	2g	32	ARG	4.0
1	1A	1555	C	4.0
1	1A	2150	C	4.0
1	1A	2165	C	4.0
50	2s	27	GLU	4.0
38	2g	79	ARG	4.0
40	2i	127	LYS	4.0
41	2j	41	PRO	4.0
32	2a	1358	U	4.0
7	2H	33	LEU	4.0
1	2A	2155	G	4.0
45	2n	30	ALA	4.0
7	2H	36	PRO	4.0
45	2n	29	ARG	4.0
45	2n	7	ILE	4.0
1	2A	2173	A	4.0
56	1y	21	A	4.0
40	2i	19	LEU	4.0
29	17	48	LYS	4.0
35	2d	34	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	1A	2134	G	4.0
32	1a	1036	G	4.0
1	1A	1142	A	3.9
33	2b	97	TRP	3.9
6	2G	35	GLU	3.9
50	2s	79	THR	3.9
21	2Z	146	ILE	3.9
3	2D	276	LYS	3.9
7	2H	6	ARG	3.9
6	2G	28	VAL	3.9
36	2e	53	LEU	3.9
7	2H	125	VAL	3.9
56	2y	71	G	3.9
1	1A	1144	A	3.9
53	1v	14	A	3.9
6	2G	34	LEU	3.8
7	2H	169	VAL	3.8
1	1A	2166	U	3.8
56	1y	12	U	3.8
56	2y	70	G	3.8
33	2b	92	TYR	3.8
21	2Z	152	ALA	3.8
33	2b	146	GLN	3.8
53	2v	13	A	3.8
7	2H	100	GLY	3.8
42	2k	13	GLN	3.8
40	2i	88	TYR	3.8
1	1A	1140	U	3.8
54	1w	20	U	3.8
7	2H	48	GLY	3.8
41	2j	46	ARG	3.8
44	2m	71	ARG	3.8
34	2c	167	TRP	3.8
1	1A	942	A	3.8
1	2A	2110	G	3.8
1	2A	2160	G	3.8
7	2H	107	VAL	3.8
35	2d	49	ARG	3.8
33	2b	120	ALA	3.7
7	2H	13	LYS	3.7
7	2H	171	LEU	3.7
45	2n	17	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
45	2n	50	LYS	3.7
7	2H	113	VAL	3.7
32	2a	1021	G	3.7
40	2i	7	THR	3.7
51	1t	9	ASN	3.7
34	2c	117	ALA	3.7
41	2j	56	HIS	3.7
45	2n	6	LEU	3.7
2	2B	59	A	3.7
6	2G	149	VAL	3.7
40	2i	10	ARG	3.7
1	1A	1112	U	3.7
56	1y	62	C	3.7
1	1A	930	G	3.7
1	1A	2182	G	3.7
9	2N	8	GLN	3.7
38	2g	40	ALA	3.7
40	2i	110	GLU	3.7
41	2j	55	LYS	3.7
40	2i	42	ARG	3.7
40	2i	17	VAL	3.7
32	2a	1002	G	3.7
32	2a	1030(A)	G	3.7
56	1y	1	G	3.7
40	2i	126	SER	3.7
50	2s	71	LEU	3.7
21	2Z	106	GLY	3.7
6	2G	181	ARG	3.6
12	2Q	32	TYR	3.6
14	2S	31	SER	3.6
1	1A	2161	C	3.6
51	1t	72	LEU	3.6
1	1A	2175	G	3.6
48	2q	23	VAL	3.6
32	2a	1531	A	3.6
45	2n	27	CYS	3.6
1	1A	1145	G	3.6
56	2y	28	G	3.6
22	20	75	LEU	3.6
34	2c	189	ALA	3.6
47	1p	7	ALA	3.6
26	24	63	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
34	2c	196	LEU	3.6
1	2A	2154	G	3.6
1	2A	2157	G	3.6
12	2Q	22	LYS	3.6
7	2H	99	VAL	3.6
43	2l	7	ILE	3.6
1	2A	2142	C	3.6
7	2H	67	LEU	3.6
44	2m	12	ASN	3.6
51	1t	14	LYS	3.6
56	2y	33	U	3.6
1	1A	2137	G	3.6
32	2a	1003	G	3.6
7	2H	124	GLU	3.6
12	2Q	96	VAL	3.6
44	2m	73	GLU	3.6
38	2g	156	TRP	3.6
14	2S	54	LEU	3.6
50	2s	84	GLY	3.6
52	2u	7	ARG	3.5
26	24	53	GLU	3.5
32	1a	204	U	3.5
7	2H	76	VAL	3.5
51	1t	18	GLN	3.5
1	1A	1113	A	3.5
40	2i	18	PHE	3.5
1	1A	2211	U	3.5
33	1b	133	LYS	3.5
12	2Q	33	GLY	3.5
56	2y	5	G	3.5
1	1A	1110	C	3.5
56	1y	13	C	3.5
18	1W	112	GLY	3.5
32	1a	1447	A	3.5
1	1A	2210	C	3.5
44	2m	63	THR	3.5
50	2s	14	HIS	3.5
7	2H	75	ALA	3.5
7	2H	102	ALA	3.5
6	2G	17	PRO	3.5
56	2y	72	C	3.5
52	2u	11	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	1A	935	C	3.5
1	1A	2178	G	3.5
1	1A	2196	C	3.5
32	1a	162	A	3.5
56	2y	18	G	3.5
7	2H	32	GLU	3.5
44	2m	120	LYS	3.5
34	2c	180	ALA	3.5
41	2j	36	GLY	3.5
44	1m	124	PRO	3.5
7	2H	105	LEU	3.5
1	1A	943	C	3.4
56	2y	64	A	3.4
12	2Q	59	ARG	3.4
47	1p	1	MET	3.4
1	1A	2173	G	3.4
34	1c	80	GLY	3.4
45	2n	49	HIS	3.4
21	2Z	145	GLU	3.4
48	2q	36	ILE	3.4
32	1a	1030(A)	G	3.4
34	2c	45	LYS	3.4
12	2Q	60	ARG	3.4
1	2A	2141	G	3.4
34	2c	184	TYR	3.4
31	29	16	VAL	3.4
41	2j	63	PHE	3.4
50	2s	80	TYR	3.4
1	2A	2159	G	3.4
32	2a	1187	G	3.4
32	2a	1202	G	3.4
56	2y	53	G	3.4
43	2l	95	GLY	3.4
41	2j	43	ARG	3.4
44	2m	88	ARG	3.4
39	1h	4	ASP	3.4
14	2S	36	TYR	3.4
47	1p	38	TYR	3.4
9	2N	73	THR	3.3
1	1A	2139	A	3.3
45	2n	37	PHE	3.3
7	2H	159	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
56	1y	27	G	3.3
21	2Z	50	GLN	3.3
38	2g	4	ARG	3.3
52	2u	15	ARG	3.3
28	26	54	ILE	3.3
1	1A	2192	A	3.3
1	1A	2172	U	3.3
8	2I	61	ARG	3.3
6	2G	166	ASP	3.3
21	2Z	42	VAL	3.3
12	2Q	104	PHE	3.3
32	1a	161	A	3.3
32	2a	1035	A	3.3
1	1A	2188	G	3.3
34	2c	7	PRO	3.3
44	2m	97	PRO	3.3
35	2d	176	LEU	3.3
1	2A	2170	A	3.3
38	1g	84	ASN	3.3
48	1q	27	PHE	3.3
1	1A	1139	G	3.3
1	1A	2203	G	3.3
1	1A	1146	C	3.3
1	1A	2133	C	3.3
7	2H	119	GLU	3.3
33	2b	132	LYS	3.3
26	24	46	GLN	3.3
26	24	42	PHE	3.3
33	2b	227	GLY	3.3
33	2b	188	ALA	3.3
1	1A	2122	G	3.3
1	1A	2177	G	3.3
7	2H	103	LEU	3.3
25	23	37	LEU	3.3
40	2i	123	PRO	3.3
56	2y	69	G	3.3
14	2S	17	ARG	3.3
34	1c	21	ARG	3.3
1	2A	2174	C	3.2
23	11	2	SER	3.2
41	2j	96	ILE	3.2
7	2H	43	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
7	2H	144	VAL	3.2
32	1a	1002	G	3.2
50	2s	58	VAL	3.2
34	2c	44	GLU	3.2
47	1p	65	GLN	3.2
7	2H	25	LYS	3.2
45	2n	32	SER	3.2
7	2H	166	GLY	3.2
32	2a	1356	G	3.2
21	2Z	173	ALA	3.2
44	2m	5	ALA	3.2
48	1q	99	SER	3.2
7	2H	161	GLY	3.2
26	24	50	VAL	3.2
36	2e	24	ARG	3.2
52	1u	15	ARG	3.2
45	2n	11	LYS	3.2
1	2A	888	C	3.2
32	2a	1030	C	3.2
32	1a	1003	G	3.2
32	1a	1030(C)	G	3.2
32	2a	1030(C)	G	3.2
45	2n	46	GLU	3.2
33	2b	99	GLY	3.2
7	2H	114	VAL	3.2
14	2S	3	ARG	3.2
21	2Z	139	VAL	3.2
35	2d	110	PHE	3.2
8	2I	68	LEU	3.2
45	2n	53	LEU	3.2
1	2A	2319	G	3.2
9	2N	84	LYS	3.2
44	1m	122	LYS	3.2
45	2n	22	THR	3.2
6	2G	169	ALA	3.2
40	2i	67	GLY	3.2
43	2l	48	PRO	3.2
51	1t	62	LEU	3.2
32	2a	1287	A	3.2
1	1A	2168	C	3.2
35	2d	167	GLY	3.2
48	1q	98	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
45	2n	57	ARG	3.2
49	2r	87	ARG	3.2
26	24	40	HIS	3.1
40	2i	81	ILE	3.1
45	2n	9	LYS	3.1
33	2b	115	LEU	3.1
34	2c	174	PRO	3.1
54	2w	71	G	3.1
56	2y	63	G	3.1
1	2A	2113	U	3.1
7	2H	133	VAL	3.1
54	2w	13	C	3.1
56	1y	4	C	3.1
33	1b	129	GLU	3.1
22	20	3	HIS	3.1
50	2s	28	LYS	3.1
56	1y	19	G	3.1
34	2c	145	GLY	3.1
45	2n	12	ARG	3.1
1	1A	2180	A	3.1
6	2G	3	LEU	3.1
50	2s	50	ALA	3.1
51	1t	13	LEU	3.1
7	2H	24	VAL	3.1
36	2e	20	GLN	3.1
42	2k	119	CYS	3.1
45	2n	45	ARG	3.1
1	2A	881	G	3.1
32	1a	1001(A)	G	3.1
32	2a	1196	U	3.1
44	2m	90	LEU	3.1
7	2H	21	PRO	3.1
38	1g	153	HIS	3.1
53	2v	24	A	3.1
56	2y	38	A	3.1
26	24	44	THR	3.1
26	24	56	VAL	3.1
51	1t	71	THR	3.1
34	2c	194	GLY	3.1
29	27	48	LYS	3.1
35	2d	194	LEU	3.1
8	2I	85	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
42	1k	13	GLN	3.1
22	20	76	GLY	3.1
44	2m	95	GLY	3.1
25	23	23	LEU	3.1
50	2s	12	ASP	3.1
35	1d	209	ARG	3.1
48	1q	37	LYS	3.1
14	2S	29	PHE	3.1
28	26	52	VAL	3.1
21	2Z	149	SER	3.1
8	2I	41	GLU	3.1
34	2c	21	ARG	3.1
42	1k	25	TYR	3.0
56	2y	6	G	3.0
7	2H	57	ASP	3.0
56	1y	56	C	3.0
1	1A	934	A	3.0
1	2A	2117	A	3.0
32	1a	344	A	3.0
21	2Z	38	TYR	3.0
52	2u	21	TYR	3.0
6	2G	19	LEU	3.0
34	2c	33	LEU	3.0
34	2c	91	LEU	3.0
1	2A	1042	G	3.0
33	2b	133	LYS	3.0
14	2S	5	THR	3.0
41	2j	48	THR	3.0
47	1p	2	VAL	3.0
51	1t	24	LEU	3.0
51	1t	55	ILE	3.0
1	1A	2184	G	3.0
14	2S	35	ILE	3.0
50	2s	62	ILE	3.0
42	1k	75	TYR	3.0
1	1A	2160	C	3.0
8	2I	65	ALA	3.0
41	2j	32	ALA	3.0
1	1A	1124	U	3.0
39	2h	72	PRO	3.0
40	2i	90	PRO	3.0
47	1p	19	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
6	2G	115	ARG	3.0
7	2H	7	LEU	3.0
40	2i	122	ALA	3.0
44	1m	2	ALA	3.0
1	2A	2115	G	3.0
32	1a	1034	G	3.0
1	2A	2132	U	3.0
34	2c	39	ILE	3.0
32	1a	160	A	3.0
41	2j	61	GLU	3.0
25	23	35	ARG	3.0
48	2q	44	ALA	3.0
40	1i	81	ILE	2.9
1	1A	1109	G	2.9
1	1A	2204	G	2.9
51	2t	30	LYS	2.9
54	1w	44	G	2.9
34	2c	23	TYR	2.9
52	2u	18	TYR	2.9
53	2v	23	A	2.9
6	2G	160	VAL	2.9
26	14	50	VAL	2.9
40	2i	26	VAL	2.9
6	2G	110	ALA	2.9
1	1A	1143	U	2.9
1	2A	2145	C	2.9
32	1a	92	C	2.9
1	2A	2162	G	2.9
8	2I	86	THR	2.9
33	2b	36	ARG	2.9
41	2j	74	ILE	2.9
41	2j	59	SER	2.9
26	14	52	THR	2.9
32	1a	1027	C	2.9
35	2d	47	ARG	2.9
39	1h	84	ARG	2.9
32	2a	1033	G	2.9
13	2R	68	ARG	2.9
34	2c	154	SER	2.9
44	2m	102	ARG	2.9
1	2A	1041	C	2.9
32	2a	1115	C	2.9

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Mol	Chain	Res	Type	RSRZ
47	1p	62	VAL	2.9
56	1y	22	G	2.9
56	2y	24	G	2.9
50	2s	10	PHE	2.9
47	1p	41	PRO	2.9
36	2e	14	ARG	2.9
39	2h	38	ILE	2.9
1	1A	2143	G	2.9
2	2B	56	G	2.9
39	2h	22	GLU	2.9
36	2e	16	THR	2.9
41	1j	16	LEU	2.9
53	1v	12	A	2.9
20	2Y	1	MET	2.9
34	2c	6	HIS	2.9
7	2H	134	SER	2.9
56	2y	2	C	2.9
34	2c	10	PHE	2.9
35	1d	140	VAL	2.9
56	2y	21	A	2.8
33	2b	19	HIS	2.8
6	2G	176	LEU	2.8
8	2I	72	LEU	2.8
34	2c	188	LEU	2.8
44	2m	48	LEU	2.8
7	2H	122	THR	2.8
37	1f	16	GLN	2.8
48	2q	42	TYR	2.8
40	2i	116	LYS	2.8
1	1A	1114	G	2.8
12	2Q	64	ILE	2.8
32	2a	982	U	2.8
48	2q	27	PHE	2.8
31	29	24	TYR	2.8
1	2A	1026	U	2.8
34	2c	164	ARG	2.8
51	2t	41	ILE	2.8
56	2y	27	G	2.8
56	2y	29	G	2.8
56	2y	66	U	2.8
12	2Q	113	GLN	2.8
32	2a	1248	A	2.8

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Mol	Chain	Res	Type	RSRZ
32	2a	1363(A)	A	2.8
7	2H	49	VAL	2.8
21	2Z	161	VAL	2.8
41	2j	72	VAL	2.8
52	2u	23	PRO	2.8
34	1c	190	ARG	2.8
51	1t	22	ARG	2.8
7	2H	89	ILE	2.8
8	2I	71	ILE	2.8
56	1y	20	U	2.8
1	1A	2187	G	2.8
1	2A	2123	G	2.8
1	2A	2124	G	2.8
6	2G	163	ALA	2.8
54	2w	14	A	2.8
54	2w	44	G	2.8
54	2w	70	G	2.8
36	2e	25	ARG	2.8
56	1y	2	C	2.8
40	2i	124	GLN	2.8
12	2Q	29	PHE	2.8
34	2c	17	ASP	2.8
1	1A	1072	U	2.8
21	2Z	96	VAL	2.8
35	2d	140	VAL	2.8
31	29	19	ARG	2.8
26	24	32	TYR	2.8
32	2a	1256	A	2.8
34	2c	182	ILE	2.8
1	2A	2144	U	2.8
1	2A	2189	U	2.8
34	1c	65	ALA	2.8
41	2j	26	ALA	2.8
50	2s	45	VAL	2.8
49	2r	85	LEU	2.8
42	1k	76	GLY	2.8
52	2u	16	GLY	2.8
33	2b	101	MET	2.7
14	2S	34	HIS	2.7
11	2P	45	LEU	2.7
36	2e	84	PHE	2.7
1	1A	2141	A	2.7

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Mol	Chain	Res	Type	RSRZ
56	1y	38	A	2.7
1	2A	882	G	2.7
1	2A	2156	G	2.7
56	1y	70	G	2.7
7	2H	29	PRO	2.7
36	2e	105	VAL	2.7
36	2e	10	MET	2.7
1	1A	2135	U	2.7
32	1a	1532	U	2.7
7	2H	51	ARG	2.7
7	2H	82	GLY	2.7
34	2c	201	TYR	2.7
51	2t	100	ILE	2.7
6	2G	26	GLN	2.7
33	2b	124	SER	2.7
48	2q	100	LYS	2.7
50	2s	38	SER	2.7
1	2A	2138	C	2.7
1	2A	2166	G	2.7
56	1y	15	G	2.7
33	2b	203	GLY	2.7
7	2H	88	LEU	2.7
33	2b	118	LEU	2.7
6	2G	39	ILE	2.7
7	2H	79	VAL	2.7
23	2i	2	SER	2.7
34	2c	187	ALA	2.7
47	1p	61	SER	2.7
1	1A	1138	C	2.7
55	2x	34	C	2.7
56	2y	26	A	2.7
47	2p	49	LEU	2.7
32	1a	1025	U	2.7
56	2y	57	G	2.7
34	2c	144	SER	2.7
40	2i	106	ALA	2.7
43	2l	68	ALA	2.7
35	2d	198	VAL	2.7
12	2Q	5	ARG	2.7
22	20	80	HIS	2.7
7	2H	74	ASN	2.7
37	1f	21	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
48	2q	37	LYS	2.7
1	2A	2111	C	2.7
1	2A	2143	C	2.7
32	2a	1249	C	2.7
56	1y	61	C	2.7
26	24	31	ILE	2.7
31	29	26	ILE	2.7
41	2j	50	ILE	2.7
1	1A	2145	G	2.7
7	2H	16	SER	2.7
12	2Q	6	ARG	2.7
40	2i	119	ALA	2.7
12	2Q	42	ILE	2.7
34	2c	157	ILE	2.7
1	1A	2186	C	2.7
8	2I	108	THR	2.7
32	2a	1446	U	2.7
44	2m	65	LYS	2.7
7	2H	17	VAL	2.7
29	17	46	VAL	2.7
34	1c	78	GLY	2.7
36	2e	90	VAL	2.7
40	2i	117	HIS	2.7
41	2j	49	VAL	2.7
7	2H	53	GLU	2.7
40	1i	111	ARG	2.7
1	1A	2197	C	2.6
7	2H	165	ALA	2.6
44	2m	107	ALA	2.6
48	1q	35	VAL	2.6
50	2s	69	HIS	2.6
7	2H	129	THR	2.6
7	2H	45	VAL	2.6
1	1A	2130	C	2.6
1	2A	2128	C	2.6
26	24	9	LEU	2.6
48	1q	6	LEU	2.6
1	2A	2114	A	2.6
32	2a	998	G	2.6
32	2a	1186	G	2.6
34	2c	159	GLY	2.6
25	23	6	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
11	1P	15	ARG	2.6
25	23	29	ARG	2.6
12	2Q	65	PHE	2.6
54	2w	3	C	2.6
42	1k	15	ALA	2.6
12	2Q	2	LEU	2.6
26	24	64	GLY	2.6
34	2c	185	GLY	2.6
37	1f	58	GLY	2.6
56	1y	11	C	2.6
7	2H	47	GLU	2.6
8	2I	4	ILE	2.6
6	2G	128	ARG	2.6
7	2H	95	ARG	2.6
15	1T	115	ARG	2.6
43	1l	89	ARG	2.6
43	2l	51	ALA	2.6
22	20	12	ASN	2.6
7	2H	98	LEU	2.6
43	2l	60	LEU	2.6
3	1D	38	LYS	2.6
1	1A	1106	U	2.6
32	1a	1446	U	2.6
40	2i	69	GLY	2.6
56	2y	51	U	2.6
44	2m	103	THR	2.6
47	2p	48	TRP	2.6
38	2g	44	TYR	2.6
43	1l	18	VAL	2.6
40	2i	101	PHE	2.6
21	2Z	82	ARG	2.6
53	2v	22	U	2.6
55	2x	20	U	2.6
56	1y	65	G	2.6
29	27	45	ALA	2.6
33	2b	77	ALA	2.6
34	2c	37	GLN	2.6
26	14	57	GLU	2.6
38	2g	33	ASP	2.6
14	2S	12	PHE	2.6
32	2a	977	A	2.6
32	2a	1357	A	2.6

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Mol	Chain	Res	Type	RSRZ
40	2i	121	ARG	2.6
51	1t	25	ARG	2.6
1	1A	1127	U	2.5
21	2Z	170	THR	2.5
31	29	17	ILE	2.5
10	2O	11	ALA	2.5
12	2Q	121	ALA	2.5
21	2Z	164	ALA	2.5
50	2s	24	ALA	2.5
1	1A	1105	G	2.5
1	1A	2169	G	2.5
12	2Q	93	TYR	2.5
4	2E	52	LEU	2.5
7	2H	37	VAL	2.5
36	2e	107	ARG	2.5
43	2l	32	PHE	2.5
48	2q	65	ILE	2.5
37	1f	83	ASP	2.5
6	2G	152	LEU	2.5
38	2g	34	GLY	2.5
40	2i	53	VAL	2.5
1	2A	2165	G	2.5
25	23	30	ARG	2.5
32	1a	1529	G	2.5
1	1A	933	C	2.5
1	2A	645	C	2.5
55	1x	67	C	2.5
7	2H	10	PRO	2.5
14	2S	18	ILE	2.5
1	1A	1878	A	2.5
7	2H	141	VAL	2.5
8	2I	19	VAL	2.5
56	2y	14	A	2.5
12	2Q	12	GLN	2.5
51	1t	19	SER	2.5
1	2A	2140	C	2.5
6	2G	108	ASN	2.5
32	2a	1114	C	2.5
5	2F	21	ALA	2.5
40	2i	107	ARG	2.5
21	2Z	163	LEU	2.5
26	24	33	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
38	2g	12	LEU	2.5
12	2Q	103	MET	2.5
33	2b	113	HIS	2.5
34	2c	95	THR	2.5
50	2s	36	ARG	2.5
1	1A	929	G	2.5
1	1A	2171	G	2.5
1	2A	2152	G	2.5
32	1a	79	G	2.5
39	2h	134	ILE	2.5
51	1t	33	ILE	2.5
56	1y	49	C	2.5
6	2G	120	LEU	2.5
8	2I	38	LEU	2.5
34	1c	42	LEU	2.5
35	1d	157	LEU	2.5
44	2m	70	LEU	2.5
20	2Y	55	TYR	2.5
21	2Z	169	GLU	2.5
25	23	60	GLU	2.5
7	2H	55	PRO	2.5
44	2m	64	TRP	2.5
35	2d	26	CYS	2.5
56	2y	56	C	2.5
1	1A	2149	G	2.5
21	2Z	14	LYS	2.5
40	2i	71	SER	2.5
43	2l	64	TYR	2.5
1	1A	2140	U	2.5
48	2q	8	GLY	2.5
26	24	57	GLU	2.5
1	1A	218	A	2.5
39	2h	39	LEU	2.5
7	2H	164	TYR	2.5
15	2T	108	ARG	2.5
32	2a	1028	C	2.5
38	2g	41	ARG	2.5
15	1T	109	GLU	2.4
40	2i	72	GLY	2.4
56	1y	45	U	2.4
14	2S	33	LYS	2.4
8	2I	44	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	1A	2191	A	2.4
9	2N	140	VAL	2.4
7	2H	3	ARG	2.4
10	1O	49	ARG	2.4
53	2v	15	A	2.4
54	2w	31	A	2.4
6	1G	146	TYR	2.4
7	2H	18	GLU	2.4
7	2H	118	PRO	2.4
32	1a	104	G	2.4
44	1m	123	ALA	2.4
17	2V	5	VAL	2.4
45	2n	18	VAL	2.4
21	1Z	168	GLU	2.4
33	1b	17	PHE	2.4
26	24	43	TYR	2.4
40	2i	113	LYS	2.4
44	2m	13	LYS	2.4
32	2a	1030(D)	A	2.4
6	2G	112	PRO	2.4
7	2H	128	PRO	2.4
32	2a	984	C	2.4
44	2m	92	HIS	2.4
54	2w	72	C	2.4
39	1h	35	ILE	2.4
45	2n	47	LEU	2.4
12	2Q	106	VAL	2.4
13	2R	69	ASP	2.4
30	28	34	TRP	2.4
52	2u	5	ASP	2.4
54	1w	1	G	2.4
56	1y	63	G	2.4
1	1A	2157	A	2.4
32	2a	1251	A	2.4
34	2c	165	THR	2.4
42	2k	96	ARG	2.4
48	2q	53	LEU	2.4
51	1t	28	ALA	2.4
34	1c	14	ILE	2.4
40	2i	112	LYS	2.4
50	2s	35	SER	2.4
56	1y	25	C	2.4

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Mol	Chain	Res	Type	RSRZ
6	2G	109	VAL	2.4
1	1A	2123	G	2.4
1	2A	2153	G	2.4
41	2j	45	ARG	2.4
51	2t	22	ARG	2.4
12	2Q	87	LYS	2.4
33	1b	128	GLU	2.4
7	2H	87	LEU	2.4
1	2A	2753	A	2.4
21	1Z	148	ASP	2.4
52	1u	13	ILE	2.4
19	2X	43	VAL	2.4
44	2m	119	GLY	2.4
33	2b	209	ARG	2.4
40	1i	113	LYS	2.4
51	1t	68	LYS	2.4
1	1A	2147	G	2.4
32	2a	1220	G	2.4
48	2q	84	LEU	2.4
56	2y	22	G	2.4
6	2G	157	ILE	2.4
21	2Z	128	VAL	2.4
38	2g	105	VAL	2.4
1	2A	2129	C	2.4
12	2Q	10	ARG	2.4
54	1w	73	A	2.4
32	1a	1029	C	2.4
34	2c	89	GLU	2.4
35	2d	4	TYR	2.4
35	1d	162	LEU	2.4
36	2e	146	ALA	2.4
38	2g	7	ALA	2.4
25	23	24	LYS	2.4
12	2Q	132	VAL	2.4
14	2S	10	ARG	2.4
15	1T	112	ARG	2.4
15	2T	111	ARG	2.4
1	1A	2156	A	2.3
6	2G	2	PRO	2.3
8	2I	133	HIS	2.3
31	29	30	PRO	2.3
56	2y	73	A	2.3

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Mol	Chain	Res	Type	RSRZ
21	2Z	17	ALA	2.3
21	2Z	172	ALA	2.3
33	2b	216	SER	2.3
34	2c	178	LEU	2.3
40	2i	27	THR	2.3
34	2c	2	GLY	2.3
41	2j	52	GLY	2.3
35	2d	70	ILE	2.3
42	1k	92	GLU	2.3
7	2H	109	PHE	2.3
39	2h	61	VAL	2.3
1	2A	2127	G	2.3
32	1a	78	G	2.3
1	1A	2189	U	2.3
6	2G	49	ASP	2.3
6	2G	135	LEU	2.3
11	2P	88	LEU	2.3
21	2Z	125	LEU	2.3
39	2h	2	LEU	2.3
6	2G	161	THR	2.3
8	2I	117	GLU	2.3
12	2Q	108	GLY	2.3
32	2a	1039	C	2.3
54	2w	4	C	2.3
55	2x	65	C	2.3
21	2Z	49	ARG	2.3
21	2Z	79	ARG	2.3
38	2g	78	ARG	2.3
35	2d	67	ILE	2.3
12	2Q	63	LYS	2.3
42	1k	123	LYS	2.3
1	1A	2209	G	2.3
32	2a	1026	G	2.3
6	2G	33	ARG	2.3
22	20	82	ARG	2.3
32	2a	1000	U	2.3
33	2b	210	SER	2.3
44	2m	42	ALA	2.3
51	1t	17	ARG	2.3
1	1A	2200	C	2.3
35	1d	158	ILE	2.3
50	1s	40	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
56	2y	3	C	2.3
6	2G	84	LYS	2.3
23	21	23	LYS	2.3
33	2b	164	VAL	2.3
42	2k	58	PRO	2.3
21	1Z	149	SER	2.3
25	23	53	LEU	2.3
33	2b	177	ALA	2.3
42	2k	89	ALA	2.3
45	2n	2	ALA	2.3
1	2A	2131	G	2.3
2	2B	24	G	2.3
11	2P	76	LYS	2.3
56	1y	28	G	2.3
56	1y	71	G	2.3
1	1A	2159	C	2.3
1	1A	2185	C	2.3
43	2l	90	VAL	2.3
7	2H	116	GLU	2.3
45	2n	8	GLU	2.3
12	2Q	56	ARG	2.3
33	2b	220	ASP	2.3
11	2P	109	GLY	2.3
41	2j	10	GLY	2.3
9	2N	116	LEU	2.3
48	2q	74	LEU	2.3
50	2s	52	TYR	2.3
32	2a	1150	U	2.3
33	2b	108	ILE	2.3
21	1Z	141	VAL	2.3
38	2g	8	GLU	2.3
48	2q	24	GLU	2.3
1	1A	2132	G	2.3
32	2a	1368	G	2.3
40	1i	128	ARG	2.3
56	1y	53	G	2.3
34	1c	18	TRP	2.3
2	2B	58	A	2.3
42	2k	117	ASN	2.3
50	1s	27	GLU	2.3
45	1n	33	VAL	2.3
48	2q	38	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
54	2w	45	U	2.3
51	1t	64	ASP	2.3
7	2H	78	GLY	2.3
34	2c	205	GLY	2.3
1	2A	2148	G	2.3
33	2b	51	LEU	2.3
35	2d	108	LEU	2.3
45	2n	54	PRO	2.3
48	2q	31	LEU	2.3
51	2t	42	GLN	2.3
43	1l	61	THR	2.3
6	2G	15	VAL	2.3
6	2G	97	ASP	2.3
47	1p	59	TRP	2.2
19	2X	66	LEU	2.2
1	2A	1118	C	2.2
32	2a	1027	C	2.2
32	2a	1193	G	2.2
44	2m	23	TYR	2.2
31	29	25	VAL	2.2
51	2t	63	ILE	2.2
1	1A	1111	U	2.2
39	1h	2	LEU	2.2
40	2i	21	PRO	2.2
50	2s	57	HIS	2.2
38	2g	149	ARG	2.2
51	1t	67	ALA	2.2
41	2j	58	ASP	2.2
32	1a	1033	G	2.2
39	1h	6	ILE	2.2
45	1n	18	VAL	2.2
17	2V	50	PRO	2.2
32	1a	1035	A	2.2
12	2Q	20	ALA	2.2
52	2u	8	THR	2.2
51	2t	69	GLY	2.2
12	2Q	91	GLU	2.2
25	23	59	VAL	2.2
48	2q	21	VAL	2.2
1	2A	2161	C	2.2
7	2H	38	SER	2.2
6	2G	179	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
21	2Z	80	ARG	2.2
25	23	52	HIS	2.2
32	2a	1258	G	2.2
32	2a	1355	G	2.2
35	1d	58	LEU	2.2
39	2h	112	LEU	2.2
41	1j	40	LEU	2.2
50	2s	42	PRO	2.2
1	1A	945	A	2.2
1	1A	2136	A	2.2
1	1A	2195	A	2.2
1	2A	2118	U	2.2
12	2Q	7	MET	2.2
12	2Q	136	ALA	2.2
8	2I	20	ASP	2.2
41	2j	42	THR	2.2
21	2Z	22	GLY	2.2
45	2n	21	TYR	2.2
12	2Q	47	ILE	2.2
48	2q	5	VAL	2.2
48	2q	10	VAL	2.2
48	1q	68	ARG	2.2
14	2S	58	LEU	2.2
25	23	26	LEU	2.2
56	1y	43	C	2.2
34	2c	58	GLU	2.2
40	2i	105	ASP	2.2
1	1A	2194	U	2.2
1	1A	2212	G	2.2
49	1r	25	THR	2.2
45	2n	16	PHE	2.2
34	2c	152	ILE	2.2
38	1g	76	ARG	2.2
39	1h	92	ARG	2.2
40	2i	83	ARG	2.2
8	2I	74	ASN	2.2
8	1I	5	LEU	2.2
8	1I	114	LEU	2.2
8	2I	134	PRO	2.2
42	1k	39	PRO	2.2
8	2I	17	GLN	2.2
34	2c	162	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
7	2H	41	MET	2.2
33	2b	152	PHE	2.2
33	2b	163	PHE	2.2
48	1q	63	ARG	2.2
1	1A	1120	G	2.2
1	1A	2142	G	2.2
44	2m	69	GLU	2.2
50	2s	15	LEU	2.2
47	2p	9	PHE	2.2
22	20	5	LYS	2.1
8	2I	79	ILE	2.1
26	14	46	GLN	2.1
36	2e	31	LEU	2.1
41	2j	90	LEU	2.1
32	2a	1224	G	2.1
56	1y	52	G	2.1
8	2I	34	GLY	2.1
32	2a	969	A	2.1
45	2n	55	GLY	2.1
56	1y	7	A	2.1
34	2c	60	ALA	2.1
35	1d	111	ALA	2.1
45	1n	10	ALA	2.1
3	2D	38	LYS	2.1
7	2H	27	LYS	2.1
1	1A	2199	C	2.1
10	2O	7	TYR	2.1
31	29	6	SER	2.1
32	1a	201	C	2.1
1	1A	2131	U	2.1
8	2I	18	VAL	2.1
32	1a	164	U	2.1
32	2a	981	U	2.1
32	2a	1219	U	2.1
39	1h	134	ILE	2.1
56	1y	51	U	2.1
7	2H	142	GLY	2.1
36	1e	96	PRO	2.1
15	1T	111	ARG	2.1
28	26	28	ARG	2.1
32	1a	1026	G	2.1
32	2a	973	G	2.1

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Mol	Chain	Res	Type	RSRZ
33	1b	27	LYS	2.1
25	23	47	VAL	2.1
7	2H	137	ASP	2.1
9	2N	105	GLY	2.1
21	2Z	102	LEU	2.1
38	1g	16	LEU	2.1
38	2g	120	ILE	2.1
1	2A	2122	U	2.1
25	23	12	PRO	2.1
32	2a	1066	C	2.1
33	2b	173	ALA	2.1
41	2j	64	GLU	2.1
18	2W	101	SER	2.1
32	2a	1288	A	2.1
6	2G	16	ARG	2.1
14	2S	110	LEU	2.1
25	23	9	VAL	2.1
33	2b	33	TYR	2.1
40	2i	70	LYS	2.1
47	1p	42	ARG	2.1
47	2p	21	VAL	2.1
50	2s	60	VAL	2.1
12	2Q	28	ALA	2.1
56	2y	4	C	2.1
15	1T	108	ARG	2.1
43	2l	87	GLY	2.1
48	1q	75	ARG	2.1
6	2G	106	LEU	2.1
9	2N	46	VAL	2.1
47	1p	73	LEU	2.1
49	1r	78	LEU	2.1
6	2G	48	GLU	2.1
32	2a	1009	G	2.1
56	2y	19	G	2.1
7	2H	145	ALA	2.1
36	1e	98	THR	2.1
56	1y	3	C	2.1
26	24	59	PHE	2.1
51	1t	8	ARG	2.1
7	2H	50	VAL	2.1
34	2c	87	LEU	2.1
15	2T	48	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
39	2h	81	HIS	2.1
41	1j	94	VAL	2.1
44	2m	78	ILE	2.1
9	2N	47	ALA	2.1
12	2Q	114	ALA	2.1
32	1a	70	G	2.1
32	2a	1221	G	2.1
33	1b	29	ALA	2.1
40	2i	52	ALA	2.1
54	2w	34	G	2.1
54	2w	38	A	2.1
56	1y	69	G	2.1
31	29	29	ASN	2.1
44	2m	62	ASN	2.1
31	29	28	GLU	2.1
32	2a	1192	C	2.1
32	2a	1254	C	2.1
7	2H	64	LEU	2.1
34	2c	204	LEU	2.1
37	1f	43	LEU	2.1
50	2s	70	LYS	2.1
22	20	18	ALA	2.1
38	2g	108	ALA	2.1
51	1t	75	ASN	2.1
33	2b	128	GLU	2.1
34	2c	122	GLU	2.1
6	2G	177	GLY	2.1
6	2G	178	PHE	2.1
7	2H	31	GLY	2.1
12	2Q	92	GLY	2.1
32	1a	1385	G	2.0
33	2b	228	GLY	2.1
51	1t	96	GLY	2.1
56	1y	60	U	2.0
4	2E	195	LEU	2.0
4	2E	72	VAL	2.0
14	2S	85	VAL	2.0
32	2a	1203	C	2.0
53	2v	21	C	2.0
7	2H	162	ILE	2.0
47	1p	15	PRO	2.0
50	2s	40	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
7	2H	146	ALA	2.0
42	2k	92	GLU	2.0
34	2c	41	GLY	2.0
36	2e	59	GLY	2.0
37	1f	55	ASP	2.0
51	1t	74	LYS	2.0
33	2b	215	LEU	2.0
40	1i	19	LEU	2.0
48	1q	74	LEU	2.0
56	1y	66	U	2.0
7	2H	11	VAL	2.0
27	15	60	VAL	2.0
32	2a	965	A	2.0
32	2a	983	A	2.0
7	2H	12	PRO	2.0
32	2a	1370	G	2.0
14	2S	13	ARG	2.0
32	1a	103	C	2.0
40	2i	61	ALA	2.0
8	1I	40	THR	2.0
22	20	71	ASP	2.0
50	2s	54	GLY	2.0
34	2c	18	TRP	2.0
48	2q	26	GLN	2.0
21	2Z	150	LEU	2.0
6	2G	37	VAL	2.0
34	2c	127	ARG	2.0
34	2c	153	VAL	2.0
39	1h	91	ARG	2.0
40	2i	66	ARG	2.0
56	1y	50	U	2.0
56	2y	12	U	2.0
14	2S	82	ILE	2.0
16	2U	17	ILE	2.0
1	1A	1130	A	2.0
1	2A	900	A	2.0
32	2a	1004	A	2.0
32	2a	1447	A	2.0
38	2g	46	ALA	2.0
42	2k	25	TYR	2.0
2	2B	17	C	2.0
32	2a	1195	C	2.0

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Mol	Chain	Res	Type	RSRZ
54	2w	40	C	2.0
12	2Q	75	THR	2.0
42	1k	87	THR	2.0
14	2S	26	LEU	2.0
34	2c	206	GLU	2.0
44	2m	93	ARG	2.0
44	2m	94	ARG	2.0
6	2G	5	VAL	2.0
12	2Q	35	VAL	2.0
45	1n	14	PRO	2.0
50	1s	67	VAL	2.0
51	1t	88	VAL	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
56	PSU	2y	32	20/21	0.68	0.40	76,83,98,98	0
56	7MG	2y	46	24/25	0.70	0.31	80,93,98,110	0
56	7MG	1y	46	24/25	0.73	0.33	78,90,96,108	0
56	MIA	2y	37	22/30	0.73	0.43	73,83,93,106	0
56	PSU	1y	55	20/21	0.75	0.31	80,86,94,107	0
56	MIA	1y	37	22/30	0.78	0.37	71,81,88,101	0
56	4SU	2y	8	20/21	0.79	0.17	80,89,100,105	0
56	5MU	2y	54	21/22	0.79	0.40	81,86,90,105	0
56	PSU	2y	39	20/21	0.80	0.39	81,86,99,110	0
54	7MG	2w	46	24/25	0.80	0.24	71,82,92,104	0
56	5MU	1y	54	21/22	0.80	0.32	76,82,87,92	0
54	7MG	1w	46	24/25	0.81	0.17	60,71,82,103	0
56	PSU	1y	32	20/21	0.82	0.34	71,77,90,107	0
56	PSU	2y	55	20/21	0.83	0.34	82,85,106,108	0
56	PSU	1y	39	20/21	0.84	0.30	66,76,89,99	0
56	4SU	1y	8	20/21	0.84	0.25	81,88,96,101	0
55	PSU	2x	55	20/21	0.87	0.18	64,68,76,77	0
54	PSU	1w	55	20/21	0.88	0.18	45,57,68,73	0
32	M2G	2a	966	25/26	0.89	0.26	53,62,70,75	0
54	PSU	2w	55	20/21	0.89	0.17	55,69,77,79	0
43	0TD	2l	92	10/11	0.89	0.19	57,63,66,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	4SU	2w	8	20/21	0.89	0.22	73,78,84,85	0
32	2MG	2a	1207	24/25	0.90	0.25	66,73,79,82	0
43	0TD	1l	92	10/11	0.90	0.21	37,46,49,64	0
55	4SU	2x	8	20/21	0.90	0.18	68,74,80,82	0
32	5MC	2a	967	21/22	0.92	0.25	56,62,70,72	0
54	5MU	2w	54	21/22	0.92	0.16	51,60,67,74	0
55	5MU	2x	54	21/22	0.92	0.23	61,69,73,76	0
32	PSU	2a	516	20/21	0.93	0.21	47,62,72,73	0
55	5MU	1x	54	21/22	0.93	0.17	54,59,65,70	0
55	5MC	2x	32	21/22	0.93	0.23	61,67,71,76	0
54	PSU	2w	32	20/21	0.93	0.29	63,71,87,87	0
54	MIA	2w	37	25/30	0.93	0.26	58,67,73,74	0
32	5MC	2a	1404	21/22	0.94	0.23	50,56,61,61	0
1	5MU	2A	1915	21/22	0.94	0.19	55,60,65,73	0
54	PSU	2w	39	20/21	0.94	0.32	55,72,78,79	0
32	7MG	2a	527	24/25	0.94	0.21	50,62,71,73	0
32	PSU	1a	516	20/21	0.94	0.20	48,54,59,61	0
32	5MC	2a	1407	21/22	0.94	0.20	46,55,59,73	0
54	4SU	1w	8	20/21	0.94	0.15	57,66,71,71	0
54	PSU	1w	32	20/21	0.94	0.20	54,60,65,67	0
55	4SU	1x	8	20/21	0.94	0.15	44,52,59,63	0
32	MA6	2a	1519	24/25	0.94	0.27	53,59,64,64	0
32	4OC	2a	1402	22/23	0.94	0.20	54,61,64,66	0
32	MA6	2a	1518	24/25	0.95	0.25	51,58,63,63	0
1	4OC	2A	1920	21/23	0.95	0.23	48,53,59,63	0
1	PSU	2A	1911	20/21	0.95	0.18	47,55,61,61	0
32	2MG	1a	1207	24/25	0.95	0.16	47,54,58,64	0
54	PSU	1w	39	20/21	0.95	0.18	45,49,56,59	0
1	5MC	2A	1962	21/22	0.95	0.19	40,45,50,58	0
55	PSU	1x	55	20/21	0.95	0.15	51,56,67,68	0
32	5MC	2a	1400	21/22	0.95	0.25	56,61,65,68	0
54	MIA	1w	37	29/30	0.95	0.22	39,46,53,55	0
54	F3N	2w	76	33/34	0.96	0.26	31,39,44,53	0
54	5MU	1w	54	21/22	0.96	0.22	34,39,52,59	0
32	UR3	2a	1498	21/22	0.96	0.18	48,54,59,61	0
32	5MC	1a	967	21/22	0.96	0.21	38,45,52,54	0
1	5MU	1A	1937	21/22	0.96	0.21	38,44,52,53	0
32	M2G	1a	966	25/26	0.96	0.19	34,39,45,46	0
1	PSU	2A	1917	20/21	0.96	0.20	46,55,61,66	0
32	5MC	1a	1407	21/22	0.96	0.19	29,36,42,45	0
1	5MC	2A	1942	21/22	0.96	0.20	36,51,59,60	0
1	PSU	1A	1933	20/21	0.96	0.19	31,41,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	4OC	1a	1402	22/23	0.97	0.22	35,41,44,45	0
1	5MU	2A	1939	21/22	0.97	0.19	29,36,40,42	0
1	5MC	1A	1964	21/22	0.97	0.18	29,34,37,40	0
32	7MG	1a	527	24/25	0.97	0.16	38,45,50,57	0
1	5MU	1A	1961	21/22	0.97	0.22	19,25,31,36	0
32	5MC	1a	1400	21/22	0.97	0.17	29,36,43,47	0
1	OMG	2A	2251	24/25	0.97	0.20	30,36,41,41	0
1	PSU	1A	1939	20/21	0.97	0.20	32,40,46,47	0
55	5MC	1x	32	21/22	0.97	0.19	38,45,48,52	0
32	MA6	1a	1519	24/25	0.97	0.22	33,38,42,45	0
54	F3N	1w	76	33/34	0.97	0.22	12,20,26,33	0
32	MA6	1a	1518	24/25	0.97	0.22	32,38,40,42	0
1	OMG	1A	2263	24/25	0.98	0.21	14,22,26,28	0
1	2MA	1A	2515	23/24	0.98	0.21	14,18,25,27	0
1	5MC	1A	1984	21/22	0.98	0.21	25,30,35,42	0
1	4OC	1A	1942	21/23	0.98	0.20	32,38,40,41	0
1	2MU	2A	2552	21/23	0.98	0.19	34,41,44,47	0
1	PSU	2A	2605	20/21	0.98	0.19	21,30,36,37	0
32	UR3	1a	1498	21/22	0.98	0.20	27,37,41,44	0
1	2MA	2A	2503	23/24	0.98	0.20	26,32,35,36	0
32	5MC	1a	1404	21/22	0.98	0.20	25,35,39,42	0
1	2MU	1A	2564	21/23	0.98	0.19	17,25,30,30	0
1	PSU	1A	2617	20/21	0.98	0.18	15,21,26,26	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
57	MG	2A	3156	1/1	0.38	0.21	64,64,64,64	0
57	MG	2A	3305	1/1	0.39	2.36	78,78,78,78	0
57	MG	1a	3037	1/1	0.41	0.20	57,57,57,57	0
57	MG	2Z	8001	1/1	0.42	0.37	80,80,80,80	0
57	MG	1y	3002	1/1	0.52	0.15	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	3200	1/1	0.55	0.28	85,85,85,85	0
57	MG	2j	8002	1/1	0.55	0.46	82,82,82,82	0
57	MG	1a	3061	1/1	0.56	0.20	59,59,59,59	0
57	MG	2a	3047	1/1	0.57	0.13	69,69,69,69	0
57	MG	1A	3782	1/1	0.57	0.19	25,25,25,25	0
57	MG	2x	103	1/1	0.58	0.25	73,73,73,73	0
57	MG	2A	3055	1/1	0.60	0.22	63,63,63,63	0
57	MG	1A	3945	1/1	0.60	0.34	58,58,58,58	0
57	MG	1a	3183	1/1	0.60	0.16	52,52,52,52	0
57	MG	2A	3553	1/1	0.61	0.27	58,58,58,58	0
57	MG	1A	3662	1/1	0.61	0.19	54,54,54,54	0
57	MG	2a	3052	1/1	0.61	0.15	69,69,69,69	0
57	MG	2A	3509	1/1	0.62	0.16	64,64,64,64	0
57	MG	2A	3272	1/1	0.62	0.16	53,53,53,53	0
57	MG	2A	3595	1/1	0.63	0.27	38,38,38,38	0
57	MG	1a	3084	1/1	0.63	0.19	54,54,54,54	0
57	MG	1A	3334	1/1	0.64	0.24	47,47,47,47	0
57	MG	1A	3414	1/1	0.64	0.19	35,35,35,35	0
57	MG	1A	3425	1/1	0.64	0.17	53,53,53,53	0
57	MG	2A	3528	1/1	0.66	0.12	58,58,58,58	0
57	MG	2a	3163	1/1	0.66	0.25	72,72,72,72	0
57	MG	2A	3154	1/1	0.66	0.29	60,60,60,60	0
57	MG	1A	3541	1/1	0.66	0.22	48,48,48,48	0
57	MG	1A	3243	1/1	0.66	0.20	56,56,56,56	0
57	MG	2A	3444	1/1	0.67	0.11	58,58,58,58	0
57	MG	2l	201	1/1	0.67	0.37	63,63,63,63	0
57	MG	1A	3604	1/1	0.67	0.19	17,17,17,17	0
57	MG	2A	3628	1/1	0.68	0.29	38,38,38,38	0
57	MG	1A	3660	1/1	0.68	0.07	39,39,39,39	0
57	MG	1A	3381	1/1	0.68	0.15	56,56,56,56	0
57	MG	1A	3661	1/1	0.68	0.16	55,55,55,55	0
57	MG	2a	3046	1/1	0.69	0.28	66,66,66,66	0
57	MG	2a	3016	1/1	0.69	0.13	78,78,78,78	0
57	MG	2A	3339	1/1	0.69	0.14	54,54,54,54	0
57	MG	2A	3331	1/1	0.69	0.14	39,39,39,39	0
57	MG	2A	3200	1/1	0.69	0.89	60,60,60,60	0
57	MG	2a	3059	1/1	0.69	0.27	50,50,50,50	0
57	MG	2A	3185	1/1	0.69	0.13	51,51,51,51	0
57	MG	1A	3784	1/1	0.69	0.11	39,39,39,39	0
57	MG	2a	3129	1/1	0.70	0.09	71,71,71,71	0
57	MG	2A	3354	1/1	0.70	0.18	52,52,52,52	0
57	MG	1Q	204	1/1	0.70	0.20	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	3081	1/1	0.70	0.21	67,67,67,67	0
57	MG	2A	3526	1/1	0.70	0.19	59,59,59,59	0
57	MG	2A	3594	1/1	0.70	0.24	46,46,46,46	0
57	MG	1a	3092	1/1	0.70	0.24	60,60,60,60	0
57	MG	2a	3004	1/1	0.70	0.10	67,67,67,67	0
57	MG	2A	3495	1/1	0.71	0.13	61,61,61,61	0
57	MG	2a	3060	1/1	0.71	0.18	66,66,66,66	0
57	MG	1A	3826	1/1	0.71	0.12	50,50,50,50	0
57	MG	1A	3291	1/1	0.71	0.28	36,36,36,36	0
57	MG	2a	3192	1/1	0.71	0.13	51,51,51,51	0
57	MG	1B	3007	1/1	0.71	0.17	38,38,38,38	0
57	MG	20	3002	1/1	0.71	0.40	64,64,64,64	0
57	MG	1A	3491	1/1	0.71	0.21	29,29,29,29	0
57	MG	2a	3087	1/1	0.71	0.12	69,69,69,69	0
57	MG	1A	3744	1/1	0.72	0.19	47,47,47,47	0
57	MG	1a	3204	1/1	0.72	0.14	75,75,75,75	0
57	MG	2a	3061	1/1	0.72	0.14	57,57,57,57	0
57	MG	1A	3338	1/1	0.72	0.33	35,35,35,35	0
57	MG	1a	3140	1/1	0.72	0.14	48,48,48,48	0
57	MG	1a	3006	1/1	0.72	0.15	55,55,55,55	0
57	MG	2A	3574	1/1	0.72	0.11	60,60,60,60	0
57	MG	2A	3284	1/1	0.73	0.12	36,36,36,36	0
57	MG	1O	202	1/1	0.73	0.45	67,67,67,67	0
57	MG	2a	3074	1/1	0.73	0.13	62,62,62,62	0
57	MG	1A	3478	1/1	0.73	0.16	17,17,17,17	0
57	MG	2A	3342	1/1	0.73	0.15	31,31,31,31	0
57	MG	2A	3603	1/1	0.73	0.11	77,77,77,77	0
57	MG	2a	3175	1/1	0.73	0.14	63,63,63,63	0
57	MG	2a	3079	1/1	0.73	0.13	63,63,63,63	0
57	MG	2a	3172	1/1	0.73	0.31	73,73,73,73	0
57	MG	2t	3001	1/1	0.73	0.16	55,55,55,55	0
57	MG	1A	3005	1/1	0.74	0.19	46,46,46,46	0
57	MG	2a	3178	1/1	0.74	0.09	59,59,59,59	0
57	MG	1a	3005	1/1	0.74	0.19	53,53,53,53	0
57	MG	2A	3604	1/1	0.74	0.20	56,56,56,56	0
57	MG	2A	3165	1/1	0.74	0.35	53,53,53,53	0
57	MG	2A	3670	1/1	0.75	0.56	49,49,49,49	0
57	MG	2a	3120	1/1	0.75	0.24	70,70,70,70	0
57	MG	1A	3834	1/1	0.75	0.18	60,60,60,60	0
57	MG	2A	3201	1/1	0.75	0.14	51,51,51,51	0
57	MG	2a	3022	1/1	0.75	0.17	59,59,59,59	0
57	MG	2A	3399	1/1	0.75	0.15	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	3134	1/1	0.75	0.13	77,77,77,77	0
57	MG	2x	102	1/1	0.75	0.10	66,66,66,66	0
57	MG	2A	3115	1/1	0.75	0.20	62,62,62,62	0
57	MG	1A	3626	1/1	0.76	0.30	61,61,61,61	0
57	MG	1a	3150	1/1	0.76	0.22	56,56,56,56	0
57	MG	2a	3036	1/1	0.76	0.08	65,65,65,65	0
57	MG	1a	3189	1/1	0.76	0.10	69,69,69,69	0
57	MG	1A	3096	1/1	0.76	0.27	56,56,56,56	0
57	MG	1A	3002	1/1	0.76	0.17	40,40,40,40	0
57	MG	2a	3043	1/1	0.76	0.18	65,65,65,65	0
57	MG	2a	3066	1/1	0.76	0.18	73,73,73,73	0
57	MG	2A	3478	1/1	0.76	0.20	64,64,64,64	0
57	MG	1A	3830	1/1	0.76	0.15	39,39,39,39	0
57	MG	2q	3003	1/1	0.76	0.14	70,70,70,70	0
57	MG	1A	3519	1/1	0.76	0.14	38,38,38,38	0
57	MG	2A	3052	1/1	0.76	0.47	61,61,61,61	0
57	MG	1A	3301	1/1	0.77	0.21	51,51,51,51	0
57	MG	1A	3490	1/1	0.77	0.18	25,25,25,25	0
57	MG	1a	3019	1/1	0.77	0.13	47,47,47,47	0
57	MG	2A	3205	1/1	0.77	0.23	46,46,46,46	0
57	MG	1a	3025	1/1	0.77	0.13	62,62,62,62	0
57	MG	1G	203	1/1	0.77	0.11	52,52,52,52	0
57	MG	2A	3195	1/1	0.77	0.21	53,53,53,53	0
57	MG	1a	3044	1/1	0.77	0.25	57,57,57,57	0
57	MG	1a	3001	1/1	0.77	0.17	50,50,50,50	0
57	MG	1a	3222	1/1	0.77	0.15	64,64,64,64	0
57	MG	20	3001	1/1	0.78	0.13	61,61,61,61	0
57	MG	2A	3680	1/1	0.78	0.23	49,49,49,49	0
57	MG	2a	3156	1/1	0.78	0.12	44,44,44,44	0
57	MG	1a	3045	1/1	0.78	0.14	63,63,63,63	0
57	MG	1A	3640	1/1	0.78	0.14	21,21,21,21	0
57	MG	2A	3121	1/1	0.78	0.53	65,65,65,65	0
57	MG	2e	3001	1/1	0.78	0.15	69,69,69,69	0
57	MG	2A	3668	1/1	0.78	0.15	47,47,47,47	0
57	MG	2A	3485	1/1	0.78	0.13	42,42,42,42	0
57	MG	2A	3469	1/1	0.78	0.20	64,64,64,64	0
57	MG	1A	3465	1/1	0.78	0.15	28,28,28,28	0
57	MG	1A	3930	1/1	0.78	0.13	25,25,25,25	0
57	MG	2A	3189	1/1	0.78	0.47	64,64,64,64	0
57	MG	2a	3177	1/1	0.78	0.18	60,60,60,60	0
57	MG	2w	101	1/1	0.78	0.17	59,59,59,59	0
57	MG	1a	3022	1/1	0.78	0.20	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	3042	1/1	0.78	0.13	44,44,44,44	0
57	MG	1A	3854	1/1	0.79	0.18	49,49,49,49	0
57	MG	1a	3115	1/1	0.79	0.15	49,49,49,49	0
57	MG	1a	3095	1/1	0.79	0.30	58,58,58,58	0
57	MG	1a	3102	1/1	0.79	0.18	43,43,43,43	0
57	MG	2A	3004	1/1	0.79	0.12	58,58,58,58	0
57	MG	2A	3319	1/1	0.79	0.18	31,31,31,31	0
57	MG	2a	3126	1/1	0.79	0.12	63,63,63,63	0
57	MG	1A	3728	1/1	0.79	0.23	45,45,45,45	0
57	MG	2a	3071	1/1	0.79	0.15	49,49,49,49	0
57	MG	2A	3369	1/1	0.79	0.12	66,66,66,66	0
57	MG	1A	3313	1/1	0.79	0.22	49,49,49,49	0
57	MG	2A	3211	1/1	0.79	0.11	51,51,51,51	0
57	MG	2A	3288	1/1	0.79	0.08	48,48,48,48	0
57	MG	2a	3162	1/1	0.79	0.11	53,53,53,53	0
57	MG	1A	3980	1/1	0.79	0.35	35,35,35,35	0
57	MG	1A	3447	1/1	0.79	0.21	26,26,26,26	0
57	MG	1A	3653	1/1	0.80	0.21	18,18,18,18	0
57	MG	2a	3166	1/1	0.80	0.20	62,62,62,62	0
57	MG	2A	3247	1/1	0.80	0.15	40,40,40,40	0
57	MG	2A	3389	1/1	0.80	0.20	57,57,57,57	0
57	MG	2a	3045	1/1	0.80	0.19	44,44,44,44	0
57	MG	2a	3165	1/1	0.80	0.21	60,60,60,60	0
57	MG	2v	8002	1/1	0.80	0.21	66,66,66,66	0
57	MG	2A	3462	1/1	0.80	0.19	41,41,41,41	0
57	MG	2A	3568	1/1	0.80	0.15	45,45,45,45	0
57	MG	2A	3294	1/1	0.80	0.17	55,55,55,55	0
57	MG	2A	3560	1/1	0.80	0.22	51,51,51,51	0
57	MG	1A	3595	1/1	0.80	0.12	14,14,14,14	0
57	MG	2A	3482	1/1	0.80	0.12	71,71,71,71	0
57	MG	1a	3058	1/1	0.80	0.21	50,50,50,50	0
57	MG	1G	204	1/1	0.80	0.12	56,56,56,56	0
57	MG	2A	3155	1/1	0.80	0.20	54,54,54,54	0
57	MG	1A	3709	1/1	0.80	0.15	31,31,31,31	0
57	MG	1A	3391	1/1	0.80	0.12	50,50,50,50	0
57	MG	2a	3137	1/1	0.80	0.18	51,51,51,51	0
57	MG	20	3003	1/1	0.80	0.20	53,53,53,53	0
57	MG	2A	3246	1/1	0.80	0.11	47,47,47,47	0
57	MG	2A	3411	1/1	0.80	0.17	40,40,40,40	0
57	MG	2a	3028	1/1	0.80	0.16	56,56,56,56	0
57	MG	2A	3418	1/1	0.80	0.26	57,57,57,57	0
57	MG	1A	3006	1/1	0.80	0.24	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3460	1/1	0.81	0.17	35,35,35,35	0
57	MG	2A	3655	1/1	0.81	0.18	51,51,51,51	0
57	MG	1A	3263	1/1	0.81	0.24	35,35,35,35	0
57	MG	2A	3593	1/1	0.81	0.17	44,44,44,44	0
57	MG	2A	3353	1/1	0.81	0.15	65,65,65,65	0
57	MG	2A	3089	1/1	0.81	0.17	63,63,63,63	0
57	MG	2A	3262	1/1	0.81	0.18	60,60,60,60	0
57	MG	1a	3075	1/1	0.81	0.11	55,55,55,55	0
57	MG	2a	3110	1/1	0.81	0.14	57,57,57,57	0
57	MG	2A	3128	1/1	0.81	0.15	35,35,35,35	0
57	MG	2a	3024	1/1	0.81	0.16	56,56,56,56	0
57	MG	2a	3029	1/1	0.81	0.14	72,72,72,72	0
57	MG	1A	3428	1/1	0.81	0.10	41,41,41,41	0
57	MG	2A	3129	1/1	0.81	0.23	50,50,50,50	0
57	MG	1A	3484	1/1	0.81	0.18	35,35,35,35	0
57	MG	2A	3217	1/1	0.81	0.22	57,57,57,57	0
57	MG	2A	3291	1/1	0.81	0.13	24,24,24,24	0
57	MG	1E	307	1/1	0.81	0.14	31,31,31,31	0
57	MG	2a	3003	1/1	0.81	0.12	57,57,57,57	0
57	MG	1A	3874	1/1	0.81	0.22	62,62,62,62	0
57	MG	1B	3021	1/1	0.81	0.15	48,48,48,48	0
57	MG	1a	3123	1/1	0.81	0.12	35,35,35,35	0
57	MG	1A	3884	1/1	0.81	0.09	40,40,40,40	0
57	MG	2a	3195	1/1	0.81	0.23	84,84,84,84	0
57	MG	1A	3185	1/1	0.81	0.20	49,49,49,49	0
57	MG	1A	3725	1/1	0.81	0.28	50,50,50,50	0
57	MG	1A	3148	1/1	0.81	0.21	52,52,52,52	0
57	MG	2A	3390	1/1	0.82	0.13	65,65,65,65	0
57	MG	1E	308	1/1	0.82	0.12	48,48,48,48	0
57	MG	1A	3312	1/1	0.82	0.24	30,30,30,30	0
57	MG	1a	3174	1/1	0.82	0.13	57,57,57,57	0
57	MG	2A	3598	1/1	0.82	0.21	52,52,52,52	0
57	MG	2a	3115	1/1	0.82	0.10	66,66,66,66	0
57	MG	2A	3274	1/1	0.82	0.17	40,40,40,40	0
57	MG	1A	3601	1/1	0.82	0.15	34,34,34,34	0
57	MG	17	102	1/1	0.82	0.26	48,48,48,48	0
57	MG	1A	3266	1/1	0.82	0.27	39,39,39,39	0
57	MG	2A	3400	1/1	0.82	0.12	55,55,55,55	0
57	MG	1A	3740	1/1	0.82	0.15	47,47,47,47	0
57	MG	1B	3027	1/1	0.82	0.09	53,53,53,53	0
57	MG	1A	3822	1/1	0.82	0.14	40,40,40,40	0
57	MG	2A	3474	1/1	0.82	0.31	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	3131	1/1	0.82	0.17	61,61,61,61	0
57	MG	2a	3006	1/1	0.82	0.15	57,57,57,57	0
57	MG	2A	3046	1/1	0.82	0.13	55,55,55,55	0
57	MG	1A	3727	1/1	0.82	0.12	46,46,46,46	0
57	MG	1E	303	1/1	0.82	0.15	22,22,22,22	0
57	MG	1A	3802	1/1	0.82	0.12	46,46,46,46	0
57	MG	2B	3009	1/1	0.82	0.15	48,48,48,48	0
57	MG	2A	3127	1/1	0.82	0.20	52,52,52,52	0
57	MG	2A	3009	1/1	0.82	0.10	59,59,59,59	0
57	MG	2w	102	1/1	0.82	0.58	61,61,61,61	0
57	MG	1A	3722	1/1	0.82	0.32	42,42,42,42	0
57	MG	2a	3053	1/1	0.82	0.14	49,49,49,49	0
57	MG	2A	3347	1/1	0.82	0.19	27,27,27,27	0
57	MG	1a	3011	1/1	0.82	0.12	50,50,50,50	0
57	MG	1a	3077	1/1	0.82	0.16	39,39,39,39	0
57	MG	1A	3299	1/1	0.82	0.11	40,40,40,40	0
57	MG	2A	3174	1/1	0.83	0.32	59,59,59,59	0
57	MG	1A	3583	1/1	0.83	0.17	15,15,15,15	0
57	MG	2A	3175	1/1	0.83	0.20	49,49,49,49	0
57	MG	2A	3051	1/1	0.83	0.26	60,60,60,60	0
57	MG	1A	3126	1/1	0.83	0.12	62,62,62,62	0
57	MG	2A	3576	1/1	0.83	0.20	60,60,60,60	0
57	MG	2a	3035	1/1	0.83	0.18	61,61,61,61	0
57	MG	2A	3582	1/1	0.83	0.12	52,52,52,52	0
57	MG	2B	3001	1/1	0.83	0.15	54,54,54,54	0
57	MG	1A	3614	1/1	0.83	0.19	23,23,23,23	0
57	MG	2q	3002	1/1	0.83	0.30	71,71,71,71	0
57	MG	2A	3190	1/1	0.83	0.17	66,66,66,66	0
57	MG	1A	3951	1/1	0.83	0.18	49,49,49,49	0
57	MG	2a	3147	1/1	0.83	0.12	56,56,56,56	0
57	MG	2A	3601	1/1	0.83	0.15	55,55,55,55	0
57	MG	2A	3536	1/1	0.83	0.09	60,60,60,60	0
57	MG	2A	3116	1/1	0.83	0.16	43,43,43,43	0
57	MG	2A	3475	1/1	0.83	0.14	61,61,61,61	0
57	MG	2A	3435	1/1	0.83	0.17	59,59,59,59	0
57	MG	1A	3207	1/1	0.83	0.18	42,42,42,42	0
57	MG	2a	3020	1/1	0.83	0.11	65,65,65,65	0
57	MG	2A	3446	1/1	0.83	0.14	41,41,41,41	0
57	MG	2a	3039	1/1	0.83	0.11	57,57,57,57	0
57	MG	1A	3460	1/1	0.83	0.12	26,26,26,26	0
57	MG	1A	3902	1/1	0.83	0.32	44,44,44,44	0
57	MG	2A	3095	1/1	0.83	0.31	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2B	3007	1/1	0.83	0.14	61,61,61,61	0
57	MG	1A	3825	1/1	0.83	0.39	37,37,37,37	0
57	MG	2A	3176	1/1	0.83	0.14	44,44,44,44	0
57	MG	2A	3039	1/1	0.83	0.27	58,58,58,58	0
57	MG	2A	3657	1/1	0.83	0.28	63,63,63,63	0
57	MG	1A	3808	1/1	0.83	0.12	41,41,41,41	0
57	MG	1a	3147	1/1	0.83	0.16	47,47,47,47	0
57	MG	2a	3153	1/1	0.83	0.08	59,59,59,59	0
57	MG	1a	3227	1/1	0.83	0.25	52,52,52,52	0
57	MG	2A	3605	1/1	0.83	0.19	49,49,49,49	0
57	MG	2A	3263	1/1	0.83	0.19	34,34,34,34	0
57	MG	1A	3812	1/1	0.84	0.18	21,21,21,21	0
57	MG	2A	3578	1/1	0.84	0.13	56,56,56,56	0
57	MG	1a	3099	1/1	0.84	0.24	48,48,48,48	0
57	MG	2a	3048	1/1	0.84	0.10	57,57,57,57	0
57	MG	1a	3057	1/1	0.84	0.11	55,55,55,55	0
57	MG	1A	3302	1/1	0.84	0.25	40,40,40,40	0
57	MG	2a	3167	1/1	0.84	0.20	64,64,64,64	0
57	MG	2a	3155	1/1	0.84	0.14	63,63,63,63	0
57	MG	2A	3643	1/1	0.84	0.15	51,51,51,51	0
57	MG	2a	3180	1/1	0.84	0.11	62,62,62,62	0
57	MG	2A	3239	1/1	0.84	0.13	48,48,48,48	0
57	MG	1A	3872	1/1	0.84	0.52	56,56,56,56	0
57	MG	2A	3340	1/1	0.84	0.12	36,36,36,36	0
57	MG	1A	3050	1/1	0.84	0.16	32,32,32,32	0
57	MG	1x	102	1/1	0.84	0.20	54,54,54,54	0
57	MG	2a	3138	1/1	0.84	0.17	62,62,62,62	0
57	MG	1a	3156	1/1	0.84	0.12	42,42,42,42	0
57	MG	1a	3169	1/1	0.84	0.16	70,70,70,70	0
57	MG	1A	3855	1/1	0.84	0.16	46,46,46,46	0
57	MG	13	101	1/1	0.84	0.31	36,36,36,36	0
57	MG	1A	3178	1/1	0.84	0.28	39,39,39,39	0
57	MG	2l	202	1/1	0.84	0.18	62,62,62,62	0
57	MG	2A	3218	1/1	0.84	0.25	57,57,57,57	0
57	MG	1A	3101	1/1	0.84	0.20	25,25,25,25	0
57	MG	1a	3206	1/1	0.84	0.15	46,46,46,46	0
57	MG	2a	3023	1/1	0.84	0.25	66,66,66,66	0
57	MG	1a	3067	1/1	0.84	0.09	56,56,56,56	0
57	MG	1A	3253	1/1	0.84	0.18	36,36,36,36	0
57	MG	2a	3095	1/1	0.84	0.15	46,46,46,46	0
57	MG	1Y	204	1/1	0.84	0.33	52,52,52,52	0
57	MG	1A	3820	1/1	0.84	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3530	1/1	0.84	0.13	55,55,55,55	0
57	MG	2A	3212	1/1	0.84	0.16	39,39,39,39	0
57	MG	1A	3715	1/1	0.84	0.12	60,60,60,60	0
57	MG	1A	3949	1/1	0.84	0.13	53,53,53,53	0
57	MG	1A	3081	1/1	0.84	0.12	41,41,41,41	0
57	MG	2a	3144	1/1	0.84	0.12	70,70,70,70	0
57	MG	2A	3638	1/1	0.84	0.14	57,57,57,57	0
57	MG	1A	3017	1/1	0.84	0.12	37,37,37,37	0
57	MG	14	502	1/1	0.84	0.15	54,54,54,54	0
57	MG	2A	3627	1/1	0.84	0.11	55,55,55,55	0
57	MG	1A	3204	1/1	0.84	0.15	32,32,32,32	0
57	MG	2A	3569	1/1	0.84	0.10	60,60,60,60	0
57	MG	2A	3226	1/1	0.84	0.27	42,42,42,42	0
57	MG	1A	3239	1/1	0.84	0.22	60,60,60,60	0
57	MG	1a	3105	1/1	0.84	0.20	59,59,59,59	0
57	MG	2A	3362	1/1	0.85	0.24	41,41,41,41	0
57	MG	1A	3794	1/1	0.85	0.50	30,30,30,30	0
57	MG	1A	3220	1/1	0.85	0.23	41,41,41,41	0
57	MG	1A	3770	1/1	0.85	0.10	28,28,28,28	0
57	MG	2A	3193	1/1	0.85	0.14	50,50,50,50	0
57	MG	2A	3094	1/1	0.85	0.25	40,40,40,40	0
57	MG	2A	3209	1/1	0.85	0.19	47,47,47,47	0
57	MG	1A	3654	1/1	0.85	0.10	36,36,36,36	0
57	MG	2A	3266	1/1	0.85	0.10	53,53,53,53	0
57	MG	1a	3018	1/1	0.85	0.10	44,44,44,44	0
57	MG	1A	3527	1/1	0.85	0.18	31,31,31,31	0
57	MG	2A	3661	1/1	0.85	0.31	37,37,37,37	0
57	MG	1A	3520	1/1	0.85	0.20	45,45,45,45	0
57	MG	1a	3205	1/1	0.85	0.18	55,55,55,55	0
57	MG	1A	3097	1/1	0.85	0.32	42,42,42,42	0
57	MG	2E	301	1/1	0.85	0.11	34,34,34,34	0
57	MG	1a	3122	1/1	0.85	0.13	27,27,27,27	0
57	MG	1A	3963	1/1	0.85	0.14	33,33,33,33	0
57	MG	2A	3138	1/1	0.85	0.15	50,50,50,50	0
57	MG	2A	3523	1/1	0.85	0.21	68,68,68,68	0
57	MG	2A	3144	1/1	0.85	0.32	53,53,53,53	0
57	MG	1A	3100	1/1	0.85	0.18	28,28,28,28	0
57	MG	1A	3598	1/1	0.85	0.25	38,38,38,38	0
57	MG	2A	3583	1/1	0.85	0.24	62,62,62,62	0
57	MG	2A	3332	1/1	0.85	0.16	34,34,34,34	0
57	MG	1a	3079	1/1	0.85	0.22	42,42,42,42	0
57	MG	1A	3677	1/1	0.85	0.09	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3516	1/1	0.85	0.24	65,65,65,65	0
57	MG	1a	3096	1/1	0.85	0.42	54,54,54,54	0
57	MG	25	502	1/1	0.85	0.22	54,54,54,54	0
57	MG	2A	3455	1/1	0.85	0.10	39,39,39,39	0
57	MG	1A	3374	1/1	0.85	0.22	39,39,39,39	0
57	MG	2A	3609	1/1	0.85	0.09	59,59,59,59	0
57	MG	1B	3023	1/1	0.85	0.22	51,51,51,51	0
57	MG	2a	3038	1/1	0.85	0.25	53,53,53,53	0
57	MG	2A	3038	1/1	0.85	0.35	52,52,52,52	0
57	MG	1A	3245	1/1	0.85	0.36	24,24,24,24	0
57	MG	1A	3948	1/1	0.85	0.21	44,44,44,44	0
57	MG	1A	3088	1/1	0.85	0.19	40,40,40,40	0
57	MG	1A	3681	1/1	0.85	0.14	42,42,42,42	0
57	MG	1A	3297	1/1	0.85	0.19	47,47,47,47	0
57	MG	2A	3391	1/1	0.85	0.20	26,26,26,26	0
57	MG	1A	3922	1/1	0.85	0.19	52,52,52,52	0
57	MG	1A	3468	1/1	0.85	0.13	60,60,60,60	0
57	MG	1A	3582	1/1	0.85	0.17	20,20,20,20	0
57	MG	2A	3103	1/1	0.85	0.23	58,58,58,58	0
57	MG	1A	3412	1/1	0.85	0.21	30,30,30,30	0
57	MG	1A	3734	1/1	0.85	0.14	58,58,58,58	0
57	MG	1V	202	1/1	0.85	0.35	42,42,42,42	0
57	MG	1a	3076	1/1	0.85	0.12	47,47,47,47	0
57	MG	1a	3041	1/1	0.85	0.13	50,50,50,50	0
57	MG	1D	311	1/1	0.86	0.20	49,49,49,49	0
57	MG	2a	3119	1/1	0.86	0.12	64,64,64,64	0
57	MG	2A	3472	1/1	0.86	0.25	65,65,65,65	0
57	MG	1A	3124	1/1	0.86	0.16	33,33,33,33	0
57	MG	1a	3132	1/1	0.86	0.13	45,45,45,45	0
57	MG	1a	3215	1/1	0.86	0.17	62,62,62,62	0
57	MG	1a	3210	1/1	0.86	0.18	61,61,61,61	0
57	MG	1r	3001	1/1	0.86	0.23	51,51,51,51	0
57	MG	2A	3580	1/1	0.86	0.14	41,41,41,41	0
57	MG	1A	3189	1/1	0.86	0.47	35,35,35,35	0
57	MG	2a	3067	1/1	0.86	0.17	64,64,64,64	0
57	MG	2A	3620	1/1	0.86	0.17	59,59,59,59	0
57	MG	1A	3080	1/1	0.86	0.14	40,40,40,40	0
57	MG	1A	3290	1/1	0.86	0.17	40,40,40,40	0
57	MG	2A	3037	1/1	0.86	0.41	49,49,49,49	0
57	MG	2A	3648	1/1	0.86	0.14	52,52,52,52	0
57	MG	1A	3208	1/1	0.86	0.22	38,38,38,38	0
57	MG	2A	3214	1/1	0.86	0.19	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3077	1/1	0.86	0.16	45,45,45,45	0
57	MG	1a	3161	1/1	0.86	0.07	52,52,52,52	0
57	MG	1A	3955	1/1	0.86	0.27	34,34,34,34	0
57	MG	1a	3009	1/1	0.86	0.18	53,53,53,53	0
57	MG	1A	3474	1/1	0.86	0.12	48,48,48,48	0
57	MG	1a	3221	1/1	0.86	0.16	57,57,57,57	0
57	MG	2a	3136	1/1	0.86	0.14	67,67,67,67	0
57	MG	2A	3316	1/1	0.86	0.15	32,32,32,32	0
57	MG	1a	3155	1/1	0.86	0.25	40,40,40,40	0
57	MG	1a	3048	1/1	0.86	0.15	40,40,40,40	0
57	MG	2A	3234	1/1	0.86	0.18	54,54,54,54	0
57	MG	2A	3257	1/1	0.86	0.17	51,51,51,51	0
57	MG	1A	3655	1/1	0.86	0.12	26,26,26,26	0
57	MG	1a	3158	1/1	0.86	0.18	41,41,41,41	0
57	MG	1A	3049	1/1	0.86	0.15	46,46,46,46	0
57	MG	1a	3085	1/1	0.86	0.19	41,41,41,41	0
57	MG	2A	3063	1/1	0.86	0.20	56,56,56,56	0
57	MG	2A	3386	1/1	0.86	0.14	46,46,46,46	0
57	MG	1A	3396	1/1	0.86	0.15	30,30,30,30	0
57	MG	2A	3143	1/1	0.86	0.17	50,50,50,50	0
57	MG	2a	3100	1/1	0.86	0.08	57,57,57,57	0
57	MG	1A	3850	1/1	0.86	0.16	33,33,33,33	0
57	MG	2A	3619	1/1	0.86	0.30	43,43,43,43	0
57	MG	1a	3040	1/1	0.86	0.08	60,60,60,60	0
57	MG	2A	3287	1/1	0.86	0.12	38,38,38,38	0
57	MG	1a	3087	1/1	0.86	0.11	51,51,51,51	0
57	MG	2A	3163	1/1	0.86	0.14	58,58,58,58	0
57	MG	1a	3133	1/1	0.86	0.16	48,48,48,48	0
57	MG	2A	3180	1/1	0.86	0.33	47,47,47,47	0
57	MG	1A	3947	1/1	0.86	0.20	53,53,53,53	0
57	MG	2A	3080	1/1	0.86	0.18	47,47,47,47	0
57	MG	1A	3284	1/1	0.86	0.12	49,49,49,49	0
57	MG	2A	3556	1/1	0.87	0.09	51,51,51,51	0
57	MG	1A	3641	1/1	0.87	0.17	64,64,64,64	0
57	MG	1A	3508	1/1	0.87	0.11	51,51,51,51	0
57	MG	1A	3863	1/1	0.87	0.16	60,60,60,60	0
57	MG	1A	3639	1/1	0.87	0.11	29,29,29,29	0
57	MG	2A	3501	1/1	0.87	0.12	57,57,57,57	0
57	MG	2a	3051	1/1	0.87	0.18	46,46,46,46	0
57	MG	1A	3256	1/1	0.87	0.23	55,55,55,55	0
57	MG	1E	302	1/1	0.87	0.18	52,52,52,52	0
57	MG	1n	503	1/1	0.87	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3836	1/1	0.87	0.37	61,61,61,61	0
57	MG	2A	3081	1/1	0.87	0.38	44,44,44,44	0
57	MG	2A	3518	1/1	0.87	0.24	55,55,55,55	0
57	MG	2a	3082	1/1	0.87	0.17	61,61,61,61	0
57	MG	2A	3363	1/1	0.87	0.18	39,39,39,39	0
57	MG	2A	3139	1/1	0.87	0.22	50,50,50,50	0
57	MG	1A	3849	1/1	0.87	0.15	50,50,50,50	0
57	MG	1D	309	1/1	0.87	0.12	38,38,38,38	0
57	MG	1a	3030	1/1	0.87	0.10	48,48,48,48	0
57	MG	1A	3667	1/1	0.87	0.18	50,50,50,50	0
57	MG	2A	3168	1/1	0.87	0.37	38,38,38,38	0
57	MG	2a	3026	1/1	0.87	0.15	65,65,65,65	0
57	MG	1E	310	1/1	0.87	0.14	63,63,63,63	0
57	MG	2A	3146	1/1	0.87	0.14	61,61,61,61	0
57	MG	2A	3310	1/1	0.87	0.21	56,56,56,56	0
57	MG	2a	3174	1/1	0.87	0.15	62,62,62,62	0
57	MG	1A	3551	1/1	0.87	0.14	38,38,38,38	0
57	MG	2A	3542	1/1	0.87	0.15	53,53,53,53	0
57	MG	2A	3383	1/1	0.87	0.09	38,38,38,38	0
57	MG	2A	3505	1/1	0.87	0.14	45,45,45,45	0
57	MG	2d	503	1/1	0.87	0.16	50,50,50,50	0
59	AQJ	2A	3677	37/37	0.87	0.49	35,55,68,73	0
57	MG	2a	3140	1/1	0.87	0.20	55,55,55,55	0
57	MG	1A	3670	1/1	0.87	0.19	40,40,40,40	0
57	MG	2A	3647	1/1	0.87	0.19	62,62,62,62	0
57	MG	1A	3571	1/1	0.87	0.12	37,37,37,37	0
57	MG	1B	3010	1/1	0.87	0.20	45,45,45,45	0
57	MG	1a	3220	1/1	0.87	0.17	63,63,63,63	0
57	MG	2A	3208	1/1	0.87	0.11	42,42,42,42	0
57	MG	1A	3172	1/1	0.87	0.12	46,46,46,46	0
57	MG	2a	3135	1/1	0.87	0.13	56,56,56,56	0
57	MG	2A	3491	1/1	0.87	0.12	59,59,59,59	0
57	MG	2A	3210	1/1	0.87	0.15	35,35,35,35	0
57	MG	1A	3398	1/1	0.87	0.15	29,29,29,29	0
57	MG	1a	3035	1/1	0.87	0.21	53,53,53,53	0
57	MG	2A	3591	1/1	0.87	0.79	73,73,73,73	0
57	MG	1a	3197	1/1	0.87	0.10	78,78,78,78	0
57	MG	2a	3200	1/1	0.87	0.10	69,69,69,69	0
57	MG	2A	3275	1/1	0.88	0.11	71,71,71,71	0
57	MG	2A	3567	1/1	0.88	0.16	34,34,34,34	0
57	MG	1T	8001	1/1	0.88	0.11	40,40,40,40	0
57	MG	1A	3553	1/1	0.88	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
57	MG	1A	3841	1/1	0.88	0.55	40,40,40,40	0
57	MG	1A	3175	1/1	0.88	0.28	37,37,37,37	0
57	MG	1A	3695	1/1	0.88	0.17	52,52,52,52	0
57	MG	2A	3243	1/1	0.88	0.14	45,45,45,45	0
57	MG	1A	3538	1/1	0.88	0.10	30,30,30,30	0
57	MG	2a	3146	1/1	0.88	0.20	55,55,55,55	0
57	MG	1A	3407	1/1	0.88	0.19	20,20,20,20	0
57	MG	1A	3657	1/1	0.88	0.21	50,50,50,50	0
57	MG	1A	3723	1/1	0.88	0.12	36,36,36,36	0
57	MG	1x	104	1/1	0.88	0.18	50,50,50,50	0
57	MG	2A	3024	1/1	0.88	0.23	49,49,49,49	0
57	MG	2A	3279	1/1	0.88	0.19	41,41,41,41	0
57	MG	1A	3735	1/1	0.88	0.26	46,46,46,46	0
57	MG	2a	3185	1/1	0.88	0.23	60,60,60,60	0
57	MG	1A	3625	1/1	0.88	0.12	49,49,49,49	0
57	MG	1A	3558	1/1	0.88	0.13	20,20,20,20	0
57	MG	2a	3056	1/1	0.88	0.16	66,66,66,66	0
57	MG	2A	3415	1/1	0.88	0.11	50,50,50,50	0
57	MG	1A	3749	1/1	0.88	0.14	61,61,61,61	0
57	MG	2A	3075	1/1	0.88	0.19	48,48,48,48	0
57	MG	1A	3763	1/1	0.88	0.16	54,54,54,54	0
57	MG	1A	4002	1/1	0.88	0.19	35,35,35,35	0
57	MG	2A	3407	1/1	0.88	0.15	42,42,42,42	0
57	MG	2A	3206	1/1	0.88	0.09	59,59,59,59	0
57	MG	1S	3001	1/1	0.88	0.24	37,37,37,37	0
57	MG	1A	3149	1/1	0.88	0.22	28,28,28,28	0
57	MG	2A	3558	1/1	0.88	0.11	38,38,38,38	0
57	MG	1a	3056	1/1	0.88	0.17	44,44,44,44	0
57	MG	2A	3065	1/1	0.88	0.17	50,50,50,50	0
57	MG	1A	3879	1/1	0.88	0.14	23,23,23,23	0
57	MG	2a	3142	1/1	0.88	0.28	54,54,54,54	0
57	MG	1A	3487	1/1	0.88	0.17	23,23,23,23	0
57	MG	1A	3873	1/1	0.88	0.13	47,47,47,47	0
57	MG	1E	304	1/1	0.88	0.19	42,42,42,42	0
57	MG	2A	3245	1/1	0.88	0.13	45,45,45,45	0
57	MG	1A	3449	1/1	0.88	0.15	45,45,45,45	0
57	MG	2A	3306	1/1	0.88	0.11	46,46,46,46	0
57	MG	1A	3648	1/1	0.88	0.16	17,17,17,17	0
57	MG	1A	3910	1/1	0.88	0.15	56,56,56,56	0
57	MG	1A	3255	1/1	0.88	0.10	50,50,50,50	0
57	MG	2a	3012	1/1	0.88	0.18	57,57,57,57	0
59	AQJ	1A	3969	37/37	0.88	0.39	21,45,62,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	3093	1/1	0.88	0.08	59,59,59,59	0
57	MG	1A	3592	1/1	0.88	0.16	37,37,37,37	0
57	MG	1A	3751	1/1	0.88	0.15	35,35,35,35	0
57	MG	1I	3001	1/1	0.88	0.17	60,60,60,60	0
57	MG	1a	3135	1/1	0.88	0.17	34,34,34,34	0
57	MG	2a	3116	1/1	0.88	0.08	63,63,63,63	0
57	MG	1A	3276	1/1	0.88	0.24	21,21,21,21	0
57	MG	2A	3067	1/1	0.88	0.20	46,46,46,46	0
57	MG	2A	3502	1/1	0.88	0.19	49,49,49,49	0
57	MG	2A	3130	1/1	0.88	0.19	38,38,38,38	0
57	MG	2D	303	1/1	0.88	0.24	46,46,46,46	0
57	MG	1A	3919	1/1	0.88	0.53	36,36,36,36	0
57	MG	1A	3611	1/1	0.88	0.15	20,20,20,20	0
57	MG	2A	3225	1/1	0.88	0.26	54,54,54,54	0
57	MG	1W	203	1/1	0.88	0.33	47,47,47,47	0
57	MG	1A	3216	1/1	0.88	0.13	42,42,42,42	0
57	MG	2A	3611	1/1	0.88	0.21	51,51,51,51	0
57	MG	2A	3682	1/1	0.88	0.17	33,33,33,33	0
57	MG	1A	3994	1/1	0.88	0.40	46,46,46,46	0
57	MG	1a	3070	1/1	0.88	0.25	50,50,50,50	0
57	MG	1O	204	1/1	0.88	0.08	40,40,40,40	0
57	MG	2a	3125	1/1	0.88	0.13	58,58,58,58	0
57	MG	1A	3431	1/1	0.88	0.06	61,61,61,61	0
57	MG	1A	3328	1/1	0.88	0.17	33,33,33,33	0
57	MG	1A	3824	1/1	0.88	0.19	34,34,34,34	0
57	MG	1P	201	1/1	0.88	0.30	24,24,24,24	0
57	MG	1G	205	1/1	0.88	0.13	61,61,61,61	0
57	MG	2A	3596	1/1	0.88	0.31	46,46,46,46	0
57	MG	1a	3159	1/1	0.88	0.12	67,67,67,67	0
57	MG	1A	3534	1/1	0.88	0.19	48,48,48,48	0
57	MG	2A	3666	1/1	0.88	0.20	49,49,49,49	0
57	MG	2A	3258	1/1	0.88	0.13	50,50,50,50	0
57	MG	1A	3352	1/1	0.88	0.17	37,37,37,37	0
57	MG	2A	3085	1/1	0.88	0.13	57,57,57,57	0
57	MG	1y	3001	1/1	0.88	0.14	78,78,78,78	0
57	MG	15	103	1/1	0.88	0.14	37,37,37,37	0
57	MG	2a	3189	1/1	0.89	0.10	49,49,49,49	0
57	MG	1Q	206	1/1	0.89	0.11	45,45,45,45	0
57	MG	2a	3019	1/1	0.89	0.15	47,47,47,47	0
57	MG	2A	3375	1/1	0.89	0.13	47,47,47,47	0
57	MG	2x	105	1/1	0.89	0.12	45,45,45,45	0
57	MG	2a	3102	1/1	0.89	0.09	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	3007	1/1	0.89	0.10	53,53,53,53	0
57	MG	2Q	3002	1/1	0.89	0.18	44,44,44,44	0
57	MG	2a	3159	1/1	0.89	0.17	61,61,61,61	0
57	MG	2E	304	1/1	0.89	0.20	29,29,29,29	0
57	MG	1A	3111	1/1	0.89	0.17	31,31,31,31	0
57	MG	2A	3506	1/1	0.89	0.17	43,43,43,43	0
57	MG	1A	3828	1/1	0.89	0.13	30,30,30,30	0
57	MG	1A	3510	1/1	0.89	0.29	39,39,39,39	0
57	MG	2A	3500	1/1	0.89	0.30	62,62,62,62	0
57	MG	2x	104	1/1	0.89	0.18	54,54,54,54	0
57	MG	1A	3685	1/1	0.89	0.13	42,42,42,42	0
57	MG	1A	3750	1/1	0.89	0.15	18,18,18,18	0
57	MG	2A	3237	1/1	0.89	0.29	46,46,46,46	0
57	MG	1A	3673	1/1	0.89	0.14	49,49,49,49	0
57	MG	2a	3201	1/1	0.89	0.18	55,55,55,55	0
57	MG	1O	205	1/1	0.89	0.11	43,43,43,43	0
57	MG	2A	3420	1/1	0.89	0.20	47,47,47,47	0
57	MG	1A	3129	1/1	0.89	0.20	29,29,29,29	0
57	MG	1S	3003	1/1	0.89	0.10	52,52,52,52	0
57	MG	2A	3494	1/1	0.89	0.18	34,34,34,34	0
57	MG	2A	3387	1/1	0.89	0.12	44,44,44,44	0
57	MG	1A	3712	1/1	0.89	0.15	56,56,56,56	0
57	MG	2A	3100	1/1	0.89	0.08	52,52,52,52	0
60	ZN	24	501	1/1	0.89	0.05	115,115,115,115	0
57	MG	2A	3289	1/1	0.89	0.18	23,23,23,23	0
57	MG	1A	3018	1/1	0.89	0.18	27,27,27,27	0
57	MG	2A	3137	1/1	0.89	0.14	34,34,34,34	0
57	MG	1a	3029	1/1	0.89	0.20	53,53,53,53	0
57	MG	1B	3009	1/1	0.89	0.27	48,48,48,48	0
57	MG	2A	3527	1/1	0.89	0.14	48,48,48,48	0
57	MG	2g	8001	1/1	0.89	0.12	71,71,71,71	0
57	MG	1A	3536	1/1	0.89	0.15	23,23,23,23	0
57	MG	2A	3356	1/1	0.89	0.14	52,52,52,52	0
57	MG	1A	3430	1/1	0.89	0.20	27,27,27,27	0
57	MG	1A	3623	1/1	0.89	0.15	22,22,22,22	0
57	MG	1a	3224	1/1	0.89	0.14	45,45,45,45	0
57	MG	1N	3004	1/1	0.89	0.29	54,54,54,54	0
57	MG	2A	3293	1/1	0.89	0.17	58,58,58,58	0
57	MG	1A	3452	1/1	0.89	0.10	45,45,45,45	0
57	MG	1A	3554	1/1	0.89	0.19	38,38,38,38	0
57	MG	2A	3106	1/1	0.89	0.14	51,51,51,51	0
57	MG	1A	3631	1/1	0.89	0.14	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3295	1/1	0.89	0.16	66,66,66,66	0
57	MG	1A	3916	1/1	0.89	0.18	39,39,39,39	0
57	MG	1A	3394	1/1	0.89	0.13	43,43,43,43	0
57	MG	2B	3008	1/1	0.89	0.08	53,53,53,53	0
57	MG	1F	306	1/1	0.89	0.19	50,50,50,50	0
57	MG	10	103	1/1	0.89	0.32	47,47,47,47	0
57	MG	2A	3379	1/1	0.89	0.12	48,48,48,48	0
57	MG	1A	3586	1/1	0.89	0.18	28,28,28,28	0
57	MG	1A	3014	1/1	0.89	0.16	26,26,26,26	0
57	MG	10	102	1/1	0.89	0.58	44,44,44,44	0
57	MG	2A	3230	1/1	0.89	0.17	48,48,48,48	0
57	MG	2A	3652	1/1	0.89	0.10	35,35,35,35	0
57	MG	2q	3001	1/1	0.89	0.17	42,42,42,42	0
57	MG	2a	3103	1/1	0.89	0.14	51,51,51,51	0
57	MG	1Z	303	1/1	0.89	0.17	51,51,51,51	0
57	MG	2a	3173	1/1	0.89	0.30	68,68,68,68	0
57	MG	2A	3178	1/1	0.89	0.14	59,59,59,59	0
57	MG	1A	3008	1/1	0.89	0.27	43,43,43,43	0
57	MG	2x	101	1/1	0.89	0.09	57,57,57,57	0
57	MG	2A	3493	1/1	0.89	0.13	55,55,55,55	0
57	MG	1A	3206	1/1	0.89	0.09	33,33,33,33	0
57	MG	2a	3062	1/1	0.89	0.10	62,62,62,62	0
57	MG	1A	3260	1/1	0.89	0.13	45,45,45,45	0
57	MG	2a	3002	1/1	0.89	0.12	49,49,49,49	0
57	MG	1A	3072	1/1	0.89	0.16	36,36,36,36	0
57	MG	2A	3417	1/1	0.89	0.24	45,45,45,45	0
57	MG	1F	307	1/1	0.89	0.25	40,40,40,40	0
57	MG	2A	3465	1/1	0.89	0.21	47,47,47,47	0
57	MG	2A	3549	1/1	0.89	0.22	48,48,48,48	0
57	MG	2A	3071	1/1	0.89	0.12	46,46,46,46	0
57	MG	1A	3252	1/1	0.89	0.25	31,31,31,31	0
57	MG	1A	3645	1/1	0.89	0.07	45,45,45,45	0
57	MG	2A	3334	1/1	0.89	0.26	50,50,50,50	0
57	MG	1A	3702	1/1	0.89	0.23	25,25,25,25	0
57	MG	2B	3014	1/1	0.89	0.16	68,68,68,68	0
57	MG	1A	3814	1/1	0.89	0.20	38,38,38,38	0
57	MG	1a	3017	1/1	0.89	0.13	51,51,51,51	0
57	MG	16	502	1/1	0.89	0.17	34,34,34,34	0
57	MG	1A	3356	1/1	0.89	0.13	19,19,19,19	0
57	MG	2A	3589	1/1	0.89	0.21	59,59,59,59	0
57	MG	1A	3679	1/1	0.89	0.15	37,37,37,37	0
57	MG	1a	3074	1/1	0.89	0.32	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3246	1/1	0.90	0.19	40,40,40,40	0
57	MG	2A	3131	1/1	0.90	0.24	46,46,46,46	0
57	MG	2a	3055	1/1	0.90	0.24	60,60,60,60	0
57	MG	1A	3876	1/1	0.90	0.20	24,24,24,24	0
57	MG	1l	103	1/1	0.90	0.13	52,52,52,52	0
57	MG	1A	3742	1/1	0.90	0.12	57,57,57,57	0
57	MG	1A	3273	1/1	0.90	0.44	36,36,36,36	0
57	MG	1A	3924	1/1	0.90	0.13	34,34,34,34	0
57	MG	2A	3618	1/1	0.90	0.15	32,32,32,32	0
57	MG	1Z	302	1/1	0.90	0.17	45,45,45,45	0
57	MG	1A	3931	1/1	0.90	0.15	53,53,53,53	0
57	MG	1A	3754	1/1	0.90	0.18	31,31,31,31	0
57	MG	1A	3905	1/1	0.90	0.14	25,25,25,25	0
57	MG	1A	3964	1/1	0.90	0.20	33,33,33,33	0
57	MG	1A	3839	1/1	0.90	0.21	24,24,24,24	0
57	MG	1A	3665	1/1	0.90	0.15	52,52,52,52	0
57	MG	2a	3001	1/1	0.90	0.14	45,45,45,45	0
57	MG	1A	3652	1/1	0.90	0.20	13,13,13,13	0
57	MG	1A	3406	1/1	0.90	0.18	27,27,27,27	0
57	MG	1A	3837	1/1	0.90	0.14	35,35,35,35	0
57	MG	1A	3483	1/1	0.90	0.21	30,30,30,30	0
57	MG	1b	3001	1/1	0.90	0.16	68,68,68,68	0
57	MG	2A	3017	1/1	0.90	0.17	53,53,53,53	0
57	MG	2A	3419	1/1	0.90	0.16	54,54,54,54	0
57	MG	2a	3084	1/1	0.90	0.18	58,58,58,58	0
57	MG	1A	3720	1/1	0.90	0.12	23,23,23,23	0
57	MG	1A	3638	1/1	0.90	0.18	36,36,36,36	0
57	MG	1N	3002	1/1	0.90	0.15	38,38,38,38	0
57	MG	1A	3692	1/1	0.90	0.23	58,58,58,58	0
57	MG	1A	3232	1/1	0.90	0.10	31,31,31,31	0
57	MG	1A	3967	1/1	0.90	0.34	45,45,45,45	0
57	MG	1A	3543	1/1	0.90	0.16	44,44,44,44	0
57	MG	1A	3244	1/1	0.90	0.26	40,40,40,40	0
57	MG	2G	3001	1/1	0.90	0.12	64,64,64,64	0
57	MG	1A	3731	1/1	0.90	0.13	50,50,50,50	0
57	MG	2A	3573	1/1	0.90	0.30	71,71,71,71	0
57	MG	2A	3367	1/1	0.90	0.16	42,42,42,42	0
57	MG	1A	3242	1/1	0.90	0.22	40,40,40,40	0
57	MG	1A	3241	1/1	0.90	0.17	28,28,28,28	0
57	MG	2A	3292	1/1	0.90	0.10	56,56,56,56	0
57	MG	1A	3330	1/1	0.90	0.12	33,33,33,33	0
57	MG	2D	301	1/1	0.90	0.36	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	3091	1/1	0.90	0.12	49,49,49,49	0
57	MG	1A	3562	1/1	0.90	0.12	37,37,37,37	0
57	MG	1A	3140	1/1	0.90	0.15	35,35,35,35	0
57	MG	1A	3073	1/1	0.90	0.18	25,25,25,25	0
57	MG	2a	3198	1/1	0.90	0.14	60,60,60,60	0
57	MG	1A	3117	1/1	0.90	0.42	51,51,51,51	0
57	MG	1A	3061	1/1	0.90	0.16	22,22,22,22	0
57	MG	1A	3052	1/1	0.90	0.10	45,45,45,45	0
57	MG	1A	3158	1/1	0.90	0.21	30,30,30,30	0
57	MG	1a	3196	1/1	0.90	0.09	58,58,58,58	0
57	MG	2A	3370	1/1	0.90	0.24	54,54,54,54	0
57	MG	2A	3644	1/1	0.90	0.06	70,70,70,70	0
57	MG	2A	3607	1/1	0.90	0.10	50,50,50,50	0
57	MG	1A	3861	1/1	0.90	0.15	30,30,30,30	0
57	MG	2A	3408	1/1	0.90	0.13	25,25,25,25	0
57	MG	1A	3370	1/1	0.90	0.13	21,21,21,21	0
57	MG	1A	3632	1/1	0.90	0.13	49,49,49,49	0
57	MG	2a	3145	1/1	0.90	0.11	64,64,64,64	0
57	MG	2a	3158	1/1	0.90	0.17	65,65,65,65	0
57	MG	1A	3865	1/1	0.90	0.19	24,24,24,24	0
57	MG	1A	3086	1/1	0.90	0.13	51,51,51,51	0
57	MG	1A	3344	1/1	0.90	0.34	29,29,29,29	0
57	MG	1A	3011	1/1	0.90	0.18	42,42,42,42	0
57	MG	2A	3204	1/1	0.90	0.29	53,53,53,53	0
57	MG	2P	3001	1/1	0.90	0.12	59,59,59,59	0
57	MG	1A	3424	1/1	0.90	0.20	38,38,38,38	0
57	MG	1a	3188	1/1	0.90	0.18	57,57,57,57	0
57	MG	1A	3348	1/1	0.90	0.24	38,38,38,38	0
57	MG	1B	3002	1/1	0.90	0.25	42,42,42,42	0
57	MG	1A	3578	1/1	0.90	0.17	53,53,53,53	0
57	MG	1A	3320	1/1	0.90	0.30	46,46,46,46	0
57	MG	2a	3049	1/1	0.90	0.10	52,52,52,52	0
57	MG	2a	3041	1/1	0.90	0.17	52,52,52,52	0
57	MG	1a	3026	1/1	0.90	0.14	43,43,43,43	0
57	MG	1A	3613	1/1	0.90	0.22	16,16,16,16	0
57	MG	1A	3548	1/1	0.90	0.11	37,37,37,37	0
57	MG	2A	3072	1/1	0.90	0.11	58,58,58,58	0
57	MG	2A	3250	1/1	0.90	0.13	43,43,43,43	0
57	MG	2A	3186	1/1	0.90	0.14	53,53,53,53	0
57	MG	1A	3746	1/1	0.90	0.23	44,44,44,44	0
57	MG	2A	3088	1/1	0.90	0.34	48,48,48,48	0
57	MG	1A	3051	1/1	0.90	0.12	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	3131	1/1	0.90	0.19	46,46,46,46	0
57	MG	1A	3225	1/1	0.90	0.15	45,45,45,45	0
57	MG	2E	303	1/1	0.90	0.12	30,30,30,30	0
57	MG	2A	3392	1/1	0.90	0.11	45,45,45,45	0
57	MG	2a	3130	1/1	0.90	0.28	51,51,51,51	0
57	MG	1A	3318	1/1	0.90	0.08	39,39,39,39	0
57	MG	1A	3388	1/1	0.90	0.34	32,32,32,32	0
57	MG	2B	3021	1/1	0.90	0.09	57,57,57,57	0
57	MG	2A	3613	1/1	0.90	0.10	55,55,55,55	0
57	MG	1A	3390	1/1	0.90	0.60	46,46,46,46	0
57	MG	1W	205	1/1	0.90	0.31	31,31,31,31	0
57	MG	1a	3190	1/1	0.90	0.11	65,65,65,65	0
57	MG	1A	3736	1/1	0.90	0.14	46,46,46,46	0
57	MG	1A	3691	1/1	0.90	0.12	48,48,48,48	0
57	MG	1A	3547	1/1	0.90	0.10	47,47,47,47	0
57	MG	2a	3069	1/1	0.90	0.08	60,60,60,60	0
57	MG	2A	3118	1/1	0.90	0.14	50,50,50,50	0
57	MG	2A	3096	1/1	0.90	0.09	54,54,54,54	0
57	MG	2a	3104	1/1	0.90	0.13	56,56,56,56	0
57	MG	1A	3212	1/1	0.90	0.19	28,28,28,28	0
57	MG	2A	3134	1/1	0.90	0.08	34,34,34,34	0
57	MG	1B	3028	1/1	0.90	0.26	53,53,53,53	0
57	MG	2A	3079	1/1	0.90	0.14	39,39,39,39	0
57	MG	1A	3710	1/1	0.90	0.12	32,32,32,32	0
57	MG	1A	3644	1/1	0.91	0.09	44,44,44,44	0
57	MG	2A	3124	1/1	0.91	0.10	61,61,61,61	0
57	MG	1A	3953	1/1	0.91	0.11	53,53,53,53	0
57	MG	2A	3413	1/1	0.91	0.15	44,44,44,44	0
57	MG	2A	3083	1/1	0.91	0.21	39,39,39,39	0
57	MG	2a	3150	1/1	0.91	0.12	69,69,69,69	0
57	MG	2A	3473	1/1	0.91	0.12	47,47,47,47	0
57	MG	1A	3929	1/1	0.91	0.21	25,25,25,25	0
57	MG	2a	3149	1/1	0.91	0.16	53,53,53,53	0
57	MG	2A	3220	1/1	0.91	0.15	45,45,45,45	0
57	MG	1A	3602	1/1	0.91	0.16	13,13,13,13	0
57	MG	2A	3625	1/1	0.91	0.15	68,68,68,68	0
57	MG	1A	3392	1/1	0.91	0.12	27,27,27,27	0
57	MG	1A	3818	1/1	0.91	0.16	28,28,28,28	0
57	MG	1A	3851	1/1	0.91	0.13	38,38,38,38	0
57	MG	1A	3144	1/1	0.91	0.15	19,19,19,19	0
57	MG	1Y	201	1/1	0.91	0.29	44,44,44,44	0
57	MG	1D	304	1/1	0.91	0.11	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3425	1/1	0.91	0.28	41,41,41,41	0
57	MG	1G	202	1/1	0.91	0.26	46,46,46,46	0
57	MG	1A	3769	1/1	0.91	0.13	49,49,49,49	0
57	MG	2A	3678	1/1	0.91	0.21	44,44,44,44	0
57	MG	1A	3229	1/1	0.91	0.18	55,55,55,55	0
57	MG	1A	3114	1/1	0.91	0.15	36,36,36,36	0
57	MG	2A	3539	1/1	0.91	0.24	43,43,43,43	0
57	MG	1A	3618	1/1	0.91	0.16	31,31,31,31	0
57	MG	2a	3118	1/1	0.91	0.09	57,57,57,57	0
57	MG	1a	3101	1/1	0.91	0.11	50,50,50,50	0
57	MG	2A	3563	1/1	0.91	0.17	48,48,48,48	0
57	MG	1D	308	1/1	0.91	0.17	38,38,38,38	0
57	MG	1A	3384	1/1	0.91	0.21	39,39,39,39	0
57	MG	2A	3358	1/1	0.91	0.17	54,54,54,54	0
57	MG	2A	3268	1/1	0.91	0.19	44,44,44,44	0
57	MG	2A	3410	1/1	0.91	0.33	58,58,58,58	0
57	MG	2a	3114	1/1	0.91	0.07	57,57,57,57	0
57	MG	1a	3090	1/1	0.91	0.11	63,63,63,63	0
57	MG	2A	3629	1/1	0.91	0.11	59,59,59,59	0
57	MG	1A	3007	1/1	0.91	0.21	19,19,19,19	0
57	MG	2A	3270	1/1	0.91	0.10	66,66,66,66	0
57	MG	1A	3523	1/1	0.91	0.19	20,20,20,20	0
57	MG	1A	3560	1/1	0.91	0.10	35,35,35,35	0
57	MG	1a	3059	1/1	0.91	0.17	50,50,50,50	0
57	MG	2A	3182	1/1	0.91	0.15	43,43,43,43	0
57	MG	2A	3136	1/1	0.91	0.27	35,35,35,35	0
57	MG	1A	3025	1/1	0.91	0.22	51,51,51,51	0
57	MG	1A	3572	1/1	0.91	0.10	51,51,51,51	0
57	MG	1A	3445	1/1	0.91	0.14	30,30,30,30	0
57	MG	2A	3373	1/1	0.91	0.29	43,43,43,43	0
57	MG	25	503	1/1	0.91	0.27	51,51,51,51	0
57	MG	1a	3175	1/1	0.91	0.13	36,36,36,36	0
57	MG	1a	3052	1/1	0.91	0.36	52,52,52,52	0
57	MG	1A	3104	1/1	0.91	0.20	33,33,33,33	0
57	MG	2A	3228	1/1	0.91	0.17	35,35,35,35	0
57	MG	1A	3277	1/1	0.91	0.21	29,29,29,29	0
57	MG	2A	3378	1/1	0.91	0.10	53,53,53,53	0
57	MG	2A	3035	1/1	0.91	0.15	52,52,52,52	0
57	MG	1A	3886	1/1	0.91	0.17	51,51,51,51	0
57	MG	1A	3827	1/1	0.91	0.17	37,37,37,37	0
57	MG	2A	3227	1/1	0.91	0.25	51,51,51,51	0
57	MG	2A	3238	1/1	0.91	0.17	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	15	105	1/1	0.91	0.11	41,41,41,41	0
57	MG	1w	3002	1/1	0.91	0.14	34,34,34,34	0
57	MG	2A	3374	1/1	0.91	0.12	38,38,38,38	0
57	MG	1A	3036	1/1	0.91	0.21	38,38,38,38	0
57	MG	2A	3057	1/1	0.91	0.13	54,54,54,54	0
57	MG	1A	3195	1/1	0.91	0.10	27,27,27,27	0
57	MG	1A	3585	1/1	0.91	0.19	28,28,28,28	0
57	MG	1a	3078	1/1	0.91	0.17	37,37,37,37	0
57	MG	1A	3257	1/1	0.91	0.11	47,47,47,47	0
57	MG	2A	3351	1/1	0.91	0.20	60,60,60,60	0
57	MG	1a	3180	1/1	0.91	0.14	40,40,40,40	0
57	MG	1a	3015	1/1	0.91	0.11	46,46,46,46	0
57	MG	2j	8001	1/1	0.91	0.10	61,61,61,61	0
57	MG	2A	3602	1/1	0.91	0.21	44,44,44,44	0
57	MG	1A	3894	1/1	0.91	0.30	31,31,31,31	0
57	MG	2a	3190	1/1	0.91	0.18	64,64,64,64	0
57	MG	1x	107	1/1	0.91	0.11	54,54,54,54	0
57	MG	1a	3201	1/1	0.91	0.09	50,50,50,50	0
57	MG	1A	3234	1/1	0.91	0.11	40,40,40,40	0
57	MG	2A	3074	1/1	0.91	0.30	48,48,48,48	0
57	MG	1a	3214	1/1	0.91	0.10	58,58,58,58	0
57	MG	2A	3675	1/1	0.91	0.12	49,49,49,49	0
57	MG	2A	3649	1/1	0.91	0.23	56,56,56,56	0
57	MG	1a	3023	1/1	0.91	0.19	45,45,45,45	0
57	MG	2A	3404	1/1	0.91	0.25	56,56,56,56	0
57	MG	1A	3119	1/1	0.91	0.15	25,25,25,25	0
57	MG	1A	3717	1/1	0.91	0.32	54,54,54,54	0
57	MG	1A	3377	1/1	0.91	0.25	31,31,31,31	0
57	MG	1A	3831	1/1	0.91	0.17	45,45,45,45	0
57	MG	2B	3020	1/1	0.91	0.11	53,53,53,53	0
57	MG	1A	3580	1/1	0.91	0.20	14,14,14,14	0
57	MG	1A	3797	1/1	0.91	0.15	58,58,58,58	0
57	MG	25	504	1/1	0.91	0.40	38,38,38,38	0
57	MG	2A	3365	1/1	0.91	0.19	59,59,59,59	0
57	MG	1A	3063	1/1	0.91	0.21	22,22,22,22	0
57	MG	1A	3191	1/1	0.91	0.21	43,43,43,43	0
57	MG	2A	3532	1/1	0.91	0.13	66,66,66,66	0
57	MG	1A	3805	1/1	0.91	0.16	22,22,22,22	0
57	MG	2A	3621	1/1	0.91	0.22	48,48,48,48	0
57	MG	1A	3470	1/1	0.91	0.06	35,35,35,35	0
57	MG	1A	3333	1/1	0.91	0.21	36,36,36,36	0
57	MG	1A	3811	1/1	0.91	0.14	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	3132	1/1	0.91	0.09	61,61,61,61	0
57	MG	1A	3914	1/1	0.91	0.13	37,37,37,37	0
57	MG	2A	3140	1/1	0.91	0.11	51,51,51,51	0
57	MG	1Q	203	1/1	0.91	0.26	37,37,37,37	0
57	MG	1A	3437	1/1	0.91	0.12	26,26,26,26	0
57	MG	2A	3381	1/1	0.91	0.08	51,51,51,51	0
57	MG	2A	3049	1/1	0.91	0.30	52,52,52,52	0
57	MG	2a	3157	1/1	0.91	0.10	50,50,50,50	0
57	MG	1B	3025	1/1	0.91	0.20	54,54,54,54	0
57	MG	2A	3559	1/1	0.91	0.18	28,28,28,28	0
57	MG	1A	3906	1/1	0.91	0.26	36,36,36,36	0
57	MG	2A	3172	1/1	0.91	0.26	55,55,55,55	0
57	MG	2a	3025	1/1	0.91	0.16	59,59,59,59	0
57	MG	2A	3042	1/1	0.91	0.20	61,61,61,61	0
57	MG	2A	3244	1/1	0.91	0.24	34,34,34,34	0
57	MG	1A	3943	1/1	0.91	0.13	36,36,36,36	0
57	MG	2A	3551	1/1	0.91	0.42	68,68,68,68	0
57	MG	2A	3153	1/1	0.91	0.23	37,37,37,37	0
57	MG	1Z	301	1/1	0.91	0.25	37,37,37,37	0
57	MG	2A	3355	1/1	0.91	0.20	47,47,47,47	0
57	MG	2a	3009	1/1	0.91	0.14	66,66,66,66	0
57	MG	2a	3063	1/1	0.91	0.32	60,60,60,60	0
57	MG	1a	3117	1/1	0.91	0.12	44,44,44,44	0
57	MG	2a	3010	1/1	0.91	0.09	47,47,47,47	0
57	MG	2A	3561	1/1	0.91	0.12	41,41,41,41	0
57	MG	2A	3663	1/1	0.91	0.14	31,31,31,31	0
57	MG	2A	3223	1/1	0.91	0.29	48,48,48,48	0
57	MG	2a	3033	1/1	0.91	0.14	53,53,53,53	0
60	ZN	2Y	501	1/1	0.91	0.10	92,92,92,92	0
57	MG	2A	3606	1/1	0.91	0.24	51,51,51,51	0
57	MG	1a	3187	1/1	0.91	0.27	58,58,58,58	0
57	MG	1P	204	1/1	0.91	0.15	34,34,34,34	0
57	MG	2a	3108	1/1	0.91	0.14	64,64,64,64	0
57	MG	2A	3421	1/1	0.91	0.11	43,43,43,43	0
57	MG	2A	3278	1/1	0.91	0.21	59,59,59,59	0
57	MG	1A	3862	1/1	0.91	0.14	22,22,22,22	0
57	MG	1A	3628	1/1	0.91	0.10	44,44,44,44	0
57	MG	1A	3368	1/1	0.91	0.19	35,35,35,35	0
57	MG	1A	3164	1/1	0.91	0.23	26,26,26,26	0
57	MG	2a	3008	1/1	0.92	0.24	41,41,41,41	0
57	MG	1A	3743	1/1	0.92	0.16	20,20,20,20	0
57	MG	2A	3617	1/1	0.92	0.12	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3338	1/1	0.92	0.17	42,42,42,42	0
57	MG	2A	3522	1/1	0.92	0.10	68,68,68,68	0
57	MG	1A	3020	1/1	0.92	0.12	41,41,41,41	0
57	MG	2B	3015	1/1	0.92	0.15	69,69,69,69	0
57	MG	1a	3008	1/1	0.92	0.22	50,50,50,50	0
57	MG	2d	502	1/1	0.92	0.10	63,63,63,63	0
57	MG	2A	3256	1/1	0.92	0.15	43,43,43,43	0
57	MG	1A	3620	1/1	0.92	0.09	55,55,55,55	0
57	MG	1A	3537	1/1	0.92	0.17	38,38,38,38	0
57	MG	2A	3548	1/1	0.92	0.15	36,36,36,36	0
57	MG	2A	3538	1/1	0.92	0.14	62,62,62,62	0
57	MG	2A	3126	1/1	0.92	0.20	39,39,39,39	0
57	MG	2A	3260	1/1	0.92	0.07	63,63,63,63	0
57	MG	2a	3179	1/1	0.92	0.15	37,37,37,37	0
57	MG	1a	3055	1/1	0.92	0.10	38,38,38,38	0
57	MG	1A	3674	1/1	0.92	0.13	49,49,49,49	0
57	MG	1A	3878	1/1	0.92	0.11	36,36,36,36	0
57	MG	1q	3001	1/1	0.92	0.08	43,43,43,43	0
57	MG	2A	3490	1/1	0.92	0.18	61,61,61,61	0
57	MG	1A	3976	1/1	0.92	0.17	25,25,25,25	0
57	MG	1A	3533	1/1	0.92	0.22	38,38,38,38	0
57	MG	2A	3344	1/1	0.92	0.16	35,35,35,35	0
57	MG	2A	3587	1/1	0.92	0.09	50,50,50,50	0
57	MG	1A	3135	1/1	0.92	0.25	49,49,49,49	0
57	MG	2A	3349	1/1	0.92	0.20	30,30,30,30	0
57	MG	1A	3761	1/1	0.92	0.22	31,31,31,31	0
57	MG	1A	3840	1/1	0.92	0.13	46,46,46,46	0
57	MG	2A	3471	1/1	0.92	0.12	29,29,29,29	0
57	MG	1A	3603	1/1	0.92	0.18	19,19,19,19	0
57	MG	1A	3193	1/1	0.92	0.21	32,32,32,32	0
57	MG	1A	3566	1/1	0.92	0.10	19,19,19,19	0
57	MG	2a	3032	1/1	0.92	0.11	48,48,48,48	0
57	MG	2A	3403	1/1	0.92	0.19	40,40,40,40	0
57	MG	1A	3171	1/1	0.92	0.16	47,47,47,47	0
57	MG	1A	3238	1/1	0.92	0.18	43,43,43,43	0
57	MG	1A	3847	1/1	0.92	0.43	67,67,67,67	0
57	MG	1x	111	1/1	0.92	0.20	56,56,56,56	0
57	MG	2A	3099	1/1	0.92	0.08	62,62,62,62	0
57	MG	1A	3429	1/1	0.92	0.04	26,26,26,26	0
57	MG	2A	3028	1/1	0.92	0.16	36,36,36,36	0
57	MG	1A	3174	1/1	0.92	0.14	26,26,26,26	0
57	MG	1B	3014	1/1	0.92	0.17	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3956	1/1	0.92	0.14	58,58,58,58	0
57	MG	2A	3299	1/1	0.92	0.17	31,31,31,31	0
57	MG	2A	3194	1/1	0.92	0.18	56,56,56,56	0
57	MG	1A	3383	1/1	0.92	0.28	28,28,28,28	0
57	MG	1A	3882	1/1	0.92	0.07	38,38,38,38	0
57	MG	1A	3889	1/1	0.92	0.15	19,19,19,19	0
57	MG	1A	3015	1/1	0.92	0.16	45,45,45,45	0
57	MG	2A	3224	1/1	0.92	0.14	39,39,39,39	0
57	MG	2a	3007	1/1	0.92	0.13	49,49,49,49	0
57	MG	1A	3479	1/1	0.92	0.24	25,25,25,25	0
57	MG	1A	3635	1/1	0.92	0.09	30,30,30,30	0
57	MG	1A	3087	1/1	0.92	0.21	32,32,32,32	0
57	MG	2a	3078	1/1	0.92	0.29	61,61,61,61	0
57	MG	2a	3015	1/1	0.92	0.18	46,46,46,46	0
57	MG	1a	3207	1/1	0.92	0.09	51,51,51,51	0
57	MG	1A	3587	1/1	0.92	0.16	29,29,29,29	0
57	MG	2A	3562	1/1	0.92	0.12	31,31,31,31	0
57	MG	2A	3631	1/1	0.92	0.19	55,55,55,55	0
57	MG	1a	3034	1/1	0.92	0.28	42,42,42,42	0
57	MG	1A	3739	1/1	0.92	0.11	31,31,31,31	0
57	MG	1A	3605	1/1	0.92	0.13	22,22,22,22	0
57	MG	2a	3065	1/1	0.92	0.15	70,70,70,70	0
57	MG	1A	3724	1/1	0.92	0.11	40,40,40,40	0
57	MG	1A	3920	1/1	0.92	0.20	73,73,73,73	0
57	MG	2A	3335	1/1	0.92	0.20	24,24,24,24	0
57	MG	2A	3622	1/1	0.92	0.24	61,61,61,61	0
57	MG	1A	3979	1/1	0.92	0.23	20,20,20,20	0
57	MG	2a	3187	1/1	0.92	0.15	74,74,74,74	0
57	MG	1t	3001	1/1	0.92	0.09	46,46,46,46	0
57	MG	1A	3194	1/1	0.92	0.14	29,29,29,29	0
57	MG	2A	3068	1/1	0.92	0.18	49,49,49,49	0
57	MG	1A	3610	1/1	0.92	0.13	25,25,25,25	0
57	MG	1A	3267	1/1	0.92	0.10	36,36,36,36	0
57	MG	1A	3529	1/1	0.92	0.15	29,29,29,29	0
57	MG	2A	3557	1/1	0.92	0.09	55,55,55,55	0
57	MG	1A	3705	1/1	0.92	0.19	29,29,29,29	0
57	MG	1A	3565	1/1	0.92	0.14	45,45,45,45	0
57	MG	2A	3188	1/1	0.92	0.11	43,43,43,43	0
57	MG	1A	3410	1/1	0.92	0.07	18,18,18,18	0
57	MG	1A	3561	1/1	0.92	0.10	49,49,49,49	0
57	MG	1A	3268	1/1	0.92	0.37	32,32,32,32	0
57	MG	2A	3610	1/1	0.92	0.16	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3458	1/1	0.92	0.07	40,40,40,40	0
57	MG	2A	3524	1/1	0.92	0.11	51,51,51,51	0
57	MG	2a	3171	1/1	0.92	0.11	64,64,64,64	0
57	MG	1A	3214	1/1	0.92	0.29	43,43,43,43	0
57	MG	1a	3051	1/1	0.92	0.24	48,48,48,48	0
57	MG	1A	3298	1/1	0.92	0.19	30,30,30,30	0
57	MG	1X	102	1/1	0.92	0.19	22,22,22,22	0
57	MG	2A	3162	1/1	0.92	0.18	64,64,64,64	0
57	MG	1A	3389	1/1	0.92	0.17	35,35,35,35	0
57	MG	1A	3923	1/1	0.92	0.16	37,37,37,37	0
57	MG	1B	3012	1/1	0.92	0.34	60,60,60,60	0
57	MG	2A	3600	1/1	0.92	0.19	33,33,33,33	0
57	MG	1A	3211	1/1	0.92	0.17	24,24,24,24	0
57	MG	2A	3133	1/1	0.92	0.18	45,45,45,45	0
57	MG	1A	3952	1/1	0.92	0.13	51,51,51,51	0
57	MG	1a	3066	1/1	0.92	0.11	34,34,34,34	0
57	MG	1A	3810	1/1	0.92	0.12	40,40,40,40	0
57	MG	2E	302	1/1	0.92	0.20	44,44,44,44	0
57	MG	1A	3926	1/1	0.92	0.07	32,32,32,32	0
57	MG	1a	3068	1/1	0.92	0.09	46,46,46,46	0
57	MG	2A	3119	1/1	0.92	0.12	37,37,37,37	0
57	MG	2A	3687	1/1	0.92	0.10	53,53,53,53	0
57	MG	1a	3162	1/1	0.92	0.14	32,32,32,32	0
57	MG	2A	3160	1/1	0.92	0.16	40,40,40,40	0
57	MG	1a	3125	1/1	0.92	0.20	68,68,68,68	0
57	MG	1A	3157	1/1	0.92	0.21	27,27,27,27	0
57	MG	2A	3241	1/1	0.92	0.09	42,42,42,42	0
57	MG	1A	3589	1/1	0.92	0.25	33,33,33,33	0
57	MG	1A	3134	1/1	0.92	0.13	25,25,25,25	0
57	MG	2A	3401	1/1	0.92	0.26	50,50,50,50	0
57	MG	2A	3653	1/1	0.92	0.16	56,56,56,56	0
57	MG	1A	3954	1/1	0.92	0.18	22,22,22,22	0
57	MG	1x	106	1/1	0.92	0.19	43,43,43,43	0
57	MG	1a	3231	1/1	0.92	0.08	53,53,53,53	0
57	MG	1a	3145	1/1	0.92	0.07	45,45,45,45	0
57	MG	1A	3682	1/1	0.92	0.31	43,43,43,43	0
57	MG	2A	3467	1/1	0.92	0.14	38,38,38,38	0
57	MG	2A	3496	1/1	0.92	0.15	42,42,42,42	0
57	MG	2a	3182	1/1	0.92	0.18	48,48,48,48	0
57	MG	2A	3026	1/1	0.92	0.17	46,46,46,46	0
57	MG	2f	3001	1/1	0.92	0.24	43,43,43,43	0
57	MG	1a	3038	1/1	0.92	0.17	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	3100	1/1	0.92	0.15	50,50,50,50	0
57	MG	2a	3139	1/1	0.92	0.21	51,51,51,51	0
57	MG	2A	3504	1/1	0.92	0.24	69,69,69,69	0
57	MG	1A	3759	1/1	0.92	0.08	43,43,43,43	0
57	MG	1A	3459	1/1	0.92	0.18	51,51,51,51	0
57	MG	1a	3004	1/1	0.92	0.13	55,55,55,55	0
57	MG	2R	201	1/1	0.92	0.11	50,50,50,50	0
57	MG	1B	3008	1/1	0.92	0.24	46,46,46,46	0
57	MG	1a	3176	1/1	0.92	0.19	34,34,34,34	0
57	MG	2A	3167	1/1	0.92	0.22	38,38,38,38	0
57	MG	2A	3514	1/1	0.92	0.15	32,32,32,32	0
57	MG	1A	3404	1/1	0.92	0.17	33,33,33,33	0
57	MG	2a	3191	1/1	0.92	0.20	55,55,55,55	0
57	MG	2A	3092	1/1	0.92	0.43	43,43,43,43	0
57	MG	2a	3186	1/1	0.92	0.19	56,56,56,56	0
57	MG	2F	3001	1/1	0.92	0.17	47,47,47,47	0
57	MG	2A	3656	1/1	0.92	0.12	36,36,36,36	0
57	MG	1A	3801	1/1	0.92	0.10	28,28,28,28	0
57	MG	2A	3481	1/1	0.92	0.09	52,52,52,52	0
57	MG	1w	3004	1/1	0.92	0.08	51,51,51,51	0
57	MG	1A	3781	1/1	0.92	0.08	58,58,58,58	0
57	MG	1a	3191	1/1	0.92	0.11	54,54,54,54	0
57	MG	1F	302	1/1	0.92	0.15	22,22,22,22	0
57	MG	1A	3549	1/1	0.92	0.09	55,55,55,55	0
57	MG	2A	3597	1/1	0.92	0.34	41,41,41,41	0
58	K	2A	3676	1/1	0.92	0.08	50,50,50,50	0
57	MG	1A	3940	1/1	0.92	0.12	45,45,45,45	0
57	MG	1A	3838	1/1	0.92	0.26	36,36,36,36	0
57	MG	1A	3019	1/1	0.92	0.17	43,43,43,43	0
57	MG	2A	3142	1/1	0.92	0.24	37,37,37,37	0
57	MG	2A	3248	1/1	0.92	0.31	47,47,47,47	0
57	MG	1A	3265	1/1	0.92	0.23	45,45,45,45	0
57	MG	2A	3181	1/1	0.92	0.15	33,33,33,33	0
57	MG	1A	3376	1/1	0.92	0.28	43,43,43,43	0
57	MG	2A	3166	1/1	0.92	0.19	49,49,49,49	0
57	MG	2a	3160	1/1	0.93	0.23	51,51,51,51	0
57	MG	1A	3187	1/1	0.93	0.22	20,20,20,20	0
57	MG	1a	3228	1/1	0.93	0.19	38,38,38,38	0
57	MG	1B	3030	1/1	0.93	0.16	25,25,25,25	0
57	MG	1A	3823	1/1	0.93	0.20	25,25,25,25	0
57	MG	1A	3085	1/1	0.93	0.13	40,40,40,40	0
57	MG	1f	3001	1/1	0.93	0.13	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3328	1/1	0.93	0.28	37,37,37,37	0
57	MG	1A	3535	1/1	0.93	0.17	44,44,44,44	0
57	MG	1A	3254	1/1	0.93	0.13	28,28,28,28	0
57	MG	1A	3517	1/1	0.93	0.14	30,30,30,30	0
57	MG	2a	3181	1/1	0.93	0.20	72,72,72,72	0
57	MG	2A	3031	1/1	0.93	0.14	35,35,35,35	0
57	MG	1A	3944	1/1	0.93	0.16	20,20,20,20	0
57	MG	1A	3651	1/1	0.93	0.14	19,19,19,19	0
57	MG	1a	3107	1/1	0.93	0.20	39,39,39,39	0
57	MG	1A	3004	1/1	0.93	0.14	17,17,17,17	0
57	MG	2A	3267	1/1	0.93	0.15	32,32,32,32	0
57	MG	1U	204	1/1	0.93	0.21	28,28,28,28	0
57	MG	2A	3665	1/1	0.93	0.26	43,43,43,43	0
57	MG	2A	3259	1/1	0.93	0.11	56,56,56,56	0
57	MG	1A	3393	1/1	0.93	0.16	41,41,41,41	0
57	MG	1A	3875	1/1	0.93	0.17	34,34,34,34	0
57	MG	1A	3896	1/1	0.93	0.11	27,27,27,27	0
57	MG	2A	3346	1/1	0.93	0.12	45,45,45,45	0
57	MG	2A	3114	1/1	0.93	0.34	44,44,44,44	0
57	MG	1A	3166	1/1	0.93	0.18	24,24,24,24	0
57	MG	2A	3614	1/1	0.93	0.32	38,38,38,38	0
57	MG	2A	3659	1/1	0.93	0.06	58,58,58,58	0
57	MG	1A	3442	1/1	0.93	0.18	35,35,35,35	0
57	MG	1A	3776	1/1	0.93	0.09	34,34,34,34	0
57	MG	1a	3160	1/1	0.93	0.08	51,51,51,51	0
57	MG	2A	3216	1/1	0.93	0.20	51,51,51,51	0
57	MG	2a	3093	1/1	0.93	0.11	40,40,40,40	0
57	MG	1a	3192	1/1	0.93	0.14	51,51,51,51	0
57	MG	2a	3124	1/1	0.93	0.25	61,61,61,61	0
57	MG	1A	3120	1/1	0.93	0.25	35,35,35,35	0
57	MG	1A	3380	1/1	0.93	0.44	30,30,30,30	0
57	MG	1A	3900	1/1	0.93	0.06	39,39,39,39	0
57	MG	1a	3113	1/1	0.93	0.18	59,59,59,59	0
57	MG	1A	3064	1/1	0.93	0.19	22,22,22,22	0
57	MG	1N	3003	1/1	0.93	0.20	32,32,32,32	0
57	MG	1A	3125	1/1	0.93	0.18	31,31,31,31	0
57	MG	1a	3086	1/1	0.93	0.18	52,52,52,52	0
57	MG	2A	3436	1/1	0.93	0.16	52,52,52,52	0
57	MG	1A	3515	1/1	0.93	0.24	45,45,45,45	0
57	MG	1A	3504	1/1	0.93	0.19	39,39,39,39	0
57	MG	1a	3060	1/1	0.93	0.25	45,45,45,45	0
57	MG	1a	3185	1/1	0.93	0.17	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3442	1/1	0.93	0.19	45,45,45,45	0
57	MG	1A	3173	1/1	0.93	0.31	46,46,46,46	0
57	MG	1O	206	1/1	0.93	0.15	35,35,35,35	0
57	MG	1a	3106	1/1	0.93	0.25	47,47,47,47	0
57	MG	2a	3113	1/1	0.93	0.11	55,55,55,55	0
57	MG	2A	3453	1/1	0.93	0.20	58,58,58,58	0
57	MG	1A	3341	1/1	0.93	0.29	36,36,36,36	0
57	MG	2A	3672	1/1	0.93	0.28	36,36,36,36	0
57	MG	2A	3592	1/1	0.93	0.16	49,49,49,49	0
57	MG	2A	3207	1/1	0.93	0.13	52,52,52,52	0
57	MG	1A	3998	1/1	0.93	0.11	33,33,33,33	0
57	MG	2A	3242	1/1	0.93	0.17	45,45,45,45	0
57	MG	1A	3908	1/1	0.93	0.12	15,15,15,15	0
57	MG	2a	3058	1/1	0.93	0.14	62,62,62,62	0
57	MG	1A	3636	1/1	0.93	0.15	32,32,32,32	0
57	MG	1a	3171	1/1	0.93	0.08	66,66,66,66	0
57	MG	2A	3276	1/1	0.93	0.17	36,36,36,36	0
57	MG	2A	3388	1/1	0.93	0.10	48,48,48,48	0
57	MG	1a	3049	1/1	0.93	0.24	41,41,41,41	0
57	MG	1B	3020	1/1	0.93	0.15	18,18,18,18	0
57	MG	1A	3800	1/1	0.93	0.14	47,47,47,47	0
57	MG	2A	3261	1/1	0.93	0.19	54,54,54,54	0
57	MG	1a	3032	1/1	0.93	0.21	55,55,55,55	0
57	MG	2A	3321	1/1	0.93	0.11	60,60,60,60	0
57	MG	2A	3187	1/1	0.93	0.09	58,58,58,58	0
57	MG	1A	3512	1/1	0.93	0.19	21,21,21,21	0
57	MG	2a	3099	1/1	0.93	0.18	58,58,58,58	0
57	MG	2A	3030	1/1	0.93	0.31	51,51,51,51	0
57	MG	1A	3345	1/1	0.93	0.14	53,53,53,53	0
57	MG	1A	3765	1/1	0.93	0.12	44,44,44,44	0
57	MG	1A	3925	1/1	0.93	0.09	39,39,39,39	0
57	MG	1a	3195	1/1	0.93	0.07	42,42,42,42	0
57	MG	1T	8002	1/1	0.93	0.29	43,43,43,43	0
57	MG	1A	3198	1/1	0.93	0.11	37,37,37,37	0
57	MG	1A	3573	1/1	0.93	0.16	44,44,44,44	0
57	MG	2X	102	1/1	0.93	0.16	58,58,58,58	0
57	MG	2A	3525	1/1	0.93	0.14	37,37,37,37	0
57	MG	2A	3309	1/1	0.93	0.19	51,51,51,51	0
57	MG	1A	3859	1/1	0.93	0.26	33,33,33,33	0
57	MG	1A	3074	1/1	0.93	0.36	26,26,26,26	0
57	MG	2a	3109	1/1	0.93	0.15	47,47,47,47	0
57	MG	1A	3526	1/1	0.93	0.12	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3477	1/1	0.93	0.21	19,19,19,19	0
57	MG	1R	203	1/1	0.93	0.24	25,25,25,25	0
57	MG	1A	3359	1/1	0.93	0.15	35,35,35,35	0
57	MG	2A	3199	1/1	0.93	0.12	41,41,41,41	0
57	MG	1A	3372	1/1	0.93	0.15	25,25,25,25	0
57	MG	2D	305	1/1	0.93	0.23	47,47,47,47	0
57	MG	2A	3466	1/1	0.93	0.29	51,51,51,51	0
57	MG	2A	3064	1/1	0.93	0.21	44,44,44,44	0
57	MG	1A	3957	1/1	0.93	0.08	38,38,38,38	0
57	MG	1a	3137	1/1	0.93	0.09	37,37,37,37	0
57	MG	1a	3212	1/1	0.93	0.19	58,58,58,58	0
57	MG	1A	3669	1/1	0.93	0.18	37,37,37,37	0
57	MG	1A	3331	1/1	0.93	0.24	51,51,51,51	0
57	MG	1A	3077	1/1	0.93	0.47	24,24,24,24	0
57	MG	2A	3470	1/1	0.93	0.21	44,44,44,44	0
57	MG	2A	3191	1/1	0.93	0.19	44,44,44,44	0
57	MG	2w	104	1/1	0.93	0.12	58,58,58,58	0
57	MG	1a	3063	1/1	0.93	0.17	44,44,44,44	0
57	MG	2A	3069	1/1	0.93	0.18	32,32,32,32	0
57	MG	1O	203	1/1	0.93	0.41	54,54,54,54	0
57	MG	1A	3961	1/1	0.93	0.30	28,28,28,28	0
57	MG	2A	3053	1/1	0.93	0.20	47,47,47,47	0
57	MG	2A	3550	1/1	0.93	0.09	42,42,42,42	0
57	MG	2A	3432	1/1	0.93	0.13	64,64,64,64	0
57	MG	2A	3451	1/1	0.93	0.18	56,56,56,56	0
57	MG	2A	3098	1/1	0.93	0.16	38,38,38,38	0
57	MG	2a	3169	1/1	0.93	0.17	48,48,48,48	0
57	MG	1A	3199	1/1	0.93	0.15	16,16,16,16	0
57	MG	1a	3002	1/1	0.93	0.13	38,38,38,38	0
57	MG	1A	3505	1/1	0.93	0.17	52,52,52,52	0
57	MG	2A	3634	1/1	0.93	0.16	41,41,41,41	0
57	MG	2A	3070	1/1	0.93	0.21	41,41,41,41	0
57	MG	1X	101	1/1	0.93	0.18	34,34,34,34	0
57	MG	1A	3248	1/1	0.93	0.16	44,44,44,44	0
57	MG	2a	3123	1/1	0.93	0.08	47,47,47,47	0
57	MG	1A	3511	1/1	0.93	0.10	45,45,45,45	0
57	MG	2A	3302	1/1	0.93	0.22	56,56,56,56	0
57	MG	1A	3179	1/1	0.93	0.24	26,26,26,26	0
57	MG	2a	3176	1/1	0.93	0.14	53,53,53,53	0
57	MG	2A	3102	1/1	0.93	0.23	28,28,28,28	0
57	MG	2B	3011	1/1	0.93	0.11	68,68,68,68	0
57	MG	2A	3301	1/1	0.93	0.36	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	3184	1/1	0.93	0.25	65,65,65,65	0
57	MG	1a	3024	1/1	0.93	0.12	55,55,55,55	0
57	MG	1A	3016	1/1	0.93	0.26	33,33,33,33	0
57	MG	2A	3681	1/1	0.93	0.18	38,38,38,38	0
57	MG	2A	3546	1/1	0.93	0.07	45,45,45,45	0
57	MG	18	102	1/1	0.93	0.30	43,43,43,43	0
57	MG	2A	3454	1/1	0.93	0.26	43,43,43,43	0
57	MG	2A	3202	1/1	0.93	0.25	49,49,49,49	0
57	MG	1A	3154	1/1	0.93	0.11	41,41,41,41	0
57	MG	2A	3448	1/1	0.93	0.10	44,44,44,44	0
57	MG	1A	3369	1/1	0.93	0.15	37,37,37,37	0
57	MG	2A	3406	1/1	0.93	0.16	50,50,50,50	0
57	MG	2X	101	1/1	0.93	0.13	52,52,52,52	0
57	MG	1A	3466	1/1	0.93	0.12	40,40,40,40	0
57	MG	1A	3796	1/1	0.93	0.14	20,20,20,20	0
57	MG	1A	3346	1/1	0.93	0.11	30,30,30,30	0
57	MG	1A	3310	1/1	0.93	0.24	32,32,32,32	0
57	MG	1A	3176	1/1	0.93	0.14	61,61,61,61	0
57	MG	1A	3856	1/1	0.93	0.20	45,45,45,45	0
57	MG	1a	3129	1/1	0.93	0.10	50,50,50,50	0
57	MG	1a	3121	1/1	0.93	0.16	36,36,36,36	0
57	MG	2B	3016	1/1	0.93	0.23	64,64,64,64	0
57	MG	2a	3085	1/1	0.93	0.15	50,50,50,50	0
57	MG	1a	3088	1/1	0.93	0.07	59,59,59,59	0
57	MG	1w	3003	1/1	0.93	0.14	27,27,27,27	0
57	MG	1b	3002	1/1	0.93	0.21	67,67,67,67	0
57	MG	1A	3887	1/1	0.93	0.15	32,32,32,32	0
57	MG	1B	3018	1/1	0.93	0.16	26,26,26,26	0
57	MG	2A	3215	1/1	0.93	0.16	38,38,38,38	0
57	MG	2A	3105	1/1	0.93	0.12	46,46,46,46	0
57	MG	1a	3198	1/1	0.93	0.12	51,51,51,51	0
57	MG	1A	3488	1/1	0.93	0.12	33,33,33,33	0
57	MG	2a	3183	1/1	0.93	0.17	34,34,34,34	0
57	MG	2A	3062	1/1	0.93	0.15	46,46,46,46	0
57	MG	1a	3157	1/1	0.93	0.06	50,50,50,50	0
57	MG	1A	3131	1/1	0.93	0.11	37,37,37,37	0
57	MG	11	101	1/1	0.93	0.15	35,35,35,35	0
57	MG	2A	3426	1/1	0.93	0.12	44,44,44,44	0
57	MG	1A	3792	1/1	0.93	0.52	39,39,39,39	0
57	MG	1A	3454	1/1	0.93	0.18	24,24,24,24	0
57	MG	1N	3007	1/1	0.93	0.24	25,25,25,25	0
57	MG	2a	3030	1/1	0.93	0.10	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3432	1/1	0.93	0.06	25,25,25,25	0
57	MG	2A	3327	1/1	0.93	0.18	30,30,30,30	0
57	MG	1A	3296	1/1	0.93	0.19	40,40,40,40	0
57	MG	1a	3146	1/1	0.93	0.14	60,60,60,60	0
57	MG	1A	3281	1/1	0.93	0.24	17,17,17,17	0
57	MG	2A	3508	1/1	0.93	0.09	57,57,57,57	0
57	MG	23	3001	1/1	0.93	0.14	46,46,46,46	0
57	MG	1A	3127	1/1	0.93	0.21	28,28,28,28	0
57	MG	1A	3259	1/1	0.94	0.13	45,45,45,45	0
57	MG	2A	3632	1/1	0.94	0.11	62,62,62,62	0
57	MG	2A	3147	1/1	0.94	0.20	40,40,40,40	0
57	MG	2A	3540	1/1	0.94	0.16	58,58,58,58	0
57	MG	2A	3654	1/1	0.94	0.08	46,46,46,46	0
57	MG	2F	3002	1/1	0.94	0.10	43,43,43,43	0
57	MG	1x	108	1/1	0.94	0.10	41,41,41,41	0
57	MG	1A	3913	1/1	0.94	0.16	23,23,23,23	0
57	MG	2A	3170	1/1	0.94	0.11	43,43,43,43	0
57	MG	1O	201	1/1	0.94	0.19	41,41,41,41	0
57	MG	2A	3322	1/1	0.94	0.11	30,30,30,30	0
57	MG	2a	3098	1/1	0.94	0.09	57,57,57,57	0
57	MG	2A	3360	1/1	0.94	0.13	29,29,29,29	0
57	MG	1A	3210	1/1	0.94	0.20	27,27,27,27	0
57	MG	1A	3350	1/1	0.94	0.11	26,26,26,26	0
57	MG	1A	3989	1/1	0.94	0.21	37,37,37,37	0
57	MG	1a	3021	1/1	0.94	0.15	38,38,38,38	0
57	MG	1A	3037	1/1	0.94	0.15	24,24,24,24	0
57	MG	2A	3664	1/1	0.94	0.27	45,45,45,45	0
57	MG	2A	3584	1/1	0.94	0.16	35,35,35,35	0
57	MG	1A	3806	1/1	0.94	0.10	35,35,35,35	0
57	MG	2B	3019	1/1	0.94	0.15	59,59,59,59	0
57	MG	1A	3373	1/1	0.94	0.20	9,9,9,9	0
57	MG	2A	3122	1/1	0.94	0.25	43,43,43,43	0
57	MG	2D	304	1/1	0.94	0.19	49,49,49,49	0
57	MG	1a	3047	1/1	0.94	0.15	23,23,23,23	0
57	MG	1E	301	1/1	0.94	0.23	33,33,33,33	0
57	MG	2A	3313	1/1	0.94	0.19	53,53,53,53	0
57	MG	2A	3459	1/1	0.94	0.17	38,38,38,38	0
57	MG	1A	3912	1/1	0.94	0.08	51,51,51,51	0
57	MG	1A	3482	1/1	0.94	0.09	44,44,44,44	0
57	MG	2A	3125	1/1	0.94	0.14	51,51,51,51	0
57	MG	2B	3003	1/1	0.94	0.05	55,55,55,55	0
57	MG	2A	3269	1/1	0.94	0.08	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	3197	1/1	0.94	0.16	52,52,52,52	0
57	MG	2A	3010	1/1	0.94	0.13	32,32,32,32	0
57	MG	1W	204	1/1	0.94	0.15	32,32,32,32	0
57	MG	2A	3398	1/1	0.94	0.07	46,46,46,46	0
57	MG	18	103	1/1	0.94	0.15	35,35,35,35	0
57	MG	1A	3001	1/1	0.94	0.14	24,24,24,24	0
57	MG	2A	3091	1/1	0.94	0.24	49,49,49,49	0
57	MG	1A	3439	1/1	0.94	0.11	49,49,49,49	0
57	MG	1a	3209	1/1	0.94	0.12	43,43,43,43	0
57	MG	2A	3636	1/1	0.94	0.62	57,57,57,57	0
57	MG	1A	3323	1/1	0.94	0.19	54,54,54,54	0
57	MG	1A	3283	1/1	0.94	0.16	38,38,38,38	0
57	MG	1A	3760	1/1	0.94	0.19	51,51,51,51	0
57	MG	1A	3958	1/1	0.94	0.38	31,31,31,31	0
57	MG	1x	103	1/1	0.94	0.16	37,37,37,37	0
57	MG	1A	3461	1/1	0.94	0.15	19,19,19,19	0
57	MG	2a	3194	1/1	0.94	0.15	44,44,44,44	0
57	MG	1a	3110	1/1	0.94	0.26	45,45,45,45	0
57	MG	2A	3585	1/1	0.94	0.14	45,45,45,45	0
57	MG	2a	3105	1/1	0.94	0.12	37,37,37,37	0
57	MG	2A	3345	1/1	0.94	0.14	28,28,28,28	0
57	MG	1a	3181	1/1	0.94	0.24	42,42,42,42	0
57	MG	1A	3203	1/1	0.94	0.18	24,24,24,24	0
57	MG	1A	3371	1/1	0.94	0.13	24,24,24,24	0
57	MG	2A	3533	1/1	0.94	0.20	55,55,55,55	0
57	MG	2A	3479	1/1	0.94	0.12	47,47,47,47	0
57	MG	1R	201	1/1	0.94	0.15	26,26,26,26	0
57	MG	1A	3574	1/1	0.94	0.14	34,34,34,34	0
57	MG	1A	3659	1/1	0.94	0.24	21,21,21,21	0
57	MG	1A	3787	1/1	0.94	0.23	47,47,47,47	0
57	MG	1A	3155	1/1	0.94	0.41	33,33,33,33	0
57	MG	1A	3375	1/1	0.94	0.11	32,32,32,32	0
57	MG	1A	3701	1/1	0.94	0.17	25,25,25,25	0
57	MG	1A	3278	1/1	0.94	0.17	35,35,35,35	0
57	MG	2A	3281	1/1	0.94	0.15	39,39,39,39	0
57	MG	1A	3646	1/1	0.94	0.12	37,37,37,37	0
57	MG	1A	3463	1/1	0.94	0.18	47,47,47,47	0
57	MG	2A	3641	1/1	0.94	0.16	48,48,48,48	0
57	MG	2A	3255	1/1	0.94	0.14	48,48,48,48	0
57	MG	1A	3683	1/1	0.94	0.18	52,52,52,52	0
57	MG	1A	3615	1/1	0.94	0.14	36,36,36,36	0
57	MG	2A	3050	1/1	0.94	0.11	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3608	1/1	0.94	0.38	61,61,61,61	0
57	MG	1A	3433	1/1	0.94	0.17	10,10,10,10	0
57	MG	1A	3110	1/1	0.94	0.18	30,30,30,30	0
57	MG	1A	3904	1/1	0.94	0.22	38,38,38,38	0
57	MG	1A	3271	1/1	0.94	0.24	35,35,35,35	0
57	MG	1A	3502	1/1	0.94	0.18	31,31,31,31	0
57	MG	1I	102	1/1	0.94	0.19	40,40,40,40	0
57	MG	1A	3881	1/1	0.94	0.11	30,30,30,30	0
57	MG	1B	3004	1/1	0.94	0.12	37,37,37,37	0
57	MG	2A	3145	1/1	0.94	0.09	37,37,37,37	0
57	MG	1A	3419	1/1	0.94	0.14	23,23,23,23	0
57	MG	1A	3152	1/1	0.94	0.16	24,24,24,24	0
57	MG	2A	3376	1/1	0.94	0.17	37,37,37,37	0
57	MG	1A	3938	1/1	0.94	0.18	22,22,22,22	0
57	MG	1A	3637	1/1	0.94	0.08	43,43,43,43	0
57	MG	1U	201	1/1	0.94	0.10	26,26,26,26	0
57	MG	2A	3402	1/1	0.94	0.14	39,39,39,39	0
57	MG	2A	3317	1/1	0.94	0.09	52,52,52,52	0
57	MG	2a	3094	1/1	0.94	0.12	62,62,62,62	0
57	MG	2A	3397	1/1	0.94	0.18	62,62,62,62	0
57	MG	1A	3055	1/1	0.94	0.28	30,30,30,30	0
57	MG	1A	3901	1/1	0.94	0.11	40,40,40,40	0
57	MG	1O	207	1/1	0.94	0.14	80,80,80,80	0
57	MG	1A	3607	1/1	0.94	0.18	17,17,17,17	0
57	MG	1A	3986	1/1	0.94	0.31	27,27,27,27	0
57	MG	2w	103	1/1	0.94	0.27	61,61,61,61	0
57	MG	1A	3184	1/1	0.94	0.17	28,28,28,28	0
57	MG	1a	3010	1/1	0.94	0.19	47,47,47,47	0
57	MG	1A	3577	1/1	0.94	0.09	47,47,47,47	0
57	MG	2A	3090	1/1	0.94	0.22	52,52,52,52	0
57	MG	2A	3612	1/1	0.94	0.08	42,42,42,42	0
57	MG	1D	305	1/1	0.94	0.19	28,28,28,28	0
57	MG	1A	3762	1/1	0.94	0.09	45,45,45,45	0
57	MG	1B	3019	1/1	0.94	0.23	44,44,44,44	0
57	MG	2a	3090	1/1	0.94	0.17	44,44,44,44	0
57	MG	1A	3771	1/1	0.94	0.08	28,28,28,28	0
57	MG	1A	3456	1/1	0.94	0.14	18,18,18,18	0
57	MG	2A	3427	1/1	0.94	0.12	38,38,38,38	0
57	MG	1A	3106	1/1	0.94	0.28	26,26,26,26	0
57	MG	2a	3170	1/1	0.94	0.12	46,46,46,46	0
57	MG	1A	3492	1/1	0.94	0.15	24,24,24,24	0
57	MG	2B	3012	1/1	0.94	0.14	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3099	1/1	0.94	0.08	58,58,58,58	0
57	MG	2V	202	1/1	0.94	0.10	38,38,38,38	0
57	MG	1A	3324	1/1	0.94	0.19	59,59,59,59	0
57	MG	2a	3077	1/1	0.94	0.17	55,55,55,55	0
57	MG	1A	3809	1/1	0.94	0.15	32,32,32,32	0
57	MG	1a	3065	1/1	0.94	0.15	64,64,64,64	0
57	MG	1A	3503	1/1	0.94	0.19	20,20,20,20	0
57	MG	1A	3897	1/1	0.94	0.12	18,18,18,18	0
57	MG	1A	3680	1/1	0.94	0.20	49,49,49,49	0
57	MG	1A	3060	1/1	0.94	0.25	41,41,41,41	0
57	MG	1a	3170	1/1	0.94	0.20	52,52,52,52	0
57	MG	2A	3441	1/1	0.94	0.13	49,49,49,49	0
60	ZN	2n	501	1/1	0.94	0.07	91,91,91,91	0
57	MG	1A	3177	1/1	0.94	0.21	20,20,20,20	0
57	MG	1A	3192	1/1	0.94	0.20	32,32,32,32	0
57	MG	2A	3073	1/1	0.94	0.11	48,48,48,48	0
57	MG	1B	3001	1/1	0.94	0.18	41,41,41,41	0
57	MG	2B	3005	1/1	0.94	0.14	34,34,34,34	0
57	MG	1A	3469	1/1	0.94	0.12	60,60,60,60	0
57	MG	1A	3151	1/1	0.94	0.15	19,19,19,19	0
57	MG	1A	3668	1/1	0.94	0.09	22,22,22,22	0
57	MG	2A	3008	1/1	0.94	0.17	37,37,37,37	0
57	MG	1A	3440	1/1	0.94	0.11	27,27,27,27	0
57	MG	2A	3011	1/1	0.94	0.21	33,33,33,33	0
57	MG	2A	3633	1/1	0.94	0.12	46,46,46,46	0
57	MG	1A	3303	1/1	0.94	0.14	29,29,29,29	0
57	MG	2A	3027	1/1	0.94	0.13	37,37,37,37	0
57	MG	1A	3991	1/1	0.94	0.16	30,30,30,30	0
57	MG	1A	3401	1/1	0.94	0.14	48,48,48,48	0
57	MG	1A	3403	1/1	0.94	0.16	16,16,16,16	0
57	MG	2A	3141	1/1	0.94	0.30	40,40,40,40	0
57	MG	1A	3434	1/1	0.94	0.12	13,13,13,13	0
57	MG	1A	3868	1/1	0.94	0.12	24,24,24,24	0
57	MG	1A	3693	1/1	0.94	0.15	60,60,60,60	0
57	MG	1B	3031	1/1	0.94	0.25	26,26,26,26	0
57	MG	2A	3673	1/1	0.94	0.27	38,38,38,38	0
57	MG	1A	3485	1/1	0.94	0.13	33,33,33,33	0
57	MG	2A	3285	1/1	0.94	0.17	50,50,50,50	0
57	MG	1B	3005	1/1	0.94	0.43	46,46,46,46	0
57	MG	1A	3054	1/1	0.94	0.28	44,44,44,44	0
57	MG	2A	3456	1/1	0.94	0.10	38,38,38,38	0
57	MG	2a	3081	1/1	0.94	0.09	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3183	1/1	0.94	0.21	26,26,26,26	0
57	MG	2A	3060	1/1	0.94	0.17	47,47,47,47	0
57	MG	1A	3342	1/1	0.94	0.20	24,24,24,24	0
57	MG	2A	3161	1/1	0.94	0.16	33,33,33,33	0
57	MG	2A	3364	1/1	0.94	0.14	53,53,53,53	0
57	MG	1A	3870	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3133	1/1	0.94	0.14	23,23,23,23	0
57	MG	2A	3544	1/1	0.94	0.07	41,41,41,41	0
57	MG	1G	201	1/1	0.94	0.14	28,28,28,28	0
57	MG	2A	3662	1/1	0.94	0.13	49,49,49,49	0
57	MG	1A	3888	1/1	0.94	0.22	57,57,57,57	0
57	MG	2A	3264	1/1	0.94	0.22	46,46,46,46	0
57	MG	2A	3488	1/1	0.94	0.12	53,53,53,53	0
57	MG	2W	201	1/1	0.94	0.40	59,59,59,59	0
57	MG	2A	3056	1/1	0.94	0.18	57,57,57,57	0
57	MG	1a	3111	1/1	0.94	0.07	55,55,55,55	0
57	MG	1A	3402	1/1	0.94	0.11	33,33,33,33	0
57	MG	1A	3977	1/1	0.94	0.24	30,30,30,30	0
57	MG	2A	3219	1/1	0.94	0.14	45,45,45,45	0
57	MG	2A	3439	1/1	0.94	0.20	46,46,46,46	0
57	MG	2a	3083	1/1	0.94	0.12	41,41,41,41	0
57	MG	2A	3337	1/1	0.94	0.21	56,56,56,56	0
57	MG	2A	3086	1/1	0.94	0.12	35,35,35,35	0
57	MG	1a	3130	1/1	0.94	0.06	45,45,45,45	0
57	MG	2a	3107	1/1	0.94	0.11	52,52,52,52	0
57	MG	1A	3497	1/1	0.94	0.17	8,8,8,8	0
57	MG	1A	3778	1/1	0.94	0.09	30,30,30,30	0
57	MG	1A	3799	1/1	0.94	0.13	30,30,30,30	0
57	MG	2A	3623	1/1	0.94	0.12	50,50,50,50	0
57	MG	1A	3542	1/1	0.94	0.12	41,41,41,41	0
57	MG	2Q	3001	1/1	0.94	0.20	63,63,63,63	0
57	MG	2A	3084	1/1	0.94	0.29	45,45,45,45	0
57	MG	1a	3062	1/1	0.94	0.09	39,39,39,39	0
57	MG	1A	3773	1/1	0.94	0.14	53,53,53,53	0
57	MG	1A	3546	1/1	0.94	0.19	39,39,39,39	0
57	MG	1A	3169	1/1	0.94	0.19	22,22,22,22	0
57	MG	1a	3016	1/1	0.94	0.21	45,45,45,45	0
57	MG	1A	3361	1/1	0.94	0.13	39,39,39,39	0
57	MG	1A	3411	1/1	0.94	0.12	39,39,39,39	0
57	MG	2D	307	1/1	0.94	0.30	38,38,38,38	0
57	MG	1A	3043	1/1	0.94	0.10	18,18,18,18	0
57	MG	1A	3737	1/1	0.94	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
57	MG	1a	3229	1/1	0.94	0.41	51,51,51,51	0
57	MG	1A	3688	1/1	0.94	0.09	46,46,46,46	0
57	MG	2A	3123	1/1	0.94	0.18	32,32,32,32	0
57	MG	1A	3985	1/1	0.94	0.47	27,27,27,27	0
57	MG	1a	3144	1/1	0.94	0.14	40,40,40,40	0
57	MG	2B	3013	1/1	0.94	0.10	61,61,61,61	0
57	MG	1A	3981	1/1	0.94	0.37	29,29,29,29	0
57	MG	1A	3274	1/1	0.94	0.14	32,32,32,32	0
57	MG	1A	3385	1/1	0.94	0.14	44,44,44,44	0
57	MG	1A	3795	1/1	0.94	0.20	33,33,33,33	0
57	MG	2A	3320	1/1	0.94	0.12	45,45,45,45	0
57	MG	1B	3013	1/1	0.94	0.21	32,32,32,32	0
57	MG	1A	3408	1/1	0.94	0.19	35,35,35,35	0
57	MG	1a	3154	1/1	0.94	0.22	58,58,58,58	0
57	MG	1A	3798	1/1	0.94	0.19	36,36,36,36	0
57	MG	1A	3455	1/1	0.94	0.14	27,27,27,27	0
57	MG	1A	3843	1/1	0.94	0.20	43,43,43,43	0
57	MG	1A	3486	1/1	0.94	0.16	35,35,35,35	0
57	MG	1B	3022	1/1	0.94	0.11	48,48,48,48	0
57	MG	1A	3240	1/1	0.94	0.15	33,33,33,33	0
57	MG	1A	3999	1/1	0.94	0.25	32,32,32,32	0
57	MG	2A	3564	1/1	0.94	0.16	46,46,46,46	0
57	MG	1a	3083	1/1	0.94	0.18	34,34,34,34	0
57	MG	1A	3575	1/1	0.94	0.13	29,29,29,29	0
57	MG	1A	3518	1/1	0.94	0.12	19,19,19,19	0
57	MG	1A	3706	1/1	0.94	0.20	60,60,60,60	0
57	MG	1A	3010	1/1	0.94	0.15	30,30,30,30	0
57	MG	1A	3416	1/1	0.94	0.12	46,46,46,46	0
57	MG	1A	3475	1/1	0.95	0.13	23,23,23,23	0
57	MG	1A	3264	1/1	0.95	0.14	21,21,21,21	0
57	MG	1A	3687	1/1	0.95	0.17	31,31,31,31	0
57	MG	1A	3180	1/1	0.95	0.29	33,33,33,33	0
57	MG	1A	3426	1/1	0.95	0.17	23,23,23,23	0
57	MG	1A	3634	1/1	0.95	0.09	54,54,54,54	0
57	MG	2A	3013	1/1	0.95	0.11	29,29,29,29	0
57	MG	1A	3642	1/1	0.95	0.14	29,29,29,29	0
57	MG	2A	3265	1/1	0.95	0.07	58,58,58,58	0
57	MG	1a	3097	1/1	0.95	0.15	43,43,43,43	0
57	MG	1A	3247	1/1	0.95	0.12	49,49,49,49	0
57	MG	1A	3867	1/1	0.95	0.12	26,26,26,26	0
57	MG	2a	3011	1/1	0.95	0.15	35,35,35,35	0
57	MG	2A	3059	1/1	0.95	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	3203	1/1	0.95	0.14	67,67,67,67	0
57	MG	1A	3094	1/1	0.95	0.17	31,31,31,31	0
57	MG	1A	3852	1/1	0.95	0.17	22,22,22,22	0
57	MG	1a	3050	1/1	0.95	0.34	57,57,57,57	0
57	MG	1A	3145	1/1	0.95	0.21	34,34,34,34	0
57	MG	1A	3251	1/1	0.95	0.15	45,45,45,45	0
57	MG	1A	3262	1/1	0.95	0.21	30,30,30,30	0
57	MG	1A	3202	1/1	0.95	0.17	49,49,49,49	0
57	MG	2A	3040	1/1	0.95	0.15	53,53,53,53	0
57	MG	1B	3015	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3684	1/1	0.95	0.12	25,25,25,25	0
58	K	1A	3968	1/1	0.95	0.14	31,31,31,31	0
57	MG	1A	3450	1/1	0.95	0.16	54,54,54,54	0
57	MG	1A	3617	1/1	0.95	0.17	14,14,14,14	0
57	MG	1A	3444	1/1	0.95	0.24	31,31,31,31	0
57	MG	1A	3893	1/1	0.95	0.16	40,40,40,40	0
57	MG	1A	3630	1/1	0.95	0.13	33,33,33,33	0
57	MG	1A	3182	1/1	0.95	0.18	22,22,22,22	0
57	MG	1a	3184	1/1	0.95	0.14	38,38,38,38	0
57	MG	1X	105	1/1	0.95	0.15	33,33,33,33	0
57	MG	2A	3452	1/1	0.95	0.15	24,24,24,24	0
57	MG	2A	3280	1/1	0.95	0.14	49,49,49,49	0
57	MG	1A	3540	1/1	0.95	0.11	41,41,41,41	0
57	MG	2A	3422	1/1	0.95	0.15	44,44,44,44	0
57	MG	2A	3642	1/1	0.95	0.16	46,46,46,46	0
57	MG	1a	3128	1/1	0.95	0.07	36,36,36,36	0
57	MG	2A	3489	1/1	0.95	0.10	45,45,45,45	0
57	MG	2A	3251	1/1	0.95	0.15	58,58,58,58	0
57	MG	2A	3307	1/1	0.95	0.11	47,47,47,47	0
57	MG	2A	3566	1/1	0.95	0.12	34,34,34,34	0
57	MG	2A	3222	1/1	0.95	0.10	41,41,41,41	0
57	MG	1A	3552	1/1	0.95	0.17	40,40,40,40	0
57	MG	1A	3057	1/1	0.95	0.10	57,57,57,57	0
57	MG	2A	3012	1/1	0.95	0.13	27,27,27,27	0
57	MG	1A	3386	1/1	0.95	0.12	36,36,36,36	0
57	MG	1B	3026	1/1	0.95	0.09	42,42,42,42	0
57	MG	1A	3972	1/1	0.95	0.37	23,23,23,23	0
57	MG	2A	3650	1/1	0.95	0.19	30,30,30,30	0
57	MG	2A	3290	1/1	0.95	0.12	48,48,48,48	0
57	MG	2a	3072	1/1	0.95	0.09	62,62,62,62	0
57	MG	1A	3521	1/1	0.95	0.09	20,20,20,20	0
57	MG	1A	3339	1/1	0.95	0.20	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3348	1/1	0.95	0.14	45,45,45,45	0
57	MG	2A	3308	1/1	0.95	0.11	51,51,51,51	0
57	MG	1A	3141	1/1	0.95	0.18	44,44,44,44	0
57	MG	2A	3283	1/1	0.95	0.22	51,51,51,51	0
57	MG	2A	3377	1/1	0.95	0.12	47,47,47,47	0
57	MG	1A	3355	1/1	0.95	0.20	19,19,19,19	0
57	MG	2A	3132	1/1	0.95	0.16	43,43,43,43	0
57	MG	1A	3347	1/1	0.95	0.14	27,27,27,27	0
57	MG	1A	3672	1/1	0.95	0.24	24,24,24,24	0
57	MG	1w	3001	1/1	0.95	0.12	52,52,52,52	0
57	MG	1a	3142	1/1	0.95	0.10	51,51,51,51	0
57	MG	1A	3509	1/1	0.95	0.16	15,15,15,15	0
57	MG	1A	3082	1/1	0.95	0.19	25,25,25,25	0
57	MG	1P	203	1/1	0.95	0.18	34,34,34,34	0
57	MG	2D	302	1/1	0.95	0.16	48,48,48,48	0
57	MG	2A	3359	1/1	0.95	0.22	35,35,35,35	0
57	MG	2A	3111	1/1	0.95	0.19	42,42,42,42	0
57	MG	1A	3076	1/1	0.95	0.22	26,26,26,26	0
57	MG	1A	3013	1/1	0.95	0.13	16,16,16,16	0
57	MG	2A	3431	1/1	0.95	0.10	42,42,42,42	0
57	MG	1A	3567	1/1	0.95	0.17	17,17,17,17	0
57	MG	2A	3394	1/1	0.95	0.19	32,32,32,32	0
57	MG	2A	3101	1/1	0.95	0.11	35,35,35,35	0
57	MG	2A	3032	1/1	0.95	0.21	40,40,40,40	0
57	MG	1A	3748	1/1	0.95	0.12	59,59,59,59	0
57	MG	1A	3079	1/1	0.95	0.18	41,41,41,41	0
57	MG	1A	3741	1/1	0.95	0.28	47,47,47,47	0
57	MG	1A	3883	1/1	0.95	0.15	35,35,35,35	0
57	MG	1a	3064	1/1	0.95	0.18	58,58,58,58	0
57	MG	1A	3819	1/1	0.95	0.14	8,8,8,8	0
57	MG	2A	3326	1/1	0.95	0.15	21,21,21,21	0
57	MG	2A	3107	1/1	0.95	0.26	52,52,52,52	0
57	MG	1A	3105	1/1	0.95	0.15	18,18,18,18	0
57	MG	2A	3001	1/1	0.95	0.12	43,43,43,43	0
57	MG	2A	3232	1/1	0.95	0.06	55,55,55,55	0
57	MG	1A	3095	1/1	0.95	0.16	35,35,35,35	0
57	MG	1A	3700	1/1	0.95	0.12	20,20,20,20	0
57	MG	1a	3216	1/1	0.95	0.17	53,53,53,53	0
57	MG	1A	3832	1/1	0.95	0.21	37,37,37,37	0
57	MG	1a	3014	1/1	0.95	0.12	54,54,54,54	0
57	MG	1A	3622	1/1	0.95	0.11	27,27,27,27	0
57	MG	2A	3044	1/1	0.95	0.22	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	3012	1/1	0.95	0.11	29,29,29,29	0
57	MG	1A	3309	1/1	0.95	0.09	24,24,24,24	0
57	MG	2a	3199	1/1	0.95	0.14	45,45,45,45	0
57	MG	2h	8001	1/1	0.95	0.14	41,41,41,41	0
57	MG	1A	3090	1/1	0.95	0.13	45,45,45,45	0
57	MG	2A	3109	1/1	0.95	0.22	42,42,42,42	0
57	MG	1A	3421	1/1	0.95	0.14	34,34,34,34	0
57	MG	1A	3568	1/1	0.95	0.12	13,13,13,13	0
57	MG	2A	3430	1/1	0.95	0.17	42,42,42,42	0
57	MG	2A	3203	1/1	0.95	0.12	43,43,43,43	0
57	MG	2r	3001	1/1	0.95	0.17	73,73,73,73	0
57	MG	2A	3087	1/1	0.95	0.22	40,40,40,40	0
57	MG	1A	3544	1/1	0.95	0.31	50,50,50,50	0
57	MG	2A	3249	1/1	0.95	0.18	48,48,48,48	0
57	MG	2F	3004	1/1	0.95	0.30	36,36,36,36	0
57	MG	2A	3480	1/1	0.95	0.09	49,49,49,49	0
57	MG	2a	3096	1/1	0.95	0.17	53,53,53,53	0
57	MG	1A	3522	1/1	0.95	0.22	51,51,51,51	0
57	MG	1a	3028	1/1	0.95	0.18	41,41,41,41	0
57	MG	1a	3168	1/1	0.95	0.15	46,46,46,46	0
57	MG	1A	3599	1/1	0.95	0.18	8,8,8,8	0
57	MG	1A	3235	1/1	0.95	0.44	26,26,26,26	0
57	MG	1a	3013	1/1	0.95	0.17	39,39,39,39	0
57	MG	2A	3689	1/1	0.95	0.18	47,47,47,47	0
57	MG	1A	3143	1/1	0.95	0.38	34,34,34,34	0
57	MG	1A	3499	1/1	0.95	0.15	21,21,21,21	0
57	MG	2a	3121	1/1	0.95	0.07	68,68,68,68	0
57	MG	2A	3371	1/1	0.95	0.21	46,46,46,46	0
57	MG	2A	3157	1/1	0.95	0.18	35,35,35,35	0
57	MG	2F	3003	1/1	0.95	0.17	43,43,43,43	0
57	MG	2A	3586	1/1	0.95	0.26	35,35,35,35	0
57	MG	1A	3821	1/1	0.95	0.10	40,40,40,40	0
57	MG	2A	3231	1/1	0.95	0.17	39,39,39,39	0
57	MG	2A	3599	1/1	0.95	0.06	46,46,46,46	0
57	MG	1A	3890	1/1	0.95	0.18	40,40,40,40	0
57	MG	1a	3098	1/1	0.95	0.14	56,56,56,56	0
57	MG	1A	3621	1/1	0.95	0.08	38,38,38,38	0
57	MG	2v	8001	1/1	0.95	0.14	61,61,61,61	0
57	MG	1A	3078	1/1	0.95	0.18	18,18,18,18	0
57	MG	18	101	1/1	0.95	0.12	35,35,35,35	0
57	MG	1A	3788	1/1	0.95	0.17	36,36,36,36	0
57	MG	2V	201	1/1	0.95	0.38	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	4003	1/1	0.95	0.12	19,19,19,19	0
57	MG	1A	3190	1/1	0.95	0.09	40,40,40,40	0
57	MG	1A	3858	1/1	0.95	0.27	26,26,26,26	0
57	MG	2A	3221	1/1	0.95	0.13	43,43,43,43	0
57	MG	2A	3616	1/1	0.95	0.13	52,52,52,52	0
57	MG	2A	3385	1/1	0.95	0.15	34,34,34,34	0
57	MG	2F	3006	1/1	0.95	0.24	63,63,63,63	0
57	MG	1A	3321	1/1	0.95	0.10	47,47,47,47	0
57	MG	2A	3135	1/1	0.95	0.18	34,34,34,34	0
57	MG	1A	3343	1/1	0.95	0.19	49,49,49,49	0
57	MG	2A	3324	1/1	0.95	0.14	35,35,35,35	0
57	MG	2A	3667	1/1	0.95	0.13	34,34,34,34	0
57	MG	1A	3942	1/1	0.95	0.14	16,16,16,16	0
57	MG	1A	3142	1/1	0.95	0.32	24,24,24,24	0
57	MG	1A	3041	1/1	0.95	0.21	26,26,26,26	0
57	MG	1A	3196	1/1	0.95	0.24	26,26,26,26	0
57	MG	1A	3596	1/1	0.95	0.16	34,34,34,34	0
57	MG	1A	3286	1/1	0.95	0.24	31,31,31,31	0
57	MG	2A	3637	1/1	0.95	0.14	63,63,63,63	0
57	MG	1A	3965	1/1	0.95	0.23	29,29,29,29	0
57	MG	1A	3791	1/1	0.95	0.41	28,28,28,28	0
57	MG	1A	3501	1/1	0.95	0.09	34,34,34,34	0
57	MG	1A	3993	1/1	0.95	0.15	22,22,22,22	0
57	MG	2A	3329	1/1	0.95	0.14	50,50,50,50	0
57	MG	2a	3112	1/1	0.95	0.09	43,43,43,43	0
57	MG	1A	3319	1/1	0.95	0.12	42,42,42,42	0
57	MG	2A	3113	1/1	0.95	0.09	54,54,54,54	0
57	MG	2a	3148	1/1	0.95	0.09	64,64,64,64	0
57	MG	1A	3755	1/1	0.95	0.19	21,21,21,21	0
57	MG	1A	3995	1/1	0.95	0.18	30,30,30,30	0
57	MG	1A	3597	1/1	0.95	0.26	37,37,37,37	0
57	MG	2D	308	1/1	0.95	0.35	51,51,51,51	0
57	MG	1R	202	1/1	0.95	0.19	39,39,39,39	0
57	MG	1A	3864	1/1	0.95	0.21	32,32,32,32	0
57	MG	1A	3779	1/1	0.95	0.25	45,45,45,45	0
57	MG	1A	3676	1/1	0.95	0.16	28,28,28,28	0
57	MG	1B	3003	1/1	0.95	0.22	24,24,24,24	0
57	MG	2A	3368	1/1	0.95	0.18	44,44,44,44	0
57	MG	2O	8001	1/1	0.95	0.24	55,55,55,55	0
57	MG	2A	3511	1/1	0.95	0.13	52,52,52,52	0
57	MG	2A	3007	1/1	0.95	0.11	36,36,36,36	0
57	MG	2a	3193	1/1	0.95	0.09	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	3054	1/1	0.95	0.10	40,40,40,40	0
57	MG	2B	3010	1/1	0.95	0.12	48,48,48,48	0
57	MG	2A	3450	1/1	0.95	0.25	54,54,54,54	0
57	MG	1X	104	1/1	0.95	0.24	33,33,33,33	0
57	MG	2A	3025	1/1	0.95	0.09	40,40,40,40	0
57	MG	1A	3288	1/1	0.95	0.11	36,36,36,36	0
57	MG	2A	3507	1/1	0.95	0.28	46,46,46,46	0
57	MG	1A	3570	1/1	0.95	0.07	31,31,31,31	0
57	MG	2a	3127	1/1	0.95	0.10	56,56,56,56	0
57	MG	1A	3663	1/1	0.95	0.12	24,24,24,24	0
57	MG	1A	3767	1/1	0.95	0.12	19,19,19,19	0
57	MG	1A	3280	1/1	0.95	0.44	37,37,37,37	0
57	MG	12	3002	1/1	0.95	0.20	29,29,29,29	0
57	MG	15	104	1/1	0.95	0.30	33,33,33,33	0
57	MG	2A	3229	1/1	0.95	0.17	42,42,42,42	0
57	MG	1A	3317	1/1	0.95	0.20	48,48,48,48	0
57	MG	2a	3089	1/1	0.95	0.22	47,47,47,47	0
57	MG	2A	3252	1/1	0.95	0.18	37,37,37,37	0
57	MG	2A	3660	1/1	0.95	0.06	56,56,56,56	0
57	MG	2a	3027	1/1	0.95	0.19	60,60,60,60	0
57	MG	2a	3017	1/1	0.95	0.12	44,44,44,44	0
57	MG	1A	3757	1/1	0.95	0.08	34,34,34,34	0
57	MG	2A	3547	1/1	0.95	0.13	37,37,37,37	0
57	MG	1x	110	1/1	0.95	0.06	57,57,57,57	0
57	MG	2A	3640	1/1	0.95	0.10	43,43,43,43	0
57	MG	1a	3202	1/1	0.95	0.14	45,45,45,45	0
57	MG	2A	3150	1/1	0.95	0.22	43,43,43,43	0
57	MG	2A	3352	1/1	0.95	0.15	35,35,35,35	0
57	MG	1X	106	1/1	0.95	0.39	33,33,33,33	0
57	MG	2A	3254	1/1	0.95	0.11	55,55,55,55	0
57	MG	2a	3005	1/1	0.95	0.12	53,53,53,53	0
57	MG	12	3001	1/1	0.95	0.18	30,30,30,30	0
57	MG	1A	3576	1/1	0.95	0.11	31,31,31,31	0
57	MG	2R	202	1/1	0.95	0.17	48,48,48,48	0
57	MG	1a	3120	1/1	0.95	0.07	52,52,52,52	0
57	MG	1A	3869	1/1	0.95	0.10	35,35,35,35	0
57	MG	1A	3921	1/1	0.95	0.16	27,27,27,27	0
57	MG	1A	3217	1/1	0.95	0.17	21,21,21,21	0
57	MG	2A	3483	1/1	0.95	0.12	60,60,60,60	0
57	MG	2a	3042	1/1	0.95	0.14	47,47,47,47	0
57	MG	1A	3844	1/1	0.95	0.15	30,30,30,30	0
57	MG	1A	3753	1/1	0.95	0.24	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3829	1/1	0.95	0.14	25,25,25,25	0
57	MG	2a	3143	1/1	0.95	0.17	59,59,59,59	0
57	MG	2A	3018	1/1	0.95	0.28	45,45,45,45	0
57	MG	2a	3128	1/1	0.95	0.14	51,51,51,51	0
57	MG	1A	3228	1/1	0.95	0.26	31,31,31,31	0
57	MG	2A	3519	1/1	0.95	0.17	54,54,54,54	0
57	MG	2A	3330	1/1	0.95	0.22	30,30,30,30	0
57	MG	1A	3040	1/1	0.95	0.15	27,27,27,27	0
57	MG	1X	103	1/1	0.95	0.19	46,46,46,46	0
57	MG	2a	3141	1/1	0.95	0.14	70,70,70,70	0
57	MG	2A	3476	1/1	0.95	0.07	65,65,65,65	0
57	MG	2A	3120	1/1	0.95	0.09	59,59,59,59	0
57	MG	1W	202	1/1	0.95	0.11	34,34,34,34	0
57	MG	2A	3499	1/1	0.95	0.18	45,45,45,45	0
57	MG	2A	3311	1/1	0.95	0.10	45,45,45,45	0
57	MG	1A	3071	1/1	0.95	0.19	20,20,20,20	0
57	MG	10	101	1/1	0.95	0.10	24,24,24,24	0
57	MG	2a	3106	1/1	0.95	0.13	62,62,62,62	0
57	MG	1A	3480	1/1	0.95	0.19	16,16,16,16	0
57	MG	1A	3137	1/1	0.95	0.07	32,32,32,32	0
57	MG	2A	3213	1/1	0.95	0.13	58,58,58,58	0
57	MG	1A	3793	1/1	0.95	0.12	24,24,24,24	0
57	MG	2A	3423	1/1	0.95	0.21	54,54,54,54	0
57	MG	1a	3139	1/1	0.95	0.17	38,38,38,38	0
57	MG	2U	202	1/1	0.95	0.15	56,56,56,56	0
57	MG	1A	3462	1/1	0.96	0.11	27,27,27,27	0
57	MG	2B	3018	1/1	0.96	0.12	58,58,58,58	0
57	MG	2a	3037	1/1	0.96	0.17	52,52,52,52	0
57	MG	2A	3282	1/1	0.96	0.14	38,38,38,38	0
57	MG	1A	3846	1/1	0.96	0.13	30,30,30,30	0
57	MG	2A	3022	1/1	0.96	0.11	29,29,29,29	0
57	MG	1A	3109	1/1	0.96	0.19	23,23,23,23	0
57	MG	1A	3335	1/1	0.96	0.16	29,29,29,29	0
57	MG	1a	3141	1/1	0.96	0.23	44,44,44,44	0
57	MG	1A	3909	1/1	0.96	0.11	42,42,42,42	0
57	MG	1A	3857	1/1	0.96	0.08	40,40,40,40	0
57	MG	1F	308	1/1	0.96	0.26	34,34,34,34	0
57	MG	2A	3341	1/1	0.96	0.18	46,46,46,46	0
57	MG	2A	3303	1/1	0.96	0.06	43,43,43,43	0
57	MG	1A	3675	1/1	0.96	0.20	31,31,31,31	0
57	MG	2A	3041	1/1	0.96	0.15	44,44,44,44	0
57	MG	1A	3756	1/1	0.96	0.21	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	3057	1/1	0.96	0.39	73,73,73,73	0
57	MG	2B	3002	1/1	0.96	0.12	66,66,66,66	0
57	MG	1W	206	1/1	0.96	0.15	26,26,26,26	0
57	MG	1a	3226	1/1	0.96	0.17	41,41,41,41	0
57	MG	2A	3019	1/1	0.96	1.20	54,54,54,54	0
57	MG	1A	3272	1/1	0.96	0.12	36,36,36,36	0
57	MG	1A	3997	1/1	0.96	0.14	27,27,27,27	0
57	MG	1A	3531	1/1	0.96	0.17	13,13,13,13	0
57	MG	1A	3222	1/1	0.96	0.17	21,21,21,21	0
57	MG	1A	3816	1/1	0.96	0.12	13,13,13,13	0
57	MG	2A	3447	1/1	0.96	0.20	31,31,31,31	0
57	MG	1A	3495	1/1	0.96	0.21	16,16,16,16	0
57	MG	2A	3624	1/1	0.96	0.15	44,44,44,44	0
57	MG	1A	3423	1/1	0.96	0.18	30,30,30,30	0
57	MG	1A	3236	1/1	0.96	0.20	38,38,38,38	0
57	MG	1A	3295	1/1	0.96	0.15	32,32,32,32	0
57	MG	1A	3417	1/1	0.96	0.17	23,23,23,23	0
57	MG	1A	3934	1/1	0.96	0.15	27,27,27,27	0
57	MG	1A	3028	1/1	0.96	0.14	14,14,14,14	0
57	MG	1F	303	1/1	0.96	0.16	22,22,22,22	0
57	MG	1l	201	1/1	0.96	0.13	31,31,31,31	0
57	MG	2A	3477	1/1	0.96	0.14	46,46,46,46	0
57	MG	1a	3033	1/1	0.96	0.20	50,50,50,50	0
57	MG	2A	3048	1/1	0.96	0.17	25,25,25,25	0
57	MG	1A	3038	1/1	0.96	0.27	28,28,28,28	0
57	MG	1a	3069	1/1	0.96	0.07	39,39,39,39	0
57	MG	2Q	3003	1/1	0.96	0.16	38,38,38,38	0
57	MG	1A	3747	1/1	0.96	0.13	55,55,55,55	0
57	MG	1A	3594	1/1	0.96	0.15	15,15,15,15	0
57	MG	2a	3164	1/1	0.96	0.09	45,45,45,45	0
57	MG	2A	3635	1/1	0.96	0.20	44,44,44,44	0
57	MG	1a	3194	1/1	0.96	0.21	49,49,49,49	0
57	MG	17	101	1/1	0.96	0.26	29,29,29,29	0
57	MG	2E	306	1/1	0.96	0.14	40,40,40,40	0
57	MG	1A	3209	1/1	0.96	0.19	25,25,25,25	0
57	MG	1A	3842	1/1	0.96	0.11	44,44,44,44	0
57	MG	1N	3001	1/1	0.96	0.14	28,28,28,28	0
57	MG	1A	3218	1/1	0.96	0.17	33,33,33,33	0
57	MG	1a	3053	1/1	0.96	0.09	41,41,41,41	0
57	MG	1a	3182	1/1	0.96	0.12	48,48,48,48	0
57	MG	1A	3420	1/1	0.96	0.13	22,22,22,22	0
57	MG	1a	3094	1/1	0.96	0.14	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	3072	1/1	0.96	0.14	41,41,41,41	0
57	MG	1A	3311	1/1	0.96	0.24	31,31,31,31	0
57	MG	1A	3365	1/1	0.96	0.07	19,19,19,19	0
57	MG	1a	3043	1/1	0.96	0.16	44,44,44,44	0
57	MG	2A	3393	1/1	0.96	0.19	50,50,50,50	0
57	MG	2A	3372	1/1	0.96	0.17	29,29,29,29	0
57	MG	1a	3199	1/1	0.96	0.11	52,52,52,52	0
57	MG	2a	3134	1/1	0.96	0.17	44,44,44,44	0
57	MG	1a	3230	1/1	0.96	0.13	33,33,33,33	0
57	MG	2A	3630	1/1	0.96	0.22	47,47,47,47	0
57	MG	1a	3186	1/1	0.96	0.08	55,55,55,55	0
57	MG	2a	3088	1/1	0.96	0.14	46,46,46,46	0
57	MG	1A	3362	1/1	0.96	0.29	19,19,19,19	0
60	ZN	29	501	1/1	0.96	0.07	64,64,64,64	0
57	MG	2A	3416	1/1	0.96	0.16	37,37,37,37	0
57	MG	1a	3003	1/1	0.96	0.16	46,46,46,46	0
57	MG	2A	3171	1/1	0.96	0.35	53,53,53,53	0
57	MG	2A	3541	1/1	0.96	0.21	50,50,50,50	0
57	MG	1A	3885	1/1	0.96	0.14	58,58,58,58	0
57	MG	1a	3211	1/1	0.96	0.15	62,62,62,62	0
57	MG	2A	3570	1/1	0.96	0.12	44,44,44,44	0
57	MG	2A	3034	1/1	0.96	0.13	31,31,31,31	0
57	MG	1A	3579	1/1	0.96	0.21	35,35,35,35	0
57	MG	2A	3484	1/1	0.96	0.27	39,39,39,39	0
57	MG	2A	3626	1/1	0.96	0.10	44,44,44,44	0
57	MG	1A	3911	1/1	0.96	0.30	35,35,35,35	0
57	MG	1A	3056	1/1	0.96	0.11	19,19,19,19	0
57	MG	1Y	203	1/1	0.96	0.27	39,39,39,39	0
57	MG	2a	3076	1/1	0.96	0.12	29,29,29,29	0
57	MG	1A	3436	1/1	0.96	0.11	36,36,36,36	0
57	MG	2A	3679	1/1	0.96	0.12	29,29,29,29	0
57	MG	1A	3261	1/1	0.96	0.14	34,34,34,34	0
57	MG	1V	203	1/1	0.96	0.11	50,50,50,50	0
57	MG	2A	3314	1/1	0.96	0.15	52,52,52,52	0
57	MG	1A	3915	1/1	0.96	0.14	35,35,35,35	0
57	MG	2A	3651	1/1	0.96	0.12	47,47,47,47	0
57	MG	1A	3159	1/1	0.96	0.17	37,37,37,37	0
57	MG	1a	3218	1/1	0.96	0.14	36,36,36,36	0
57	MG	1a	3089	1/1	0.96	0.62	42,42,42,42	0
57	MG	1A	3231	1/1	0.96	0.18	23,23,23,23	0
57	MG	2a	3073	1/1	0.96	0.09	51,51,51,51	0
57	MG	1A	3305	1/1	0.96	0.07	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3197	1/1	0.96	0.19	48,48,48,48	0
57	MG	1A	3108	1/1	0.96	0.12	30,30,30,30	0
57	MG	2A	3078	1/1	0.96	0.22	25,25,25,25	0
57	MG	1E	305	1/1	0.96	0.13	16,16,16,16	0
57	MG	1a	3031	1/1	0.96	0.12	39,39,39,39	0
57	MG	1a	3217	1/1	0.96	0.09	56,56,56,56	0
57	MG	1A	3591	1/1	0.96	0.12	32,32,32,32	0
57	MG	2A	3112	1/1	0.96	0.21	59,59,59,59	0
57	MG	1A	3035	1/1	0.96	0.16	25,25,25,25	0
57	MG	1A	3903	1/1	0.96	0.13	57,57,57,57	0
57	MG	1a	3167	1/1	0.96	0.12	36,36,36,36	0
57	MG	1A	3092	1/1	0.96	0.15	17,17,17,17	0
57	MG	2A	3534	1/1	0.96	0.12	37,37,37,37	0
57	MG	1A	3066	1/1	0.96	0.14	24,24,24,24	0
57	MG	1A	3224	1/1	0.96	0.23	25,25,25,25	0
57	MG	1A	3058	1/1	0.96	0.17	30,30,30,30	0
57	MG	1A	3569	1/1	0.96	0.15	25,25,25,25	0
57	MG	2A	3054	1/1	0.96	0.09	47,47,47,47	0
57	MG	1A	3107	1/1	0.96	0.17	17,17,17,17	0
57	MG	1B	3006	1/1	0.96	0.10	54,54,54,54	0
57	MG	2A	3645	1/1	0.96	0.08	50,50,50,50	0
57	MG	2A	3382	1/1	0.96	0.27	31,31,31,31	0
57	MG	1A	3336	1/1	0.96	0.15	22,22,22,22	0
57	MG	1A	3783	1/1	0.96	0.16	27,27,27,27	0
57	MG	1A	3716	1/1	0.96	0.13	26,26,26,26	0
57	MG	2B	3017	1/1	0.96	0.09	47,47,47,47	0
57	MG	2A	3646	1/1	0.96	0.13	57,57,57,57	0
57	MG	1A	3258	1/1	0.96	0.11	38,38,38,38	0
57	MG	1A	3936	1/1	0.96	0.22	38,38,38,38	0
57	MG	1A	3138	1/1	0.96	0.62	26,26,26,26	0
57	MG	2A	3449	1/1	0.96	0.15	34,34,34,34	0
57	MG	2A	3047	1/1	0.96	0.13	28,28,28,28	0
57	MG	1A	3250	1/1	0.96	0.16	26,26,26,26	0
57	MG	2a	3117	1/1	0.96	0.11	48,48,48,48	0
57	MG	2A	3463	1/1	0.96	0.14	34,34,34,34	0
57	MG	1A	3835	1/1	0.96	0.09	43,43,43,43	0
57	MG	1A	3917	1/1	0.96	0.12	35,35,35,35	0
57	MG	2A	3240	1/1	0.96	0.24	44,44,44,44	0
57	MG	2f	3002	1/1	0.96	0.14	71,71,71,71	0
57	MG	2a	3064	1/1	0.96	0.07	59,59,59,59	0
57	MG	2A	3271	1/1	0.96	0.27	53,53,53,53	0
57	MG	2a	3068	1/1	0.96	0.08	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3113	1/1	0.96	0.09	36,36,36,36	0
57	MG	1A	3853	1/1	0.96	0.24	49,49,49,49	0
57	MG	1A	3223	1/1	0.96	0.16	27,27,27,27	0
57	MG	2A	3045	1/1	0.96	0.14	34,34,34,34	0
57	MG	1a	3193	1/1	0.96	0.15	43,43,43,43	0
57	MG	1A	3730	1/1	0.96	0.17	42,42,42,42	0
57	MG	1A	3513	1/1	0.96	0.06	28,28,28,28	0
57	MG	1a	3225	1/1	0.96	0.15	35,35,35,35	0
57	MG	2A	3152	1/1	0.96	0.22	40,40,40,40	0
57	MG	1a	3177	1/1	0.96	0.16	49,49,49,49	0
57	MG	2a	3040	1/1	0.96	0.15	44,44,44,44	0
57	MG	1A	3322	1/1	0.96	0.15	40,40,40,40	0
57	MG	1A	3443	1/1	0.96	0.16	9,9,9,9	0
57	MG	1A	3358	1/1	0.96	0.23	36,36,36,36	0
57	MG	2A	3005	1/1	0.96	0.20	37,37,37,37	0
57	MG	1A	3413	1/1	0.96	0.14	8,8,8,8	0
57	MG	1a	3082	1/1	0.96	0.07	53,53,53,53	0
57	MG	2A	3179	1/1	0.96	0.17	35,35,35,35	0
57	MG	1a	3148	1/1	0.96	0.11	56,56,56,56	0
57	MG	1A	3962	1/1	0.96	0.13	10,10,10,10	0
57	MG	1A	3379	1/1	0.96	0.13	33,33,33,33	0
57	MG	1A	3337	1/1	0.96	0.15	36,36,36,36	0
57	MG	1a	3126	1/1	0.96	0.12	48,48,48,48	0
57	MG	1A	3083	1/1	0.96	0.12	54,54,54,54	0
57	MG	1A	3116	1/1	0.96	0.19	21,21,21,21	0
57	MG	1Q	205	1/1	0.96	0.17	30,30,30,30	0
57	MG	1F	301	1/1	0.96	0.15	47,47,47,47	0
57	MG	1A	3786	1/1	0.96	0.18	21,21,21,21	0
57	MG	1a	3054	1/1	0.96	0.11	38,38,38,38	0
57	MG	1A	3351	1/1	0.96	0.20	39,39,39,39	0
57	MG	28	102	1/1	0.96	0.16	52,52,52,52	0
57	MG	18	104	1/1	0.96	0.20	26,26,26,26	0
57	MG	1A	3895	1/1	0.96	0.14	28,28,28,28	0
57	MG	2A	3006	1/1	0.96	0.38	52,52,52,52	0
57	MG	1A	3721	1/1	0.96	0.14	24,24,24,24	0
57	MG	1a	3179	1/1	0.96	0.06	41,41,41,41	0
57	MG	2A	3579	1/1	0.96	0.08	39,39,39,39	0
57	MG	1A	3689	1/1	0.96	0.15	53,53,53,53	0
57	MG	1Q	201	1/1	0.96	0.22	28,28,28,28	0
57	MG	2A	3298	1/1	0.96	0.09	45,45,45,45	0
57	MG	2A	3671	1/1	0.96	0.52	46,46,46,46	0
57	MG	2A	3104	1/1	0.96	0.12	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3177	1/1	0.96	0.32	44,44,44,44	0
57	MG	1A	3168	1/1	0.96	0.15	10,10,10,10	0
57	MG	1A	3395	1/1	0.96	0.17	21,21,21,21	0
57	MG	1A	3249	1/1	0.96	0.16	21,21,21,21	0
57	MG	1A	3777	1/1	0.96	0.12	36,36,36,36	0
57	MG	1A	3732	1/1	0.96	0.17	24,24,24,24	0
57	MG	1A	3698	1/1	0.96	0.21	36,36,36,36	0
57	MG	1A	3031	1/1	0.96	0.21	24,24,24,24	0
57	MG	2A	3350	1/1	0.96	0.16	32,32,32,32	0
57	MG	1A	3233	1/1	0.96	0.20	23,23,23,23	0
57	MG	2U	201	1/1	0.96	0.23	29,29,29,29	0
57	MG	2a	3161	1/1	0.96	0.26	58,58,58,58	0
57	MG	1A	3121	1/1	0.96	0.13	19,19,19,19	0
57	MG	2A	3066	1/1	0.96	0.16	33,33,33,33	0
57	MG	2a	3021	1/1	0.96	0.09	37,37,37,37	0
57	MG	1A	3833	1/1	0.96	0.16	46,46,46,46	0
57	MG	2a	3013	1/1	0.96	0.17	51,51,51,51	0
57	MG	1A	3287	1/1	0.96	0.13	53,53,53,53	0
57	MG	1A	3405	1/1	0.96	0.12	20,20,20,20	0
57	MG	1A	3471	1/1	0.96	0.10	46,46,46,46	0
57	MG	1U	202	1/1	0.96	0.17	24,24,24,24	0
57	MG	2a	3075	1/1	0.96	0.21	38,38,38,38	0
57	MG	1A	3974	1/1	0.96	0.17	29,29,29,29	0
57	MG	2B	3004	1/1	0.96	0.12	65,65,65,65	0
57	MG	1a	3046	1/1	0.96	0.23	37,37,37,37	0
57	MG	1A	3525	1/1	0.96	0.11	26,26,26,26	0
57	MG	2A	3023	1/1	0.96	0.28	34,34,34,34	0
57	MG	1A	3289	1/1	0.96	0.14	30,30,30,30	0
57	MG	1A	3170	1/1	0.96	0.18	24,24,24,24	0
57	MG	1A	3848	1/1	0.96	0.16	28,28,28,28	0
57	MG	1A	3514	1/1	0.96	0.15	22,22,22,22	0
57	MG	1B	3024	1/1	0.96	0.16	37,37,37,37	0
57	MG	1A	3563	1/1	0.96	0.11	25,25,25,25	0
57	MG	1A	3382	1/1	0.96	0.12	38,38,38,38	0
57	MG	1A	3643	1/1	0.96	0.29	57,57,57,57	0
57	MG	1A	3500	1/1	0.96	0.21	21,21,21,21	0
57	MG	2A	3183	1/1	0.96	0.12	41,41,41,41	0
57	MG	2D	306	1/1	0.96	0.14	29,29,29,29	0
57	MG	1A	3918	1/1	0.96	0.16	38,38,38,38	0
57	MG	2A	3414	1/1	0.96	0.17	58,58,58,58	0
57	MG	1A	3711	1/1	0.96	0.18	39,39,39,39	0
57	MG	1a	3108	1/1	0.96	0.24	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3367	1/1	0.96	0.24	27,27,27,27	0
57	MG	1A	3971	1/1	0.96	0.16	12,12,12,12	0
57	MG	1A	3866	1/1	0.96	0.23	50,50,50,50	0
57	MG	1A	3671	1/1	0.96	0.10	16,16,16,16	0
57	MG	1A	3729	1/1	0.96	0.11	30,30,30,30	0
57	MG	1A	3032	1/1	0.96	0.11	27,27,27,27	0
57	MG	2A	3588	1/1	0.96	0.14	45,45,45,45	0
57	MG	1n	502	1/1	0.96	0.29	33,33,33,33	0
57	MG	2a	3014	1/1	0.96	0.08	51,51,51,51	0
57	MG	1A	3899	1/1	0.96	0.19	40,40,40,40	0
57	MG	1A	3308	1/1	0.96	0.20	36,36,36,36	0
57	MG	1A	3435	1/1	0.96	0.17	19,19,19,19	0
57	MG	2A	3236	1/1	0.96	0.16	40,40,40,40	0
57	MG	1A	3400	1/1	0.96	0.17	20,20,20,20	0
57	MG	1a	3149	1/1	0.96	0.16	35,35,35,35	0
57	MG	1A	3427	1/1	0.96	0.14	36,36,36,36	0
57	MG	2A	3434	1/1	0.96	0.10	34,34,34,34	0
57	MG	2a	3188	1/1	0.96	0.09	47,47,47,47	0
57	MG	1A	3713	1/1	0.96	0.21	49,49,49,49	0
57	MG	2A	3688	1/1	0.96	0.32	57,57,57,57	0
57	MG	1a	3112	1/1	0.96	0.15	42,42,42,42	0
57	MG	1A	3726	1/1	0.96	0.13	35,35,35,35	0
57	MG	1A	3633	1/1	0.96	0.17	28,28,28,28	0
57	MG	1a	3080	1/1	0.96	0.24	45,45,45,45	0
57	MG	1A	3966	1/1	0.96	0.12	50,50,50,50	0
57	MG	1A	3774	1/1	0.96	0.18	25,25,25,25	0
57	MG	1A	3357	1/1	0.97	0.33	42,42,42,42	0
57	MG	2a	3151	1/1	0.97	0.14	40,40,40,40	0
57	MG	1a	3020	1/1	0.97	0.15	39,39,39,39	0
57	MG	2A	3510	1/1	0.97	0.09	43,43,43,43	0
57	MG	1a	3127	1/1	0.97	0.09	37,37,37,37	0
57	MG	1A	3624	1/1	0.97	0.06	32,32,32,32	0
57	MG	1A	3340	1/1	0.97	0.15	19,19,19,19	0
57	MG	2A	3572	1/1	0.97	0.10	47,47,47,47	0
57	MG	2a	3080	1/1	0.97	0.14	45,45,45,45	0
57	MG	1A	3970	1/1	0.97	0.27	24,24,24,24	0
57	MG	2A	3117	1/1	0.97	0.20	35,35,35,35	0
57	MG	1B	3011	1/1	0.97	0.24	37,37,37,37	0
57	MG	1A	3507	1/1	0.97	0.23	49,49,49,49	0
57	MG	2a	3097	1/1	0.97	0.16	25,25,25,25	0
57	MG	1A	3718	1/1	0.97	0.14	26,26,26,26	0
57	MG	1A	3453	1/1	0.97	0.12	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
61	SF4	2d	501	8/8	0.97	0.11	52,59,68,73	0
57	MG	1A	3932	1/1	0.97	0.24	42,42,42,42	0
57	MG	1A	3003	1/1	0.97	0.11	19,19,19,19	0
57	MG	1A	3307	1/1	0.97	0.15	29,29,29,29	0
57	MG	1A	3557	1/1	0.97	0.09	48,48,48,48	0
57	MG	1a	3027	1/1	0.97	0.07	39,39,39,39	0
57	MG	1A	3960	1/1	0.97	0.46	29,29,29,29	0
57	MG	10	104	1/1	0.97	0.12	51,51,51,51	0
57	MG	1A	3197	1/1	0.97	0.11	26,26,26,26	0
57	MG	2A	3468	1/1	0.97	0.12	38,38,38,38	0
57	MG	2A	3021	1/1	0.97	0.17	39,39,39,39	0
57	MG	1a	3165	1/1	0.97	0.13	48,48,48,48	0
57	MG	2A	3014	1/1	0.97	0.15	37,37,37,37	0
57	MG	1A	3457	1/1	0.97	0.09	26,26,26,26	0
57	MG	2A	3076	1/1	0.97	0.33	40,40,40,40	0
57	MG	1A	3409	1/1	0.97	0.17	35,35,35,35	0
57	MG	2A	3669	1/1	0.97	0.09	39,39,39,39	0
57	MG	1A	3524	1/1	0.97	0.16	28,28,28,28	0
57	MG	1A	3768	1/1	0.97	0.14	42,42,42,42	0
57	MG	1A	3353	1/1	0.97	0.15	24,24,24,24	0
57	MG	1A	3593	1/1	0.97	0.19	29,29,29,29	0
57	MG	1A	3069	1/1	0.97	0.18	20,20,20,20	0
57	MG	1A	3397	1/1	0.97	0.21	22,22,22,22	0
57	MG	1A	3559	1/1	0.97	0.10	52,52,52,52	0
57	MG	2A	3535	1/1	0.97	0.19	49,49,49,49	0
57	MG	2a	3050	1/1	0.97	0.15	55,55,55,55	0
57	MG	1D	301	1/1	0.97	0.18	36,36,36,36	0
57	MG	2A	3357	1/1	0.97	0.13	41,41,41,41	0
57	MG	1A	3871	1/1	0.97	0.10	41,41,41,41	0
57	MG	1a	3138	1/1	0.97	0.11	29,29,29,29	0
57	MG	2A	3458	1/1	0.97	0.16	30,30,30,30	0
57	MG	1A	3354	1/1	0.97	0.15	15,15,15,15	0
57	MG	1A	3366	1/1	0.97	0.12	19,19,19,19	0
57	MG	1A	3758	1/1	0.97	0.10	33,33,33,33	0
57	MG	2A	3384	1/1	0.97	0.15	31,31,31,31	0
57	MG	2A	3575	1/1	0.97	0.11	36,36,36,36	0
57	MG	1A	3112	1/1	0.97	0.20	24,24,24,24	0
57	MG	2A	3110	1/1	0.97	0.14	47,47,47,47	0
57	MG	1A	3467	1/1	0.97	0.20	17,17,17,17	0
60	ZN	25	501	1/1	0.97	0.19	48,48,48,48	0
57	MG	2A	3333	1/1	0.97	0.17	32,32,32,32	0
57	MG	1A	3790	1/1	0.97	0.24	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1a	3091	1/1	0.97	0.13	39,39,39,39	0
57	MG	1A	3493	1/1	0.97	0.09	24,24,24,24	0
57	MG	1A	3332	1/1	0.97	0.12	39,39,39,39	0
57	MG	1A	3446	1/1	0.97	0.10	38,38,38,38	0
57	MG	1A	3973	1/1	0.97	0.34	25,25,25,25	0
57	MG	1A	3600	1/1	0.97	0.22	34,34,34,34	0
57	MG	2A	3457	1/1	0.97	0.16	32,32,32,32	0
57	MG	2A	3639	1/1	0.97	0.11	41,41,41,41	0
57	MG	1A	3167	1/1	0.97	0.15	28,28,28,28	0
57	MG	1A	3975	1/1	0.97	0.18	29,29,29,29	0
57	MG	1A	3123	1/1	0.97	0.31	27,27,27,27	0
57	MG	1A	3294	1/1	0.97	0.13	20,20,20,20	0
57	MG	1B	3017	1/1	0.97	0.20	39,39,39,39	0
57	MG	2A	3366	1/1	0.97	0.14	18,18,18,18	0
57	MG	2A	3513	1/1	0.97	0.08	44,44,44,44	0
57	MG	2A	3498	1/1	0.97	0.17	46,46,46,46	0
57	MG	1A	3627	1/1	0.97	0.24	16,16,16,16	0
57	MG	2A	3336	1/1	0.97	0.18	47,47,47,47	0
57	MG	1A	3581	1/1	0.97	0.21	20,20,20,20	0
57	MG	1A	3062	1/1	0.97	0.07	21,21,21,21	0
57	MG	2a	3133	1/1	0.97	0.13	33,33,33,33	0
57	MG	1A	3156	1/1	0.97	0.25	29,29,29,29	0
57	MG	2A	3464	1/1	0.97	0.16	33,33,33,33	0
57	MG	2A	3159	1/1	0.97	0.17	53,53,53,53	0
57	MG	2A	3487	1/1	0.97	0.18	50,50,50,50	0
57	MG	1A	3516	1/1	0.97	0.16	18,18,18,18	0
57	MG	2A	3486	1/1	0.97	0.08	29,29,29,29	0
57	MG	1A	3506	1/1	0.97	0.09	24,24,24,24	0
57	MG	1A	3270	1/1	0.97	0.25	22,22,22,22	0
57	MG	2A	3169	1/1	0.97	0.17	23,23,23,23	0
57	MG	1A	3978	1/1	0.97	0.37	28,28,28,28	0
57	MG	1A	3785	1/1	0.97	0.22	24,24,24,24	0
57	MG	2A	3036	1/1	0.97	0.21	52,52,52,52	0
57	MG	1A	3329	1/1	0.97	0.32	29,29,29,29	0
57	MG	2A	3433	1/1	0.97	0.18	30,30,30,30	0
57	MG	1A	3609	1/1	0.97	0.19	25,25,25,25	0
57	MG	2A	3151	1/1	0.97	0.30	32,32,32,32	0
57	MG	1A	3550	1/1	0.97	0.19	25,25,25,25	0
57	MG	1A	3686	1/1	0.97	0.13	34,34,34,34	0
57	MG	1D	306	1/1	0.97	0.18	27,27,27,27	0
57	MG	1B	3029	1/1	0.97	0.14	54,54,54,54	0
57	MG	1A	3619	1/1	0.97	0.09	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	ZN	26	501	1/1	0.97	0.17	56,56,56,56	0
57	MG	10	105	1/1	0.97	0.15	55,55,55,55	0
57	MG	1a	3103	1/1	0.97	0.22	34,34,34,34	0
57	MG	1A	3845	1/1	0.97	0.16	39,39,39,39	0
57	MG	2a	3034	1/1	0.97	0.12	53,53,53,53	0
57	MG	1a	3164	1/1	0.97	0.12	55,55,55,55	0
57	MG	2A	3554	1/1	0.97	0.16	56,56,56,56	0
57	MG	1A	3817	1/1	0.97	0.16	20,20,20,20	0
57	MG	1A	3012	1/1	0.97	0.16	17,17,17,17	0
57	MG	1A	3150	1/1	0.97	0.12	39,39,39,39	0
57	MG	2F	3005	1/1	0.97	0.30	39,39,39,39	0
57	MG	1A	3708	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3118	1/1	0.97	0.37	34,34,34,34	0
57	MG	2A	3173	1/1	0.97	0.12	37,37,37,37	0
57	MG	2A	3503	1/1	0.97	0.20	45,45,45,45	0
57	MG	2A	3184	1/1	0.97	0.26	40,40,40,40	0
57	MG	1a	3114	1/1	0.97	0.17	42,42,42,42	0
57	MG	2A	3515	1/1	0.97	0.30	36,36,36,36	0
57	MG	1a	3124	1/1	0.97	0.09	56,56,56,56	0
57	MG	1A	3387	1/1	0.97	0.13	23,23,23,23	0
57	MG	1A	3939	1/1	0.97	0.17	31,31,31,31	0
57	MG	2A	3429	1/1	0.97	0.11	42,42,42,42	0
57	MG	1A	3102	1/1	0.97	0.15	22,22,22,22	0
57	MG	1A	3880	1/1	0.97	0.20	37,37,37,37	0
60	ZN	14	501	1/1	0.97	0.10	68,68,68,68	0
57	MG	1A	3315	1/1	0.97	0.13	31,31,31,31	0
57	MG	1D	302	1/1	0.97	0.27	31,31,31,31	0
57	MG	1A	3719	1/1	0.97	0.10	37,37,37,37	0
57	MG	15	102	1/1	0.97	0.45	36,36,36,36	0
57	MG	2A	3443	1/1	0.97	0.22	31,31,31,31	0
57	MG	2a	3086	1/1	0.97	0.27	38,38,38,38	0
57	MG	1A	3163	1/1	0.97	0.13	37,37,37,37	0
57	MG	1A	3033	1/1	0.97	0.28	23,23,23,23	0
57	MG	1A	3213	1/1	0.97	0.12	21,21,21,21	0
57	MG	2A	3552	1/1	0.97	0.35	37,37,37,37	0
57	MG	2E	305	1/1	0.97	0.11	48,48,48,48	0
57	MG	1a	3071	1/1	0.97	0.18	30,30,30,30	0
57	MG	1a	3208	1/1	0.97	0.18	31,31,31,31	0
57	MG	1A	3226	1/1	0.97	0.15	40,40,40,40	0
57	MG	1D	303	1/1	0.97	0.19	29,29,29,29	0
57	MG	2A	3686	1/1	0.97	0.16	48,48,48,48	0
57	MG	2A	3016	1/1	0.97	0.18	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3684	1/1	0.97	0.15	42,42,42,42	0
57	MG	1a	3136	1/1	0.97	0.09	22,22,22,22	0
57	MG	1N	3005	1/1	0.97	0.14	27,27,27,27	0
57	MG	2A	3003	1/1	0.97	0.19	46,46,46,46	0
57	MG	1A	3987	1/1	0.97	0.20	29,29,29,29	0
57	MG	2A	3590	1/1	0.97	0.17	49,49,49,49	0
57	MG	2a	3101	1/1	0.97	0.10	60,60,60,60	0
57	MG	1A	3130	1/1	0.97	0.15	34,34,34,34	0
57	MG	2A	3529	1/1	0.97	0.10	49,49,49,49	0
57	MG	1A	3304	1/1	0.97	0.17	35,35,35,35	0
57	MG	2A	3409	1/1	0.97	0.11	51,51,51,51	0
57	MG	1A	3282	1/1	0.97	0.33	30,30,30,30	0
57	MG	28	101	1/1	0.97	0.15	43,43,43,43	0
57	MG	1A	3733	1/1	0.97	0.09	38,38,38,38	0
57	MG	2A	3461	1/1	0.97	0.14	41,41,41,41	0
57	MG	2A	3277	1/1	0.97	0.17	47,47,47,47	0
57	MG	1A	3115	1/1	0.97	0.18	24,24,24,24	0
57	MG	1A	3451	1/1	0.97	0.24	26,26,26,26	0
57	MG	2B	3006	1/1	0.97	0.21	61,61,61,61	0
57	MG	1l	202	1/1	0.97	0.16	51,51,51,51	0
57	MG	1A	3664	1/1	0.97	0.17	16,16,16,16	0
57	MG	1A	3098	1/1	0.97	0.10	33,33,33,33	0
57	MG	2A	3440	1/1	0.97	0.15	43,43,43,43	0
57	MG	1a	3219	1/1	0.97	0.14	40,40,40,40	0
57	MG	1A	3990	1/1	0.97	0.34	38,38,38,38	0
57	MG	1A	3545	1/1	0.97	0.10	9,9,9,9	0
57	MG	1A	3907	1/1	0.97	0.18	55,55,55,55	0
57	MG	2a	3122	1/1	0.97	0.12	50,50,50,50	0
57	MG	1X	107	1/1	0.97	0.16	37,37,37,37	0
57	MG	2A	3029	1/1	0.97	0.30	35,35,35,35	0
57	MG	1A	3027	1/1	0.97	0.08	30,30,30,30	0
57	MG	1A	3070	1/1	0.97	0.13	32,32,32,32	0
57	MG	1A	3472	1/1	0.97	0.21	20,20,20,20	0
57	MG	1a	3104	1/1	0.97	0.21	49,49,49,49	0
57	MG	1A	3399	1/1	0.97	0.20	44,44,44,44	0
57	MG	1A	3530	1/1	0.97	0.17	16,16,16,16	0
57	MG	1A	3201	1/1	0.97	0.21	38,38,38,38	0
57	MG	2A	3428	1/1	0.97	0.22	31,31,31,31	0
57	MG	1a	3172	1/1	0.97	0.11	32,32,32,32	0
57	MG	2A	3235	1/1	0.97	0.18	30,30,30,30	0
57	MG	2A	3565	1/1	0.97	0.09	25,25,25,25	0
57	MG	1A	3877	1/1	0.97	0.12	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3555	1/1	0.97	0.23	13,13,13,13	0
57	MG	2A	3158	1/1	0.97	0.10	50,50,50,50	0
57	MG	2A	3361	1/1	0.97	0.12	40,40,40,40	0
57	MG	1A	3813	1/1	0.97	0.14	15,15,15,15	0
57	MG	2A	3545	1/1	0.97	0.17	32,32,32,32	0
57	MG	1A	3026	1/1	0.97	0.20	21,21,21,21	0
57	MG	2A	3380	1/1	0.97	0.11	46,46,46,46	0
57	MG	1A	3047	1/1	0.97	0.14	23,23,23,23	0
57	MG	1A	3564	1/1	0.97	0.19	44,44,44,44	0
57	MG	1A	3496	1/1	0.97	0.16	14,14,14,14	0
57	MG	1A	3053	1/1	0.97	0.20	27,27,27,27	0
57	MG	1A	3048	1/1	0.97	0.21	24,24,24,24	0
57	MG	1A	3556	1/1	0.97	0.08	31,31,31,31	0
57	MG	2A	3058	1/1	0.97	0.16	47,47,47,47	0
57	MG	1A	3714	1/1	0.97	0.17	30,30,30,30	0
57	MG	1a	3073	1/1	0.97	0.08	50,50,50,50	0
57	MG	1a	3213	1/1	0.97	0.12	58,58,58,58	0
57	MG	1A	3766	1/1	0.97	0.12	41,41,41,41	0
57	MG	1F	309	1/1	0.97	0.22	39,39,39,39	0
57	MG	1e	3001	1/1	0.97	0.13	69,69,69,69	0
57	MG	1A	3584	1/1	0.97	0.24	51,51,51,51	0
57	MG	1A	3703	1/1	0.97	0.17	17,17,17,17	0
57	MG	1A	3935	1/1	0.97	0.16	44,44,44,44	0
57	MG	2A	3685	1/1	0.97	0.23	46,46,46,46	0
57	MG	1A	3928	1/1	0.97	0.15	28,28,28,28	0
57	MG	2A	3033	1/1	0.97	0.17	33,33,33,33	0
57	MG	1A	3608	1/1	0.97	0.13	15,15,15,15	0
57	MG	1V	201	1/1	0.97	0.26	24,24,24,24	0
57	MG	1A	3745	1/1	0.97	0.16	34,34,34,34	0
57	MG	1A	3039	1/1	0.97	0.40	23,23,23,23	0
57	MG	1a	3163	1/1	0.97	0.04	43,43,43,43	0
57	MG	1A	3528	1/1	0.97	0.29	20,20,20,20	0
57	MG	2A	3093	1/1	0.97	0.13	40,40,40,40	0
57	MG	2A	3196	1/1	0.97	0.10	30,30,30,30	0
57	MG	1A	3772	1/1	0.97	0.09	44,44,44,44	0
57	MG	2A	3061	1/1	0.97	0.22	50,50,50,50	0
57	MG	2A	3198	1/1	0.97	0.17	31,31,31,31	0
57	MG	2A	3571	1/1	0.97	0.17	35,35,35,35	0
57	MG	2A	3108	1/1	0.97	0.18	43,43,43,43	0
57	MG	2A	3437	1/1	0.98	0.18	31,31,31,31	0
57	MG	2A	3097	1/1	0.98	0.18	35,35,35,35	0
57	MG	2A	3325	1/1	0.98	0.14	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3186	1/1	0.98	0.23	20,20,20,20	0
57	MG	2A	3286	1/1	0.98	0.14	33,33,33,33	0
57	MG	1A	3075	1/1	0.98	0.23	39,39,39,39	0
57	MG	1A	3215	1/1	0.98	0.19	22,22,22,22	0
57	MG	1A	3029	1/1	0.98	0.14	18,18,18,18	0
57	MG	1A	3696	1/1	0.98	0.34	27,27,27,27	0
57	MG	1a	3039	1/1	0.98	0.15	41,41,41,41	0
57	MG	1A	3892	1/1	0.98	0.17	52,52,52,52	0
57	MG	2A	3002	1/1	0.98	0.21	23,23,23,23	0
57	MG	1A	3292	1/1	0.98	0.22	21,21,21,21	0
57	MG	1A	3200	1/1	0.98	0.18	20,20,20,20	0
57	MG	2A	3658	1/1	0.98	0.26	35,35,35,35	0
57	MG	2A	3543	1/1	0.98	0.09	58,58,58,58	0
57	MG	2A	3438	1/1	0.98	0.15	23,23,23,23	0
57	MG	1x	101	1/1	0.98	0.24	35,35,35,35	0
57	MG	1A	3764	1/1	0.98	0.11	35,35,35,35	0
57	MG	1A	3647	1/1	0.98	0.15	14,14,14,14	0
57	MG	1A	3030	1/1	0.98	0.22	18,18,18,18	0
57	MG	2A	3312	1/1	0.98	0.11	43,43,43,43	0
57	MG	1A	3084	1/1	0.98	0.12	15,15,15,15	0
57	MG	2A	3082	1/1	0.98	0.21	56,56,56,56	0
57	MG	1A	3539	1/1	0.98	0.15	42,42,42,42	0
57	MG	1A	3789	1/1	0.98	0.25	29,29,29,29	0
57	MG	1A	3464	1/1	0.98	0.16	49,49,49,49	0
57	MG	1A	3699	1/1	0.98	0.14	29,29,29,29	0
57	MG	2A	3424	1/1	0.98	0.18	33,33,33,33	0
57	MG	1A	3697	1/1	0.98	0.11	41,41,41,41	0
57	MG	1A	3481	1/1	0.98	0.14	29,29,29,29	0
57	MG	1A	3034	1/1	0.98	0.20	16,16,16,16	0
57	MG	2A	3445	1/1	0.98	0.23	25,25,25,25	0
57	MG	1a	3116	1/1	0.98	0.16	37,37,37,37	0
57	MG	2A	3296	1/1	0.98	0.18	29,29,29,29	0
57	MG	1A	3181	1/1	0.98	0.42	28,28,28,28	0
57	MG	1a	3153	1/1	0.98	0.10	47,47,47,47	0
57	MG	1A	3658	1/1	0.98	0.12	21,21,21,21	0
57	MG	1A	3959	1/1	0.98	0.16	31,31,31,31	0
57	MG	2A	3343	1/1	0.98	0.09	47,47,47,47	0
57	MG	1W	201	1/1	0.98	0.16	25,25,25,25	0
57	MG	1D	307	1/1	0.98	0.50	32,32,32,32	0
57	MG	1Q	202	1/1	0.98	0.22	17,17,17,17	0
57	MG	1A	3364	1/1	0.98	0.18	50,50,50,50	0
57	MG	1A	3678	1/1	0.98	0.11	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2A	3304	1/1	0.98	0.20	31,31,31,31	0
57	MG	2A	3300	1/1	0.98	0.12	21,21,21,21	0
57	MG	1a	3166	1/1	0.98	0.09	42,42,42,42	0
57	MG	1A	3996	1/1	0.98	0.27	31,31,31,31	0
57	MG	1A	3378	1/1	0.98	0.16	9,9,9,9	0
57	MG	1A	3146	1/1	0.98	0.12	26,26,26,26	0
57	MG	1A	3418	1/1	0.98	0.13	33,33,33,33	0
57	MG	1A	3160	1/1	0.98	0.17	10,10,10,10	0
57	MG	1a	3152	1/1	0.98	0.17	39,39,39,39	0
57	MG	1A	3807	1/1	0.98	0.09	20,20,20,20	0
57	MG	1A	3009	1/1	0.98	0.13	18,18,18,18	0
57	MG	1A	3588	1/1	0.98	0.25	28,28,28,28	0
57	MG	1A	3950	1/1	0.98	0.11	38,38,38,38	0
57	MG	2a	3018	1/1	0.98	0.16	43,43,43,43	0
57	MG	1F	305	1/1	0.98	0.31	26,26,26,26	0
57	MG	1A	3476	1/1	0.98	0.14	36,36,36,36	0
57	MG	1a	3119	1/1	0.98	0.06	51,51,51,51	0
57	MG	1D	310	1/1	0.98	0.15	10,10,10,10	0
57	MG	2A	3396	1/1	0.98	0.21	49,49,49,49	0
61	SF4	1d	501	8/8	0.98	0.14	46,53,55,72	0
57	MG	1A	3300	1/1	0.98	0.26	31,31,31,31	0
57	MG	1A	3132	1/1	0.98	0.53	30,30,30,30	0
57	MG	1A	3738	1/1	0.98	0.14	38,38,38,38	0
57	MG	2A	3395	1/1	0.98	0.18	36,36,36,36	0
57	MG	1A	3803	1/1	0.98	0.13	20,20,20,20	0
57	MG	1A	3023	1/1	0.98	0.12	14,14,14,14	0
57	MG	1A	3165	1/1	0.98	0.17	23,23,23,23	0
57	MG	1a	3223	1/1	0.98	0.17	37,37,37,37	0
57	MG	1A	3237	1/1	0.98	0.15	35,35,35,35	0
57	MG	2A	3297	1/1	0.98	0.14	40,40,40,40	0
57	MG	1A	3590	1/1	0.98	0.15	48,48,48,48	0
57	MG	2a	3044	1/1	0.98	0.15	64,64,64,64	0
57	MG	1A	3103	1/1	0.98	0.28	31,31,31,31	0
57	MG	1A	3147	1/1	0.98	0.19	27,27,27,27	0
57	MG	1A	3136	1/1	0.98	0.22	9,9,9,9	0
57	MG	1x	109	1/1	0.98	0.08	45,45,45,45	0
57	MG	1A	3219	1/1	0.98	0.20	33,33,33,33	0
57	MG	1A	3279	1/1	0.98	0.11	16,16,16,16	0
57	MG	2A	3233	1/1	0.98	0.14	35,35,35,35	0
57	MG	2A	3492	1/1	0.98	0.18	29,29,29,29	0
57	MG	1A	3122	1/1	0.98	0.34	31,31,31,31	0
57	MG	2a	3070	1/1	0.98	0.17	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	2a	3031	1/1	0.98	0.10	38,38,38,38	0
57	MG	2A	3273	1/1	0.98	0.13	49,49,49,49	0
60	ZN	1Y	202	1/1	0.98	0.18	61,61,61,61	0
57	MG	2A	3323	1/1	0.98	0.14	29,29,29,29	0
57	MG	1A	3694	1/1	0.98	0.21	30,30,30,30	0
57	MG	1A	3422	1/1	0.98	0.15	18,18,18,18	0
57	MG	1F	304	1/1	0.98	0.16	15,15,15,15	0
57	MG	1A	3326	1/1	0.98	0.10	26,26,26,26	0
57	MG	1A	3188	1/1	0.98	0.17	19,19,19,19	0
57	MG	1a	3178	1/1	0.98	0.16	47,47,47,47	0
57	MG	2A	3405	1/1	0.98	0.21	45,45,45,45	0
57	MG	1A	3946	1/1	0.98	0.11	19,19,19,19	0
57	MG	1a	3173	1/1	0.98	0.11	47,47,47,47	0
57	MG	1A	3089	1/1	0.98	0.10	21,21,21,21	0
57	MG	1B	3016	1/1	0.98	0.18	21,21,21,21	0
57	MG	1A	3448	1/1	0.98	0.21	11,11,11,11	0
57	MG	1A	3093	1/1	0.98	0.25	41,41,41,41	0
57	MG	1A	3314	1/1	0.98	0.54	42,42,42,42	0
57	MG	1A	3891	1/1	0.98	0.16	10,10,10,10	0
57	MG	1A	3489	1/1	0.98	0.15	14,14,14,14	0
57	MG	1A	3221	1/1	0.98	0.11	28,28,28,28	0
57	MG	1A	3441	1/1	0.98	0.17	25,25,25,25	0
57	MG	2A	3581	1/1	0.98	0.07	49,49,49,49	0
57	MG	1A	3649	1/1	0.98	0.17	19,19,19,19	0
57	MG	1A	3494	1/1	0.98	0.17	13,13,13,13	0
57	MG	1A	3044	1/1	0.98	0.23	34,34,34,34	0
57	MG	1A	3941	1/1	0.98	0.17	10,10,10,10	0
57	MG	2A	3164	1/1	0.98	0.23	31,31,31,31	0
57	MG	1A	4001	1/1	0.98	0.20	29,29,29,29	0
57	MG	1A	3415	1/1	0.98	0.16	17,17,17,17	0
57	MG	2A	3015	1/1	0.98	0.17	20,20,20,20	0
57	MG	1A	3042	1/1	0.98	0.19	27,27,27,27	0
57	MG	1A	3815	1/1	0.98	0.22	40,40,40,40	0
57	MG	2A	3512	1/1	0.98	0.06	55,55,55,55	0
57	MG	1A	3933	1/1	0.98	0.12	34,34,34,34	0
57	MG	1E	306	1/1	0.98	0.15	23,23,23,23	0
57	MG	1A	3666	1/1	0.98	0.20	16,16,16,16	0
57	MG	2A	3537	1/1	0.98	0.16	25,25,25,25	0
57	MG	1A	3927	1/1	0.98	0.13	31,31,31,31	0
57	MG	1A	3275	1/1	0.98	0.09	27,27,27,27	0
57	MG	19	502	1/1	0.98	0.18	31,31,31,31	0
57	MG	2A	3577	1/1	0.98	0.08	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3139	1/1	0.98	0.16	20,20,20,20	0
57	MG	1A	3988	1/1	0.98	0.28	22,22,22,22	0
57	MG	1A	3045	1/1	0.98	0.15	10,10,10,10	0
57	MG	2a	3154	1/1	0.98	0.12	47,47,47,47	0
57	MG	1A	3067	1/1	0.98	0.12	22,22,22,22	0
57	MG	1A	3205	1/1	0.98	0.42	25,25,25,25	0
57	MG	2a	3152	1/1	0.98	0.11	59,59,59,59	0
57	MG	2a	3111	1/1	0.98	0.14	35,35,35,35	0
57	MG	1A	3153	1/1	0.98	0.20	22,22,22,22	0
57	MG	1A	3022	1/1	0.98	0.11	33,33,33,33	0
57	MG	1A	4000	1/1	0.98	0.20	27,27,27,27	0
57	MG	1A	3293	1/1	0.98	0.18	39,39,39,39	0
57	MG	1a	3109	1/1	0.98	0.12	54,54,54,54	0
57	MG	1A	3752	1/1	0.98	0.14	18,18,18,18	0
57	MG	1A	3616	1/1	0.98	0.11	14,14,14,14	0
57	MG	1A	3704	1/1	0.98	0.12	31,31,31,31	0
57	MG	2Y	502	1/1	0.98	0.26	38,38,38,38	0
57	MG	2A	3521	1/1	0.98	0.23	36,36,36,36	0
57	MG	1A	3982	1/1	0.98	0.18	18,18,18,18	0
57	MG	1A	3612	1/1	0.98	0.18	26,26,26,26	0
57	MG	1A	3065	1/1	0.98	0.16	10,10,10,10	0
57	MG	2A	3192	1/1	0.98	0.21	26,26,26,26	0
57	MG	2A	3531	1/1	0.98	0.19	35,35,35,35	0
57	MG	2a	3092	1/1	0.98	0.12	59,59,59,59	0
57	MG	1A	3984	1/1	0.98	0.15	22,22,22,22	0
57	MG	1A	3230	1/1	0.98	0.37	21,21,21,21	0
57	MG	1A	3983	1/1	0.98	0.16	31,31,31,31	0
57	MG	1x	105	1/1	0.98	0.19	56,56,56,56	0
57	MG	1A	3898	1/1	0.98	0.20	23,23,23,23	0
57	MG	1A	3024	1/1	0.98	0.17	48,48,48,48	0
57	MG	1a	3151	1/1	0.98	0.11	38,38,38,38	0
57	MG	1A	3021	1/1	0.98	0.22	19,19,19,19	0
57	MG	1A	3269	1/1	0.98	0.16	25,25,25,25	0
57	MG	1A	3656	1/1	0.98	0.15	18,18,18,18	0
57	MG	1A	3860	1/1	0.98	0.08	27,27,27,27	0
57	MG	1A	3360	1/1	0.98	0.10	21,21,21,21	0
57	MG	1A	3629	1/1	0.98	0.15	35,35,35,35	0
57	MG	1A	3363	1/1	0.98	0.26	21,21,21,21	0
57	MG	1N	3006	1/1	0.98	0.13	31,31,31,31	0
57	MG	1A	3937	1/1	0.98	0.20	16,16,16,16	0
57	MG	1A	3316	1/1	0.98	0.19	32,32,32,32	0
57	MG	1A	3650	1/1	0.98	0.10	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3091	1/1	0.98	0.17	38,38,38,38	0
57	MG	1A	3059	1/1	0.98	0.14	16,16,16,16	0
57	MG	1A	3327	1/1	0.98	0.18	24,24,24,24	0
57	MG	2A	3555	1/1	0.98	0.11	44,44,44,44	0
57	MG	2A	3520	1/1	0.98	0.19	33,33,33,33	0
57	MG	1A	3775	1/1	0.99	0.25	26,26,26,26	0
57	MG	1a	3118	1/1	0.99	0.20	38,38,38,38	0
57	MG	1A	3532	1/1	0.99	0.16	8,8,8,8	0
57	MG	2A	3148	1/1	0.99	0.17	28,28,28,28	0
57	MG	1A	3804	1/1	0.99	0.17	16,16,16,16	0
57	MG	1A	3707	1/1	0.99	0.19	25,25,25,25	0
57	MG	2A	3043	1/1	0.99	0.23	55,55,55,55	0
57	MG	1Y	205	1/1	0.99	0.23	43,43,43,43	0
57	MG	1P	202	1/1	0.99	0.47	22,22,22,22	0
57	MG	2A	3497	1/1	0.99	0.13	36,36,36,36	0
60	ZN	19	501	1/1	0.99	0.17	40,40,40,40	0
57	MG	1A	3068	1/1	0.99	0.09	17,17,17,17	0
57	MG	2A	3674	1/1	0.99	0.17	40,40,40,40	0
57	MG	1A	3690	1/1	0.99	0.10	52,52,52,52	0
57	MG	1A	3046	1/1	0.99	0.13	15,15,15,15	0
57	MG	1A	3780	1/1	0.99	0.16	28,28,28,28	0
57	MG	1D	312	1/1	0.99	0.22	29,29,29,29	0
57	MG	1a	3143	1/1	0.99	0.19	40,40,40,40	0
57	MG	1A	3285	1/1	0.99	0.23	34,34,34,34	0
57	MG	1A	3498	1/1	0.99	0.13	17,17,17,17	0
57	MG	2A	3412	1/1	0.99	0.12	36,36,36,36	0
57	MG	1A	3227	1/1	0.99	0.13	37,37,37,37	0
57	MG	1A	3438	1/1	0.99	0.13	8,8,8,8	0
57	MG	1A	3161	1/1	0.99	0.20	34,34,34,34	0
57	MG	2A	3149	1/1	0.99	0.14	52,52,52,52	0
57	MG	1U	203	1/1	0.99	0.42	27,27,27,27	0
57	MG	1A	3325	1/1	0.99	0.18	25,25,25,25	0
57	MG	2A	3315	1/1	0.99	0.13	49,49,49,49	0
57	MG	2A	3253	1/1	0.99	0.16	47,47,47,47	0
57	MG	2a	3196	1/1	0.99	0.10	45,45,45,45	0
57	MG	2A	3615	1/1	0.99	0.09	42,42,42,42	0
57	MG	2A	3020	1/1	0.99	0.23	41,41,41,41	0
57	MG	1A	3992	1/1	0.99	0.16	25,25,25,25	0
57	MG	2A	3517	1/1	0.99	0.17	24,24,24,24	0
60	ZN	1n	501	1/1	0.99	0.15	55,55,55,55	0
57	MG	1A	3606	1/1	0.99	0.19	31,31,31,31	0
57	MG	1a	3036	1/1	0.99	0.10	38,38,38,38	0

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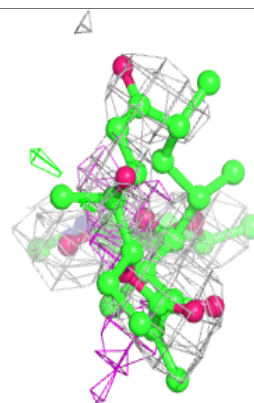
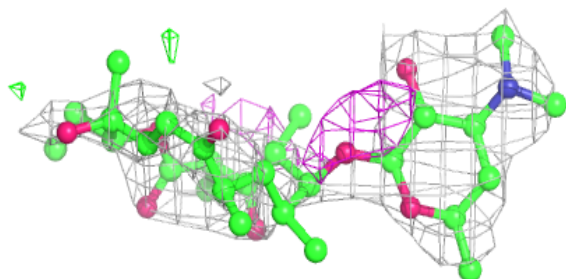
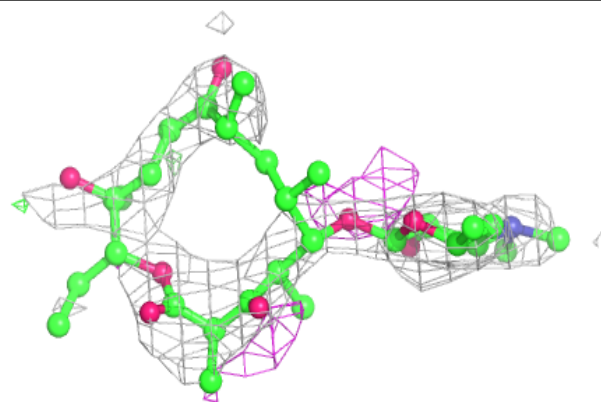
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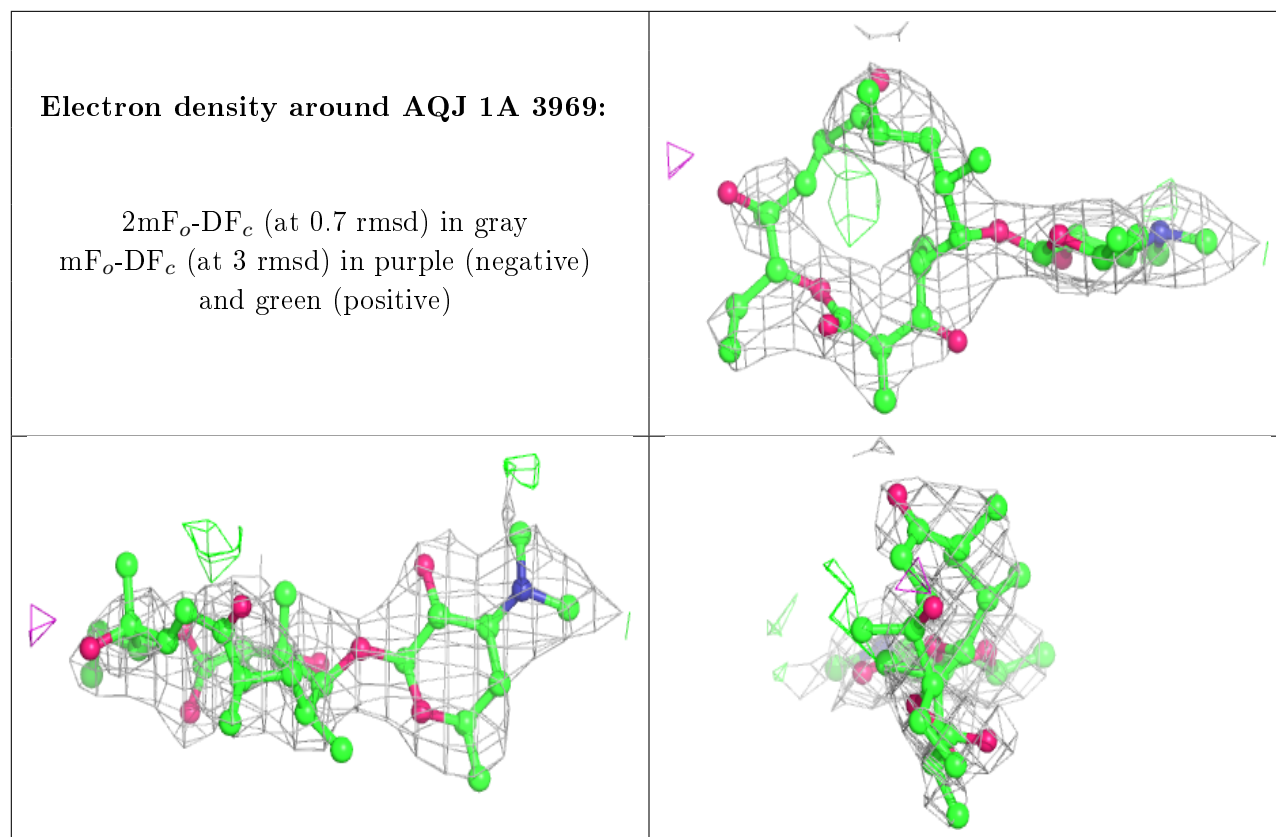
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1A	3473	1/1	0.99	0.15	21,21,21,21	0
57	MG	1A	3306	1/1	0.99	0.12	33,33,33,33	0
57	MG	2a	3168	1/1	0.99	0.17	46,46,46,46	0
57	MG	2A	3683	1/1	0.99	0.14	52,52,52,52	0
57	MG	2A	3318	1/1	0.99	0.21	39,39,39,39	0
57	MG	1S	3002	1/1	0.99	0.12	36,36,36,36	0
57	MG	1A	3128	1/1	0.99	0.15	20,20,20,20	0
57	MG	1A	3349	1/1	0.99	0.17	23,23,23,23	0
57	MG	1E	309	1/1	0.99	0.37	39,39,39,39	0
57	MG	1A	3162	1/1	0.99	0.10	18,18,18,18	0
60	ZN	16	501	1/1	1.00	0.19	34,34,34,34	0
60	ZN	15	101	1/1	1.00	0.21	35,35,35,35	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 AQJ 2A 3677:

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.