



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 04:24 PM EDT

PDB ID : 5W4K / pdb_00005w4k
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with Klebsazolicin and bound to mRNA and A-, P- and E-site tRNAs at 2.7Å resolution
Authors : Metelev, M.; Osterman, I.A.; Ghilarov, D.; Khabibullina, N.F.; Yakimov, A.; Shabalin, K.; Utkina, I.; Travin, D.Y.; Komarova, E.S.; Serebryakova, M.; Artamonova, T.; Khodorkovskii, M.; Konevega, A.L.; Sergiev, P.V.; Severinov, K.; Polikanov, Y.S.
Deposited on : 2017-06-12
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

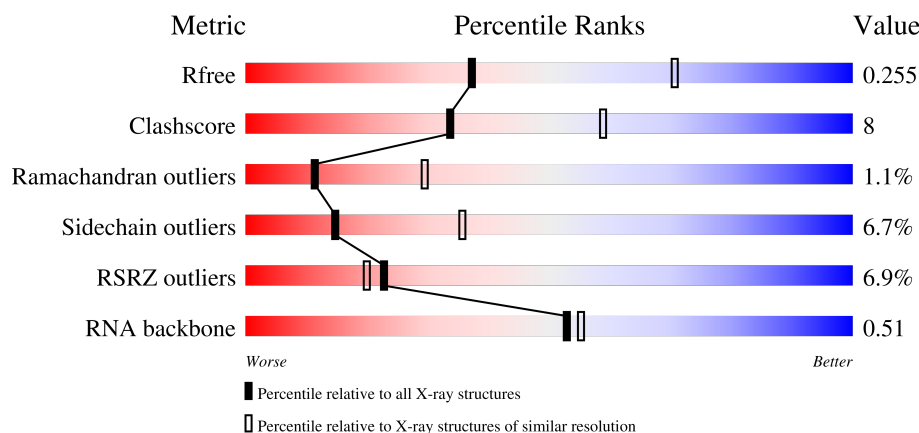
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

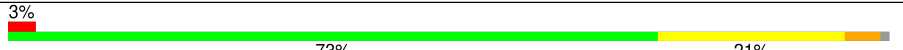
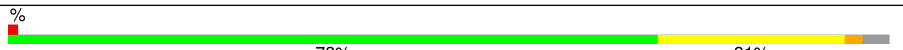
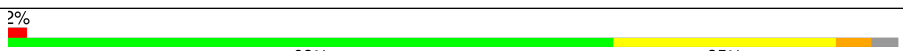
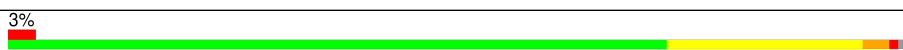
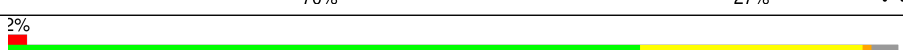
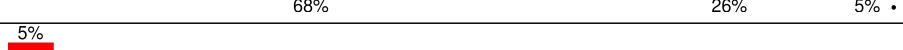
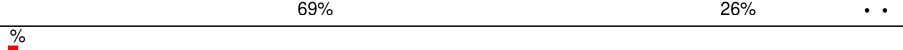
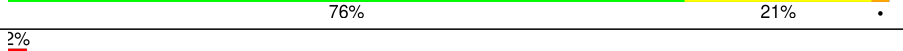
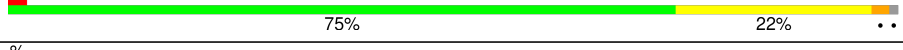
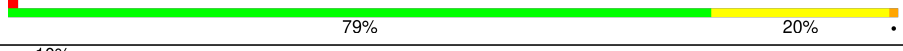
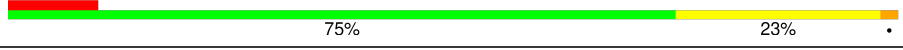
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	1A	2915	4% 68% 25% 6%
1	2A	2915	4% 59% 31% 6%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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

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

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Mol	Chain	Length	Quality of chain
27	15	60	
27	25	60	
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	

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

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Mol	Chain	Length	Quality of chain
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	2y	76	
57	2a	1521	
58	A	18	
58	B	18	

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
59	MG	1a	3435	-	-	-	X
59	MG	1y	104	-	-	-	X
59	MG	2a	3118	-	-	-	X
61	SF4	2d	501	-	-	X	-

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 302030 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1423	913	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			

- 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			

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0
			1592	713	285	518	74	2		
54	2w	72	Total	C	N	O	P	S	0	0
			1544	690	278	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 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 a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	2a	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

- Molecule 58 is a protein called Klebsazolicin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	A	18	Total	C	N	O	S	0	0	0
			115	64	23	25	3			
58	B	18	Total	C	N	O	S	0	0	0
			115	64	23	25	3			

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1229	Total Mg 1229 1229	0	0
59	1B	38	Total Mg 38 38	0	0
59	1D	13	Total Mg 13 13	0	0
59	1E	14	Total Mg 14 14	0	0
59	1F	10	Total Mg 10 10	0	0
59	1G	5	Total Mg 5 5	0	0
59	1I	1	Total Mg 1 1	0	0
59	1N	9	Total Mg 9 9	0	0
59	1O	6	Total Mg 6 6	0	0
59	1P	4	Total Mg 4 4	0	0
59	1Q	6	Total Mg 6 6	0	0
59	1R	3	Total Mg 3 3	0	0
59	1S	3	Total Mg 3 3	0	0
59	1T	2	Total Mg 2 2	0	0
59	1U	5	Total Mg 5 5	0	0
59	1V	2	Total Mg 2 2	0	0
59	1W	5	Total Mg 5 5	0	0
59	1X	5	Total Mg 5 5	0	0
59	1Y	3	Total Mg 3 3	0	0
59	1Z	4	Total Mg 4 4	0	0
59	10	8	Total Mg 8 8	0	0
59	11	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	12	2	Total 2	Mg 2	0	0
59	13	3	Total 3	Mg 3	0	0
59	15	2	Total 2	Mg 2	0	0
59	16	3	Total 3	Mg 3	0	0
59	17	2	Total 2	Mg 2	0	0
59	18	3	Total 3	Mg 3	0	0
59	19	1	Total 1	Mg 1	0	0
59	1a	278	Total 278	Mg 278	0	0
59	1b	2	Total 2	Mg 2	0	0
59	1d	1	Total 1	Mg 1	0	0
59	1e	1	Total 1	Mg 1	0	0
59	1f	3	Total 3	Mg 3	0	0
59	1k	1	Total 1	Mg 1	0	0
59	1l	3	Total 3	Mg 3	0	0
59	1n	2	Total 2	Mg 2	0	0
59	1p	1	Total 1	Mg 1	0	0
59	1s	1	Total 1	Mg 1	0	0
59	1t	1	Total 1	Mg 1	0	0
59	1v	1	Total 1	Mg 1	0	0
59	1w	12	Total 12	Mg 12	0	0
59	1x	17	Total 17	Mg 17	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1y	5	Total 5	Mg 5	0	0
59	2A	848	Total 848	Mg 848	0	0
59	2B	22	Total 22	Mg 22	0	0
59	2D	5	Total 5	Mg 5	0	0
59	2E	7	Total 7	Mg 7	0	0
59	2F	4	Total 4	Mg 4	0	0
59	2G	1	Total 1	Mg 1	0	0
59	2N	1	Total 1	Mg 1	0	0
59	2O	2	Total 2	Mg 2	0	0
59	2P	1	Total 1	Mg 1	0	0
59	2Q	4	Total 4	Mg 4	0	0
59	2R	3	Total 3	Mg 3	0	0
59	2S	1	Total 1	Mg 1	0	0
59	2T	3	Total 3	Mg 3	0	0
59	2U	4	Total 4	Mg 4	0	0
59	2V	1	Total 1	Mg 1	0	0
59	2X	2	Total 2	Mg 2	0	0
59	2Z	1	Total 1	Mg 1	0	0
59	20	3	Total 3	Mg 3	0	0
59	23	2	Total 2	Mg 2	0	0
59	25	3	Total 3	Mg 3	0	0

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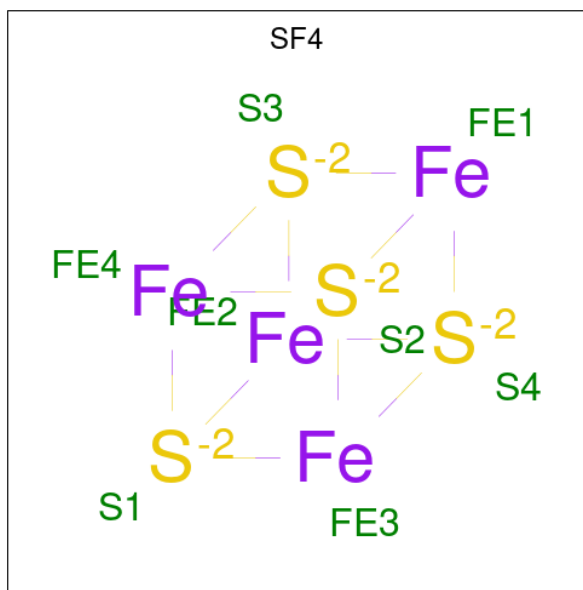
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	27	1	Total 1	Mg 1	0	0
59	28	2	Total 2	Mg 2	0	0
59	2a	239	Total 239	Mg 239	0	0
59	2d	1	Total 1	Mg 1	0	0
59	2e	1	Total 1	Mg 1	0	0
59	2f	2	Total 2	Mg 2	0	0
59	2g	1	Total 1	Mg 1	0	0
59	2j	2	Total 2	Mg 2	0	0
59	2k	1	Total 1	Mg 1	0	0
59	2l	2	Total 2	Mg 2	0	0
59	2p	1	Total 1	Mg 1	0	0
59	2q	5	Total 5	Mg 5	0	0
59	2r	1	Total 1	Mg 1	0	0
59	2t	1	Total 1	Mg 1	0	0
59	2v	4	Total 4	Mg 4	0	0
59	2w	7	Total 7	Mg 7	0	0
59	2x	4	Total 4	Mg 4	0	0
59	2y	7	Total 7	Mg 7	0	0
59	A	1	Total 1	Mg 1	0	0
59	B	1	Total 1	Mg 1	0	0

- Molecule 60 is ZINC ION (CCD ID: 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	15	1	Total Zn 1 1	0	0
60	16	1	Total Zn 1 1	0	0
60	19	1	Total Zn 1 1	0	0
60	1n	1	Total Zn 1 1	0	0
60	2Y	1	Total Zn 1 1	0	0
60	24	1	Total Zn 1 1	0	0
60	25	1	Total Zn 1 1	0	0
60	26	1	Total Zn 1 1	0	0
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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 POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2A	1	Total	K	0	0
			1	1		

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1A	2636	Total	O	0	0
			2636	2636		
63	1B	71	Total	O	0	0
			71	71		
63	1D	31	Total	O	0	0
			31	31		
63	1E	35	Total	O	0	0
			35	35		
63	1F	18	Total	O	0	0
			18	18		
63	1G	6	Total	O	0	0
			6	6		
63	1H	3	Total	O	0	0
			3	3		
63	1I	2	Total	O	0	0
			2	2		
63	1N	10	Total	O	0	0
			10	10		
63	1O	8	Total	O	0	0
			8	8		
63	1P	23	Total	O	0	0
			23	23		
63	1Q	16	Total	O	0	0
			16	16		
63	1R	14	Total	O	0	0
			14	14		
63	1S	4	Total	O	0	0
			4	4		
63	1T	9	Total	O	0	0
			9	9		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1U	13	Total 13	O 13	0	0
63	1V	9	Total 9	O 9	0	0
63	1W	11	Total 11	O 11	0	0
63	1X	8	Total 8	O 8	0	0
63	1Y	7	Total 7	O 7	0	0
63	1Z	2	Total 2	O 2	0	0
63	10	12	Total 12	O 12	0	0
63	11	13	Total 13	O 13	0	0
63	12	4	Total 4	O 4	0	0
63	13	5	Total 5	O 5	0	0
63	14	1	Total 1	O 1	0	0
63	15	5	Total 5	O 5	0	0
63	16	5	Total 5	O 5	0	0
63	17	9	Total 9	O 9	0	0
63	18	13	Total 13	O 13	0	0
63	19	1	Total 1	O 1	0	0
63	1a	523	Total 523	O 523	0	0
63	1b	1	Total 1	O 1	0	0
63	1d	3	Total 3	O 3	0	0
63	1e	3	Total 3	O 3	0	0
63	1g	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1k	3	Total 3	O 3	0	0
63	1l	10	Total 10	O 10	0	0
63	1m	1	Total 1	O 1	0	0
63	1o	2	Total 2	O 2	0	0
63	1p	1	Total 1	O 1	0	0
63	1q	4	Total 4	O 4	0	0
63	1r	1	Total 1	O 1	0	0
63	1t	2	Total 2	O 2	0	0
63	1v	6	Total 6	O 6	0	0
63	1w	26	Total 26	O 26	0	0
63	1x	18	Total 18	O 18	0	0
63	1y	2	Total 2	O 2	0	0
63	2A	1602	Total 1602	O 1602	0	0
63	2B	28	Total 28	O 28	0	0
63	2D	29	Total 29	O 29	0	0
63	2E	15	Total 15	O 15	0	0
63	2F	20	Total 20	O 20	0	0
63	2I	4	Total 4	O 4	0	0
63	2N	2	Total 2	O 2	0	0
63	2P	15	Total 15	O 15	0	0
63	2Q	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	2R	5	Total 5	O 5	0	0
63	2T	6	Total 6	O 6	0	0
63	2U	6	Total 6	O 6	0	0
63	2V	4	Total 4	O 4	0	0
63	2W	4	Total 4	O 4	0	0
63	2X	4	Total 4	O 4	0	0
63	2Y	1	Total 1	O 1	0	0
63	2Z	2	Total 2	O 2	0	0
63	20	5	Total 5	O 5	0	0
63	21	14	Total 14	O 14	0	0
63	22	1	Total 1	O 1	0	0
63	23	2	Total 2	O 2	0	0
63	25	4	Total 4	O 4	0	0
63	27	7	Total 7	O 7	0	0
63	28	7	Total 7	O 7	0	0
63	29	1	Total 1	O 1	0	0
63	2a	389	Total 389	O 389	0	0
63	2d	3	Total 3	O 3	0	0
63	2e	3	Total 3	O 3	0	0
63	2f	1	Total 1	O 1	0	0
63	2g	1	Total 1	O 1	0	0

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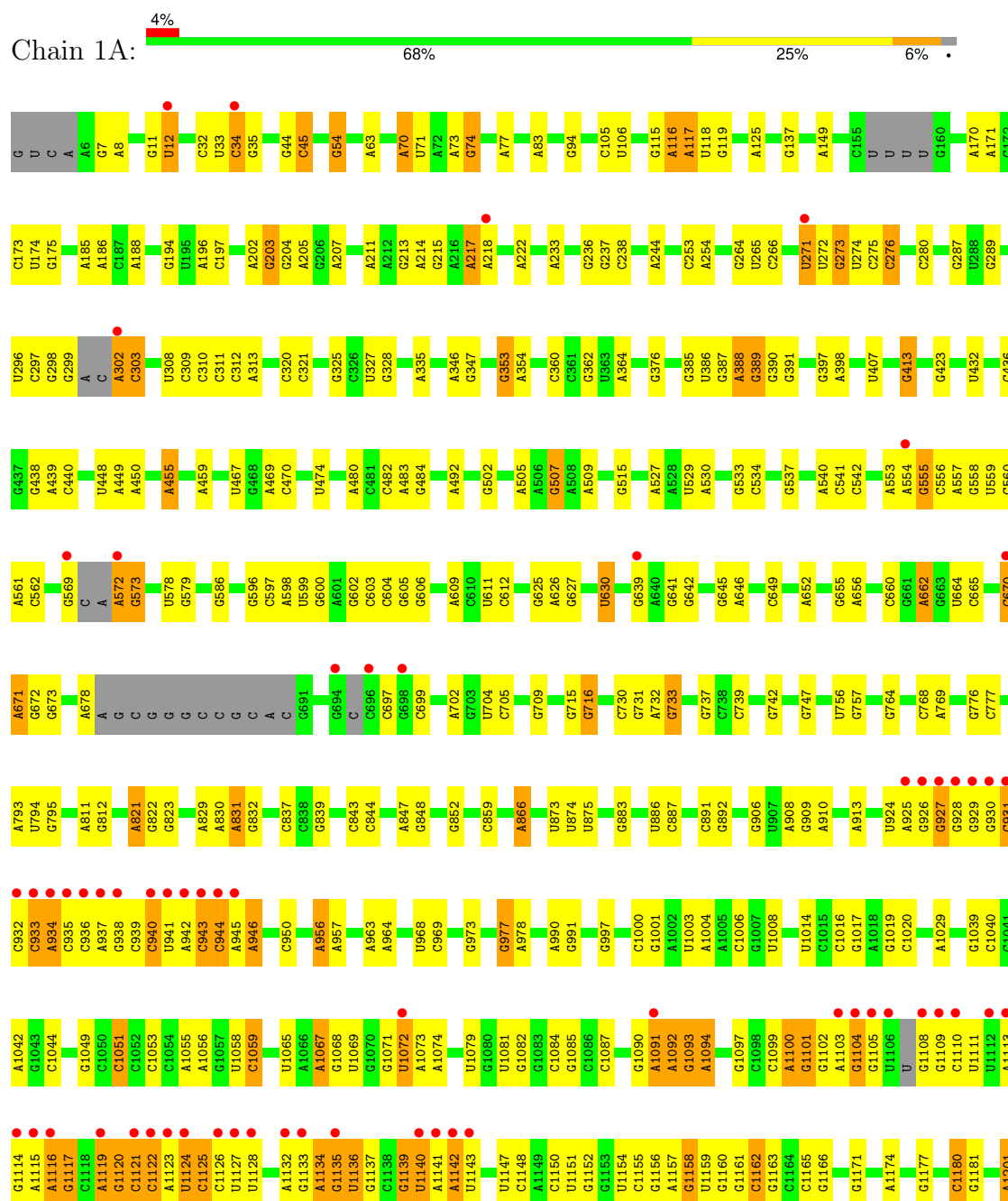
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	2h	2	Total	O	0	0
			2	2		
63	2i	1	Total	O	0	0
			1	1		
63	2j	4	Total	O	0	0
			4	4		
63	2l	5	Total	O	0	0
			5	5		
63	2o	1	Total	O	0	0
			1	1		
63	2p	3	Total	O	0	0
			3	3		
63	2q	2	Total	O	0	0
			2	2		
63	2r	1	Total	O	0	0
			1	1		
63	2t	3	Total	O	0	0
			3	3		
63	2u	1	Total	O	0	0
			1	1		
63	2v	1	Total	O	0	0
			1	1		
63	2w	3	Total	O	0	0
			3	3		
63	2x	10	Total	O	0	0
			10	10		
63	2y	20	Total	O	0	0
			20	20		
63	A	4	Total	O	0	0
			4	4		
63	B	2	Total	O	0	0
			2	2		

3 Residue-property plots

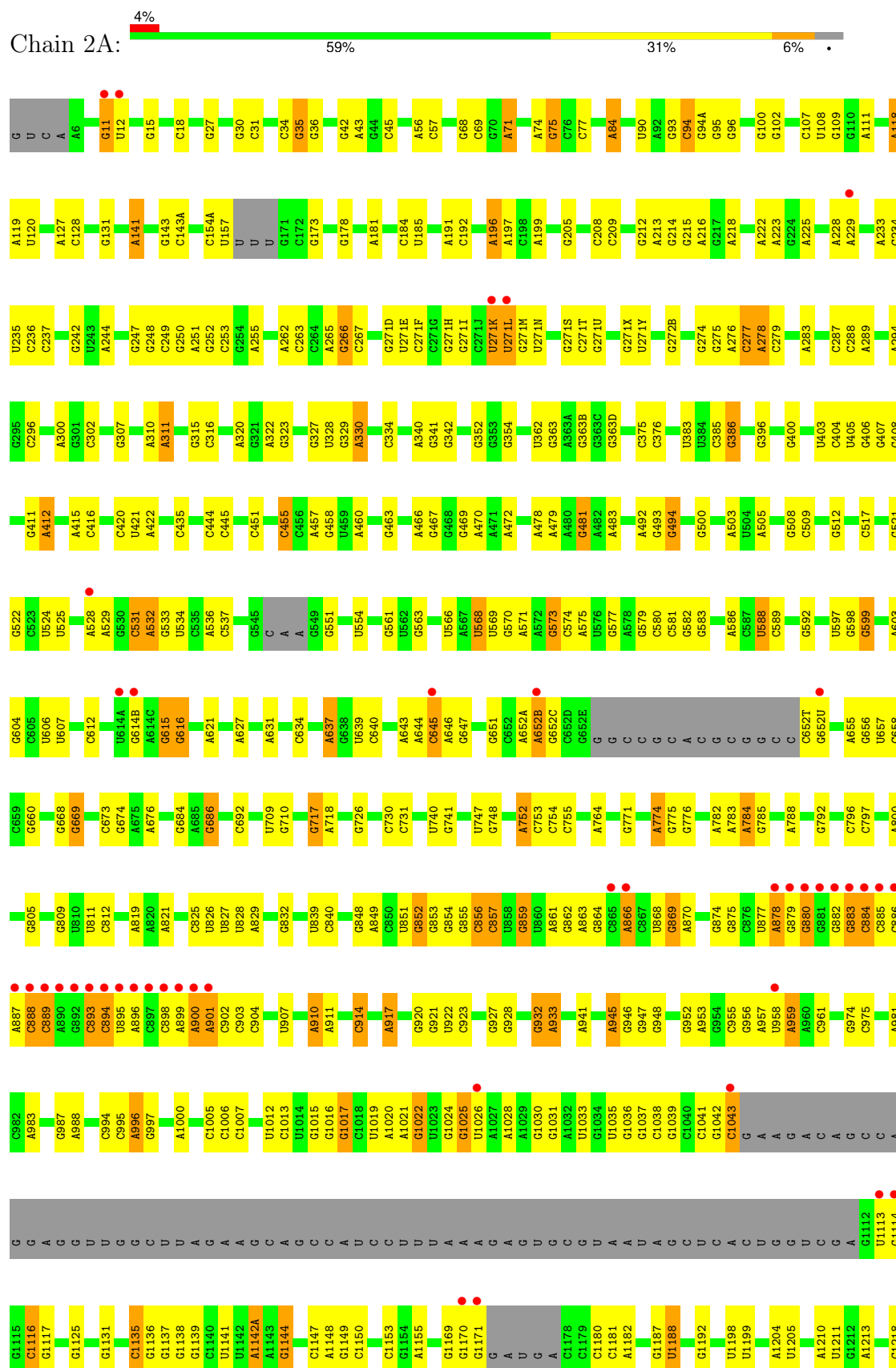
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 23S Ribosomal RNA

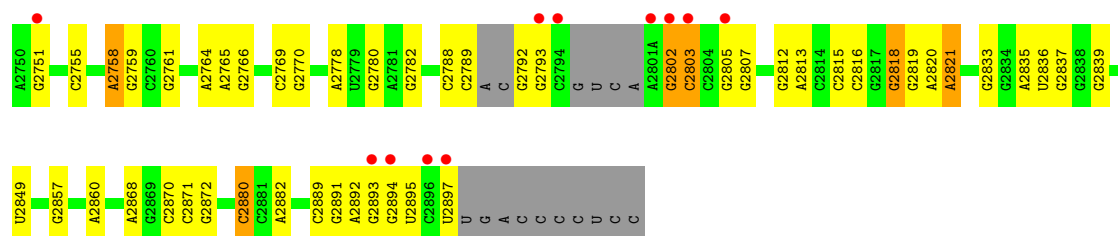




- Molecule 1: 23S Ribosomal RNA

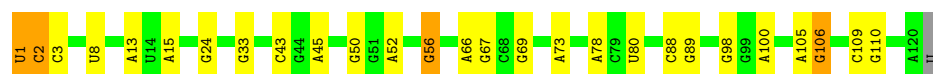


G2624	G2625	G2626	G2627	G2630	G2634	G2646	G2647	G2654	G2657	G2667	G2668	G2674	A2675	G2678	A2679	G2683	G2687	G2688	G2689	G2690	A2693	G2694	G2698	G2699	U2702	A2712A	A2713	G2714	G2718	G2719	U2726	G2727	G2732	A2733	A2741	G2745	U2746	A2748	A2749												
U2506	C2507	G2508	C2512	G2513	A2518	U2519	C2520	G2525	G2529	G2536	U2537	G2538	C2539	G2540	A2541	A2542	G2543	G2544	U2547	U2552	G2553	U2554	G2558	C2559	U2562	U2563	A2564	A2565	A2566	G2567	A2572	C2573	G2574	C2586	A2590	A2602	U2605	U2609	U2610	U2611	G2612	A2617									
G2409	A2412	U2419	U2420	A2425	G2429	A2430	U2431	A2432	A2433	A2434	A2435	U2438	A2439	G2440	G2441	G2442	G2443	G2444	G2445	A2448	U2461	U2462	G2467	G2468	A2469	G2470	G2471	G2472	U2473	G2474	G2475	A2476	G2484	G2485	G2486	G2487	A2488	G2489	G2490	G2494	G2495	G2496	A2497	G2498	G2502	A2503	U2504	G2505			
C2316	C2317	G2318	G2319	G2320	G2321	G2325	G2326	A2327	A2328	G2329	G2330	G2334	A2335	A2336	G2342	G2343	U2344	G2345	A2346	C2347	C2350	C2355	G2364	G2365	A2366	G2367	A2368	A2369	G2370	G2371	G2372	G2373	G2374	G2375	A2376	A2377	A2378	C2381	G2382	G2383	G2384	C2385	C2394	C2402	G2403	G2404	G2405	U2406	U2408		
U2197	A2198	G2206	G2207	A2208	U2218	G2219	G2224	A2225	U2233	G2238	G2239	G2242	U2243	U2244	G2248	U2249	G2250	G2251	A2268	A2269	G2270	G2271	U2272	A2273	G2274	G2275	G2276	G2277	A2278	G2279	C2283	G2284	C2285	A2286	A2287	A2288	U2291	C2292	G2293	C2294	G2295	U2296	U2297	A2298	A2299	A2305	G2308	G2315			
G2131	U2132	G2133	A2134	C2135	C2136	C2137	C2138	C2139	C2140	G2141	C2142	C2143	U2144	C2145	G2146	G2147	G2148	G2149	U2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	A2158	C2159	G2160	C2161	C2162	C2163	C2164	G2165	U2167	G2168	A2169	A2170	A2171	U2172	C2173	U2180	G2181	G2182	G2183	G2184	C2185	U2189	G2190	G2191	G2192
C2049	C2055	G2056	A2057	A2058	A2059	A2060	G2061	C2064	C2065	C2066	G2067	U2068	G2069	G2070	U2074	U2075	U2079	C2095	U2096	C2097	U2098	C2103	G2104	C2105	U2109	G2110	C2111	C2112	U2113	A2114	G2115	A2117	U2118	A2119	G2120	G2121	U2122	G2123	A2124	G2125	U2126	G2127	C2128	G2129	U2130						
G1929	G1930	U1931	G1932	G1933	G1934	G1935	A1936	A1937	A1938	U1939	C1942	U1946	C1947	U1955	C1958	C1962	U1963	G1964	C1967	A1970	A1971	A1972	G1973	U1991	G1992	U1993	G1997	G2010	A2014	G2022	G2023	G2024	C2025	C2026	G2029	A2030	A2031	G2032	G2033	U2034	G2035	C2036	G2037	G2038							
G1811	A1812	G1816	G1817	G1824	A1825	G1826	U1829	U1833	U1834	G1835	G1836	A1837	G1838	G1839	C1843	A1847	A1848	U1851	C1852	G1863	G1864	G1866	A1876	A1877	G1878	C1882	A1889	A1890	G1899	A1900	G1906	U1911	A1912	G1913	U1914	U1915	A1916	U1917	U1918	A1919	G1920	C1924	C1925	U1926	A1928						
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C1557	A1558	G1559	G1568	A1569	U1578	A1579	G1581	A1582	C1583	C1584	A1586	C1589	U1590	G1591	C1592	G1593	G1594	A1603	A1608	A1609	A1610	G1627	G1628	U1629	G1630	C1631	A1634	G1635	C1636	C1637	C1638	U1639	C1640	G1647	C1648	A1652	G1653	U1654	G1657	G1674	C1688	U1689	U1693	C1694	G1695						
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A1389	A1360	G1364	A1365	G1368	G1369	G1370	G1371	U1372	A1373	G1374	C1375	G1379	A1380	A1384	G1385	U1405	U1406	C1407	A1408	C1409	G1410	C1411	A1412	G1413	G1416	C1417	A1420	G1421	G1426	A1427	C1428	G1429	C1430	U1431	A1434	C1437	G1442	U1445	C1446A	G1446	G1447	G1448	A1449	G1450	A1452						
G1219	A1220	C1221	G1229	C1230	G1231	G1232	C1233	G1238	G1239	U1240	A1241	G1248	A1253	A1254	U1255	G1256	U1263	G1264	A1265	G1266	G1271	A1272	U1273	A1274	A1278	A1284	A1287	C1297	U1300	A1301	A1308	G1311	G1314	U1340	U1341	A1342	G1343	G1344	C1345	U1352	A1353	A1354									



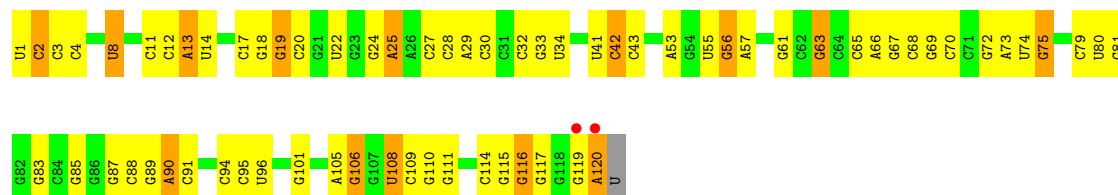
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 77% 19% ..



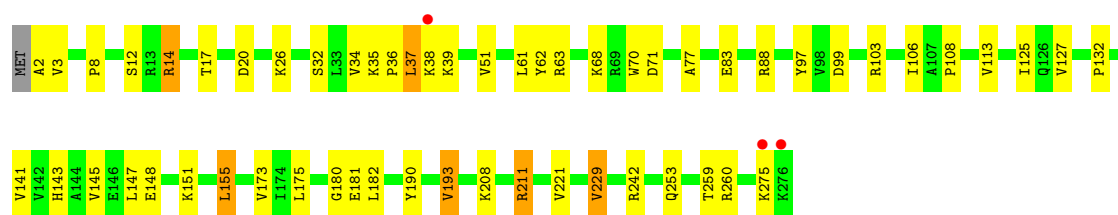
• Molecule 2: 5S Ribosomal RNA

Chain 2B: 2% 43% 45% 12% ..



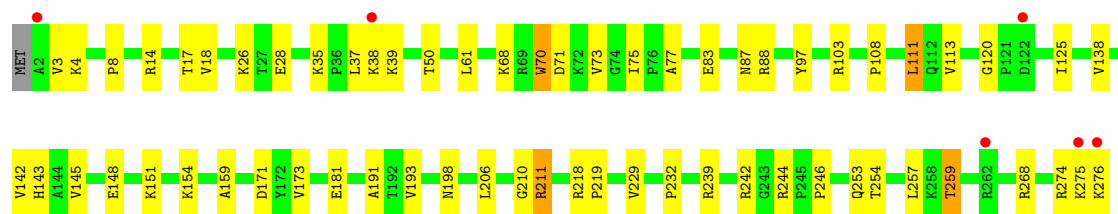
• Molecule 3: 50S ribosomal protein L2

Chain 1D: % 79% 18% ..



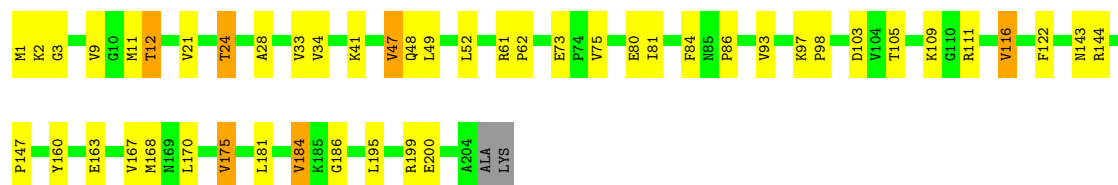
• Molecule 3: 50S ribosomal protein L2

Chain 2D: 2% 77% 21% ..

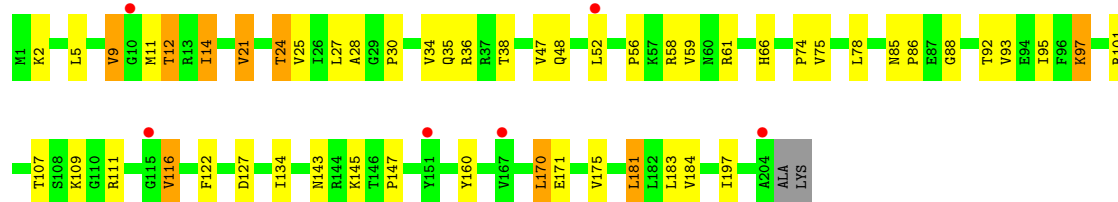
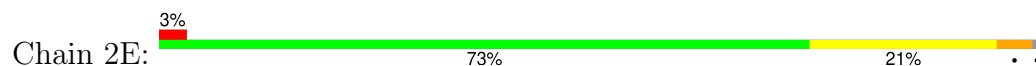


• Molecule 4: 50S ribosomal protein L3

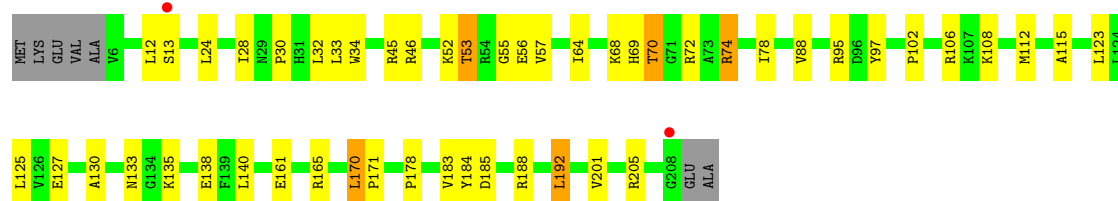
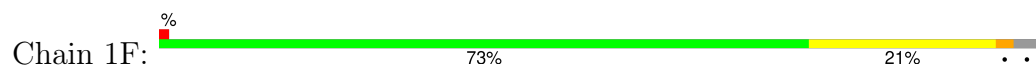
Chain 1E: 76% 20% ..



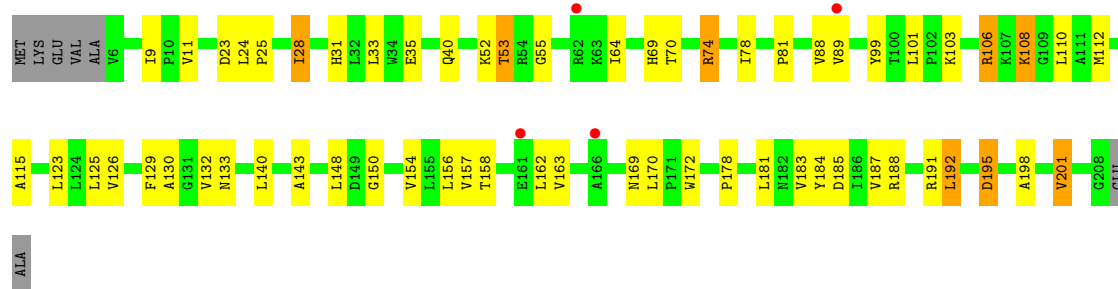
- Molecule 4: 50S ribosomal protein L3



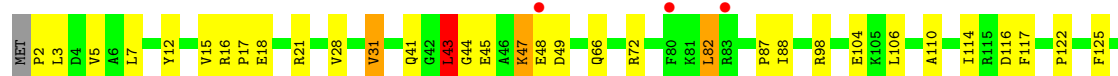
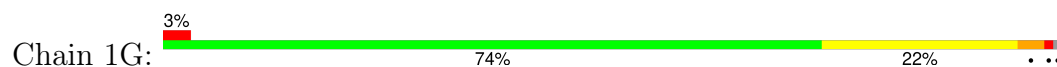
- Molecule 5: 50S ribosomal protein L4

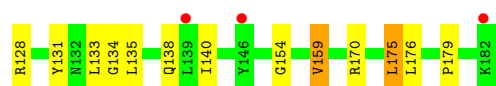


- Molecule 5: 50S ribosomal protein L4

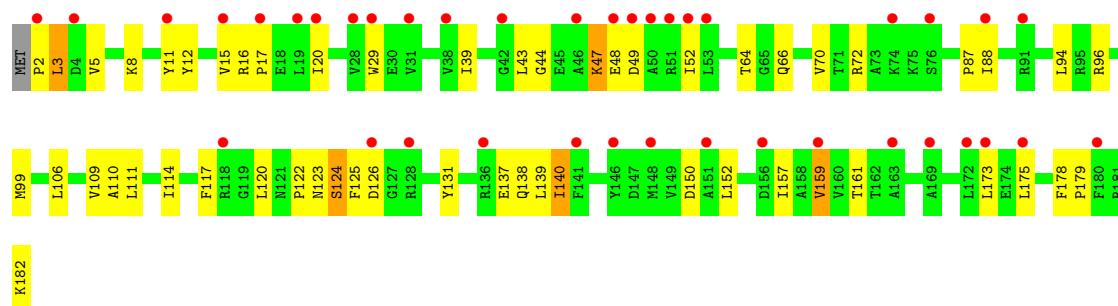


- Molecule 6: 50S ribosomal protein L5

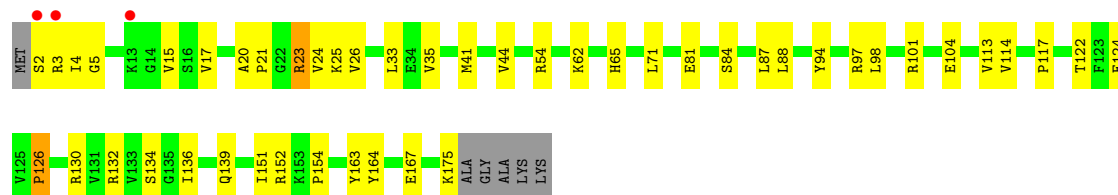




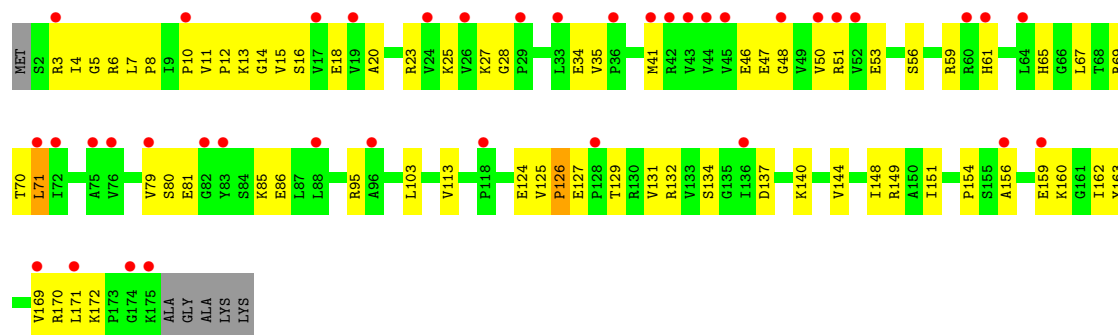
- Molecule 6: 50S ribosomal protein L5



- Molecule 7: 50S ribosomal protein L6



- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9

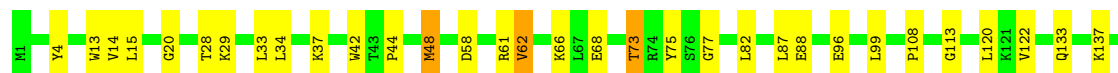
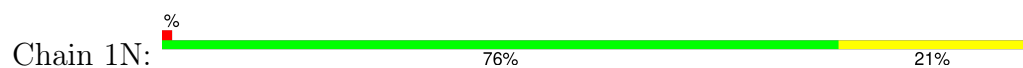




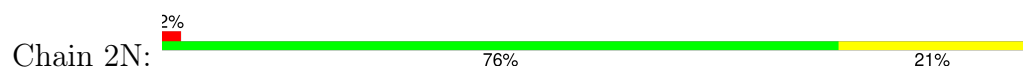
- Molecule 8: 50S ribosomal protein L9



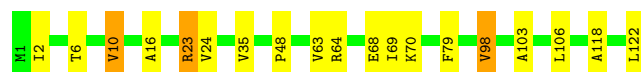
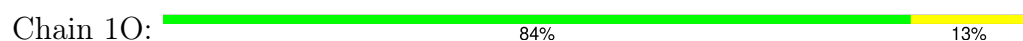
- Molecule 9: 50S ribosomal protein L13



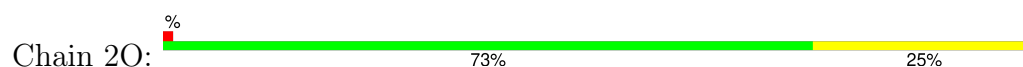
- Molecule 9: 50S ribosomal protein L13



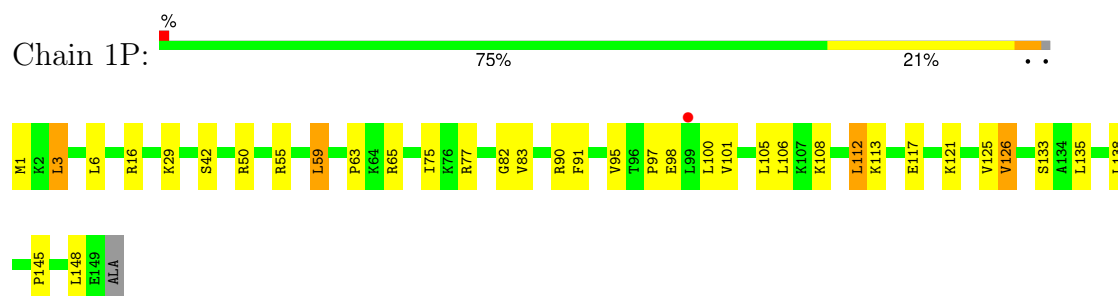
- Molecule 10: 50S ribosomal protein L14



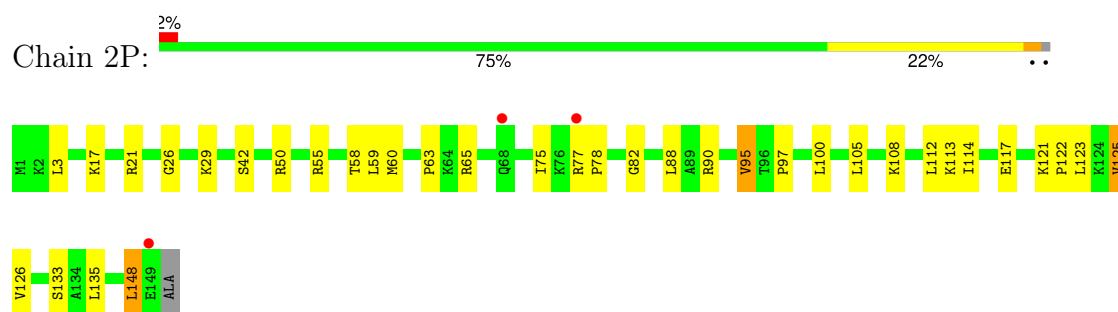
- Molecule 10: 50S ribosomal protein L14



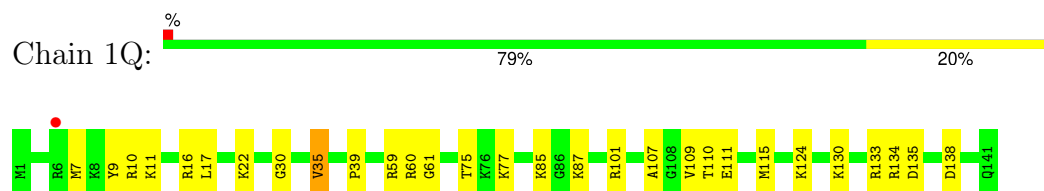
• Molecule 11: 50S ribosomal protein L15



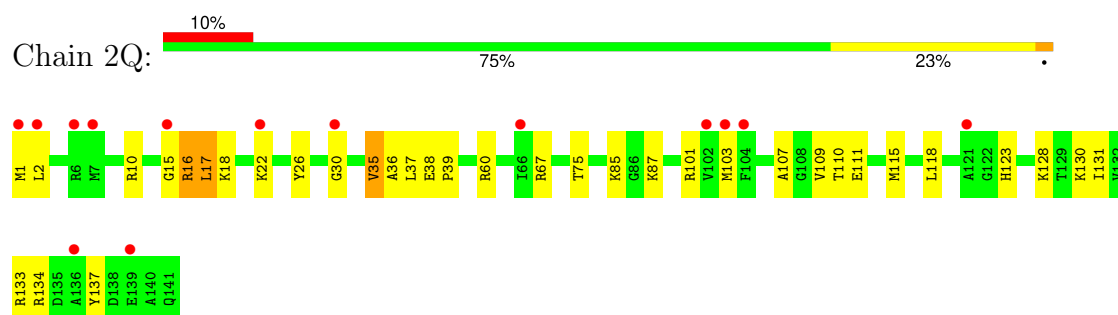
• Molecule 11: 50S ribosomal protein L15



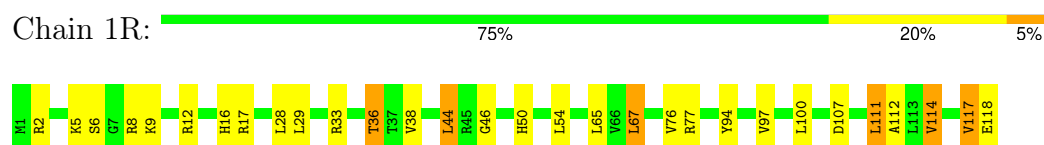
• Molecule 12: 50S ribosomal protein L16



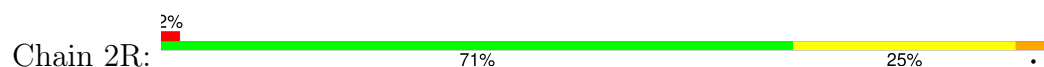
• Molecule 12: 50S ribosomal protein L16

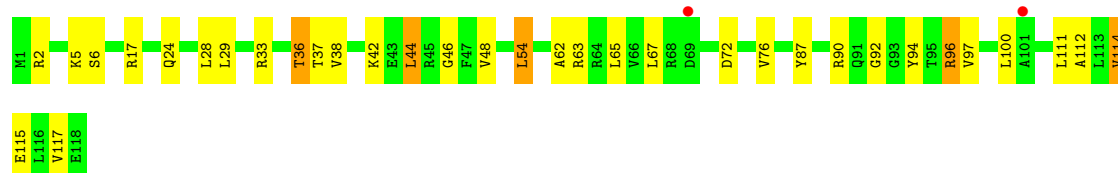


• Molecule 13: 50S ribosomal protein L17



• Molecule 13: 50S ribosomal protein L17





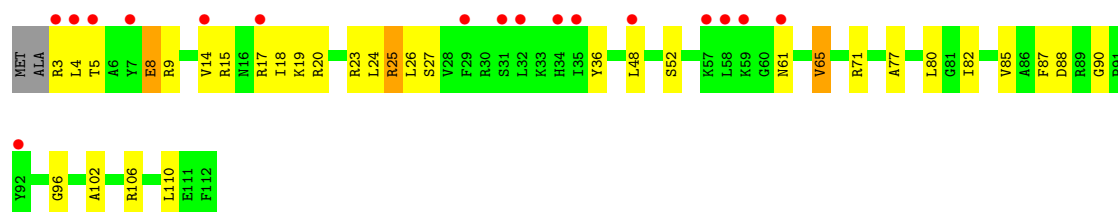
- Molecule 14: 50S ribosomal protein L18

Chain 1S: 79% 17% ..



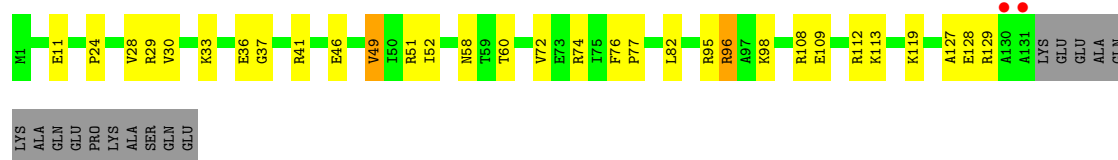
- Molecule 14: 50S ribosomal protein L18

Chain 2S: 15% 69% 27% ..



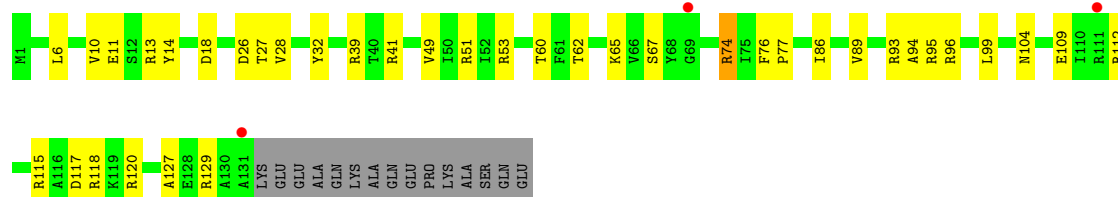
- Molecule 15: 50S ribosomal protein L19

Chain 1T: 2% 68% 20% 10%



- Molecule 15: 50S ribosomal protein L19

Chain 2T: 2% 64% 25% 10%



- Molecule 16: 50S ribosomal protein L20

Chain 1U: 77% 20% ..



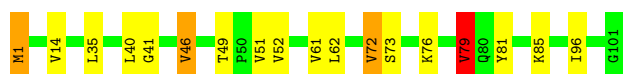
- Molecule 16: 50S ribosomal protein L20

Chain 2U: 86% 11% ..



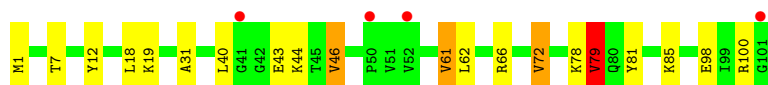
- Molecule 17: 50S ribosomal protein L21

Chain 1V: 82% 14% ..



- Molecule 17: 50S ribosomal protein L21

Chain 2V: 4% 80% 16% ..



- Molecule 18: 50S ribosomal protein L22

Chain 1W: 0% 81% 15% ..



- Molecule 18: 50S ribosomal protein L22

Chain 2W: 3% 81% 17% ..



- Molecule 19: 50S ribosomal protein L23

Chain 1X: 2% 78% 20% ..

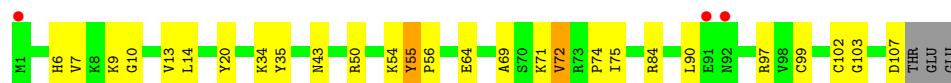
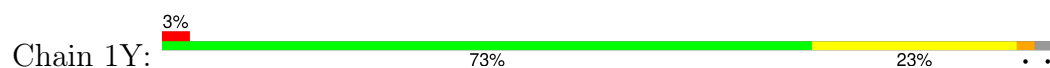


- Molecule 19: 50S ribosomal protein L23

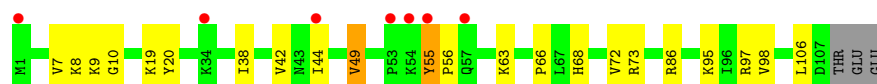
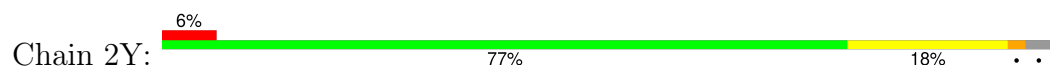
Chain 2X: 4% 75% 23% ..



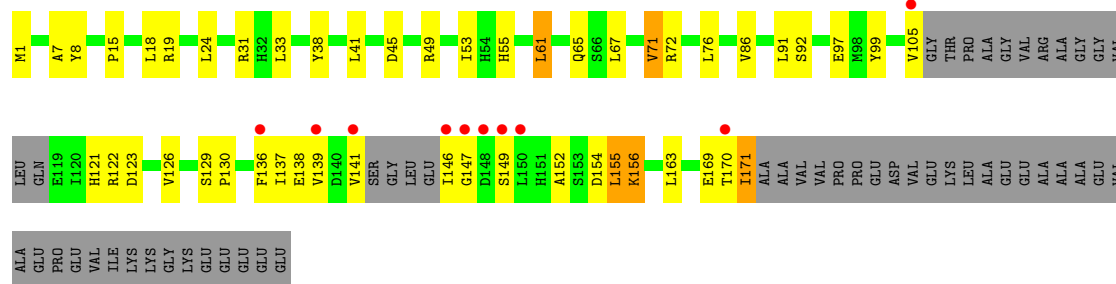
- Molecule 20: 50S ribosomal protein L24



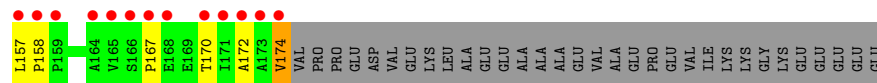
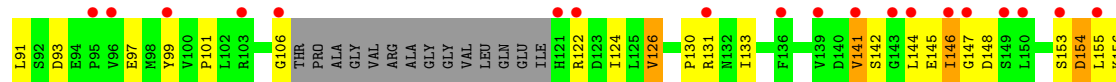
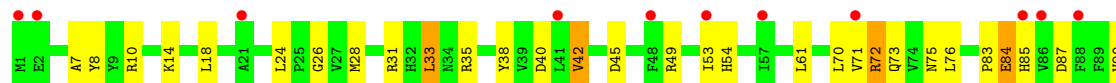
- Molecule 20: 50S ribosomal protein L24



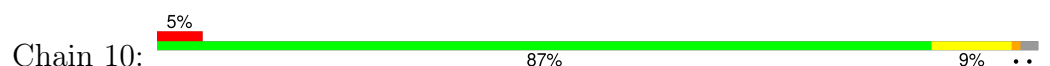
- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25

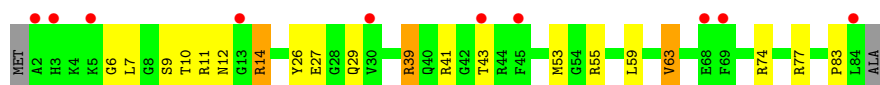
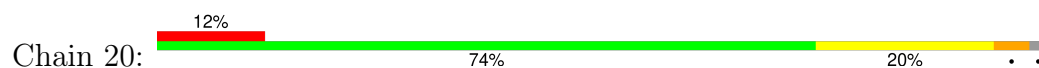


- Molecule 22: 50S ribosomal protein L27

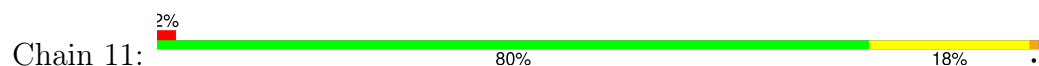




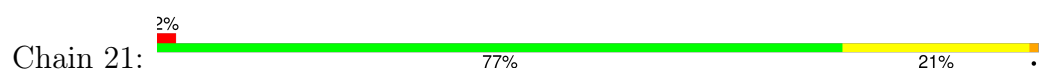
- Molecule 22: 50S ribosomal protein L27



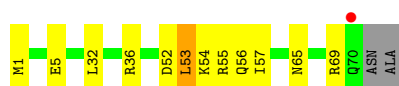
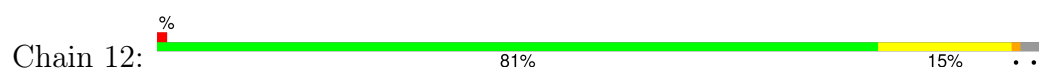
- Molecule 23: 50S ribosomal protein L28



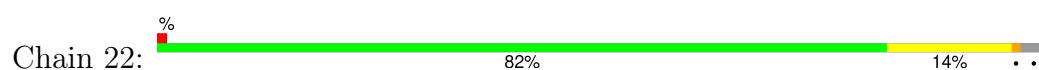
- Molecule 23: 50S ribosomal protein L28



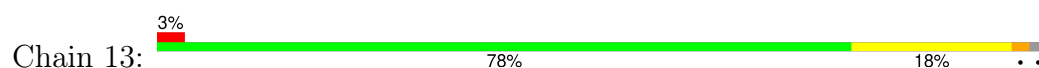
- Molecule 24: 50S ribosomal protein L29



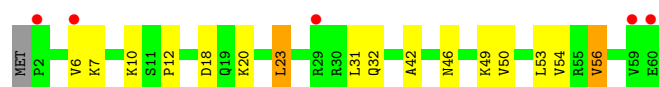
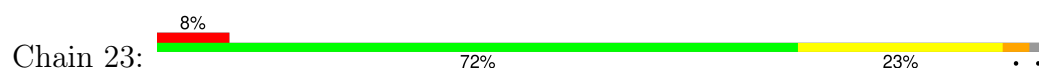
- Molecule 24: 50S ribosomal protein L29



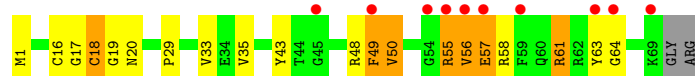
- Molecule 25: 50S ribosomal protein L30



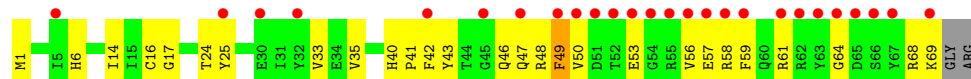
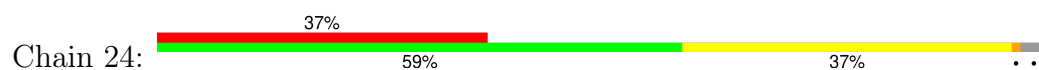
- Molecule 25: 50S ribosomal protein L30



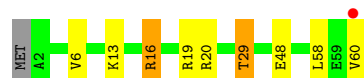
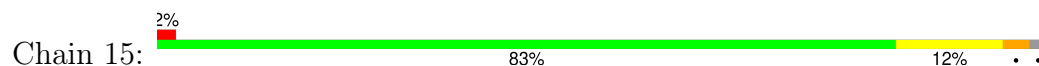
- Molecule 26: 50S ribosomal protein L31



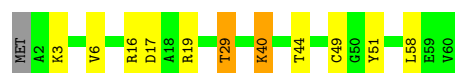
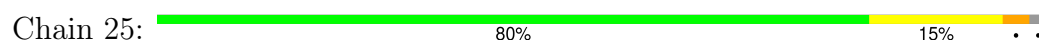
- Molecule 26: 50S ribosomal protein L31



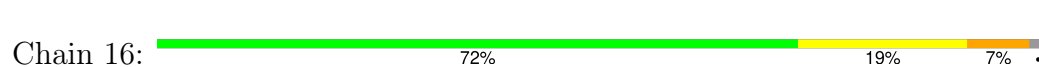
- Molecule 27: 50S ribosomal protein L32



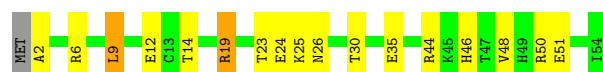
- Molecule 27: 50S ribosomal protein L32



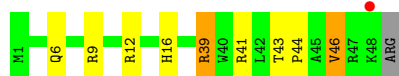
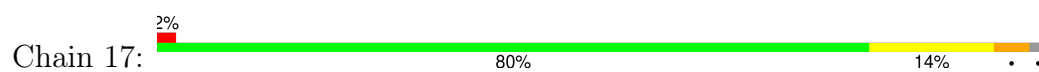
- Molecule 28: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



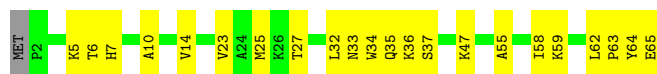
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



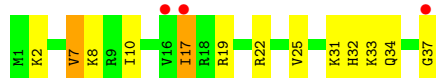
- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36



- Molecule 31: 50S ribosomal protein L36

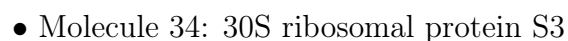
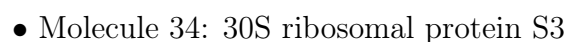


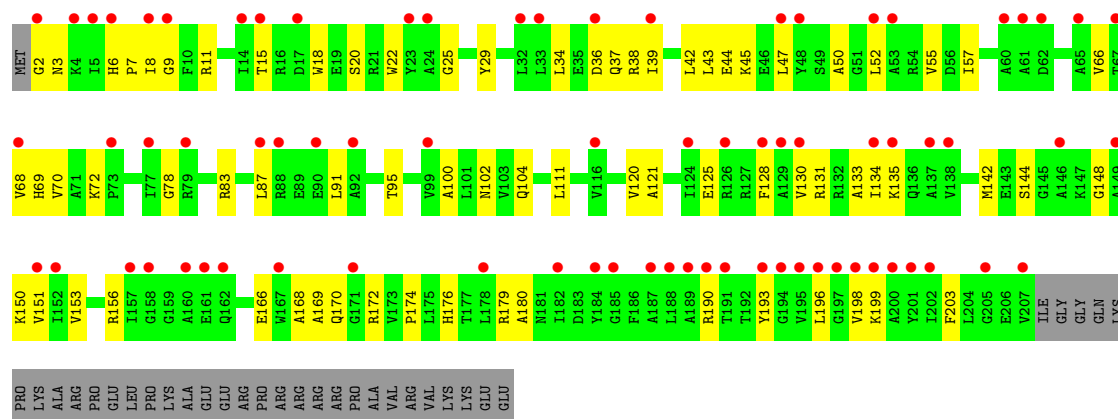
- Molecule 32: 16S Ribosomal RNA



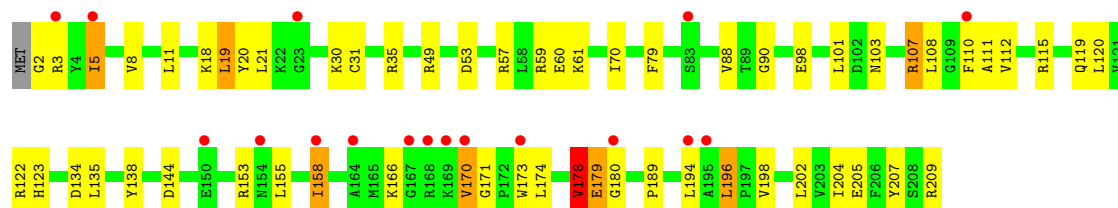
A1507	C1382	A1289	G1197	G1084	U911	U757	G650	A539	G410	G301	C189C	A101
G1508	C1383	G1290	G1198	U1085	A914	G758	A853	G540	A411	G310	U189F	G102
C1509	C1386	G1291	C1200	U1086	A918	A766	G657	G544	G412	G313	U189J	C103
U1510	G1389	A1299	G1201	U1094	A919	A767	G658	A547	U421	A133	U189K	G104
G1511	G1390	U1301	G1202	U1095	U920	A768	U659	U552	G424	C314	G189L	G105
U1512	G1391	U1302	G1203	G1099	U921	G769	G660	U557	G429	A321	C193	G106
A1513	G1392	U1303	G1204	C1100	G926	G774	G664	G557	U429	G326	C194	G107
G1517	C1397	U1304	U1205	A1101	G927	A777	A665	G558	U435	A327	A195	A109
A1518	G1400	G1305	U1206	C1107	G933	A792	G666	A559	C436	G328	A196	C110
A1519	G1401	A1213	U1212	C1118	C934	U793	G667	U561	U437	A329	A197	G111
G1529	C1402	G1309	A1218	U1125	A935	A794	U672	C562	G438	G332	G200	G115
G1530	C1403	C1314	U1219	U1126	A936	A794	G673	U561	A439	G333	G201	A116
A1531	C1404	C1317	U1220	G1127	G942	G803	G674	C562	A441	C341	U202	U118
U1532	C1407	A1318	G1221	C1128	G946	A814	U677	U565	C442	G342	U203	C121
C1533	C1412	U1319	A1225	U1128	A947	A815	U678	G568	G445	G343	U204	G131
C	A1413	C1320	C1226	C1129	G947	A816	G680	A572	G446	G344	G216	C131
C	U1414	C1321	A1227	A1130	G953	C817	C680	A573	A448	G345	C218	A134
C	G1415	C1328	C1228	G1134	G953	G821	G685	G576	A452	G346	U222	A141
C	G1419	U1330	A1236	U1135	U950	G821	U686	G577	A453	G347	U223	G144
U	G1422	A1329	C1237	U1136	U961	A828	A867	U580	C458	G351	A228	G145
U	U1427	G1331	A1238	C1137	C962	G829	G688	G581	G460	C352	G228	G148
C	A1428	C1343	A1251	U1138	A964	U833	C689	U582	A461	G353	G232	A149
U	A1429	C1344	A1252	C1140	G966	C834	G691	G584	C470	C354	G236	G149
C	C1430	U1345	U1255	C1141	C967	U835	A695	G585	G471	C355	G247	G159
G1435	G1435	A1346	A1256	C1145	A968	G836	G700	C596	G485	U367	G250	A160
U1436	U1436	U1347	U1257	A1146	A969	C840	G711	G597	A496	U368	G251	A161
G1442	G1442	U1348	U1258	C1149	G971	C848	G712	U598	U498	G376	G258	A162
G1442A	G1442A	A1350	C1259	U1150	C972	C849	G713	C599	C501	G377	G259	U172
U1446	U1446	G1353	C1260	A1151	G973	U850	G714	C600	C502	C381	U261	U173
A1447	A1447	C1354	C1263	A1152	A974	G851	G715	C601	C503	A382	A262	C174
G1452	G1452	G1355	C1264	A1157	A975	G851	A716	C613	C504	A383	A263	C175
G1456	G1456	G1356	G1265	C1158	G976	A864	A716	A614	G505	A384	G265	C176
G1457	G1457	A1357	G1266	U1159	A977	A865	C719	U619	A509	G392	G266	A179
G1458	G1458	U1358	C1270	G1160	U982	U870	U723	C620	A510	A393	C267	G181
G1469	G1469	U1363	G1271	G1166	A983	U871	G731	A621	C511	G397	C268	U180
G1470	G1470	A1363A	G1272	A1168	C984	U871	G731	A621	C511	C398	C269	U182
G1487	G1487	U1364	G1273	A1169	U992	C880	G731	A621	C511	C399	A270	G183
A1492	A1492	G1368	G1274	A1170	G993	C881	A737	U625	U516	C400	C272	A185
A1493	A1493	C1369	G1275	G1171	U1000	C882	C738	G627	G517	U405	C277	C186
G1494	G1494	G1370	G1276	C1172	A1001	G890	C739	G628	C518	G406	G289	C188
U1498	U1498	A1374	C1277	A1176	G1001A	U891	U740	G630	G524	G407	A300	G189
A1503	A1503	U1375	C1278	U1177	G1002	A892	G741	G630	G524	A533	G289	C189A
G1504	G1504	U1377	A1285	G1178	G1003	G902	C749	A642	G527	U531	G289	C189A
G1505	G1505	C1378	A1286	G1179	A1004	G906	G752	U646	U531	A533	G289	C189A
U1506	U1506	U1381	A1287	A1183	C1006	A909	G755	A648	U531	A533	G289	C189A
			A1288	G1184	C1007	A909	G755	A648	U531	A533	G289	C189A
				U1196	G1008	C910	C756	G649	U531	A533	G289	C189A

Chain 1b:

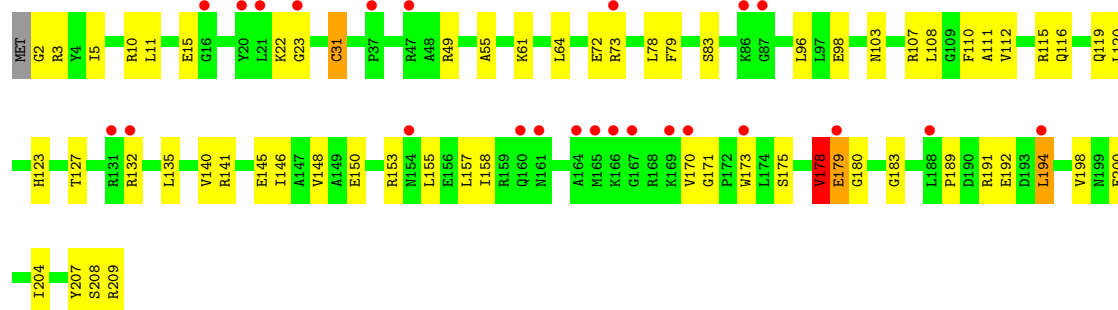
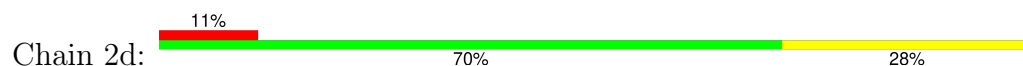




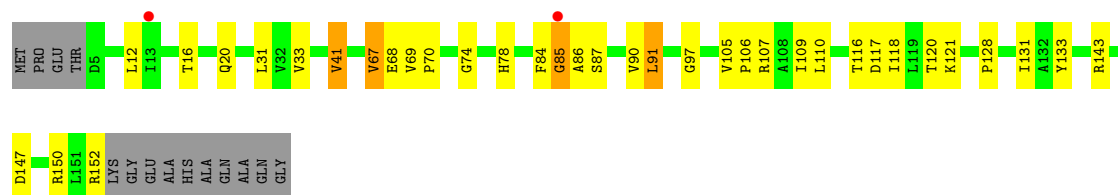
• Molecule 35: 30S ribosomal protein S4



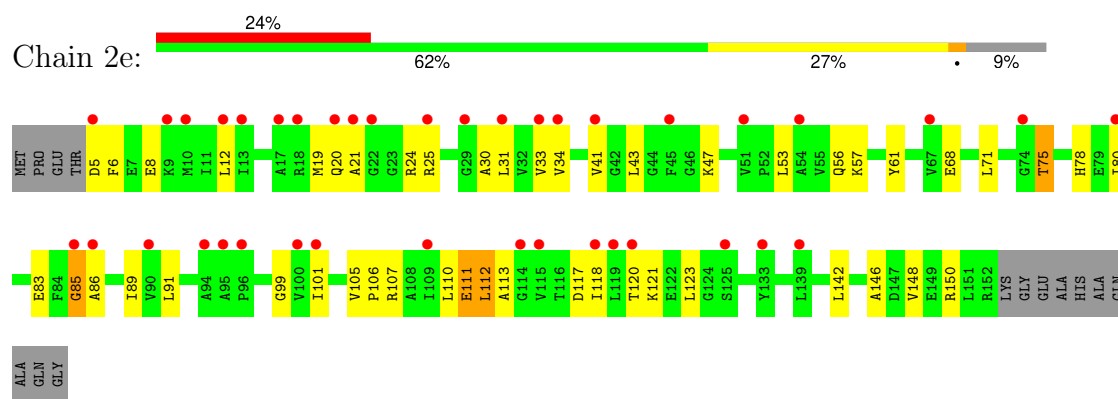
• Molecule 35: 30S ribosomal protein S4



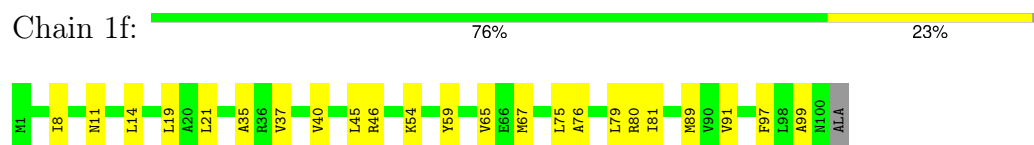
• Molecule 36: 30S ribosomal protein S5



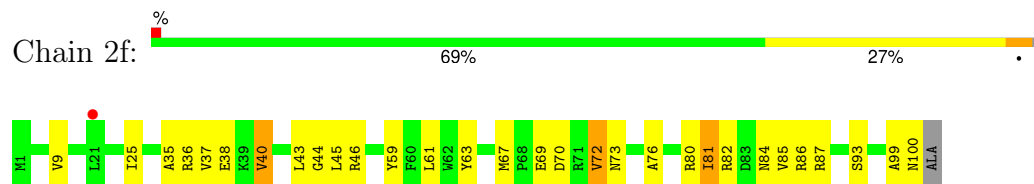
• Molecule 36: 30S ribosomal protein S5



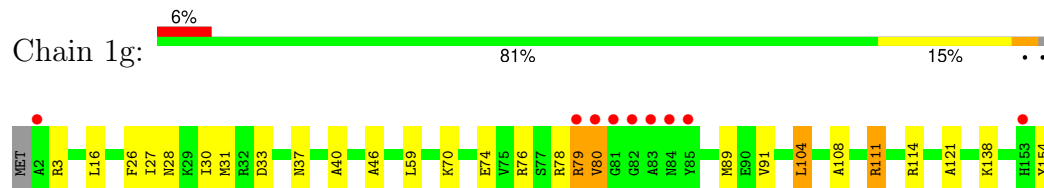
- Molecule 37: 30S ribosomal protein S6



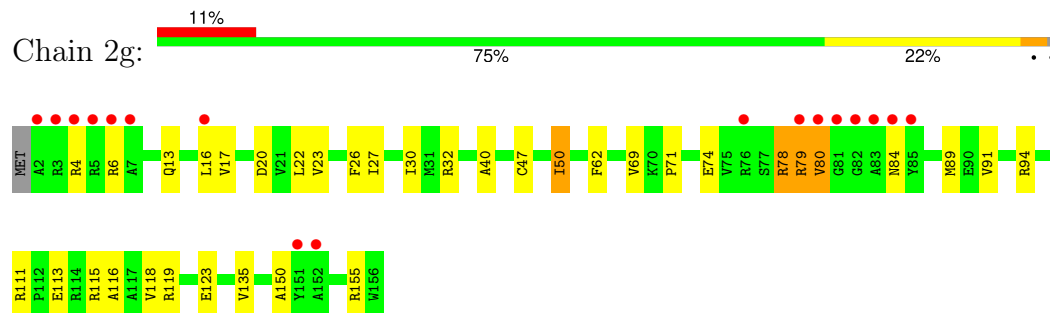
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7

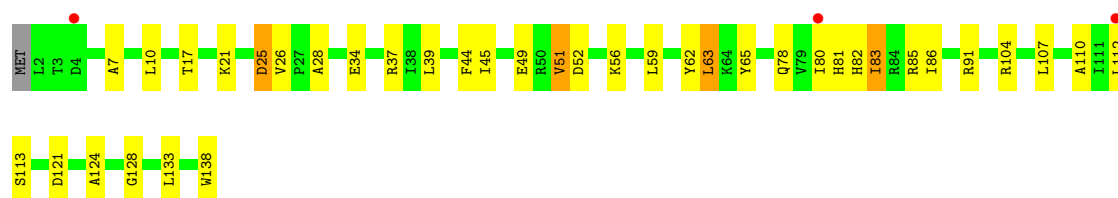


- Molecule 38: 30S ribosomal protein S7

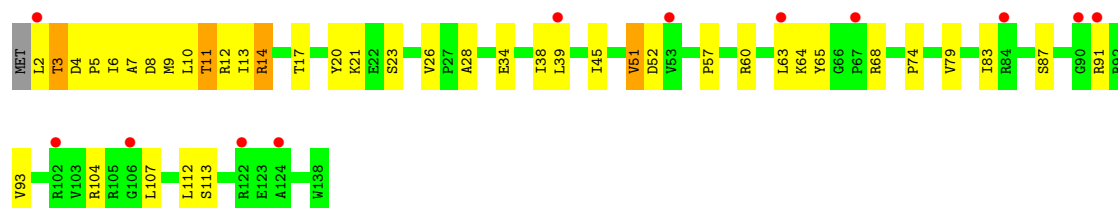


- Molecule 39: 30S ribosomal protein S8

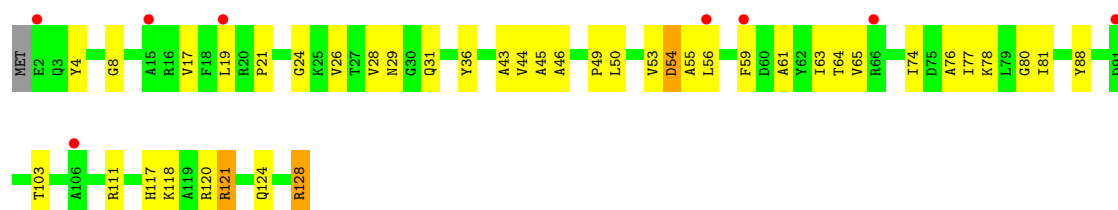




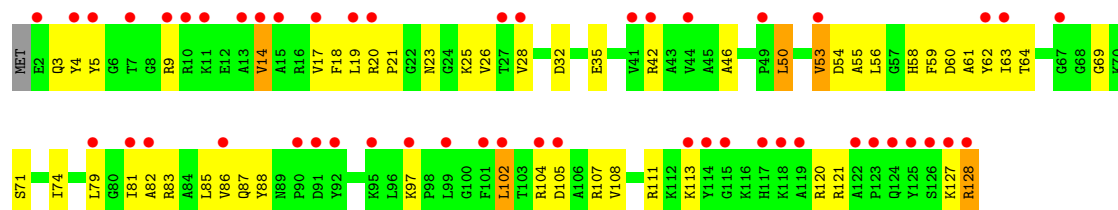
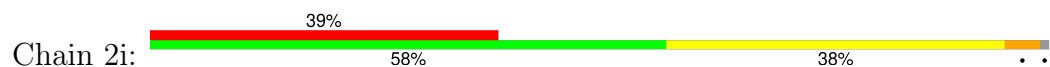
- Molecule 39: 30S ribosomal protein S8



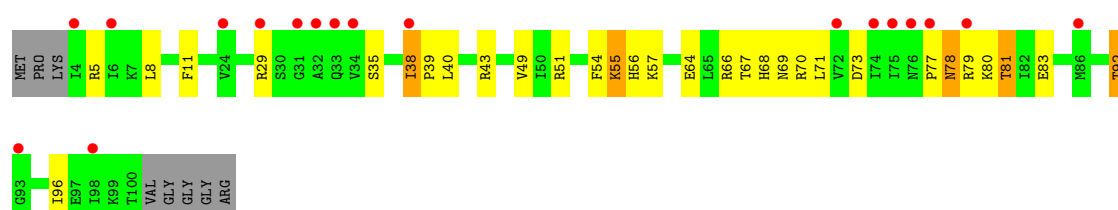
- Molecule 40: 30S ribosomal protein S9



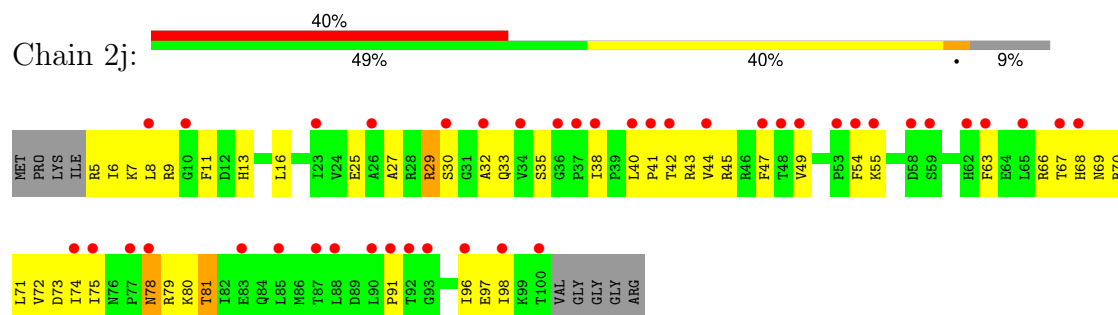
- Molecule 40: 30S ribosomal protein S9



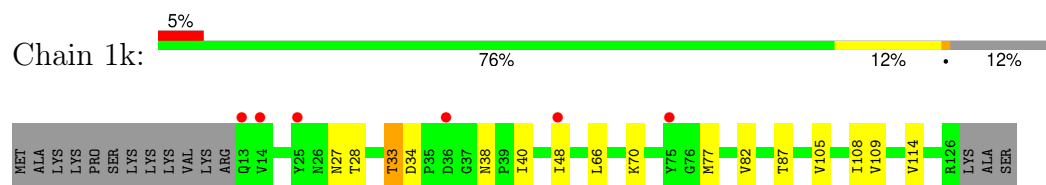
- Molecule 41: 30S ribosomal protein S10



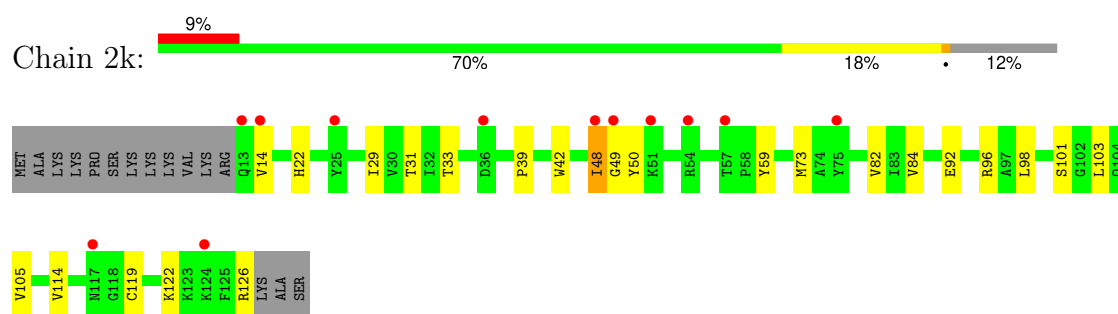
- Molecule 41: 30S ribosomal protein S10



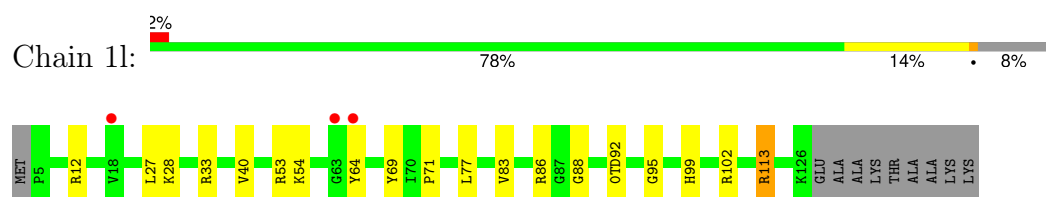
- Molecule 42: 30S ribosomal protein S11



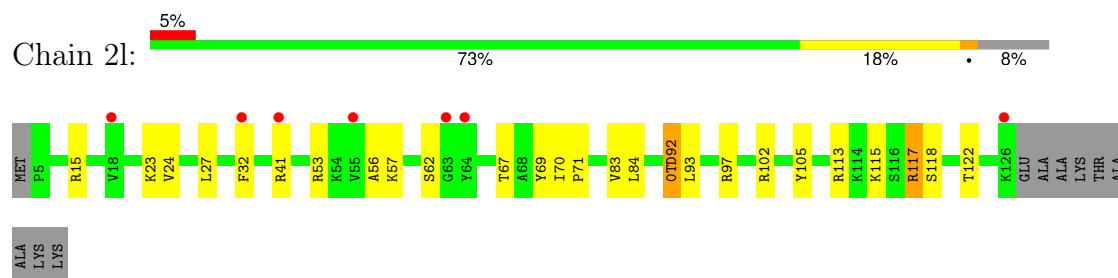
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12

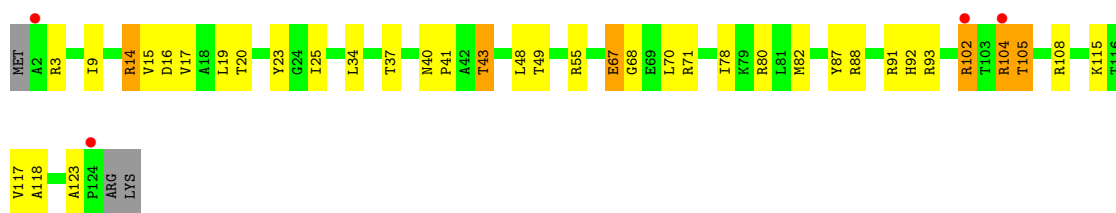


- Molecule 43: 30S ribosomal protein S12

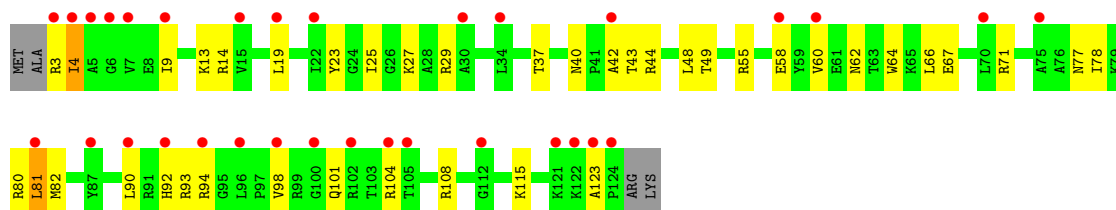


- Molecule 44: 30S ribosomal protein S13





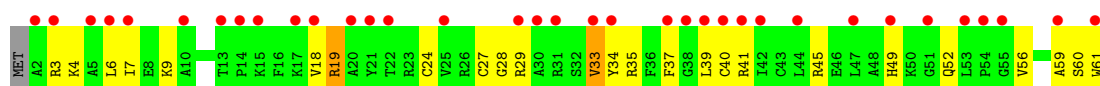
- Molecule 44: 30S ribosomal protein S13



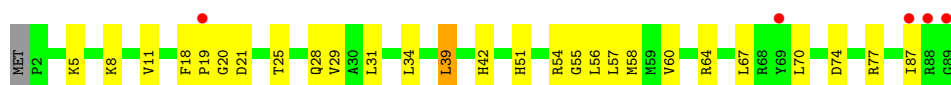
- Molecule 45: 30S ribosomal protein S14 type Z



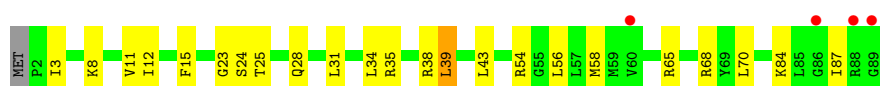
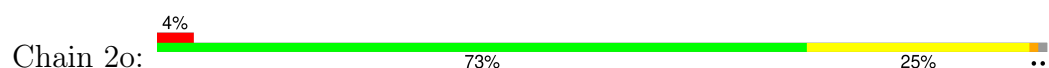
- Molecule 45: 30S ribosomal protein S14 type Z



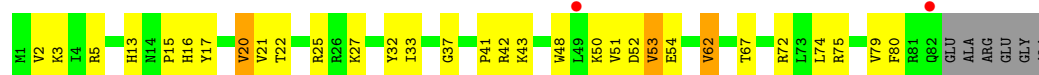
- Molecule 46: 30S ribosomal protein S15



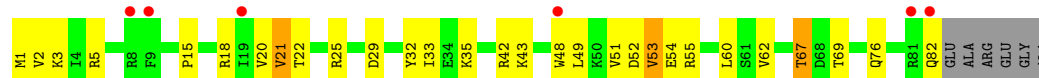
- Molecule 46: 30S ribosomal protein S15



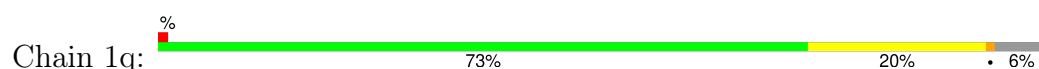
- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



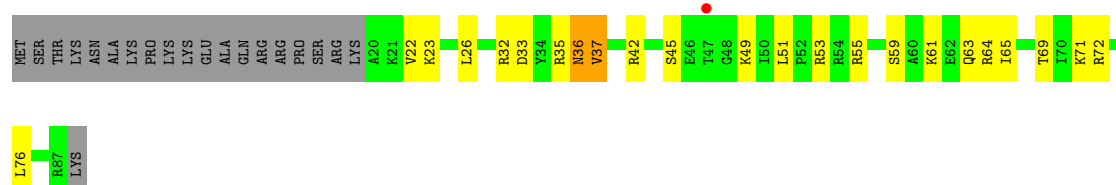
- Molecule 48: 30S ribosomal protein S17



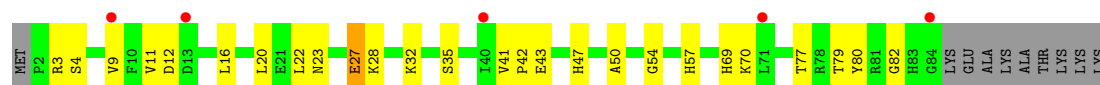
- Molecule 49: 30S ribosomal protein S18



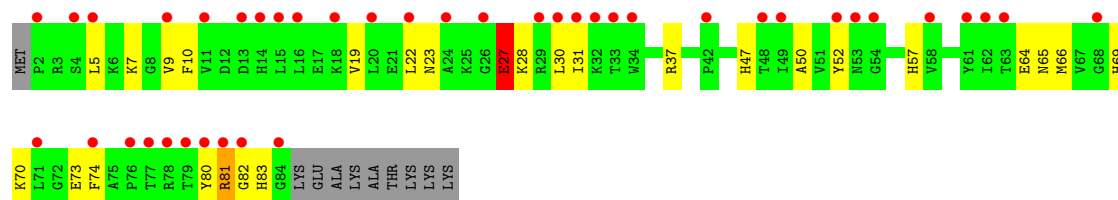
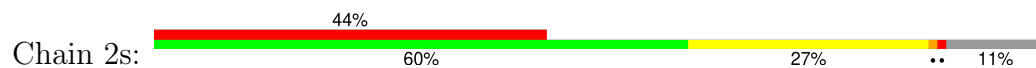
- Molecule 49: 30S ribosomal protein S18



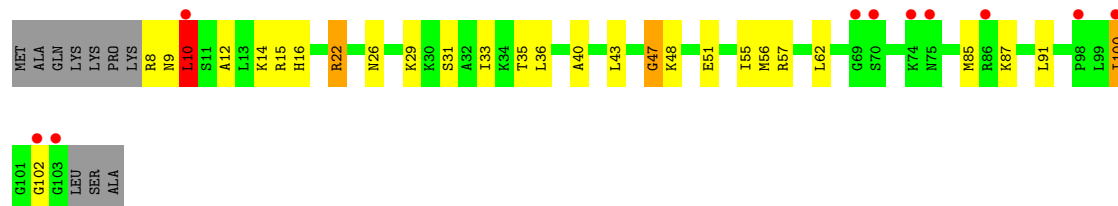
- Molecule 50: 30S ribosomal protein S19



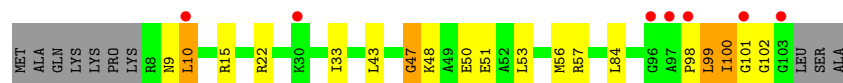
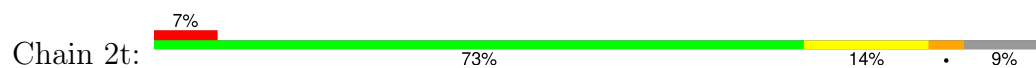
- Molecule 50: 30S ribosomal protein S19



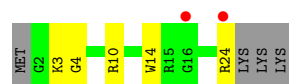
- Molecule 51: 30S ribosomal protein S20



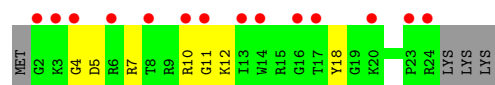
- Molecule 51: 30S ribosomal protein S20



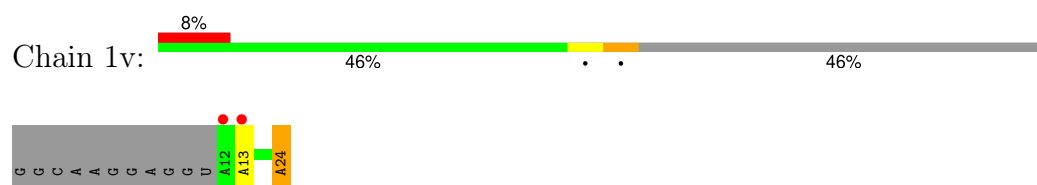
- Molecule 52: 30S ribosomal protein Thx



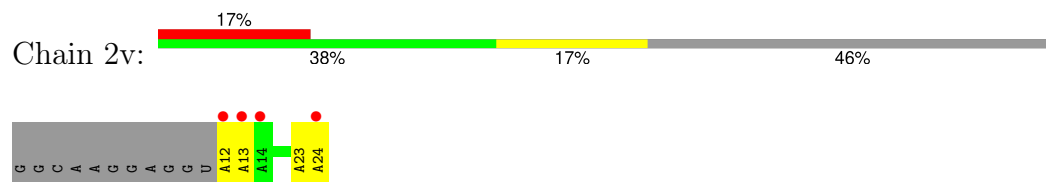
- Molecule 52: 30S ribosomal protein Thx



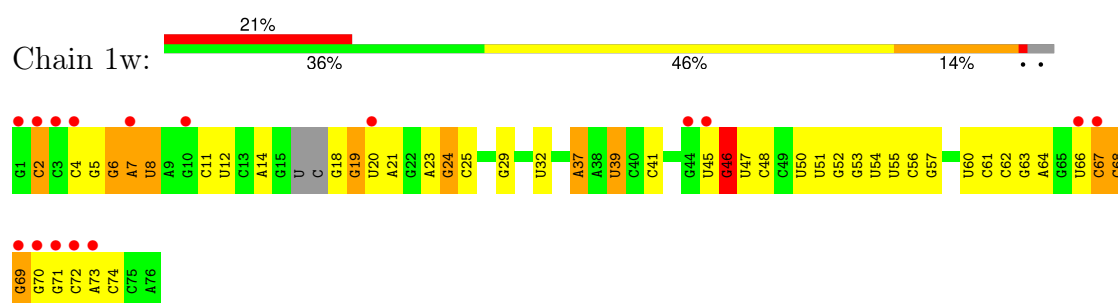
- Molecule 53: mRNA



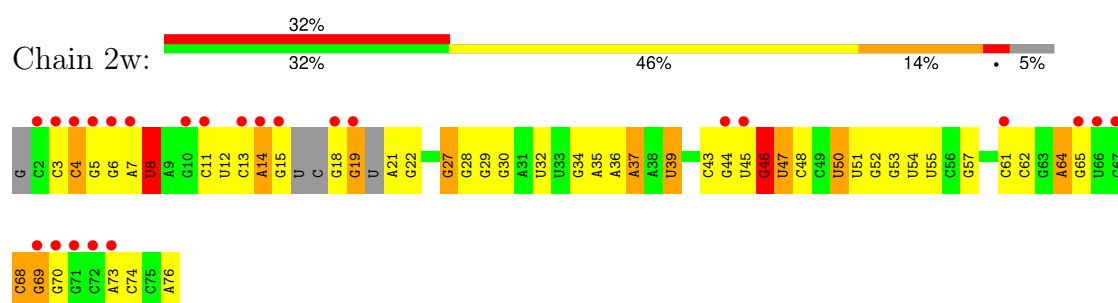
- Molecule 53: mRNA



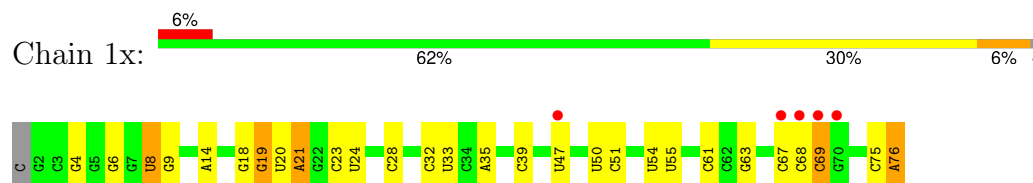
- Molecule 54: tRNA, A-site and E-site tRNAs



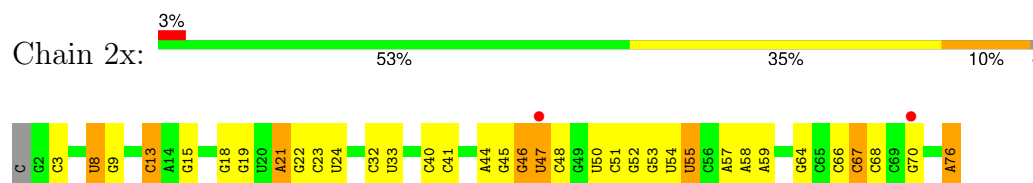
- Molecule 54: tRNA, A-site and E-site tRNAs



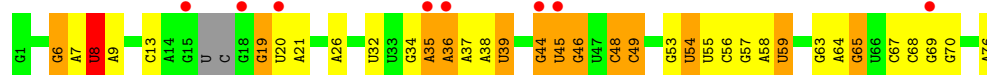
- Molecule 55: P-site tRNA



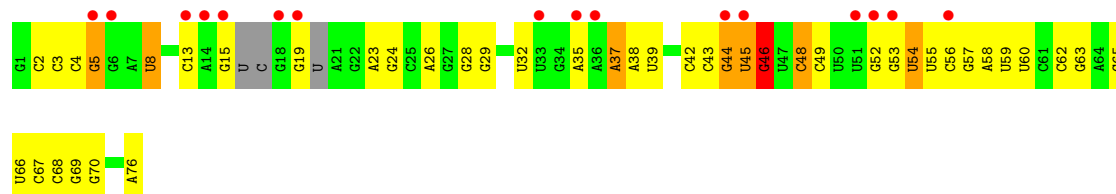
- Molecule 55: P-site tRNA



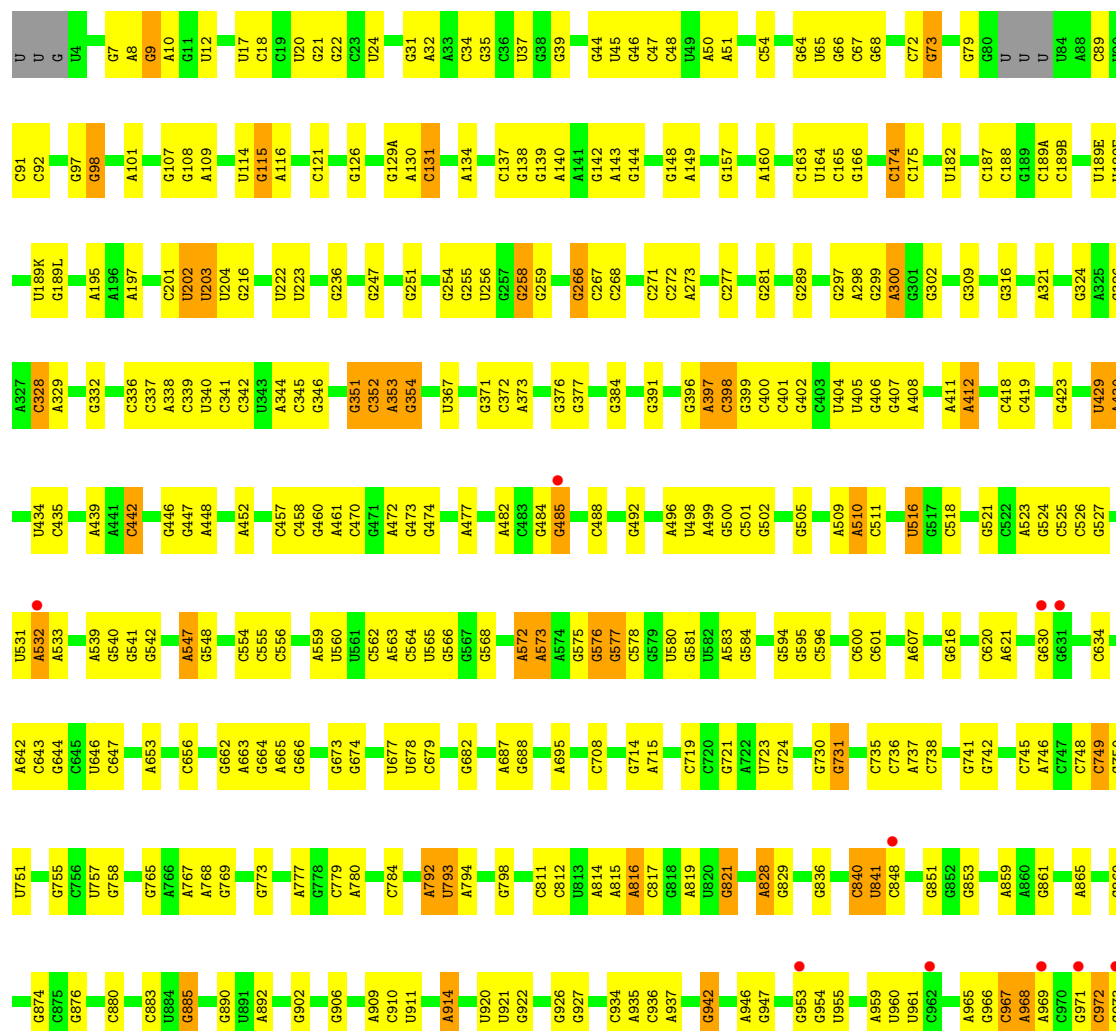
- Molecule 56: tRNA

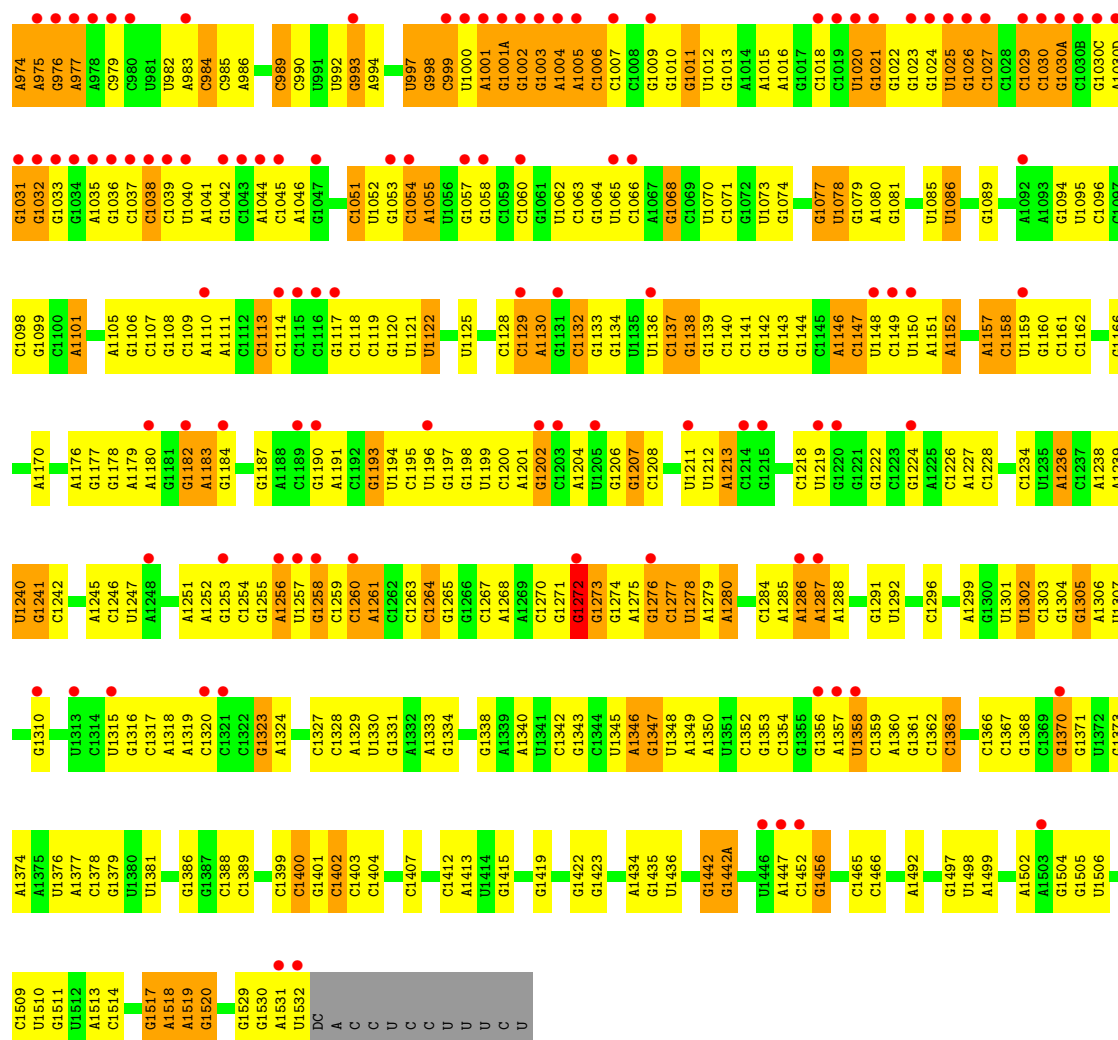


• Molecule 56: tRNA

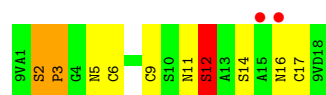
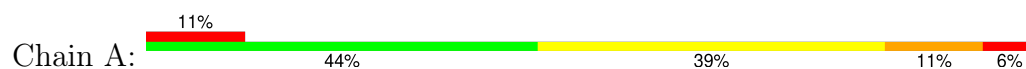


• Molecule 57: 16S Ribosomal RNA

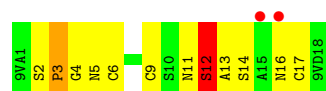




• Molecule 58: Klebsazolicin



• Molecule 58: Klebsazolicin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.64Å 449.06Å 622.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	155.50 – 2.70 155.50 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (155.50-2.70) 99.3 (155.50-2.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.207 , 0.252 0.211 , 0.255	Depositor DCC
R_{free} test set	78961 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 70.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	302030	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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: 4OC, UR3, 2MA, PSU, 4SU, K, OMG, M2G, MA6, 9VA, 9VD, MG, MIA, SF4, 5MC, ZN, 2MG, BB9, G7M, 2MU, 5MU, 0TD

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	0.30	0/69009	0.48	3/107712 (0.0%)
1	2A	0.23	0/67293	0.41	1/105034 (0.0%)
2	1B	0.23	0/2882	0.43	0/4494
2	2B	0.20	0/2879	0.39	0/4487
3	1D	0.29	0/2186	0.52	0/2944
3	2D	0.25	0/2186	0.51	1/2944 (0.0%)
4	1E	0.30	0/1592	0.53	0/2149
4	2E	0.23	0/1592	0.46	0/2149
5	1F	0.28	0/1619	0.51	0/2193
5	2F	0.20	0/1615	0.45	0/2188
6	1G	0.21	0/1448	0.45	0/1957
6	2G	0.22	0/1453	0.48	1/1963 (0.1%)
7	1H	0.24	0/1356	0.42	0/1834
7	2H	0.20	0/1356	0.38	0/1834
8	1I	0.20	0/1112	0.44	0/1514
8	2I	0.19	0/1079	0.42	0/1475
9	1N	0.28	0/1144	0.47	0/1543
9	2N	0.20	0/1144	0.40	0/1543
10	1O	0.28	0/943	0.50	0/1269
10	2O	0.23	0/943	0.47	0/1269
11	1P	0.28	0/1152	0.51	0/1533
11	2P	0.22	0/1152	0.44	0/1533
12	1Q	0.28	0/1143	0.47	0/1527
12	2Q	0.20	0/1143	0.43	0/1527
13	1R	0.28	0/982	0.50	0/1312
13	2R	0.21	0/982	0.48	0/1312
14	1S	0.23	0/883	0.49	0/1176
14	2S	0.29	1/880 (0.1%)	0.46	0/1172
15	1T	0.26	0/1105	0.51	0/1477
15	2T	0.20	0/1097	0.41	0/1468
16	1U	0.32	0/977	0.53	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.22	0/977	0.42	0/1301
17	1V	0.31	0/782	0.51	0/1049
17	2V	0.21	0/782	0.42	0/1049
18	1W	0.30	0/897	0.48	0/1205
18	2W	0.22	0/897	0.41	0/1205
19	1X	0.30	0/764	0.55	2/1025 (0.2%)
19	2X	0.21	0/764	0.42	0/1025
20	1Y	0.25	0/819	0.55	2/1095 (0.2%)
20	2Y	0.21	0/819	0.47	0/1095
21	1Z	0.24	0/1267	0.48	0/1717
21	2Z	0.23	0/1299	0.44	0/1763
22	10	0.29	0/662	0.56	0/881
22	20	0.20	0/662	0.46	0/881
23	11	0.28	0/762	0.47	0/1014
23	21	0.24	0/762	0.47	0/1014
24	12	0.26	0/590	0.48	0/781
24	22	0.19	0/590	0.42	0/781
25	13	0.27	0/474	0.45	0/635
25	23	0.19	0/469	0.41	0/630
26	14	0.28	0/565	0.55	0/761
26	24	0.26	0/545	0.58	0/737
27	15	0.27	0/469	0.57	0/635
27	25	0.21	0/469	0.44	0/635
28	16	0.30	0/460	0.52	0/613
28	26	0.22	0/456	0.45	0/608
29	17	0.30	0/426	0.54	0/561
29	27	0.26	0/426	0.54	0/561
30	18	0.27	0/525	0.49	0/691
30	28	0.22	0/525	0.41	0/691
31	19	0.27	0/310	0.48	0/407
31	29	0.20	0/310	0.44	0/407
32	1a	0.22	0/35795	0.40	0/55864
33	1b	0.22	0/1881	0.49	0/2542
33	2b	0.22	0/1860	0.44	0/2518
34	1c	0.20	0/1572	0.40	0/2126
34	2c	0.21	0/1566	0.42	0/2119
35	1d	0.21	0/1685	0.46	0/2262
35	2d	0.22	0/1704	0.46	0/2284
36	1e	0.22	0/1145	0.44	0/1543
36	2e	0.21	0/1149	0.48	0/1548
37	1f	0.20	0/823	0.38	0/1115
37	2f	0.21	0/829	0.39	0/1123
38	1g	0.19	0/1250	0.38	0/1679

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	2g	0.20	0/1254	0.41	0/1683
39	1h	0.19	0/1108	0.42	0/1494
39	2h	0.19	0/1108	0.42	0/1494
40	1i	0.21	0/1002	0.51	0/1346
40	2i	0.21	0/997	0.47	0/1343
41	1j	0.21	0/722	0.43	0/982
41	2j	0.26	0/727	0.51	0/988
42	1k	0.20	0/844	0.40	0/1145
42	2k	0.20	0/848	0.40	0/1149
43	1l	0.23	0/937	0.42	0/1260
43	2l	0.20	0/937	0.41	0/1260
44	1m	0.21	0/969	0.45	0/1302
44	2m	0.20	0/961	0.43	0/1291
45	1n	0.20	0/501	0.49	1/664 (0.2%)
45	2n	0.26	0/501	0.54	0/664
46	1o	0.19	0/739	0.39	0/985
46	2o	0.17	0/739	0.38	0/985
47	1p	0.20	0/697	0.46	0/939
47	2p	0.20	0/693	0.44	0/935
48	1q	0.22	0/836	0.42	0/1117
48	2q	0.20	0/836	0.41	0/1117
49	1r	0.20	0/560	0.42	0/746
49	2r	0.19	0/560	0.42	0/746
50	1s	0.24	0/667	0.51	0/900
50	2s	0.26	0/661	0.51	0/893
51	1t	0.22	0/730	0.48	0/965
51	2t	0.23	0/729	0.50	0/965
52	1u	0.22	0/203	0.43	0/266
52	2u	0.30	0/203	0.52	0/266
53	1v	0.22	0/310	0.34	0/480
53	2v	0.24	0/310	0.37	0/480
54	1w	0.32	2/1606 (0.1%)	0.45	0/2497
54	2w	0.32	2/1556 (0.1%)	0.43	0/2418
55	1x	0.29	0/1725	0.44	0/2689
55	2x	0.25	0/1725	0.41	0/2689
56	1y	0.35	2/1632 (0.1%)	0.43	0/2540
56	2y	0.36	1/1609 (0.1%)	0.43	0/2502
57	2a	0.21	0/35886	0.38	1/56005 (0.0%)
58	A	2.60	3/74 (4.1%)	2.92	9/97 (9.3%)
58	B	2.79	4/74 (5.4%)	2.65	7/97 (7.2%)
All	All	0.25	15/316886 (0.0%)	0.44	28/474393 (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
26	24	0	1
33	1b	0	1
50	2s	0	1
58	A	1	0
58	B	1	0
All	All	2	3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	B	12	SER	CA-C	-14.48	1.33	1.52
58	A	12	SER	CA-C	-14.01	1.34	1.52
58	B	12	SER	CA-CB	-11.91	1.33	1.53
58	A	12	SER	CA-CB	-11.47	1.34	1.53
58	A	12	SER	N-CA	-9.92	1.33	1.46
58	B	12	SER	N-CA	-9.87	1.33	1.46
58	B	3	PRO	CA-C	-8.90	1.44	1.52
54	1w	46	G7M	O3'-P	5.90	1.62	1.56
54	1w	8	4SU	O3'-P	5.41	1.61	1.56
54	2w	46	G7M	O3'-P	5.37	1.61	1.56
56	1y	8	4SU	O3'-P	5.35	1.61	1.56
56	2y	8	4SU	O3'-P	5.35	1.61	1.56
56	1y	46	G7M	O3'-P	5.25	1.61	1.56
14	2S	20	ARG	CA-C	5.20	1.59	1.52
54	2w	8	4SU	O3'-P	5.02	1.61	1.56

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	A	2	SER	CA-C-N	9.81	129.56	119.56
58	A	2	SER	C-N-CA	9.81	129.56	119.56
58	B	3	PRO	N-CA-C	9.49	126.22	114.92
58	A	11	ASN	CA-C-N	-8.66	105.00	121.54
58	A	11	ASN	C-N-CA	-8.66	105.00	121.54
58	A	3	PRO	N-CA-C	8.60	125.02	113.84
58	B	11	ASN	CA-C-N	-8.37	105.55	121.54
58	B	11	ASN	C-N-CA	-8.37	105.55	121.54
1	1A	2014	G	C2'-C3'-O3'	7.08	120.12	109.50
58	B	12	SER	N-CA-C	6.93	125.57	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	B	12	SER	CB-CA-C	6.78	123.92	110.42
58	A	12	SER	CB-CA-C	6.65	123.65	110.42
58	A	12	SER	N-CA-C	6.64	124.95	110.80
58	A	3	PRO	CA-C-N	6.46	133.32	121.70
58	A	3	PRO	C-N-CA	6.46	133.32	121.70
1	2A	1992	G	C2'-C3'-O3'	6.08	118.63	109.50
6	2G	139	LEU	N-CA-C	-5.96	106.36	113.21
3	2D	70	TRP	N-CA-C	-5.62	106.50	113.19
20	1Y	54	LYS	CA-C-N	5.60	135.46	121.80
20	1Y	54	LYS	C-N-CA	5.60	135.46	121.80
57	2a	1272	G	N1-C2-N2	-5.58	99.47	116.20
58	B	3	PRO	CA-C-N	5.57	131.73	121.70
58	B	3	PRO	C-N-CA	5.57	131.73	121.70
1	1A	2701	U	C4'-C3'-O3'	5.46	117.59	109.40
1	1A	1700	G	C2'-C3'-O3'	5.46	117.69	109.50
45	1n	38	GLY	N-CA-C	-5.24	108.01	115.30
19	1X	94	GLY	CA-C-N	5.06	130.81	121.70
19	1X	94	GLY	C-N-CA	5.06	130.81	121.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
58	A	12	SER	CA
58	B	12	SER	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	8	LYS	Peptide
26	24	56	VAL	Peptide
50	2s	27	GLU	Peptide

5.2 Too-close contacts [i](#)

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	31194	528	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2A	60322	0	30423	627	0
2	1B	2577	0	1305	15	0
2	2B	2575	0	1303	43	0
3	1D	2136	0	2218	41	0
3	2D	2136	0	2218	46	0
4	1E	1559	0	1618	27	0
4	2E	1559	0	1618	33	0
5	1F	1584	0	1625	30	0
5	2F	1580	0	1619	40	0
6	1G	1423	0	1436	27	0
6	2G	1428	0	1438	40	0
7	1H	1330	0	1407	27	0
7	2H	1330	0	1407	42	0
8	1I	1097	0	1140	28	0
8	2I	1064	0	1082	26	0
9	1N	1117	0	1184	20	0
9	2N	1117	0	1184	24	0
10	1O	933	0	996	13	0
10	2O	933	0	996	20	0
11	1P	1135	0	1212	27	0
11	2P	1135	0	1212	31	0
12	1Q	1122	0	1179	19	0
12	2Q	1122	0	1179	23	0
13	1R	968	0	1033	19	0
13	2R	968	0	1032	20	0
14	1S	873	0	927	15	0
14	2S	870	0	923	19	0
15	1T	1091	0	1151	21	0
15	2T	1083	0	1136	26	0
16	1U	959	0	1019	15	0
16	2U	959	0	1019	11	0
17	1V	771	0	830	9	0
17	2V	771	0	830	15	0
18	1W	886	0	940	12	0
18	2W	886	0	940	9	0
19	1X	750	0	814	13	0
19	2X	750	0	814	18	0
20	1Y	806	0	881	14	0
20	2Y	806	0	881	15	0
21	1Z	1240	0	1240	24	0
21	2Z	1271	0	1273	38	0
22	10	653	0	674	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	653	0	674	14	0
23	11	755	0	826	14	0
23	21	755	0	826	16	0
24	12	588	0	643	10	0
24	22	588	0	643	9	0
25	13	469	0	518	9	0
25	23	464	0	514	9	0
26	14	552	0	533	15	0
26	24	532	0	503	16	0
27	15	455	0	465	6	0
27	25	455	0	465	7	0
28	16	453	0	473	7	0
28	26	449	0	469	9	0
29	17	418	0	467	5	0
29	27	418	0	467	12	0
30	18	517	0	582	16	0
30	28	517	0	582	15	0
31	19	307	0	335	1	0
31	29	307	0	335	11	0
32	1a	32246	0	16295	357	0
33	1b	1846	0	1867	59	0
33	2b	1825	0	1828	74	0
34	1c	1548	0	1535	21	0
34	2c	1542	0	1517	44	0
35	1d	1655	0	1672	48	0
35	2d	1674	0	1714	39	0
36	1e	1129	0	1185	23	0
36	2e	1133	0	1191	33	0
37	1f	810	0	804	15	0
37	2f	816	0	808	20	0
38	1g	1231	0	1238	18	0
38	2g	1235	0	1249	23	0
39	1h	1088	0	1126	21	0
39	2h	1088	0	1126	29	0
40	1i	983	0	986	30	0
40	2i	978	0	966	37	0
41	1j	709	0	650	26	0
41	2j	714	0	672	29	0
42	1k	829	0	825	7	0
42	2k	833	0	836	12	0
43	1l	932	0	981	10	0
43	2l	932	0	981	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	1m	958	0	1002	25	0
44	2m	950	0	988	29	0
45	1n	492	0	529	11	0
45	2n	492	0	529	21	0
46	1o	728	0	760	20	0
46	2o	728	0	760	15	0
47	1p	681	0	697	23	0
47	2p	677	0	686	20	0
48	1q	823	0	891	21	0
48	2q	823	0	891	22	0
49	1r	555	0	618	13	0
49	2r	555	0	618	17	0
50	1s	652	0	662	18	0
50	2s	646	0	644	24	0
51	1t	728	0	798	20	0
51	2t	727	0	796	13	0
52	1u	199	0	208	3	0
52	2u	199	0	208	5	0
53	1v	277	0	140	1	0
53	2v	277	0	140	3	0
54	1w	1592	0	818	33	0
54	2w	1544	0	787	31	0
55	1x	1625	0	829	16	0
55	2x	1625	0	828	22	0
56	1y	1585	0	806	19	0
56	2y	1565	0	797	26	0
57	2a	32327	0	16338	465	0
58	A	115	0	72	4	0
58	B	115	0	72	7	0
59	10	8	0	0	0	0
59	11	3	0	0	0	0
59	12	2	0	0	0	0
59	13	3	0	0	0	0
59	15	2	0	0	0	0
59	16	3	0	0	0	0
59	17	2	0	0	0	0
59	18	3	0	0	0	0
59	19	1	0	0	0	0
59	1A	1229	0	0	0	0
59	1B	38	0	0	0	0
59	1D	13	0	0	0	0
59	1E	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	1F	10	0	0	0	0
59	1G	5	0	0	0	0
59	1I	1	0	0	0	0
59	1N	9	0	0	0	0
59	1O	6	0	0	0	0
59	1P	4	0	0	0	0
59	1Q	6	0	0	0	0
59	1R	3	0	0	0	0
59	1S	3	0	0	0	0
59	1T	2	0	0	0	0
59	1U	5	0	0	0	0
59	1V	2	0	0	0	0
59	1W	5	0	0	0	0
59	1X	5	0	0	0	0
59	1Y	3	0	0	0	0
59	1Z	4	0	0	0	0
59	1a	278	0	0	0	0
59	1b	2	0	0	0	0
59	1d	1	0	0	0	0
59	1e	1	0	0	0	0
59	1f	3	0	0	0	0
59	1k	1	0	0	0	0
59	1l	3	0	0	0	0
59	1n	2	0	0	0	0
59	1p	1	0	0	0	0
59	1s	1	0	0	0	0
59	1t	1	0	0	0	0
59	1v	1	0	0	0	0
59	1w	12	0	0	0	0
59	1x	17	0	0	0	0
59	1y	5	0	0	0	0
59	20	3	0	0	0	0
59	23	2	0	0	0	0
59	25	3	0	0	0	0
59	27	1	0	0	0	0
59	28	2	0	0	0	0
59	2A	848	0	0	0	0
59	2B	22	0	0	0	0
59	2D	5	0	0	0	0
59	2E	7	0	0	0	0
59	2F	4	0	0	0	0
59	2G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	2N	1	0	0	0	0
59	2O	2	0	0	0	0
59	2P	1	0	0	0	0
59	2Q	4	0	0	0	0
59	2R	3	0	0	0	0
59	2S	1	0	0	0	0
59	2T	3	0	0	0	0
59	2U	4	0	0	0	0
59	2V	1	0	0	0	0
59	2X	2	0	0	0	0
59	2Z	1	0	0	0	0
59	2a	239	0	0	0	0
59	2d	1	0	0	0	0
59	2e	1	0	0	0	0
59	2f	2	0	0	0	0
59	2g	1	0	0	0	0
59	2j	2	0	0	0	0
59	2k	1	0	0	0	0
59	2l	2	0	0	0	0
59	2p	1	0	0	0	0
59	2q	5	0	0	0	0
59	2r	1	0	0	0	0
59	2t	1	0	0	0	0
59	2v	4	0	0	0	0
59	2w	7	0	0	0	0
59	2x	4	0	0	0	0
59	2y	7	0	0	0	0
59	A	1	0	0	0	0
59	B	1	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	2	0
62	2A	1	0	0	0	0
63	10	12	0	0	1	0
63	11	13	0	0	0	0
63	12	4	0	0	1	0
63	13	5	0	0	1	0
63	14	1	0	0	0	0
63	15	5	0	0	0	0
63	16	5	0	0	1	0
63	17	9	0	0	0	0
63	18	13	0	0	1	0
63	19	1	0	0	0	0
63	1A	2636	0	0	45	0
63	1B	71	0	0	0	0
63	1D	31	0	0	0	0
63	1E	35	0	0	1	0
63	1F	18	0	0	0	0
63	1G	6	0	0	3	0
63	1H	3	0	0	0	0
63	1I	2	0	0	0	0
63	1N	10	0	0	0	0
63	1O	8	0	0	0	0
63	1P	23	0	0	1	0
63	1Q	16	0	0	0	0
63	1R	14	0	0	1	0
63	1S	4	0	0	0	0
63	1T	9	0	0	0	0
63	1U	13	0	0	0	0
63	1V	9	0	0	0	0
63	1W	11	0	0	1	0
63	1X	8	0	0	0	0
63	1Y	7	0	0	1	0
63	1Z	2	0	0	0	0
63	1a	523	0	0	11	0
63	1b	1	0	0	0	0
63	1d	3	0	0	0	0
63	1e	3	0	0	0	0
63	1g	1	0	0	0	0
63	1k	3	0	0	0	0
63	1l	10	0	0	0	0
63	1m	1	0	0	0	0
63	1o	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	1p	1	0	0	0	0
63	1q	4	0	0	0	0
63	1r	1	0	0	0	0
63	1t	2	0	0	0	0
63	1v	6	0	0	0	0
63	1w	26	0	0	1	0
63	1x	18	0	0	0	0
63	1y	2	0	0	0	0
63	20	5	0	0	0	0
63	21	14	0	0	0	0
63	22	1	0	0	0	0
63	23	2	0	0	0	0
63	25	4	0	0	0	0
63	27	7	0	0	0	0
63	28	7	0	0	0	0
63	29	1	0	0	0	0
63	2A	1602	0	0	43	0
63	2B	28	0	0	1	0
63	2D	29	0	0	0	0
63	2E	15	0	0	1	0
63	2F	20	0	0	0	0
63	2I	4	0	0	1	0
63	2N	2	0	0	0	0
63	2P	15	0	0	2	0
63	2Q	2	0	0	0	0
63	2R	5	0	0	0	0
63	2T	6	0	0	0	0
63	2U	6	0	0	0	0
63	2V	4	0	0	0	0
63	2W	4	0	0	0	0
63	2X	4	0	0	0	0
63	2Y	1	0	0	0	0
63	2Z	2	0	0	0	0
63	2a	389	0	0	10	0
63	2d	3	0	0	0	0
63	2e	3	0	0	0	0
63	2f	1	0	0	0	0
63	2g	1	0	0	0	0
63	2h	2	0	0	0	0
63	2i	1	0	0	0	0
63	2j	4	0	0	2	0
63	2l	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	2o	1	0	0	1	0
63	2p	3	0	0	0	0
63	2q	2	0	0	0	0
63	2r	1	0	0	1	0
63	2t	3	0	0	0	0
63	2u	1	0	0	0	0
63	2v	1	0	0	0	0
63	2w	3	0	0	0	0
63	2x	10	0	0	1	0
63	2y	20	0	0	0	0
63	A	4	0	0	0	0
63	B	2	0	0	0	0
All	All	302030	0	196834	3685	0

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

All (3685) 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	1.32	1.23
1:2A:2138:C:N4	1:2A:2153:G:H1	1.52	1.06
1:1A:1128:U:O4	1:1A:1132:A:N1	1.87	1.06
1:2A:2129:C:N4	1:2A:2159:G:H1	1.55	1.04
1:2A:2136:C:N4	1:2A:2155:G:H1	1.57	1.02
56:2y:15:G:N2	56:2y:48:C:H42	1.60	0.99
9:2N:123:TYR:HH	9:2N:130:HIS:HE2	1.02	0.99
1:1A:1104:G:H1	1:1A:1126:C:H42	0.98	0.98
56:2y:15:G:H22	56:2y:48:C:N4	1.63	0.96
54:1w:6:G:H1	54:1w:67:C:H42	0.94	0.93
54:2w:4:C:N4	54:2w:69:G:H1	1.66	0.93
54:1w:7:A:H61	54:1w:66:U:H3	1.14	0.93
54:2w:4:C:H42	54:2w:69:G:H1	0.96	0.92
1:1A:1104:G:H1	1:1A:1126:C:N4	1.67	0.92
57:2a:1133:G:H1	57:2a:1141:C:H42	1.17	0.91
57:2a:1025:U:H3	57:2a:1036:G:H1	1.18	0.90
1:1A:2122:G:H1	1:1A:2211:U:H3	1.18	0.90
54:1w:6:G:H1	54:1w:67:C:N4	1.68	0.89
57:2a:1264:C:H42	57:2a:1271:G:H1	1.19	0.89
57:2a:997:U:H3	57:2a:1044:A:H61	1.20	0.87
56:2y:15:G:H22	56:2y:48:C:H42	0.92	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2158:C:N3	1:1A:2177:G:N2	2.23	0.87
1:1A:929:G:H1	1:1A:940:C:H42	1.21	0.87
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.07	0.87
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.56	0.86
57:2a:1030(A):G:N2	57:2a:1030(D):A:OP2	2.07	0.86
54:2w:50:U:H3	54:2w:64:A:H61	1.19	0.86
54:2w:4:C:N3	54:2w:69:G:N2	2.24	0.86
57:2a:1271:G:N2	57:2a:1272:G:N7	2.25	0.85
33:2b:185:ILE:HG22	33:2b:199:TYR:HB2	1.58	0.85
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.59	0.85
22:20:10:THR:HG22	22:20:12:ASN:H	1.42	0.85
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.58	0.85
1:2A:1204:A:H2	1:2A:1241:A:H62	1.25	0.84
32:1a:200:G:H1	32:1a:217:C:H42	1.24	0.83
57:2a:999:C:H42	57:2a:1042:G:H1	1.26	0.83
33:2b:178:ARG:HH12	39:2h:68:ARG:HH22	1.26	0.83
32:1a:266:G:H5"	32:1a:268:C:H41	1.44	0.83
32:1a:1006:C:H42	32:1a:1023:G:H1	1.26	0.82
1:1A:2158:C:N4	1:1A:2177:G:N1	2.28	0.82
1:2A:2136:C:H42	1:2A:2155:G:H1	1.27	0.82
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.63	0.81
1:2A:2807:G:N1	1:2A:2893:G:O6	2.13	0.81
51:1t:57:ARG:HH12	51:1t:100:ILE:HD12	1.46	0.81
32:1a:407:G:H5"	35:1d:115:ARG:HG2	1.63	0.81
10:2O:48:PRO:HB3	57:2a:1422:G:H5"	1.62	0.81
41:2j:7:LYS:HE3	41:2j:9:ARG:HH12	1.46	0.80
1:2A:2127:G:N1	1:2A:2161:C:C4	2.49	0.80
1:1A:715:G:N7	63:1A:4347:HOH:O	2.14	0.80
1:1A:2801:C:OP1	4:1E:61:ARG:NH2	2.15	0.80
57:2a:1128:C:O2	57:2a:1147:C:N4	2.14	0.80
1:1A:1111:U:O2	1:1A:1119:A:N6	2.15	0.79
32:1a:664:G:H22	32:1a:741:G:H1	1.28	0.79
1:2A:2138:C:N3	1:2A:2153:G:N2	2.28	0.79
57:2a:1002:G:H1	57:2a:1038:C:H42	1.30	0.79
15:2T:39:ARG:NH2	57:2a:345:C:OP2	2.13	0.79
1:2A:2127:G:N2	1:2A:2161:C:C2	2.51	0.79
41:2j:32:ALA:HB1	41:2j:33:GLN:HA	1.62	0.79
1:2A:2079:U:OP1	23:21:21:ARG:NH2	2.15	0.79
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.64	0.79
36:1e:78:HIS:HE1	36:1e:143:ARG:H	1.30	0.79
1:2A:2127:G:C6	1:2A:2161:C:N4	2.51	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:21:PRO:HA	40:1i:59:PHE:HA	1.64	0.78
54:1w:18:G:O2'	54:1w:57:G:N2	2.14	0.78
2:2B:20:C:N4	2:2B:63:G:O6	2.17	0.78
36:2e:78:HIS:HD2	39:2h:104:ARG:HD2	1.47	0.78
1:1A:1104:G:N2	1:1A:1126:C:N3	2.30	0.78
1:2A:740:U:OP2	63:2A:3934:HOH:O	2.00	0.78
32:1a:584:G:H5'	48:1q:91:ARG:HH22	1.48	0.78
57:2a:1026:G:O6	57:2a:1036:G:N2	2.18	0.77
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.16	0.77
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.66	0.77
1:1A:325:G:OP2	20:1Y:84:ARG:NH2	2.17	0.77
1:2A:2136:C:N4	1:2A:2155:G:N1	2.32	0.77
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.66	0.77
34:1c:58:GLU:HB3	41:1j:92:THR:HG21	1.67	0.77
41:1j:49:VAL:HG23	45:1n:41:ARG:HB2	1.66	0.77
1:1A:973:G:N7	63:1A:4354:HOH:O	2.18	0.77
1:1A:2158:C:N4	1:1A:2177:G:H1	1.80	0.77
1:2A:2127:G:C2	1:2A:2161:C:N3	2.52	0.77
1:1A:1700:G:H3'	13:1R:2:ARG:HD3	1.66	0.77
40:1i:31:GLN:HE21	40:1i:36:TYR:HD1	1.30	0.77
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	1.67	0.77
1:1A:2460:A:OP1	63:1A:4304:HOH:O	2.01	0.76
1:1A:656:A:OP1	11:1P:65:ARG:NH1	2.18	0.76
1:2A:2129:C:H42	1:2A:2159:G:H1	0.80	0.76
32:1a:310:G:OP2	47:1p:27:LYS:NZ	2.18	0.76
35:1d:98:GLU:OE1	35:1d:103:ASN:ND2	2.17	0.76
1:1A:11:G:H2'	1:1A:12:U:H5''	1.68	0.76
32:1a:975:A:H4'	32:1a:976:G:H5''	1.67	0.76
1:2A:2129:C:N3	1:2A:2159:G:N2	2.31	0.76
1:2A:2287:A:H62	1:2A:2344:U:H3	1.32	0.76
1:2A:1530:C:O2'	1:2A:1531:C:O5'	2.03	0.76
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.67	0.76
21:2Z:145:GLU:H	21:2Z:148:ASP:HB2	1.50	0.76
57:2a:1347:G:N2	57:2a:1373:G:H2'	2.01	0.75
40:2i:50:LEU:HD13	40:2i:56:LEU:HA	1.67	0.75
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.67	0.75
1:2A:2586:C:N4	58:B:5:ASN:HB3	2.01	0.75
1:1A:2598:C:N4	58:A:5:ASN:HB3	2.01	0.75
54:1w:7:A:N6	54:1w:66:U:H3	1.85	0.75
57:2a:1320:C:H1'	50:2s:73:GLU:HG2	1.68	0.75
1:1A:927:G:H2'	1:1A:928:G:H8	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.51	0.75
1:2A:882:G:H1	1:2A:894:C:H42	1.34	0.75
1:1A:1166:G:O6	63:1A:4336:HOH:O	2.04	0.74
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.19	0.74
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.69	0.74
41:2j:38:ILE:HD11	41:2j:71:LEU:HD23	1.69	0.74
22:10:11:ARG:O	22:10:14:ARG:NH2	2.20	0.74
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.23	0.74
1:1A:542:C:OP1	27:15:16:ARG:NH2	2.20	0.74
1:2A:1783:A:OP1	63:2A:3934:HOH:O	2.04	0.74
1:2A:2126:A:N6	1:2A:2162:G:O2'	2.17	0.74
44:2m:37:THR:O	44:2m:55:ARG:NH1	2.20	0.74
1:1A:2149:G:H1	1:1A:2183:C:H42	1.33	0.74
3:1D:71:ASP:HB3	3:1D:103:ARG:HH12	1.53	0.74
1:1A:943:C:N3	1:1A:944:C:N4	2.36	0.74
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.23	0.73
28:16:13:CYS:SG	28:16:47:THR:HG21	2.28	0.73
1:1A:2641:A:O2'	1:1A:2642:G:OP2	2.07	0.73
10:1O:63:VAL:HG12	10:1O:106:LEU:HD11	1.70	0.73
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.21	0.73
1:2A:852:G:H2'	1:2A:853:G:H8	1.54	0.73
39:2h:64:LYS:HG2	39:2h:79:VAL:HG21	1.70	0.73
57:2a:1133:G:H1	57:2a:1141:C:N4	1.86	0.73
1:1A:2149:G:H1	1:1A:2183:C:N4	1.86	0.73
1:2A:1693:U:O2'	3:2D:14:ARG:NH2	2.22	0.73
1:2A:2104:G:H1	1:2A:2185:C:H42	1.37	0.73
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.71	0.73
57:2a:1264:C:N4	57:2a:1271:G:H1	1.86	0.73
1:1A:1053:C:OP2	63:1A:4337:HOH:O	2.07	0.73
1:1A:1165:C:N4	63:1A:4356:HOH:O	2.20	0.73
57:2a:1029:C:C4	57:2a:1032:G:N1	2.57	0.72
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.22	0.72
2:2B:22:U:H3	2:2B:61:G:H1	1.36	0.72
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.70	0.72
57:2a:1089:G:H1	57:2a:1096:C:H42	1.37	0.72
11:1P:126:VAL:HG12	11:1P:148:LEU:HD23	1.70	0.72
55:1x:4:G:H1	55:1x:69:C:H42	1.37	0.72
1:2A:1689:A:H62	1:2A:1698:A:H2	1.35	0.72
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.36	0.72
54:1w:60:U:H5''	54:1w:61:C:H5	1.53	0.72
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.22	0.72
1:1A:1613:A:OP1	3:1D:211:ARG:NH1	2.23	0.72
17:1V:40:LEU:HB2	17:1V:46:VAL:HG13	1.72	0.72
33:1b:94:ASN:HB3	33:1b:95:GLN:HG3	1.72	0.72
57:2a:953:G:H5'	57:2a:965:A:H61	1.55	0.72
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.55	0.72
11:1P:91:PHE:O	11:1P:121:LYS:NZ	2.23	0.71
32:1a:1518:MA6:N6	32:1a:1519:MA6:H103	2.05	0.71
54:2w:50:U:H3	54:2w:64:A:N6	1.88	0.71
32:1a:1255:G:N7	41:1j:43:ARG:NH2	2.39	0.71
50:1s:27:GLU:HB2	50:1s:28:LYS:HA	1.73	0.71
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.24	0.71
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.54	0.71
57:2a:134:A:H61	47:2p:25:ARG:HH12	1.38	0.71
57:2a:997:U:H3	57:2a:1044:A:N6	1.87	0.71
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.25	0.71
1:2A:531:C:OP1	1:2A:561:G:N1	2.23	0.71
19:1X:35:THR:HG22	19:1X:38:GLU:HB2	1.71	0.71
32:1a:1006:C:N3	32:1a:1023:G:N2	2.38	0.71
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.72	0.71
40:2i:128:ARG:NH2	55:2x:33:U:OP2	2.22	0.71
46:2o:39:LEU:HB3	46:2o:56:LEU:HD12	1.73	0.70
26:14:55:ARG:H	26:14:56:VAL:HA	1.56	0.70
23:21:51:VAL:HG11	23:21:74:VAL:HG21	1.72	0.70
57:2a:656:C:O2'	46:2o:28:GLN:OE1	2.09	0.70
21:2Z:106:GLY:HA3	21:2Z:141:VAL:HG22	1.74	0.70
1:2A:2782:G:OP2	63:2A:3936:HOH:O	2.09	0.70
36:2e:24:ARG:NH1	53:2v:24:A:OP2	2.25	0.70
32:1a:700:G:N7	63:1a:3623:HOH:O	2.24	0.70
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.74	0.70
2:1B:33:G:H5'	6:1G:2:PRO:HD3	1.74	0.70
6:1G:45:GLU:OE2	63:1G:5001:HOH:O	2.10	0.70
32:1a:1027:C:C2	32:1a:1034:G:N2	2.59	0.70
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.73	0.70
1:2A:2136:C:N3	1:2A:2155:G:N2	2.34	0.70
32:1a:582:U:OP1	46:1o:64:ARG:NH1	2.25	0.70
32:1a:1047:G:H5''	45:1n:4:LYS:HD3	1.72	0.70
35:1d:166:LYS:NZ	35:1d:179:GLU:OE2	2.24	0.70
40:1i:50:LEU:HD13	40:1i:56:LEU:HA	1.74	0.70
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.73	0.69
24:12:55:ARG:NH2	63:12:3101:HOH:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1g:78:ARG:NH1	38:1g:154:TYR:O	2.25	0.69
46:1o:74:ASP:HB3	46:1o:77:ARG:HB2	1.74	0.69
1:2A:2127:G:C2	1:2A:2161:C:C4	2.80	0.69
32:1a:1033:G:H2'	32:1a:1034:G:H8	1.57	0.69
1:2A:863:A:H2'	1:2A:864:G:H8	1.56	0.69
57:2a:273:A:N7	63:2a:3322:HOH:O	2.25	0.69
57:2a:1347:G:H22	57:2a:1373:G:H2'	1.57	0.69
1:1A:1044:C:OP1	63:1A:4338:HOH:O	2.09	0.69
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.74	0.69
57:2a:983:A:N1	57:2a:1222:G:N2	2.40	0.69
57:2a:1129:C:O2'	57:2a:1130:A:N7	2.26	0.69
57:2a:972:C:O2'	41:2j:55:LYS:O	2.09	0.69
34:2c:172:ARG:HG2	34:2c:174:PRO:HD3	1.73	0.69
57:2a:1255:G:OP1	41:2j:45:ARG:NH2	2.25	0.69
11:1P:100:LEU:HD12	11:1P:112:LEU:HD11	1.75	0.69
32:1a:1346:A:OP1	40:1i:120:ARG:NH1	2.23	0.69
55:2x:50:U:H3	55:2x:64:G:H1	1.38	0.69
1:1A:1485:A:OP1	63:1A:4339:HOH:O	2.10	0.69
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.75	0.69
1:2A:400:G:N7	63:2A:3974:HOH:O	2.25	0.69
44:2m:78:ILE:HA	44:2m:81:LEU:HD12	1.74	0.69
46:1o:18:PHE:O	46:1o:20:GLY:N	2.26	0.69
57:2a:1055:A:N7	57:2a:1200:C:N4	2.41	0.69
1:1A:1059:C:OP2	63:1A:4301:HOH:O	2.11	0.69
57:2a:1105:A:H2'	57:2a:1106:G:H8	1.58	0.68
32:1a:405:U:O4	35:1d:2:GLY:N	2.25	0.68
1:2A:376:C:OP1	63:2A:3937:HOH:O	2.12	0.68
1:2A:2127:G:N1	1:2A:2161:C:N4	2.41	0.68
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.29	0.68
57:2a:811:C:N4	63:2a:3323:HOH:O	2.26	0.68
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.75	0.68
48:2q:45:HIS:H	48:2q:72:ARG:HA	1.58	0.68
1:1A:2101:U:OP1	23:11:21:ARG:NH2	2.23	0.68
32:1a:953:G:H5'	32:1a:965:A:H61	1.58	0.68
1:2A:2712(A):A:OP2	63:2A:3938:HOH:O	2.12	0.68
57:2a:572:A:OP1	63:2a:3317:HOH:O	2.11	0.68
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.75	0.68
32:1a:1378:C:O2	38:1g:76:ARG:NH2	2.26	0.68
35:1d:119:GLN:HG3	35:1d:123:HIS:HD2	1.59	0.68
1:2A:994:C:O2'	1:2A:996:A:OP1	2.11	0.68
1:2A:1434:A:H61	1:2A:1558:A:H62	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:27:G:H1	54:2w:43:C:H42	1.41	0.68
1:1A:1151:U:H2'	1:1A:1152:G:H8	1.57	0.68
34:1c:8:ILE:HD12	34:1c:16:ARG:HG3	1.74	0.68
1:2A:2448:A:N6	63:2A:3982:HOH:O	2.26	0.68
33:2b:52:GLU:HG2	33:2b:56:ARG:HH21	1.58	0.68
34:2c:70:VAL:HG12	34:2c:72:LYS:H	1.58	0.68
4:2E:48:GLN:HE21	4:2E:78:LEU:HD23	1.57	0.68
23:21:50:ARG:HG2	23:21:59:THR:HG22	1.74	0.68
1:1A:2124:U:H3	1:1A:2209:G:H1	1.42	0.68
4:1E:163:GLU:OE2	63:1E:401:HOH:O	2.11	0.68
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.29	0.68
1:2A:2138:C:H42	1:2A:2153:G:H1	0.76	0.68
1:1A:2227:G:H3'	1:1A:2228:G:C8	2.29	0.67
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.25	0.67
34:2c:37:GLN:NE2	45:2n:52:GLN:OE1	2.25	0.67
1:1A:737:G:O6	63:1A:4340:HOH:O	2.11	0.67
8:1I:93:THR:H	8:1I:96:ASP:HB2	1.60	0.67
19:1X:57:LEU:HD11	19:1X:78:LYS:HE2	1.76	0.67
19:2X:35:THR:HG22	19:2X:38:GLU:H	1.59	0.67
26:24:46:GLN:HE21	26:24:48:ARG:HH21	1.40	0.67
32:1a:67:C:H2'	32:1a:68:G:C8	2.29	0.67
32:1a:642:A:N3	39:1h:113:SER:OG	2.27	0.67
6:2G:179:PRO:HB2	26:24:42:PHE:HE2	1.58	0.67
1:1A:931:C:H42	1:1A:938:G:H1	1.43	0.67
1:1A:2408:G:N7	63:1A:4382:HOH:O	2.26	0.67
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.28	0.67
41:2j:47:PHE:N	41:2j:63:PHE:O	2.26	0.67
1:1A:1069:U:OP2	63:1A:4341:HOH:O	2.11	0.67
39:1h:34:GLU:OE1	39:1h:37:ARG:NH2	2.28	0.67
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.27	0.67
57:2a:1348:U:H4'	40:2i:120:ARG:HD2	1.77	0.67
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.77	0.67
1:2A:2504:U:OP2	63:2A:3941:HOH:O	2.13	0.67
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	1.77	0.67
1:2A:2624:G:N7	63:2A:3984:HOH:O	2.26	0.67
2:2B:41:U:H5	6:2G:70:VAL:H	1.43	0.67
2:2B:106:G:H5'	21:2Z:31:ARG:HG2	1.75	0.67
1:1A:1310:G:OP1	27:15:19:ARG:NH2	2.19	0.67
26:14:16:CYS:SG	26:14:17:GLY:N	2.67	0.67
32:1a:1027:C:N4	32:1a:1034:G:C6	2.63	0.67
37:1f:8:ILE:HD11	37:1f:79:LEU:HD13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1m:40:ASN:O	44:1m:43:THR:OG1	2.12	0.67
1:2A:1253:A:OP1	63:2A:3940:HOH:O	2.12	0.67
55:2x:76:A:OP2	63:2x:3101:HOH:O	2.12	0.67
1:1A:1464:G:OP2	63:1A:4343:HOH:O	2.13	0.66
36:1e:78:HIS:CE1	36:1e:143:ARG:H	2.14	0.66
2:2B:42:C:H2'	6:2G:66:GLN:HE21	1.59	0.66
57:2a:1402:4OC:HM22	57:2a:1403:C:H5'	1.77	0.66
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.22	0.66
5:1F:108:LYS:HG2	5:1F:112:MET:HE2	1.77	0.66
28:16:37:ARG:NH1	63:16:5001:HOH:O	2.29	0.66
33:1b:118:LEU:HB3	33:1b:142:LEU:HD12	1.76	0.66
1:2A:981:A:OP1	63:2A:3939:HOH:O	2.12	0.66
35:2d:23:GLY:HA3	35:2d:112:VAL:HG12	1.77	0.66
1:1A:2362:C:OP2	63:1A:4342:HOH:O	2.12	0.66
32:1a:677:U:H3	32:1a:713:G:H22	1.43	0.66
41:1j:8:LEU:HD22	41:1j:96:ILE:HG22	1.77	0.66
1:1A:1055:A:OP2	9:1N:37:LYS:NZ	2.26	0.66
32:1a:1037:C:H2'	32:1a:1038:C:H6	1.60	0.66
3:1D:125:ILE:HB	37:1f:81:ILE:HD11	1.78	0.66
1:2A:863:A:H2'	1:2A:864:G:C8	2.31	0.66
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.26	0.66
33:2b:134:GLU:HA	33:2b:137:ARG:HE	1.60	0.66
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.29	0.66
1:2A:2755:C:H2'	31:29:19:ARG:HD3	1.78	0.66
9:2N:34:LEU:HD21	9:2N:120:LEU:HB2	1.78	0.66
23:21:3:LYS:HB2	23:21:61:ARG:HH22	1.60	0.66
42:2k:48:ILE:O	42:2k:50:TYR:N	2.29	0.66
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.67	0.66
1:2A:2148:G:H2'	1:2A:2149:G:C8	2.31	0.66
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.78	0.66
57:2a:999:C:N4	57:2a:1042:G:H1	1.92	0.66
57:2a:1003:G:N2	57:2a:1025:U:O4	2.27	0.66
1:1A:436:C:OP1	63:1A:4302:HOH:O	2.13	0.66
1:2A:276:A:H5''	1:2A:277:C:H5'	1.76	0.66
1:1A:1016:C:OP2	63:1A:4345:HOH:O	2.13	0.66
1:1A:2459:G:OP2	63:1A:4344:HOH:O	2.13	0.66
1:2A:1627:G:OP1	63:2A:3943:HOH:O	2.14	0.66
57:2a:266:G:H5''	57:2a:268:C:H41	1.60	0.66
57:2a:673:G:H2'	57:2a:674:G:C8	2.30	0.66
57:2a:1060:C:C5	34:2c:2:GLY:HA3	2.31	0.66
57:2a:1204:A:OP1	45:2n:3:ARG:NH1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:637:A:OP1	11:2P:133:SER:OG	2.14	0.65
1:2A:1125:G:H5'	31:29:37:GLY:HA2	1.77	0.65
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.28	0.65
1:1A:455:A:OP1	63:1A:4346:HOH:O	2.14	0.65
1:1A:2133:C:N3	1:1A:2167:C:O2'	2.25	0.65
1:1A:2185:C:OP1	1:1A:2187:G:N2	2.29	0.65
1:2A:2049:G:N7	63:2A:3993:HOH:O	2.29	0.65
57:2a:107:G:N7	51:2t:15:ARG:NH2	2.44	0.65
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.58	0.65
57:2a:975:A:H4'	57:2a:976:G:H5''	1.76	0.65
1:2A:2445:G:OP1	5:2F:74:ARG:NH2	2.29	0.65
18:2W:34:ASN:OD1	18:2W:37:ARG:NH2	2.29	0.65
57:2a:157:G:H1	57:2a:164:U:H3	1.42	0.65
1:1A:1101:G:H1	1:1A:1150:C:H42	1.45	0.65
32:1a:117:G:OP2	63:1a:3615:HOH:O	2.13	0.65
1:2A:1448:G:N7	63:2A:3998:HOH:O	2.29	0.65
13:2R:67:LEU:HD13	13:2R:76:VAL:HG21	1.78	0.65
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.77	0.65
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.42	0.65
1:2A:2125:G:H1'	1:2A:2173:A:H61	1.61	0.65
43:2l:71:PRO:O	43:2l:102:ARG:NH1	2.28	0.65
51:2t:43:LEU:O	51:2t:47:GLY:N	2.30	0.65
40:1i:19:LEU:HD21	40:1i:81:ILE:HG13	1.78	0.65
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.14	0.65
33:1b:69:LEU:HB3	33:1b:162:ILE:HG22	1.79	0.65
1:2A:2242:G:OP1	63:2A:3945:HOH:O	2.14	0.65
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.79	0.65
55:2x:47:U:N3	55:2x:50:U:OP1	2.29	0.65
32:1a:1030:C:H42	32:1a:1031:G:H1	1.42	0.65
1:2A:825:C:O2	11:2P:55:ARG:NH1	2.29	0.65
12:2Q:10:ARG:HH22	55:2x:64:G:H4'	1.62	0.65
32:1a:1030:C:N3	32:1a:1031:G:C2	2.65	0.64
1:2A:1568:G:N7	63:2A:4005:HOH:O	2.30	0.64
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.29	0.64
57:2a:446:G:H1	57:2a:488:C:H42	1.45	0.64
57:2a:1228:C:OP1	44:2m:115:LYS:NZ	2.30	0.64
1:1A:287:G:O2'	63:1A:4349:HOH:O	2.15	0.64
1:1A:2071:G:N7	63:1A:4394:HOH:O	2.29	0.64
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.33	0.64
1:2A:851:U:O2'	25:23:42:ALA:O	2.12	0.64
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2371:G:O2'	28:26:46:HIS:ND1	2.29	0.64
12:2Q:10:ARG:HH12	55:2x:64:G:H4'	1.62	0.64
21:2Z:154:ASP:N	21:2Z:154:ASP:OD1	2.30	0.64
36:2e:57:LYS:HG2	36:2e:61:TYR:HE2	1.61	0.64
40:2i:9:ARG:HG2	40:2i:14:VAL:HG12	1.80	0.64
32:1a:1027:C:C4	32:1a:1034:G:C2	2.85	0.64
1:2A:2060:A:N3	63:2A:4001:HOH:O	2.29	0.64
42:2k:92:GLU:HB3	42:2k:96:ARG:HH12	1.61	0.64
1:1A:2297:C:OP2	28:16:6:ARG:NH1	2.30	0.64
57:2a:1005:A:H5''	57:2a:1006:C:C5	2.33	0.64
47:2p:51:VAL:HG12	47:2p:53:VAL:H	1.62	0.64
56:2y:46:G7M:O2'	56:2y:48:C:OP2	2.14	0.64
1:1A:276:C:OP1	8:1I:45:LYS:NZ	2.22	0.64
1:1A:739:C:O2'	3:1D:38:LYS:NZ	2.30	0.64
1:1A:1072:U:OP1	63:1A:4341:HOH:O	2.14	0.64
1:1A:2150:C:H2'	1:1A:2151:C:O4'	1.97	0.64
32:1a:1314:C:OP2	50:1s:4:SER:OG	2.05	0.64
57:2a:1030:C:H42	57:2a:1031:G:H1	1.44	0.64
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.79	0.64
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.80	0.64
1:2A:1958:C:OP2	63:2A:3944:HOH:O	2.14	0.64
4:2E:48:GLN:NE2	4:2E:78:LEU:HD23	2.13	0.64
57:2a:1305:G:N2	57:2a:1331:G:H1'	2.13	0.64
33:2b:90:MET:HE3	33:2b:226:ARG:HH12	1.63	0.64
1:1A:2255:U:OP1	63:1A:4348:HOH:O	2.14	0.64
1:2A:692:C:O2'	3:2D:38:LYS:NZ	2.30	0.64
17:2V:98:GLU:OE2	17:2V:100:ARG:NH1	2.30	0.64
36:2e:33:VAL:HG13	36:2e:112:LEU:HD12	1.78	0.64
1:1A:2143:G:H1	1:1A:2199:C:H42	1.45	0.64
1:1A:2289:G:OP2	22:10:10:THR:HG21	1.97	0.64
4:1E:111:ARG:HG3	4:1E:160:TYR:CD2	2.33	0.64
1:2A:2127:G:N2	1:2A:2161:C:N3	2.46	0.64
1:2A:2448:A:OP1	63:2A:3942:HOH:O	2.13	0.64
32:1a:1029:C:H41	32:1a:1030(A):G:H21	1.44	0.64
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.79	0.64
7:2H:20:ALA:HB3	7:2H:23:ARG:HG3	1.78	0.64
1:1A:2695:C:O2	10:1O:70:LYS:NZ	2.21	0.63
1:2A:955:C:OP1	12:2Q:87:LYS:HE3	1.98	0.63
1:1A:1085:G:H1	1:1A:1162:C:H42	1.46	0.63
5:2F:143:ALA:HB1	5:2F:148:LEU:HB2	1.78	0.63
47:2p:52:ASP:O	47:2p:54:GLU:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:907:U:H4'	12:2Q:101:ARG:HH22	1.61	0.63
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.24	0.63
57:2a:34:C:H2'	57:2a:35:G:H8	1.63	0.63
35:2d:173:TRP:CD2	35:2d:189:PRO:HG3	2.33	0.63
45:2n:4:LYS:HA	45:2n:7:ILE:HG22	1.80	0.63
1:2A:752:A:H3'	29:27:1:MET:HE1	1.79	0.63
2:2B:87:G:N2	2:2B:90:A:OP2	2.30	0.63
1:1A:2803:A:H3'	1:1A:2803:A:N3	2.14	0.63
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.79	0.63
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.15	0.63
4:2E:59:VAL:HG21	4:2E:74:PRO:HB3	1.81	0.63
32:1a:1198:G:OP1	63:1a:3616:HOH:O	2.15	0.63
57:2a:1002:G:H1	57:2a:1038:C:N4	1.96	0.63
57:2a:1128:C:H1'	57:2a:1147:C:H42	1.62	0.63
1:2A:1793:C:OP1	63:2A:3946:HOH:O	2.16	0.63
57:2a:67:C:H2'	57:2a:68:G:C8	2.34	0.63
34:2c:47:LEU:HD12	34:2c:68:VAL:HG11	1.81	0.63
1:1A:1040:C:OP1	16:1U:53:ARG:NH2	2.32	0.63
7:1H:17:VAL:HG22	7:1H:26:VAL:HG22	1.81	0.63
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.32	0.63
39:2h:10:LEU:HD22	39:2h:83:ILE:HD11	1.80	0.63
32:1a:103:C:OP2	51:1t:14:LYS:NZ	2.27	0.62
5:2F:28:ILE:HG12	5:2F:112:MET:HG2	1.78	0.62
1:1A:2147:G:N1	1:1A:2194:U:OP1	2.21	0.62
32:1a:1030:C:N3	32:1a:1031:G:N2	2.47	0.62
57:2a:1273:G:H3'	57:2a:1274:G:C8	2.34	0.62
1:1A:1115:A:H4'	1:1A:1116:A:H8	1.64	0.62
1:1A:1123:A:H2'	1:1A:1124:U:H4'	1.81	0.62
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.18	0.62
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.16	0.62
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.33	0.62
1:1A:2658:C:OP2	1:1A:2745:G:O2'	2.17	0.62
46:1o:39:LEU:HD13	46:1o:56:LEU:HB2	1.80	0.62
47:1p:15:PRO:HD2	47:1p:42:ARG:HD2	1.80	0.62
1:2A:2143:C:H2'	1:2A:2144:U:O4'	1.99	0.62
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.31	0.62
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.35	0.62
1:1A:1115:A:H4'	1:1A:1116:A:C8	2.35	0.62
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.33	0.62
57:2a:750:G:N3	46:2o:23:GLY:HA3	2.15	0.62
57:2a:1239:A:H62	57:2a:1299:A:H62	1.45	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:2q:54:GLY:O	48:2q:81:ARG:N	2.31	0.62
1:1A:1346:U:H4'	1:1A:1347:A:H5''	1.82	0.62
19:1X:2:LYS:NZ	19:1X:38:GLU:OE2	2.29	0.62
2:2B:24:G:N7	2:2B:56:G:H2'	2.15	0.62
57:2a:1032:G:H2'	57:2a:1033:G:C8	2.35	0.62
32:1a:200:G:H1	32:1a:217:C:N4	1.97	0.62
32:1a:1026:G:H8	32:1a:1027:C:O2	1.83	0.62
49:1r:21:LYS:NZ	49:1r:54:ARG:O	2.31	0.62
44:2m:80:ARG:HH12	50:2s:69:HIS:HE1	1.48	0.62
1:2A:1311:G:H2'	29:27:47:ARG:HH22	1.65	0.62
1:1A:1151:U:H2'	1:1A:1152:G:C8	2.33	0.62
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.31	0.62
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.82	0.62
57:2a:516:PSU:O2	63:2a:3316:HOH:O	2.11	0.62
57:2a:664:G:H22	57:2a:741:G:H1	1.47	0.62
21:1Z:72:ARG:NH2	21:1Z:97:GLU:O	2.33	0.61
36:1e:152:ARG:NH2	39:1h:107:LEU:O	2.32	0.61
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.17	0.61
1:2A:2690:C:OP1	13:2R:17:ARG:NH2	2.32	0.61
35:2d:178:VAL:O	35:2d:180:GLY:N	2.33	0.61
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.82	0.61
10:1O:122:LEU:HD13	15:1T:72:VAL:HG11	1.81	0.61
32:1a:108:G:N1	51:1t:15:ARG:HG2	2.15	0.61
1:2A:2144:U:H1'	1:2A:2148:G:N2	2.15	0.61
44:2m:40:ASN:HB3	44:2m:43:THR:HG23	1.82	0.61
47:2p:18:ARG:HD3	47:2p:35:LYS:HD2	1.81	0.61
7:1H:3:ARG:HH22	7:1H:65:HIS:HB3	1.64	0.61
54:1w:5:G:H2'	54:1w:6:G:C8	2.34	0.61
1:2A:1631:C:H2'	63:2A:4620:HOH:O	1.99	0.61
54:2w:12:U:H3'	54:2w:13:C:H5''	1.81	0.61
32:1a:1300:G:N7	63:1a:3634:HOH:O	2.31	0.61
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.81	0.61
1:2A:900:A:O2'	1:2A:901:A:OP1	2.17	0.61
7:2H:125:VAL:HG22	7:2H:131:VAL:HG22	1.82	0.61
26:24:16:CYS:SG	26:24:17:GLY:N	2.73	0.61
35:2d:3:ARG:HG3	35:2d:5:ILE:HG23	1.81	0.61
7:2H:113:VAL:HG11	7:2H:151:ILE:HG21	1.83	0.61
1:1A:1232:G:H5''	17:1V:81:TYR:CE1	2.35	0.61
1:1A:1405:A:H2	1:1A:1418:U:O4	1.84	0.61
1:2A:2498:C:H3'	63:2A:3926:HOH:O	1.97	0.61
21:2Z:146:ILE:HG12	21:2Z:174:VAL:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2a:986:A:N3	50:2s:52:TYR:OH	2.33	0.61
1:1A:2457:G:OP1	5:1F:74:ARG:NH2	2.32	0.61
48:1q:45:HIS:HB3	48:1q:72:ARG:HB3	1.81	0.61
31:29:2:LYS:NZ	31:29:31:LYS:O	2.33	0.61
57:2a:45:U:H2'	57:2a:46:G:C8	2.36	0.61
44:2m:13:LYS:HA	44:2m:44:ARG:HH11	1.64	0.61
1:1A:928:G:N2	1:1A:943:C:O2	2.34	0.61
1:1A:1740:U:O2'	3:1D:14:ARG:NH2	2.33	0.61
3:1D:147:LEU:HD13	3:1D:155:LEU:HD21	1.82	0.61
32:1a:1006:C:N4	32:1a:1023:G:H1	1.99	0.61
32:1a:1025:U:O2	32:1a:1036:G:O6	2.18	0.61
7:2H:23:ARG:NH1	7:2H:34:GLU:OE1	2.33	0.61
57:2a:1118:C:OP1	40:2i:104:ARG:NH1	2.34	0.61
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	1.83	0.61
1:1A:1829:U:H5'	3:1D:259:THR:HG22	1.81	0.60
10:1O:48:PRO:HB3	32:1a:1422:G:H5''	1.83	0.60
24:12:32:LEU:HD22	24:12:36:ARG:HH11	1.66	0.60
32:1a:1002:G:H3'	32:1a:1003:G:C4'	2.31	0.60
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.82	0.60
1:2A:467:G:OP2	29:27:34:ARG:HD3	2.01	0.60
1:2A:2268:A:OP1	63:2A:3947:HOH:O	2.16	0.60
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.83	0.60
54:2w:8:4SU:N3	54:2w:15:G:O6	2.35	0.60
33:1b:12:GLU:HG3	33:1b:44:LEU:HD23	1.83	0.60
35:2d:98:GLU:OE1	35:2d:103:ASN:ND2	2.34	0.60
50:2s:28:LYS:HD2	50:2s:47:HIS:HA	1.82	0.60
5:1F:32:LEU:HD13	5:1F:112:MET:HE1	1.82	0.60
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.36	0.60
50:1s:32:LYS:HA	50:1s:50:ALA:HB3	1.83	0.60
1:2A:884:C:N3	1:2A:893:C:O2'	2.34	0.60
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.17	0.60
18:2W:57:ASN:HA	18:2W:61:ASN:HD22	1.65	0.60
41:2j:6:ILE:HG12	41:2j:98:ILE:HG13	1.82	0.60
21:1Z:152:ALA:HB1	21:1Z:163:LEU:HD11	1.83	0.60
32:1a:1030:C:N4	32:1a:1031:G:N1	2.44	0.60
3:2D:17:THR:O	3:2D:211:ARG:NH2	2.34	0.60
5:2F:101:LEU:O	5:2F:106:ARG:NH1	2.34	0.60
37:2f:36:ARG:NH2	37:2f:38:GLU:OE2	2.34	0.60
51:2t:57:ARG:HH12	51:2t:100:ILE:HD12	1.65	0.60
1:1A:1431:G:O2'	1:1A:1442:U:O2	2.14	0.60
32:1a:739:C:HO2'	46:1o:42:HIS:HD1	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:972:C:O2'	41:1j:55:LYS:O	2.17	0.60
32:1a:1129:C:O2	32:1a:1130:A:N6	2.26	0.60
48:1q:6:LEU:HD23	48:1q:23:VAL:HG11	1.82	0.60
56:1y:19:G:N2	56:1y:56:C:N3	2.49	0.60
15:2T:127:ALA:C	15:2T:129:ARG:H	2.10	0.60
19:2X:57:LEU:HD11	19:2X:78:LYS:HE2	1.84	0.60
57:2a:1134:G:H1	57:2a:1140:C:H42	1.48	0.60
57:2a:1286:A:C8	57:2a:1287:A:H4'	2.37	0.60
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.82	0.60
34:2c:6:HIS:HD2	34:2c:8:ILE:H	1.49	0.60
33:1b:166:ASP:HB3	33:1b:169:LYS:HB3	1.84	0.60
1:2A:1031:G:H5''	31:29:8:LYS:HE3	1.83	0.60
1:2A:2741:A:OP1	31:29:22:ARG:NH2	2.32	0.60
11:2P:26:GLY:O	63:2P:301:HOH:O	2.16	0.60
35:2d:191:ARG:NH1	35:2d:194:LEU:O	2.30	0.60
35:1d:79:PHE:HE1	35:1d:204:ILE:HD13	1.65	0.60
40:2i:5:TYR:H	40:2i:87:GLN:NE2	2.00	0.60
1:1A:2182:G:O6	1:1A:2183:C:N4	2.35	0.60
32:1a:116:A:OP1	63:1a:3615:HOH:O	2.16	0.60
32:1a:1009:G:O6	32:1a:1020:U:O2	2.19	0.60
33:1b:10:LEU:N	33:1b:48:MET:HE1	2.16	0.60
57:2a:1149:C:O2'	57:2a:1280:A:N1	2.31	0.60
36:2e:31:LEU:HD22	36:2e:43:LEU:HD11	1.82	0.60
1:1A:1219:A:H4'	1:1A:1220:U:OP1	2.01	0.60
7:1H:94:TYR:OH	7:1H:152:ARG:NH1	2.34	0.60
32:1a:1151:A:HO2'	32:1a:1152:A:H8	1.50	0.60
1:2A:854:G:H2'	1:2A:855:G:H8	1.67	0.60
57:2a:1027:C:N4	57:2a:1036:G:O6	2.35	0.60
57:2a:1202:G:O4'	45:2n:29:ARG:NH1	2.34	0.60
1:1A:625:G:O2'	1:1A:702:A:N6	2.35	0.59
1:1A:1385:G:N3	63:1A:4402:HOH:O	2.32	0.59
1:1A:2015:U:OP2	63:1A:4350:HOH:O	2.16	0.59
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.34	0.59
32:1a:1006:C:N4	32:1a:1023:G:N1	2.44	0.59
1:2A:307:G:H21	1:2A:330:A:H62	1.49	0.59
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.36	0.59
15:2T:65:LYS:HE3	15:2T:67:SER:HB2	1.84	0.59
23:21:83:GLU:OE1	23:21:83:GLU:N	2.34	0.59
35:2d:79:PHE:HE1	35:2d:204:ILE:HD13	1.66	0.59
1:1A:1104:G:N2	1:1A:1127:U:O2	2.35	0.59
39:1h:25:ASP:N	39:1h:25:ASP:OD1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:947:G:H2'	1:2A:948:G:C8	2.37	0.59
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.36	0.59
57:2a:1358:U:H5'	45:2n:34:TYR:HD1	1.67	0.59
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.34	0.59
1:2A:1452:A:OP2	63:2A:3948:HOH:O	2.16	0.59
8:2I:3:VAL:HG12	8:2I:38:LEU:HA	1.83	0.59
57:2a:165:C:H2'	57:2a:166:G:H8	1.68	0.59
57:2a:1274:G:N2	57:2a:1275:A:N7	2.49	0.59
40:2i:21:PRO:HA	40:2i:59:PHE:HA	1.83	0.59
44:1m:82:MET:HE3	44:1m:92:HIS:HB3	1.85	0.59
54:1w:66:U:H2'	54:1w:67:C:C6	2.37	0.59
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.84	0.59
1:2A:2171:A:N3	1:2A:2172:U:N3	2.50	0.59
63:2A:3946:HOH:O	57:2a:773:G:OP1	2.17	0.59
11:2P:100:LEU:HD12	11:2P:112:LEU:HD11	1.84	0.59
57:2a:1182:G:H4'	57:2a:1183:A:H5''	1.84	0.59
32:1a:1003:G:C4	32:1a:1004:A:H2	2.20	0.59
5:2F:25:PRO:HD2	5:2F:115:ALA:HB2	1.84	0.59
57:2a:1347:G:H5''	40:2i:107:ARG:HB3	1.84	0.59
47:1p:75:ARG:HE	47:1p:80:PHE:HD2	1.49	0.59
12:2Q:16:ARG:O	12:2Q:18:LYS:N	2.31	0.59
1:1A:843:C:H2'	1:1A:844:C:C6	2.38	0.59
8:1I:101:LEU:HD22	8:1I:107:VAL:HB	1.84	0.59
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.83	0.59
20:1Y:55:TYR:H	20:1Y:56:PRO:HD3	1.68	0.59
35:1d:170:VAL:HG12	35:1d:171:GLY:H	1.67	0.59
54:1w:66:U:H2'	54:1w:67:C:H6	1.68	0.59
7:2H:159:GLU:HG3	7:2H:169:VAL:HG11	1.84	0.59
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.84	0.59
1:1A:1140:U:H1'	1:1A:1143:U:H5	1.68	0.59
32:1a:1353:G:OP1	52:1u:10:ARG:NH1	2.36	0.59
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.02	0.59
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.84	0.59
57:2a:1348:U:H2'	57:2a:1349:A:H8	1.67	0.59
40:2i:28:VAL:HG22	40:2i:63:ILE:HB	1.85	0.59
1:1A:1108:G:H1	1:1A:1123:A:H61	1.49	0.59
32:1a:159:G:N2	32:1a:162:A:OP2	2.35	0.59
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.03	0.59
1:2A:2152:G:C2	1:2A:2153:G:H1'	2.38	0.59
1:2A:2857:G:N2	1:2A:2860:A:OP2	2.34	0.59
19:2X:60:ARG:HH22	29:27:47:ARG:HH12	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1000:C:OP1	12:1Q:87:LYS:HE3	2.03	0.58
1:1A:2849:G:H5'	13:1R:46:GLY:HA2	1.85	0.58
1:2A:300:A:OP2	20:2Y:86:ARG:NH2	2.36	0.58
1:2A:2355:C:H1'	22:20:39:ARG:HH21	1.68	0.58
1:1A:1117:G:H1'	1:1A:1135:G:H2'	1.83	0.58
6:1G:16:ARG:HB2	6:1G:17:PRO:HD3	1.85	0.58
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.36	0.58
25:23:6:VAL:HG22	25:23:56:VAL:HG13	1.85	0.58
57:2a:64:G:H4'	57:2a:65:U:H3'	1.86	0.58
40:2i:23:ASN:HB2	40:2i:25:LYS:HG2	1.85	0.58
1:1A:1071:G:C4	1:1A:1180:C:H1'	2.38	0.58
30:18:33:ASN:HA	30:18:36:LYS:HD2	1.85	0.58
36:1e:41:VAL:HG23	36:1e:67:VAL:HG12	1.85	0.58
44:1m:15:VAL:HG11	44:1m:48:LEU:HD21	1.86	0.58
1:2A:1634:A:OP1	63:2A:3949:HOH:O	2.16	0.58
1:2A:2749:A:OP1	7:2H:3:ARG:NH1	2.36	0.58
3:2D:71:ASP:HB2	3:2D:103:ARG:HH12	1.68	0.58
1:1A:303:C:H42	1:1A:385:G:H1	1.50	0.58
32:1a:1029:C:H41	32:1a:1030(A):G:N2	2.01	0.58
35:1d:173:TRP:CZ3	35:1d:174:LEU:HG	2.38	0.58
1:2A:2104:G:H1	1:2A:2185:C:N4	2.00	0.58
57:2a:34:C:H2'	57:2a:35:G:C8	2.38	0.58
37:2f:9:VAL:HB	37:2f:87:ARG:HB2	1.85	0.58
33:1b:178:ARG:NH1	33:1b:196:LEU:O	2.33	0.58
57:2a:920:U:H2'	57:2a:921:U:C6	2.38	0.58
33:2b:77:ALA:HB2	33:2b:211:ILE:HD13	1.84	0.58
1:1A:1115:A:H1'	1:1A:1142:A:H4'	1.86	0.58
1:1A:1398:U:OP2	63:1A:4351:HOH:O	2.17	0.58
1:1A:2798:C:OP1	4:1E:41:LYS:NZ	2.37	0.58
1:1A:2804:C:H2'	1:1A:2805:G:C8	2.39	0.58
15:1T:29:ARG:NH1	15:1T:46:GLU:OE1	2.35	0.58
22:10:27:GLU:HG3	22:10:68:GLU:HA	1.85	0.58
7:2H:3:ARG:NH1	7:2H:4:ILE:H	2.01	0.58
33:2b:187:LEU:HA	33:2b:201:ILE:HB	1.85	0.58
1:1A:2348:A:H61	22:10:43:THR:HG22	1.69	0.58
1:1A:2825:C:H5'	27:15:29:THR:HG21	1.85	0.58
40:1i:50:LEU:HD23	40:1i:81:ILE:HD11	1.84	0.58
57:2a:976:G:H5'	57:2a:1358:U:O2'	2.04	0.58
57:2a:1166:G:N2	57:2a:1170:A:OP2	2.37	0.58
57:2a:1442:G:H2'	57:2a:1442:G:N3	2.17	0.58
40:2i:3:GLN:NE2	40:2i:20:ARG:HH21	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:2q:9:VAL:HG12	48:2q:56:VAL:HG22	1.85	0.58
8:1l:75:LEU:HD22	8:1l:105:HIS:CD2	2.39	0.58
21:1Z:24:LEU:HD22	21:1Z:41:LEU:HD12	1.86	0.58
47:1p:52:ASP:O	47:1p:54:GLU:N	2.37	0.58
21:1Z:1:MET:HE2	21:1Z:55:HIS:HA	1.86	0.58
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.39	0.58
11:1P:98:GLU:O	11:1P:101:VAL:HG12	2.04	0.58
1:2A:861:A:N3	2:2B:79:C:O2'	2.35	0.58
30:28:23:VAL:HG11	30:28:47:LYS:HD3	1.86	0.58
57:2a:1187:G:H4'	40:2i:111:ARG:HH11	1.67	0.58
36:2e:8:GLU:HG2	36:2e:34:VAL:HG23	1.86	0.58
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.39	0.57
1:2A:2529:G:O6	31:29:31:LYS:NZ	2.37	0.57
56:2y:67:C:H2'	56:2y:68:C:C6	2.38	0.57
1:2A:2058:A:N7	63:2A:4016:HOH:O	2.32	0.57
33:2b:74:LYS:NZ	33:2b:205:ASP:O	2.37	0.57
34:2c:78:GLY:HA3	34:2c:83:ARG:H	1.69	0.57
1:1A:1108:G:P	1:1A:1116:A:H1'	2.44	0.57
15:1T:109:GLU:O	15:1T:113:LYS:HG2	2.05	0.57
32:1a:1226:C:N4	44:1m:104:ARG:HG2	2.19	0.57
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.39	0.57
1:2A:2317:C:N4	1:2A:2318:G:O6	2.36	0.57
57:2a:523:A:H61	43:2l:92:0TD:CG	2.18	0.57
57:2a:1207:2MG:H2'	57:2a:1208:C:C6	2.39	0.57
37:2f:45:LEU:HD12	37:2f:59:TYR:HD1	1.68	0.57
56:2y:42:C:H2'	56:2y:43:C:H6	1.68	0.57
1:1A:2486:C:OP1	63:1A:4353:HOH:O	2.17	0.57
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.86	0.57
35:1d:107:ARG:NH2	35:1d:194:LEU:HD21	2.19	0.57
54:1w:5:G:H2'	54:1w:6:G:H8	1.69	0.57
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.19	0.57
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.67	0.57
22:20:63:VAL:HG21	22:20:83:PRO:HG3	1.85	0.57
57:2a:1271:G:C2	57:2a:1272:G:N7	2.72	0.57
54:2w:8:4SU:S4	54:2w:13:C:O2'	2.53	0.57
1:1A:1140:U:H1'	1:1A:1143:U:C5	2.39	0.57
1:1A:1211:U:H2'	1:1A:1212:C:C6	2.40	0.57
15:1T:24:PRO:HA	15:1T:49:VAL:HG23	1.85	0.57
33:1b:93:VAL:HG21	33:1b:97:TRP:HD1	1.70	0.57
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.86	0.57
22:20:26:TYR:N	22:20:29:GLN:OE1	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:25:LYS:N	40:2i:60:ASP:OD1	2.34	0.57
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.52	0.57
4:2E:181:LEU:HD11	15:2T:6:LEU:HD23	1.87	0.57
35:2d:111:ALA:HB2	35:2d:120:LEU:HD12	1.87	0.57
32:1a:204:U:H4'	32:1a:216:G:O5'	2.05	0.57
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.87	0.57
48:1q:43:LEU:HD12	48:1q:68:ARG:HG2	1.87	0.57
11:2P:95:VAL:HG13	11:2P:125:VAL:HA	1.86	0.57
50:2s:19:VAL:O	50:2s:23:ASN:ND2	2.38	0.57
6:1G:18:GLU:OE2	6:1G:21:ARG:NH1	2.38	0.57
32:1a:1004:A:H5''	32:1a:1024:G:H1	1.70	0.57
1:2A:75:G:H4'	24:22:55:ARG:NH1	2.20	0.57
1:2A:2507:C:H2'	1:2A:2508:G:O4'	2.03	0.57
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.37	0.57
1:1A:957:A:H2'	12:1Q:9:TYR:OH	2.05	0.57
4:1E:12:THR:HG21	15:1T:11:GLU:OE2	2.04	0.57
20:1Y:34:LYS:NZ	63:1Y:601:HOH:O	2.36	0.57
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.87	0.57
1:2A:2590:A:O3'	3:2D:239:ARG:NH2	2.38	0.57
8:2I:93:THR:H	8:2I:96:ASP:HB2	1.69	0.57
21:2Z:10:ARG:NH2	21:2Z:26:GLY:O	2.37	0.57
57:2a:236:G:O2'	48:2q:4:LYS:NZ	2.37	0.57
34:2c:100:ALA:O	34:2c:102:ASN:ND2	2.38	0.57
39:2h:4:ASP:OD1	39:2h:7:ALA:N	2.34	0.57
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.86	0.57
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.05	0.57
14:1S:61:ASN:HB3	14:1S:64:GLU:HB2	1.87	0.57
36:1e:85:GLY:O	36:1e:87:SER:N	2.37	0.57
1:2A:1340:U:OP1	19:2X:16:LYS:NZ	2.38	0.57
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.87	0.57
5:2F:195:ASP:HB3	5:2F:198:ALA:H	1.70	0.57
50:2s:70:LYS:HB2	50:2s:73:GLU:HG3	1.85	0.57
1:1A:469:A:H1'	1:1A:1246:C:O4'	2.05	0.56
1:1A:1159:U:H2'	1:1A:1160:G:H8	1.69	0.56
1:1A:1827:U:H2'	1:1A:1828:C:C6	2.39	0.56
11:1P:42:SER:O	63:1P:301:HOH:O	2.18	0.56
21:1Z:45:ASP:CG	21:1Z:49:ARG:HE	2.13	0.56
33:1b:158:LEU:HD21	33:1b:180:LEU:HD13	1.85	0.56
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.70	0.56
57:2a:1315:U:O2'	57:2a:1360:A:N3	2.36	0.56
50:2s:27:GLU:OE1	50:2s:27:GLU:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1t:22:ARG:O	51:1t:26:ASN:ND2	2.38	0.56
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.41	0.56
44:2m:58:GLU:O	44:2m:62:ASN:ND2	2.38	0.56
1:1A:302:A:H2'	1:1A:303:C:C6	2.40	0.56
1:1A:1133:G:H2'	1:1A:1135:G:C8	2.39	0.56
1:1A:1831:C:OP1	3:1D:260:ARG:NH2	2.38	0.56
9:1N:15:LEU:HD22	9:1N:137:LYS:HD2	1.85	0.56
18:1W:58:ALA:HB1	18:1W:64:MET:HB2	1.88	0.56
32:1a:17:U:H2'	32:1a:18:C:C6	2.40	0.56
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.40	0.56
21:2Z:153:SER:HB3	21:2Z:167:PRO:HB3	1.87	0.56
33:2b:76:GLN:HB3	33:2b:208:ILE:HG13	1.87	0.56
35:2d:153:ARG:HA	35:2d:158:ILE:HD11	1.88	0.56
44:2m:3:ARG:NH2	44:2m:9:ILE:O	2.37	0.56
53:2v:23:A:H4'	53:2v:24:A:H5'	1.87	0.56
1:1A:2262:G:OP1	12:1Q:85:LYS:NZ	2.38	0.56
37:1f:46:ARG:HH22	49:1r:37:VAL:HG11	1.69	0.56
1:2A:796:C:H2'	1:2A:797:C:C6	2.40	0.56
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.39	0.56
57:2a:174:C:H2'	57:2a:175:C:H6	1.71	0.56
57:2a:1301:U:O2'	57:2a:1302:U:H5'	2.06	0.56
51:2t:53:LEU:HA	51:2t:56:MET:HG2	1.86	0.56
1:1A:297:C:H2'	1:1A:298:G:H8	1.70	0.56
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.87	0.56
5:1F:178:PRO:O	5:1F:205:ARG:NH2	2.38	0.56
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.40	0.56
47:1p:15:PRO:O	47:1p:16:HIS:ND1	2.38	0.56
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.87	0.56
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.05	0.56
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.39	0.56
26:24:41:PRO:HG3	26:24:49:PHE:CZ	2.40	0.56
57:2a:748:C:H4'	57:2a:749:C:O5'	2.05	0.56
57:2a:1030(A):G:N2	57:2a:1030(C):G:H3'	2.20	0.56
40:2i:17:VAL:HG23	40:2i:63:ILE:HG12	1.87	0.56
48:2q:45:HIS:HB2	48:2q:65:ILE:HD13	1.86	0.56
51:2t:56:MET:HB2	51:2t:84:LEU:HD21	1.87	0.56
1:1A:776:G:C6	3:1D:208:LYS:HB2	2.40	0.56
1:1A:1139:G:H3'	1:1A:1140:U:H5''	1.87	0.56
32:1a:171:A:H2'	32:1a:172:A:C8	2.41	0.56
32:1a:1033:G:H2'	32:1a:1034:G:C8	2.37	0.56
36:1e:68:GLU:HG3	36:1e:70:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1h:21:LYS:O	39:1h:65:TYR:OH	2.23	0.56
1:2A:483:A:O2'	20:2Y:49:VAL:O	2.15	0.56
1:2A:2404:C:O3'	11:2P:77:ARG:NH2	2.39	0.56
21:2Z:45:ASP:OD1	21:2Z:49:ARG:NE	2.35	0.56
57:2a:1030:C:N4	57:2a:1031:G:H1	2.04	0.56
37:2f:67:MET:HE3	37:2f:72:VAL:HG12	1.88	0.56
47:2p:52:ASP:HB3	47:2p:55:ARG:HB2	1.87	0.56
1:1A:939:C:H2'	1:1A:940:C:C6	2.40	0.56
1:1A:1102:G:H4'	1:1A:1132:A:H8	1.71	0.56
5:1F:140:LEU:HD11	5:1F:170:LEU:HD11	1.88	0.56
32:1a:328:C:H4'	32:1a:329:A:H5'	1.86	0.56
1:2A:668:G:H5'	1:2A:669:G:OP2	2.04	0.56
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.05	0.56
17:2V:1:MET:HE1	17:2V:44:LYS:H	1.70	0.56
57:2a:841:U:OP1	57:2a:841:U:H6	1.89	0.56
57:2a:936:C:H2'	57:2a:937:A:O4'	2.06	0.56
57:2a:1349:A:H2'	57:2a:1350:A:H8	1.69	0.56
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.39	0.56
50:1s:27:GLU:OE1	50:1s:27:GLU:N	2.36	0.56
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.40	0.56
1:1A:611:U:H2'	1:1A:612:C:C6	2.41	0.56
1:1A:1874:C:H5'	3:1D:253:GLN:OE1	2.05	0.56
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.06	0.56
34:1c:15:THR:HG21	34:1c:181:ASN:HA	1.87	0.56
49:1r:26:LEU:HD21	49:1r:39:VAL:HG13	1.88	0.56
1:2A:928:G:H8	1:2A:928:G:O5'	1.89	0.56
1:2A:2469:A:H5'	1:2A:2470:G:OP2	2.06	0.56
57:2a:742:G:OP2	46:2o:35:ARG:NH2	2.39	0.56
33:2b:115:LEU:O	33:2b:119:GLU:N	2.36	0.56
33:2b:118:LEU:HB3	33:2b:142:LEU:HD12	1.88	0.56
36:2e:5:ASP:N	36:2e:5:ASP:OD1	2.39	0.56
41:2j:8:LEU:HD22	41:2j:96:ILE:HG22	1.87	0.56
54:2w:18:G:O2'	54:2w:19:G:OP2	2.21	0.56
15:1T:127:ALA:C	15:1T:129:ARG:H	2.13	0.56
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.21	0.56
32:1a:649:G:H2'	32:1a:650:G:H8	1.70	0.56
41:1j:11:PHE:HE1	41:1j:67:THR:HG22	1.71	0.56
10:2O:2:ILE:HD12	10:2O:6:THR:HG21	1.87	0.56
1:1A:1159:U:H2'	1:1A:1160:G:C8	2.41	0.55
33:1b:15:VAL:HG23	33:1b:16:HIS:ND1	2.21	0.55
33:1b:204:ASN:OD1	33:1b:206:ASP:N	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:84:A:H5''	20:2Y:8:LYS:HE3	1.88	0.55
3:2D:125:ILE:HB	37:2f:81:ILE:HD11	1.89	0.55
30:28:33:ASN:HA	30:28:36:LYS:HD2	1.88	0.55
57:2a:448:A:OP2	57:2a:485:G:N1	2.22	0.55
57:2a:1119:C:H2'	57:2a:1120:G:C8	2.39	0.55
1:1A:1633:A:H2'	1:1A:1634:C:C6	2.40	0.55
36:1e:91:LEU:HD12	36:1e:120:THR:HG22	1.86	0.55
43:1l:88:GLY:O	43:1l:99:HIS:HD2	1.89	0.55
1:2A:566:U:H5''	11:2P:29:LYS:HE3	1.88	0.55
1:2A:882:G:H2'	1:2A:883:G:H8	1.71	0.55
1:2A:2439:A:N6	55:2x:76:A:OP1	2.39	0.55
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.06	0.55
1:2A:1113:U:H2'	1:2A:1114:G:C8	2.41	0.55
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.22	0.55
3:2D:8:PRO:HB3	3:2D:14:ARG:HG2	1.89	0.55
57:2a:1107:C:O2	57:2a:1191:A:O2'	2.22	0.55
57:2a:1190:G:O2'	34:2c:3:ASN:HB2	2.07	0.55
42:2k:31:THR:HG22	42:2k:42:TRP:HB2	1.87	0.55
1:1A:1475:G:H2'	1:1A:1476:C:C6	2.40	0.55
1:1A:1634:C:H2'	1:1A:1635:C:H6	1.70	0.55
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.06	0.55
32:1a:1228:C:OP1	44:1m:115:LYS:NZ	2.39	0.55
50:1s:27:GLU:CB	50:1s:28:LYS:HA	2.36	0.55
1:2A:271(K):U:O2	8:2I:50:ARG:NE	2.39	0.55
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.25	0.55
57:2a:1031:G:H2'	57:2a:1032:G:C8	2.41	0.55
57:2a:1224:G:OP1	63:2a:3318:HOH:O	2.17	0.55
46:2o:68:ARG:NH1	63:2o:101:HOH:O	2.39	0.55
3:1D:37:LEU:HD12	3:1D:62:TYR:HB2	1.87	0.55
17:1V:72:VAL:HG13	17:1V:85:LYS:HG2	1.88	0.55
44:1m:3:ARG:NH2	44:1m:9:ILE:O	2.31	0.55
1:2A:2507:C:H5''	1:2A:2573:C:N4	2.22	0.55
2:2B:14:U:OP2	2:2B:70:C:O2'	2.21	0.55
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.21	0.55
56:2y:58:A:O2'	56:2y:60:U:OP2	2.18	0.55
1:1A:1071:G:O2'	63:1A:4341:HOH:O	2.17	0.55
1:1A:2442:A:H2'	1:1A:2442:A:N3	2.21	0.55
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	1.89	0.55
18:1W:71:VAL:HA	18:1W:107:LEU:HD12	1.89	0.55
32:1a:757:U:H2'	32:1a:758:G:O4'	2.06	0.55
33:1b:80:ILE:HD11	33:1b:212:GLN:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:40:HIS:HB3	26:24:43:TYR:HB2	1.89	0.55
57:2a:353:A:H5'	57:2a:353:A:H8	1.71	0.55
57:2a:798:G:O6	63:2a:3319:HOH:O	2.18	0.55
40:2i:4:TYR:CE1	40:2i:88:TYR:HA	2.42	0.55
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.42	0.55
1:2A:2343:C:HO2'	1:2A:2373:G:HO2'	1.47	0.55
7:2H:144:VAL:O	7:2H:148:ILE:HG13	2.07	0.55
57:2a:737:A:H2'	57:2a:738:C:C6	2.42	0.55
36:2e:78:HIS:HE1	36:2e:142:LEU:HA	1.72	0.55
1:1A:1039:G:OP1	16:1U:50:ARG:NH2	2.39	0.55
32:1a:413:G:N7	35:1d:35:ARG:NH1	2.55	0.55
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.42	0.55
55:1x:4:G:H1	55:1x:69:C:N4	2.04	0.55
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.72	0.55
8:2I:129:THR:HA	8:2I:138:ILE:O	2.07	0.55
9:2N:123:TYR:HH	9:2N:130:HIS:CD2	2.22	0.55
57:2a:1273:G:H3'	57:2a:1274:G:H8	1.71	0.55
41:2j:30:SER:O	41:2j:81:THR:OG1	2.25	0.55
1:1A:215:G:H21	1:1A:217:A:H62	1.54	0.55
1:1A:1452:U:H2'	1:1A:1453:C:C6	2.42	0.55
32:1a:78:G:C6	32:1a:91:C:N4	2.75	0.55
32:1a:1386:G:N7	63:1a:3637:HOH:O	2.33	0.55
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.22	0.55
41:1j:55:LYS:O	41:1j:57:LYS:N	2.40	0.55
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.21	0.55
9:2N:30:ILE:HG22	9:2N:34:LEU:HD22	1.88	0.55
48:2q:62:SER:OG	48:2q:72:ARG:HG2	2.07	0.55
1:1A:929:G:H3'	1:1A:930:G:H8	1.72	0.55
3:1D:145:VAL:HG11	3:1D:175:LEU:HD11	1.88	0.55
8:1I:3:VAL:HG12	8:1I:38:LEU:HA	1.89	0.55
11:1P:59:LEU:HD21	30:18:10:ALA:HA	1.88	0.55
33:1b:97:TRP:HZ2	33:1b:102:LEU:HD13	1.71	0.55
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.22	0.55
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.42	0.55
57:2a:1299:A:H2'	57:2a:1299:A:N3	2.22	0.55
35:2d:107:ARG:HG2	35:2d:173:TRP:CH2	2.42	0.55
18:1W:2:GLU:OE2	18:1W:72:LYS:NZ	2.25	0.54
1:2A:223:A:O2'	1:2A:420:C:O2	2.26	0.54
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.07	0.54
57:2a:8:A:H5'	36:2e:101:ILE:HG22	1.89	0.54
34:2c:69:HIS:CD2	34:2c:104:GLN:HG2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:6:ILE:HB	41:2j:72:VAL:HG23	1.89	0.54
1:1A:173:C:H2'	1:1A:174:U:C6	2.41	0.54
1:1A:1696:G:O2'	13:1R:107:ASP:OD2	2.21	0.54
30:18:42:ARG:HD2	63:18:202:HOH:O	2.07	0.54
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.90	0.54
32:1a:1086:U:H3	32:1a:1099:G:H22	1.53	0.54
35:1d:194:LEU:HD22	35:1d:196:LEU:HD13	1.88	0.54
38:1g:74:GLU:HG2	38:1g:91:VAL:HG22	1.89	0.54
40:1i:4:TYR:CZ	40:1i:88:TYR:HD1	2.25	0.54
41:1j:78:ASN:O	41:1j:80:LYS:N	2.40	0.54
1:2A:307:G:N1	1:2A:310:A:OP2	2.37	0.54
1:2A:652(T):C:H2'	1:2A:652(U):G:H8	1.73	0.54
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.40	0.54
1:2A:859:G:N2	1:2A:917:A:OP2	2.39	0.54
57:2a:1119:C:H2'	57:2a:1120:G:H8	1.72	0.54
57:2a:1412:C:H2'	57:2a:1413:A:C8	2.42	0.54
36:2e:57:LYS:HG2	36:2e:61:TYR:CE2	2.42	0.54
21:1Z:149:SER:OG	21:1Z:171:ILE:O	2.24	0.54
32:1a:448:A:OP2	32:1a:485:G:N1	2.23	0.54
33:1b:155:LEU:HD11	33:1b:159:PRO:HG3	1.89	0.54
38:1g:78:ARG:HG2	38:1g:79:ARG:H	1.72	0.54
5:2F:140:LEU:HD11	5:2F:170:LEU:HD11	1.88	0.54
6:2G:72:ARG:NH1	6:2G:87:PRO:HG3	2.22	0.54
19:2X:60:ARG:HH22	29:27:47:ARG:NH1	2.06	0.54
57:2a:984:C:H2'	57:2a:985:C:C6	2.42	0.54
33:2b:125:PRO:O	33:2b:127:ILE:HG22	2.07	0.54
34:2c:18:TRP:HE3	34:2c:18:TRP:H	1.52	0.54
51:2t:9:ASN:O	51:2t:10:LEU:HB2	2.06	0.54
7:1H:33:LEU:HD21	7:1H:136:ILE:HG13	1.88	0.54
1:2A:2148:G:H2'	1:2A:2149:G:H8	1.72	0.54
1:2A:2698:U:H2'	1:2A:2699:C:C6	2.43	0.54
6:2G:114:ILE:HA	6:2G:140:ILE:HD11	1.90	0.54
7:2H:137:ASP:HB3	7:2H:140:LYS:HB3	1.89	0.54
57:2a:1064:G:O6	57:2a:1191:A:N6	2.41	0.54
57:2a:1251:A:N1	57:2a:1354:C:O2'	2.36	0.54
7:1H:88:LEU:HD23	7:1H:130:ARG:HG3	1.90	0.54
7:1H:126:PRO:HG2	7:1H:130:ARG:HH21	1.71	0.54
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.43	0.54
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	1.87	0.54
11:2P:42:SER:O	63:2P:302:HOH:O	2.19	0.54
57:2a:1003:G:H2'	57:2a:1004:A:O4'	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2495:C:N3	12:1Q:124:LYS:NZ	2.56	0.54
15:1T:108:ARG:HH22	15:1T:112:ARG:HD3	1.71	0.54
32:1a:184:G:H2'	32:1a:185:A:H8	1.73	0.54
32:1a:557:G:OP1	63:1a:3617:HOH:O	2.18	0.54
50:1s:27:GLU:HG3	50:1s:47:HIS:NE2	2.21	0.54
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.43	0.54
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.06	0.54
1:2A:2114:A:N6	1:2A:2115:G:H21	2.05	0.54
25:23:10:LYS:HB3	25:23:53:LEU:HA	1.89	0.54
33:2b:54:THR:HG23	33:2b:199:TYR:HB3	1.89	0.54
45:2n:24:CYS:HB2	45:2n:40:CYS:HB3	1.89	0.54
32:1a:236:G:OP1	48:1q:40:LYS:NZ	2.40	0.54
36:1e:147:ASP:OD1	36:1e:150:ARG:NH2	2.40	0.54
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.08	0.54
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.25	0.54
6:2G:137:GLU:HG2	6:2G:152:LEU:HD22	1.88	0.54
9:2N:67:LEU:HB3	9:2N:88:GLU:HG3	1.90	0.54
21:2Z:28:MET:HE1	21:2Z:61:LEU:HD21	1.88	0.54
57:2a:1020:U:H2'	57:2a:1021:G:C8	2.43	0.54
57:2a:1263:C:N3	57:2a:1272:G:O6	2.41	0.54
57:2a:1347:G:HO2'	57:2a:1373:G:H1	1.56	0.54
34:2c:50:ALA:HB1	34:2c:70:VAL:HG11	1.89	0.54
1:1A:715:G:H5'	1:1A:716:G:OP2	2.08	0.54
1:1A:1829:U:H5'	3:1D:259:THR:CG2	2.37	0.54
32:1a:920:U:H2'	32:1a:921:U:C6	2.43	0.54
1:2A:995:C:O2	9:2N:3:THR:OG1	2.22	0.54
5:2F:123:LEU:HD13	5:2F:192:LEU:HD13	1.89	0.54
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.08	0.54
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.48	0.54
57:2a:17:U:H2'	57:2a:18:C:C6	2.43	0.54
57:2a:24:U:OP1	43:2l:23:LYS:NZ	2.41	0.54
57:2a:769:G:H4'	57:2a:1513:A:H4'	1.90	0.54
37:2f:46:ARG:HH22	49:2r:37:VAL:HG11	1.72	0.54
48:2q:9:VAL:HG11	48:2q:84:LEU:HD13	1.90	0.54
32:1a:405:U:OP2	35:1d:3:ARG:NH1	2.41	0.54
1:2A:674:G:O2'	5:2F:74:ARG:HD3	2.07	0.54
7:2H:124:GLU:OE2	7:2H:132:ARG:HD2	2.07	0.54
57:2a:1133:G:N2	57:2a:1141:C:N3	2.55	0.54
57:2a:1218:C:H2'	57:2a:1219:U:C6	2.43	0.54
33:2b:97:TRP:HH2	33:2b:176:GLU:CD	2.15	0.54
41:2j:42:THR:HG23	41:2j:68:HIS:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:747:G:O2'	1:1A:1679:A:N3	2.38	0.54
33:1b:84:GLU:OE1	33:1b:87:ARG:NH1	2.41	0.54
54:1w:68:C:H2'	54:1w:69:G:H8	1.73	0.54
1:2A:236:C:H2'	1:2A:237:C:H6	1.72	0.54
2:2B:101:G:OP2	63:2B:3101:HOH:O	2.17	0.54
10:2O:49:ARG:NH1	57:2a:1422:G:O3'	2.39	0.54
1:1A:1814:A:H5'	1:1A:2620:G:H4'	1.89	0.53
44:1m:102:ARG:HH21	44:1m:105:THR:HG23	1.73	0.53
50:1s:22:LEU:HB3	50:1s:27:GLU:HB3	1.89	0.53
1:2A:451:C:H4'	5:2F:52:LYS:HE3	1.89	0.53
1:2A:888:C:H2'	1:2A:889:C:C4	2.43	0.53
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.08	0.53
57:2a:1132:C:H2'	57:2a:1133:G:C8	2.43	0.53
57:2a:1510:U:H2'	57:2a:1511:G:C8	2.43	0.53
33:2b:163:PHE:CD1	33:2b:185:ILE:HG13	2.43	0.53
46:2o:11:VAL:HG21	46:2o:34:LEU:HD22	1.89	0.53
54:2w:51:U:H2'	54:2w:52:G:C8	2.43	0.53
2:1B:2:C:H2'	2:1B:3:C:C6	2.42	0.53
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.90	0.53
15:1T:24:PRO:HD3	15:1T:52:ILE:HD12	1.90	0.53
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	1.90	0.53
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.74	0.53
51:1t:87:LYS:O	51:1t:91:LEU:HG	2.08	0.53
1:2A:568:U:H5'	1:2A:945:A:N1	2.22	0.53
1:2A:586:A:N1	1:2A:809:G:O2'	2.35	0.53
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.43	0.53
57:2a:984:C:H2'	57:2a:985:C:H6	1.73	0.53
57:2a:1239:A:H4'	57:2a:1240:U:H5'	1.89	0.53
1:1A:238:C:O2	30:18:12:LYS:NZ	2.39	0.53
9:1N:62:VAL:HG22	9:1N:66:LYS:HD2	1.89	0.53
29:17:9:ARG:HG2	29:17:46:VAL:HG23	1.90	0.53
33:1b:219:VAL:HA	33:1b:222:ILE:HD12	1.90	0.53
35:1d:111:ALA:HB2	35:1d:120:LEU:HD12	1.90	0.53
54:1w:4:C:H2'	54:1w:5:G:H8	1.73	0.53
56:1y:9:A:O3'	56:1y:45:U:O2'	2.27	0.53
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.25	0.53
1:2A:615:G:OP1	5:2F:40:GLN:NE2	2.40	0.53
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.43	0.53
2:2B:83:G:N1	2:2B:94:C:N3	2.41	0.53
6:2G:123:ASN:C	6:2G:125:PHE:H	2.17	0.53
13:2R:44:LEU:HD22	13:2R:48:VAL:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2a:953:G:H5'	57:2a:965:A:N6	2.20	0.53
57:2a:967:5MC:H2'	57:2a:968:A:C8	2.43	0.53
33:2b:40:HIS:HB3	33:2b:190:THR:HG21	1.89	0.53
33:2b:58:ILE:O	33:2b:62:ALA:N	2.37	0.53
51:2t:100:ILE:HG13	51:2t:101:GLY:H	1.72	0.53
32:1a:78:G:N1	32:1a:91:C:C4	2.76	0.53
32:1a:1442:G:O2'	32:1a:1442(A):G:H5'	2.07	0.53
1:2A:880:G:N1	1:2A:898:C:O2	2.39	0.53
10:2O:7:TYR:CZ	10:2O:44:LYS:HG3	2.44	0.53
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.90	0.53
28:26:12:GLU:OE1	28:26:19:ARG:NH1	2.42	0.53
57:2a:757:U:H2'	57:2a:758:G:O4'	2.09	0.53
57:2a:1194:U:H2'	57:2a:1195:C:C6	2.44	0.53
57:2a:1502:A:C8	57:2a:1505:G:N2	2.76	0.53
1:1A:1425:A:H4'	1:1A:1426:G:OP2	2.09	0.53
1:1A:2340:A:H2'	1:1A:2341:G:C8	2.43	0.53
4:1E:24:THR:HG23	4:1E:184:VAL:HG12	1.91	0.53
32:1a:92:C:H2'	32:1a:93:G:C8	2.44	0.53
1:2A:1446:C:H42	1:2A:1465:G:H1	1.55	0.53
57:2a:91:C:H2'	57:2a:92:C:C6	2.44	0.53
1:1A:964:A:N3	2:1B:80:U:O2'	2.38	0.53
1:1A:1941:A:O2'	32:1a:1517:G:N3	2.40	0.53
1:1A:2401:G:H5''	1:1A:2402:U:O4'	2.09	0.53
32:1a:69:G:H2'	32:1a:70:G:H8	1.73	0.53
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.39	0.53
1:2A:774:A:H2'	1:2A:774:A:N3	2.24	0.53
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.44	0.53
57:2a:222:U:H2'	57:2a:223:U:C6	2.44	0.53
57:2a:911:U:OP2	43:2l:97:ARG:NH2	2.36	0.53
33:2b:71:VAL:HA	33:2b:93:VAL:HG23	1.90	0.53
1:1A:1140:U:O2'	1:1A:1141:A:N7	2.39	0.53
1:1A:2389:A:H2'	1:1A:2390:A:C8	2.44	0.53
5:1F:34:TRP:HA	11:1P:6:LEU:HD13	1.91	0.53
12:1Q:10:ARG:HH11	12:1Q:11:LYS:HE3	1.74	0.53
21:1Z:155:LEU:HD12	21:1Z:156:LYS:H	1.74	0.53
23:11:51:VAL:HG11	23:11:74:VAL:HG21	1.90	0.53
32:1a:659:U:H2'	32:1a:660:G:H8	1.73	0.53
32:1a:1060:C:H5''	41:1j:51:ARG:HG2	1.91	0.53
36:1e:85:GLY:C	36:1e:87:SER:H	2.16	0.53
1:2A:1758:G:O2'	63:2A:3952:HOH:O	2.19	0.53
57:2a:646:U:H2'	57:2a:647:C:C6	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2a:1089:G:H1	57:2a:1096:C:N4	2.04	0.53
57:2a:1193:G:O2'	36:2e:25:ARG:NH2	2.42	0.53
1:1A:1001:G:H5''	12:1Q:77:LYS:HD2	1.91	0.53
1:1A:1105:G:H1	1:1A:1125:C:H42	1.57	0.53
1:1A:2303:U:H2'	1:1A:2304:C:C6	2.44	0.53
1:1A:2760:G:O6	1:1A:2768:C:H5''	2.07	0.53
32:1a:1239:A:H62	32:1a:1299:A:N6	2.07	0.53
44:1m:14:ARG:NH2	44:1m:16:ASP:OD2	2.39	0.53
1:2A:1218:C:H42	1:2A:1231:G:H1	1.56	0.53
1:2A:2141:G:H2'	1:2A:2142:C:O4'	2.08	0.53
3:2D:242:ARG:HG2	3:2D:246:PRO:HG3	1.91	0.53
14:2S:61:ASN:O	14:2S:65:VAL:HG23	2.09	0.53
57:2a:1263:C:N4	57:2a:1271:G:O6	2.41	0.53
1:1A:1501:U:OP1	13:1R:77:ARG:NH1	2.39	0.53
1:1A:1848:G:OP1	3:1D:88:ARG:NH2	2.41	0.53
1:1A:2013:U:H2'	1:1A:2014:G:H5''	1.91	0.53
1:1A:2227:G:H5''	1:1A:2228:G:C5	2.43	0.53
1:1A:2348:A:H61	22:10:43:THR:CG2	2.21	0.53
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.24	0.53
32:1a:333:G:H4'	51:1t:16:HIS:CE1	2.44	0.53
32:1a:1226:C:H41	44:1m:104:ARG:HG2	1.74	0.53
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.24	0.53
37:1f:97:PHE:N	49:1r:30:ASP:OD1	2.42	0.53
55:1x:39:C:O2'	56:1y:35:A:O2'	2.25	0.53
55:1x:68:C:H2'	55:1x:69:C:C6	2.44	0.53
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.41	0.53
39:2h:21:LYS:O	39:2h:65:TYR:OH	2.21	0.53
54:2w:27:G:H1	54:2w:43:C:N4	2.06	0.53
1:1A:2804:C:H2'	1:1A:2805:G:H8	1.73	0.53
14:1S:39:ILE:HB	14:1S:49:VAL:HG12	1.91	0.53
54:1w:4:C:H2'	54:1w:5:G:C8	2.44	0.53
1:2A:900:A:H2'	1:2A:901:A:C8	2.44	0.53
1:2A:1721:G:H8	1:2A:1741:A:H62	1.56	0.53
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.42	0.53
5:2F:103:LYS:HA	5:2F:106:ARG:HG3	1.90	0.53
57:2a:376:G:H5''	47:2p:5:ARG:HB2	1.91	0.53
33:2b:19:HIS:NE2	33:2b:206:ASP:OD2	2.29	0.53
32:1a:974:A:OP2	45:1n:29:ARG:NH2	2.34	0.52
33:1b:24:TRP:CZ3	33:1b:26:PRO:HA	2.44	0.52
33:1b:80:ILE:HD13	33:1b:211:ILE:HG22	1.90	0.52
36:1e:110:LEU:HD13	36:1e:118:ILE:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1h:7:ALA:HB2	39:1h:85:ARG:HG3	1.91	0.52
1:2A:987:G:O2'	1:2A:1000:A:N3	2.41	0.52
1:2A:2114:A:O2'	1:2A:2167:U:H1'	2.08	0.52
1:2A:2287:A:N6	1:2A:2344:U:H3	2.04	0.52
35:2d:116:GLN:HE21	35:2d:157:LEU:HD11	1.74	0.52
12:1Q:35:VAL:HG13	12:1Q:130:LYS:HB3	1.91	0.52
13:1R:2:ARG:HA	13:1R:5:LYS:HD2	1.91	0.52
37:1f:37:VAL:HA	37:1f:65:VAL:HG12	1.92	0.52
39:1h:17:THR:HG22	39:1h:63:LEU:HG	1.91	0.52
54:1w:6:G:N2	54:1w:67:C:N3	2.43	0.52
1:2A:2292:C:OP1	14:2S:17:ARG:NH2	2.42	0.52
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	1.91	0.52
41:2j:5:ARG:N	63:2j:8101:HOH:O	2.41	0.52
1:1A:2180:A:O2'	1:1A:2181:G:OP2	2.23	0.52
1:1A:2880:C:H2'	1:1A:2881:C:O4'	2.10	0.52
9:1N:20:GLY:HA2	9:1N:61:ARG:HG2	1.91	0.52
32:1a:544:G:OP1	35:1d:59:ARG:NH2	2.36	0.52
32:1a:584:G:H5'	48:1q:91:ARG:NH2	2.21	0.52
32:1a:667:G:H4'	46:1o:51:HIS:ND1	2.24	0.52
32:1a:1030(A):G:O2'	32:1a:1031:G:N2	2.43	0.52
44:1m:80:ARG:HH12	50:1s:69:HIS:HE1	1.57	0.52
1:2A:893:C:H2'	1:2A:894:C:C5	2.45	0.52
6:2G:11:TYR:HA	6:2G:15:VAL:HB	1.92	0.52
17:2V:40:LEU:HB2	17:2V:46:VAL:HG13	1.92	0.52
21:2Z:156:LYS:HE3	21:2Z:158:PRO:HD3	1.91	0.52
57:2a:35:G:O2'	43:2l:118:SER:O	2.22	0.52
33:1b:10:LEU:H	33:1b:10:LEU:HD12	1.73	0.52
51:1t:40:ALA:HB2	51:1t:55:ILE:HG22	1.91	0.52
55:1x:8:4SU:O2	55:1x:21:A:H2	1.92	0.52
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.73	0.52
2:2B:75:G:H1	21:2Z:73:GLN:NE2	2.08	0.52
6:2G:44:GLY:N	6:2G:88:ILE:O	2.42	0.52
29:27:9:ARG:HD3	29:27:47:ARG:HB2	1.91	0.52
57:2a:1150:U:H4'	41:2j:41:PRO:HG3	1.91	0.52
57:2a:1376:U:H2'	57:2a:1377:A:C8	2.44	0.52
35:2d:119:GLN:HG3	35:2d:123:HIS:CD2	2.44	0.52
58:A:3:PRO:HG2	58:A:12:SER:HB2	1.91	0.52
1:1A:1094:A:N1	1:1A:1158:G:O2'	2.34	0.52
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.23	0.52
8:1I:116:LEU:HD11	8:1I:120:ILE:HG13	1.90	0.52
24:12:1:MET:HE3	24:12:5:GLU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:625:G:H4'	47:1p:16:HIS:CD2	2.45	0.52
32:1a:1456:G:N1	51:1t:51:GLU:OE2	2.43	0.52
1:2A:854:G:O6	63:2A:3953:HOH:O	2.19	0.52
1:2A:1973:G:OP1	63:2A:3955:HOH:O	2.19	0.52
1:2A:2141:G:O6	1:2A:2150:U:O2	2.27	0.52
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.42	0.52
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.44	0.52
57:2a:501:C:H2'	57:2a:502:G:H8	1.75	0.52
41:2j:40:LEU:HB2	41:2j:69:ASN:HB3	1.91	0.52
44:2m:82:MET:HE3	44:2m:92:HIS:HB3	1.91	0.52
1:1A:1099:C:H42	1:1A:1152:G:H1	1.56	0.52
1:1A:2584:A:C8	4:1E:144:ARG:HD3	2.45	0.52
32:1a:382:A:H2'	32:1a:383:A:C8	2.45	0.52
32:1a:1125:U:H4'	41:1j:5:ARG:HH12	1.74	0.52
1:2A:2689:U:OP2	1:2A:2719:G:N2	2.40	0.52
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.45	0.52
7:2H:41:MET:HE2	7:2H:65:HIS:HA	1.92	0.52
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.91	0.52
57:2a:1352:C:H2'	57:2a:1353:G:C8	2.45	0.52
44:2m:3:ARG:HG3	44:2m:4:ILE:H	1.75	0.52
1:1A:2163:G:C6	1:1A:2164:C:C2	2.98	0.52
32:1a:673:G:H2'	32:1a:674:G:C8	2.43	0.52
40:1i:43:ALA:HA	40:1i:74:ILE:HD13	1.92	0.52
1:2A:1170:G:O6	1:2A:1180:C:N4	2.43	0.52
2:2B:24:G:H4'	2:2B:25:A:C8	2.45	0.52
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.24	0.52
57:2a:573:A:N3	57:2a:883:C:O2'	2.43	0.52
57:2a:989:C:H2'	57:2a:990:C:C6	2.45	0.52
34:2c:6:HIS:CG	45:2n:49:HIS:HB3	2.45	0.52
34:2c:11:ARG:HB3	34:2c:15:THR:HB	1.90	0.52
34:2c:36:ASP:HA	34:2c:39:ILE:HD12	1.91	0.52
38:2g:32:ARG:HH21	38:2g:109:ASN:ND2	2.07	0.52
1:1A:704:U:H2'	1:1A:705:C:C6	2.45	0.52
1:1A:2317:A:H5''	6:1G:134:GLY:HA3	1.90	0.52
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.92	0.52
21:1Z:53:ILE:HG22	21:1Z:71:VAL:HG12	1.92	0.52
34:1c:22:TRP:CZ2	45:1n:54:PRO:HG2	2.45	0.52
39:2h:12:ARG:HD2	39:2h:26:VAL:HG12	1.92	0.52
50:2s:22:LEU:HD12	50:2s:31:ILE:HD11	1.91	0.52
1:1A:63:A:O3'	19:1X:71:GLY:HA3	2.10	0.52
1:1A:174:U:H2'	1:1A:175:G:H8	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.91	0.52
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.45	0.52
15:1T:108:ARG:HD2	63:1a:3945:HOH:O	2.10	0.52
15:1T:108:ARG:NH2	15:1T:112:ARG:HD3	2.25	0.52
1:2A:403:U:H4'	1:2A:404:C:H5'	1.90	0.52
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.45	0.52
1:2A:2342:C:O2'	1:2A:2374:C:OP1	2.27	0.52
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.43	0.52
57:2a:562:C:H1'	43:2l:15:ARG:HB3	1.91	0.52
1:1A:2175:G:H2'	1:1A:2176:G:C8	2.45	0.52
3:1D:180:GLY:HA3	3:1D:275:LYS:HD3	1.91	0.52
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.45	0.52
33:1b:102:LEU:HB3	33:1b:180:LEU:HD12	1.92	0.52
47:1p:20:VAL:HG21	47:1p:32:TYR:CD2	2.45	0.52
1:2A:2064:C:H2'	1:2A:2065:C:C6	2.45	0.52
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.74	0.52
17:2V:72:VAL:HG13	17:2V:85:LYS:HB3	1.91	0.52
21:2Z:7:ALA:HB3	21:2Z:61:LEU:HD12	1.92	0.52
57:2a:1207:2MG:H2'	57:2a:1208:C:H6	1.75	0.52
48:2q:67:LYS:HA	48:2q:70:ARG:HH12	1.75	0.52
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.91	0.51
26:14:55:ARG:N	26:14:56:VAL:HA	2.23	0.51
43:1l:54:LYS:HD2	43:1l:54:LYS:N	2.25	0.51
44:1m:34:LEU:HD13	44:1m:41:PRO:HA	1.92	0.51
1:2A:2121:G:H1	1:2A:2177:C:H42	1.57	0.51
21:2Z:145:GLU:C	21:2Z:147:GLY:H	2.16	0.51
57:2a:1000:U:H3	57:2a:1041:A:H61	1.57	0.51
57:2a:1004:A:C8	57:2a:1005:A:H4'	2.46	0.51
39:2h:28:ALA:HB3	39:2h:57:PRO:HB2	1.92	0.51
54:2w:28:G:H2'	54:2w:29:G:O4'	2.10	0.51
1:1A:1556:A:H3'	1:1A:1557:A:H8	1.75	0.51
1:1A:2859:U:H4'	1:1A:2878:A:C2	2.46	0.51
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.93	0.51
8:1I:12:LEU:HD22	8:1I:19:VAL:HG21	1.92	0.51
20:1Y:55:TYR:H	20:1Y:56:PRO:CD	2.22	0.51
32:1a:341:C:H2'	32:1a:342:C:H6	1.74	0.51
36:1e:74:GLY:HA3	36:1e:116:THR:HG22	1.93	0.51
50:1s:43:GLU:OE1	50:1s:43:GLU:N	2.43	0.51
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.46	0.51
1:2A:2099:U:H3	1:2A:2190:G:H1	1.58	0.51
1:2A:2133:G:O2'	1:2A:2157:G:N2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:145:VAL:HG13	3:2D:191:ALA:HB2	1.90	0.51
4:2E:36:ARG:NH2	4:2E:88:GLY:O	2.43	0.51
9:2N:16:ILE:HD13	9:2N:140:VAL:HG21	1.93	0.51
21:2Z:40:ASP:OD2	21:2Z:42:VAL:HG13	2.10	0.51
56:2y:67:C:H2'	56:2y:68:C:H6	1.75	0.51
1:1A:2339:A:H2'	1:1A:2340:A:C8	2.45	0.51
32:1a:1346:A:N1	32:1a:1374:A:H5''	2.25	0.51
1:2A:287:C:H2'	1:2A:288:C:H6	1.75	0.51
1:2A:2117:A:O2'	1:2A:2118:U:H5''	2.11	0.51
1:2A:2133:G:HO2'	1:2A:2157:G:N2	2.08	0.51
2:2B:14:U:O3'	2:2B:108:U:O2'	2.27	0.51
10:2O:73:ASP:OD2	15:2T:32:TYR:OH	2.23	0.51
57:2a:1085:U:H3'	57:2a:1086:U:C6	2.45	0.51
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.10	0.51
32:1a:1458:G:H5''	51:1t:31:SER:HB2	1.91	0.51
41:1j:38:ILE:HG13	41:1j:71:LEU:HB3	1.92	0.51
1:2A:11:G:O5'	1:2A:11:G:H8	1.92	0.51
1:2A:296:C:O3'	20:2Y:95:LYS:NZ	2.44	0.51
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.11	0.51
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.45	0.51
6:2G:109:VAL:HG21	26:24:14:ILE:HD13	1.93	0.51
22:20:11:ARG:O	22:20:14:ARG:NH2	2.43	0.51
33:2b:24:TRP:CD1	33:2b:24:TRP:H	2.29	0.51
33:2b:134:GLU:O	33:2b:138:LEU:HG	2.09	0.51
55:2x:58:A:H4'	55:2x:59:A:OP1	2.10	0.51
1:1A:927:G:N2	1:1A:944:C:N3	2.58	0.51
9:1N:13:TRP:CE2	9:1N:133:GLN:HG2	2.46	0.51
20:1Y:6:HIS:HE1	20:1Y:72:VAL:O	1.93	0.51
32:1a:410:G:OP1	35:1d:30:LYS:NZ	2.43	0.51
32:1a:1036:G:H3'	32:1a:1037:C:C6	2.46	0.51
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.92	0.51
8:2I:29:TYR:HD2	8:2I:30:LEU:HD23	1.76	0.51
8:2I:124:GLY:H	8:2I:144:VAL:HG23	1.74	0.51
35:2d:127:THR:HG22	35:2d:132:ARG:HA	1.93	0.51
49:2r:33:ASP:OD2	49:2r:36:ASN:HB2	2.10	0.51
1:1A:1085:G:H1	1:1A:1162:C:N4	2.09	0.51
1:1A:2328:C:O2'	6:1G:128:ARG:NH2	2.26	0.51
4:1E:109:LYS:O	4:1E:111:ARG:NH1	2.43	0.51
5:1F:70:THR:HG23	5:1F:72:ARG:H	1.75	0.51
26:14:57:GLU:HB3	26:14:58:ARG:HD2	1.92	0.51
32:1a:445:G:H2'	32:1a:446:G:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:218:ALA:O	33:1b:222:ILE:HG13	2.11	0.51
40:1i:77:ILE:O	40:1i:81:ILE:HG22	2.10	0.51
42:1k:27:ASN:OD1	42:1k:28:THR:N	2.43	0.51
54:1w:51:U:H2'	54:1w:52:G:C8	2.45	0.51
1:2A:854:G:H2'	1:2A:855:G:C8	2.45	0.51
35:2d:61:LYS:NZ	35:2d:72:GLU:OE1	2.36	0.51
41:2j:25:GLU:OE2	41:2j:29:ARG:NH1	2.38	0.51
1:1A:264:G:H1	1:1A:280:C:H42	1.59	0.51
1:1A:1688:A:H2'	1:1A:1689:G:O4'	2.10	0.51
32:1a:613:C:H2'	32:1a:614:A:H8	1.76	0.51
1:2A:30:G:H2'	1:2A:31:C:C6	2.45	0.51
1:2A:882:G:H2'	1:2A:883:G:C8	2.45	0.51
1:2A:1017:G:N7	63:2A:4025:HOH:O	2.34	0.51
1:2A:2137:C:O2'	1:2A:2138:C:OP2	2.28	0.51
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.11	0.51
57:2a:1327:C:OP1	52:2u:12:LYS:NZ	2.31	0.51
33:2b:51:LEU:HD22	33:2b:55:PHE:HE2	1.76	0.51
32:1a:175:C:H2'	32:1a:176:C:C6	2.45	0.51
32:1a:186:C:H2'	32:1a:187:C:C6	2.46	0.51
32:1a:1037:C:H2'	32:1a:1038:C:C6	2.44	0.51
32:1a:1145:C:H4'	32:1a:1146:A:H5'	1.93	0.51
33:1b:24:TRP:CD1	33:1b:24:TRP:H	2.28	0.51
1:2A:534:U:O2'	16:2U:49:HIS:ND1	2.36	0.51
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.75	0.51
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.10	0.51
7:2H:51:ARG:NH1	7:2H:53:GLU:OE2	2.43	0.51
21:2Z:93:ASP:HB2	21:2Z:131:ARG:HH12	1.74	0.51
57:2a:922:G:H4'	36:2e:20:GLN:HA	1.93	0.51
54:2w:29:G:H2'	54:2w:30:G:H8	1.76	0.51
1:1A:742:G:OP1	1:1A:1426:G:O2'	2.27	0.51
1:1A:997:G:OP1	12:1Q:16:ARG:NH2	2.44	0.51
1:1A:1781:G:O2'	1:1A:2870:A:N1	2.36	0.51
1:1A:2417:G:O2'	1:1A:2418:U:OP1	2.27	0.51
3:1D:17:THR:O	3:1D:211:ARG:NH2	2.44	0.51
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.93	0.51
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.92	0.51
32:1a:92:C:H2'	32:1a:93:G:H8	1.76	0.51
32:1a:356:A:N3	32:1a:368:U:O2'	2.38	0.51
35:1d:107:ARG:HH21	35:1d:194:LEU:HD21	1.74	0.51
39:1h:39:LEU:HB3	39:1h:45:ILE:HG12	1.92	0.51
56:1y:63:G:H2'	56:1y:64:A:O4'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:39:ILE:HG12	6:2G:157:ILE:HG12	1.93	0.51
6:2G:124:SER:HB2	6:2G:131:TYR:CE1	2.46	0.51
7:2H:80:SER:OG	7:2H:81:GLU:OE1	2.28	0.51
57:2a:137:C:H2'	57:2a:138:G:H8	1.75	0.51
57:2a:1316:G:N7	50:2s:7:LYS:NZ	2.58	0.51
33:2b:53:ARG:O	33:2b:56:ARG:HG2	2.11	0.51
34:2c:42:LEU:HA	34:2c:45:LYS:HE2	1.92	0.51
1:1A:2168:C:H4'	1:1A:2169:G:C4	2.46	0.51
1:1A:2264:G:OP2	63:1A:4352:HOH:O	2.17	0.51
32:1a:881:G:P	43:1l:12:ARG:HH22	2.34	0.51
9:2N:67:LEU:HA	9:2N:87:LEU:HD22	1.93	0.51
57:2a:1010:G:H2'	57:2a:1011:G:H8	1.74	0.51
57:2a:1226:C:H41	44:2m:104:ARG:HG2	1.75	0.51
57:2a:1253:G:H2'	57:2a:1254:C:C6	2.46	0.51
33:2b:178:ARG:NH2	39:2h:74:PRO:HB3	2.26	0.51
42:2k:98:LEU:O	42:2k:101:SER:OG	2.19	0.51
52:2u:5:ASP:O	52:2u:11:GLY:HA3	2.11	0.51
1:1A:362:G:OP2	63:1A:4355:HOH:O	2.19	0.50
1:1A:1552:C:H2'	1:1A:1553:A:H8	1.77	0.50
1:1A:1830:G:O2'	3:1D:181:GLU:OE2	2.23	0.50
5:1F:13:SER:HB2	5:1F:127:GLU:OE1	2.11	0.50
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.59	0.50
34:1c:116:VAL:HG21	34:1c:202:ILE:HD11	1.92	0.50
35:1d:119:GLN:HG3	35:1d:123:HIS:CD2	2.44	0.50
1:2A:1364:G:P	23:21:3:LYS:HG3	2.51	0.50
1:2A:2815:C:H5'	27:25:29:THR:HG21	1.92	0.50
57:2a:134:A:N6	47:2p:25:ARG:HH12	2.06	0.50
57:2a:1070:U:H2'	57:2a:1071:C:H6	1.75	0.50
57:2a:1264:C:N4	57:2a:1265:G:O6	2.45	0.50
34:2c:148:GLY:HA3	34:2c:172:ARG:O	2.11	0.50
39:2h:9:MET:HG3	39:2h:26:VAL:HG11	1.93	0.50
49:2r:53:ARG:HG2	49:2r:63:GLN:HE21	1.75	0.50
1:1A:265:U:H2'	1:1A:266:C:C6	2.46	0.50
1:1A:1218:G:N1	1:1A:1221:G:OP2	2.43	0.50
1:1A:1550:C:H2'	1:1A:1551:C:C6	2.46	0.50
1:1A:1554:A:O2'	1:1A:1555:C:OP1	2.28	0.50
9:1N:4:TYR:HB2	16:1U:101:ARG:NH1	2.27	0.50
30:18:63:PRO:HG2	30:18:64:TYR:CE2	2.46	0.50
32:1a:250:A:H4'	32:1a:251:G:O5'	2.10	0.50
32:1a:803:G:OP1	63:1a:3618:HOH:O	2.19	0.50
32:1a:1073:U:O2'	33:1b:104:ASN:OD1	2.21	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.92	0.50
55:1x:23:C:H2'	55:1x:24:U:C6	2.47	0.50
1:2A:1181:C:H2'	1:2A:1182:A:C8	2.46	0.50
1:2A:1826:G:H4'	3:2D:242:ARG:CZ	2.41	0.50
57:2a:1011:G:H1	57:2a:1018:C:H42	1.58	0.50
40:2i:97:LYS:HA	40:2i:102:LEU:HG	1.92	0.50
44:2m:25:ILE:HD11	44:2m:66:LEU:HD13	1.93	0.50
1:1A:1110:C:H1'	1:1A:1122:C:H5	1.77	0.50
1:1A:1921:G:N3	1:1A:1921:G:H2'	2.26	0.50
1:1A:2204:G:H2'	1:1A:2205:C:C6	2.46	0.50
32:1a:532:A:N6	32:1a:1206:G:O2'	2.44	0.50
32:1a:600:C:H2'	32:1a:601:C:C6	2.45	0.50
32:1a:963:G:H5'	63:1a:3838:HOH:O	2.10	0.50
32:1a:1263:C:H2'	32:1a:1264:C:C6	2.47	0.50
35:1d:53:ASP:O	35:1d:57:ARG:HG3	2.11	0.50
1:2A:645:C:H5''	1:2A:646:A:OP2	2.11	0.50
1:2A:868:U:C4	1:2A:869:G:N7	2.79	0.50
1:2A:927:G:H2'	1:2A:928:G:O4'	2.11	0.50
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.93	0.50
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.77	0.50
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.46	0.50
26:24:46:GLN:HE21	26:24:48:ARG:NH2	2.08	0.50
26:24:57:GLU:CB	26:24:58:ARG:HA	2.42	0.50
57:2a:165:C:H2'	57:2a:166:G:C8	2.47	0.50
57:2a:401:C:O2'	57:2a:621:A:N3	2.40	0.50
51:2t:50:GLU:HB2	51:2t:99:LEU:HD23	1.93	0.50
1:1A:1210:G:H2'	1:1A:1211:U:C6	2.46	0.50
1:1A:1275:G:N7	63:1A:4416:HOH:O	2.34	0.50
1:1A:1374:G:N7	63:1A:4421:HOH:O	2.35	0.50
6:1G:106:LEU:HD12	6:1G:110:ALA:HB3	1.93	0.50
32:1a:341:C:H2'	32:1a:342:C:C6	2.47	0.50
46:1o:11:VAL:HG21	46:1o:34:LEU:HD22	1.94	0.50
1:2A:903:C:H2'	1:2A:904:C:C6	2.46	0.50
1:2A:2168:G:H8	1:2A:2170:A:N7	2.10	0.50
1:2A:2394:C:N3	56:2y:76:A:O2'	2.41	0.50
12:2Q:35:VAL:HG13	12:2Q:130:LYS:HB3	1.93	0.50
57:2a:9:G:H2'	57:2a:10:A:H8	1.76	0.50
33:2b:15:VAL:HG11	33:2b:213:LEU:HD12	1.93	0.50
33:2b:208:ILE:H	33:2b:208:ILE:HD12	1.75	0.50
34:2c:43:LEU:HD21	34:2c:91:LEU:HD13	1.94	0.50
41:2j:27:ALA:HA	41:2j:81:THR:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:2x:23:C:H2'	55:2x:24:U:C6	2.46	0.50
1:1A:1233:U:H4'	17:1V:79:VAL:HG22	1.93	0.50
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.93	0.50
32:1a:382:A:H2'	32:1a:383:A:H8	1.76	0.50
32:1a:890:G:O2'	32:1a:906:G:O6	2.29	0.50
55:1x:19:G:H4'	55:1x:20:U:OP2	2.12	0.50
1:2A:848:G:H2'	1:2A:849:A:C8	2.46	0.50
1:2A:1036:G:OP1	7:2H:59:ARG:HG3	2.12	0.50
1:2A:2330:G:O2'	22:20:41:ARG:O	2.24	0.50
57:2a:994:A:N3	57:2a:994:A:H2'	2.27	0.50
57:2a:1004:A:N3	57:2a:1038:C:C2	2.80	0.50
57:2a:1346:A:N1	57:2a:1374:A:H5''	2.27	0.50
43:2l:53:ARG:HG3	43:2l:93:LEU:HD21	1.94	0.50
1:1A:943:C:H5'	54:1w:56:C:OP1	2.12	0.50
1:1A:2576:A:C2	1:1A:2659:U:H4'	2.46	0.50
1:1A:2820:A:N6	1:1A:2900:G:O2'	2.34	0.50
21:1Z:7:ALA:HB3	21:1Z:61:LEU:HD12	1.92	0.50
1:2A:2166:G:H3'	1:2A:2167:U:H5''	1.94	0.50
1:2A:2746:U:OP1	7:2H:85:LYS:NZ	2.45	0.50
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.94	0.50
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.93	0.50
57:2a:1346:A:H5''	40:2i:120:ARG:NH1	2.27	0.50
33:2b:48:MET:HA	33:2b:51:LEU:HD12	1.93	0.50
1:1A:2044:U:O2'	1:1A:2629:C:H5'	2.11	0.50
6:1G:12:TYR:HA	6:1G:16:ARG:HG3	1.92	0.50
9:1N:29:LYS:HD2	9:1N:140:VAL:HB	1.94	0.50
21:1Z:105:VAL:N	21:1Z:139:VAL:O	2.39	0.50
32:1a:659:U:H2'	32:1a:660:G:C8	2.47	0.50
32:1a:1129:C:O2'	32:1a:1139:G:N7	2.40	0.50
32:1a:1343:G:H2'	32:1a:1344:C:C6	2.47	0.50
50:1s:11:VAL:HG11	50:1s:16:LEU:HB2	1.94	0.50
1:2A:1021:A:H62	1:2A:1141:U:H3	1.59	0.50
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.12	0.50
5:2F:110:LEU:HD11	5:2F:181:LEU:HG	1.93	0.50
57:2a:1218:C:OP2	45:2n:9:LYS:NZ	2.35	0.50
41:2j:44:VAL:HG22	41:2j:66:ARG:HG2	1.94	0.50
49:2r:61:LYS:O	49:2r:65:ILE:HG12	2.12	0.50
1:1A:215:G:N2	1:1A:217:A:H62	2.09	0.50
1:1A:909:G:H2'	1:1A:910:A:O4'	2.12	0.50
1:1A:968:U:H2'	1:1A:969:C:C6	2.46	0.50
1:1A:1817:A:H1'	1:1A:1960:A:N6	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:984:C:H42	32:1a:1221:G:H1	1.58	0.50
32:1a:1060:C:C5	34:1c:2:GLY:HA3	2.47	0.50
32:1a:1429:C:H2'	32:1a:1430:C:H6	1.76	0.50
34:1c:162:GLN:NE2	53:1v:24:A:O2'	2.45	0.50
50:1s:20:LEU:HD23	50:1s:23:ASN:HD22	1.77	0.50
1:2A:247:G:H4'	1:2A:386:G:C5	2.47	0.50
17:2V:18:LEU:HD12	17:2V:19:LYS:H	1.76	0.50
22:20:10:THR:HG22	22:20:12:ASN:N	2.20	0.50
57:2a:947:G:H1	57:2a:1234:C:H42	1.58	0.50
33:2b:100:GLY:N	33:2b:176:GLU:OE2	2.30	0.50
33:2b:122:PHE:HE2	33:2b:139:LYS:HD3	1.76	0.50
38:2g:47:CYS:O	38:2g:50:ILE:HG22	2.12	0.50
1:1A:1001:G:OP2	12:1Q:87:LYS:HE2	2.12	0.50
5:1F:24:LEU:HD23	5:1F:115:ALA:HA	1.94	0.50
14:1S:6:ALA:O	14:1S:10:ARG:HG3	2.11	0.50
32:1a:165:C:H2'	32:1a:166:G:H8	1.77	0.50
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.94	0.50
38:1g:46:ALA:HB1	38:1g:121:ALA:HB2	1.93	0.50
1:2A:118:A:N3	1:2A:178:G:H1'	2.27	0.50
1:2A:2818:G:OP2	13:2R:42:LYS:NZ	2.43	0.50
2:2B:75:G:N2	21:2Z:87:ASP:OD1	2.44	0.50
57:2a:277:C:OP1	48:2q:68:ARG:NH2	2.44	0.50
57:2a:352:C:O2'	57:2a:354:G:OP1	2.27	0.50
57:2a:1251:A:H2'	57:2a:1252:A:C8	2.46	0.50
40:2i:127:LYS:O	40:2i:128:ARG:HG2	2.12	0.50
1:1A:1121:C:C2'	1:1A:1122:C:H5'	2.42	0.49
1:1A:1634:C:H2'	1:1A:1635:C:C6	2.46	0.49
32:1a:381:C:H2'	32:1a:382:A:O4'	2.11	0.49
33:1b:174:VAL:HG13	33:1b:184:VAL:HG11	1.94	0.49
36:1e:12:LEU:HB3	36:1e:31:LEU:HB2	1.93	0.49
51:1t:9:ASN:O	51:1t:10:LEU:HB2	2.12	0.49
1:2A:458:G:O2'	1:2A:469:G:O6	2.25	0.49
1:2A:479:A:N3	1:2A:481:G:H5''	2.26	0.49
1:2A:731:C:H5''	63:2A:4039:HOH:O	2.12	0.49
1:2A:2125:G:H1'	1:2A:2173:A:N6	2.27	0.49
1:2A:2689:U:P	1:2A:2719:G:H22	2.35	0.49
1:2A:2889:C:H2'	1:2A:2891:G:O4'	2.12	0.49
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.31	0.49
9:2N:15:LEU:HB2	9:2N:135:PRO:HB2	1.93	0.49
20:2Y:55:TYR:H	20:2Y:56:PRO:HD3	1.77	0.49
57:2a:682:G:H1	57:2a:708:C:H42	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2a:1320:C:C1'	50:2s:73:GLU:HG2	2.41	0.49
33:2b:60:ASP:O	33:2b:64:ARG:HG2	2.12	0.49
39:2h:34:GLU:O	39:2h:38:ILE:HG12	2.12	0.49
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.44	0.49
50:2s:27:GLU:HB2	50:2s:28:LYS:HA	1.94	0.49
4:1E:24:THR:HG22	4:1E:186:GLY:O	2.11	0.49
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.12	0.49
32:1a:269:C:H2'	32:1a:270:A:C8	2.47	0.49
32:1a:399:G:H2'	32:1a:400:C:C6	2.47	0.49
32:1a:438:G:H4'	35:1d:123:HIS:ND1	2.27	0.49
33:1b:54:THR:HG23	33:1b:199:TYR:HB3	1.94	0.49
33:1b:105:PHE:C	33:1b:107:THR:H	2.19	0.49
47:1p:43:LYS:HG2	47:1p:48:TRP:CD2	2.46	0.49
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.47	0.49
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.47	0.49
1:2A:2154:G:H2'	1:2A:2155:G:H5'	1.94	0.49
1:2A:2882:A:OP1	13:2R:96:ARG:HD3	2.12	0.49
8:2I:5:LEU:HD11	8:2I:19:VAL:HG22	1.93	0.49
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.94	0.49
57:2a:297:G:N2	57:2a:300:A:OP2	2.45	0.49
57:2a:575:G:O2'	57:2a:821:G:H5'	2.12	0.49
57:2a:1401:G:C2	57:2a:1402:4OC:H1'	2.46	0.49
37:2f:69:GLU:CD	37:2f:69:GLU:H	2.20	0.49
1:1A:469:A:C5	5:1F:45:ARG:HD2	2.47	0.49
1:1A:1384:G:N7	19:1X:62:LYS:NZ	2.55	0.49
1:1A:2346:G:H5'	14:1S:9:ARG:HG2	1.94	0.49
1:1A:2434:A:O4'	56:1y:76:A:N6	2.44	0.49
9:1N:42:TRP:CH2	9:1N:44:PRO:HB3	2.47	0.49
30:18:23:VAL:HG11	30:18:47:LYS:HD3	1.94	0.49
55:1x:50:U:H2'	55:1x:51:C:C6	2.46	0.49
1:2A:1882:C:H5''	23:21:26:ARG:HH21	1.76	0.49
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.47	0.49
9:2N:30:ILE:HG21	9:2N:120:LEU:HD13	1.95	0.49
57:2a:1275:A:H2'	57:2a:1276:G:O4'	2.13	0.49
57:2a:1317:C:O2	50:2s:37:ARG:NH1	2.46	0.49
57:2a:1346:A:H5''	40:2i:120:ARG:HH12	1.76	0.49
46:2o:39:LEU:HD13	46:2o:56:LEU:HB2	1.94	0.49
1:1A:630:U:OP1	5:1F:102:PRO:HA	2.12	0.49
1:1A:1735:U:O2	1:1A:1747:A:H5'	2.13	0.49
1:2A:1824:G:N3	3:2D:254:THR:OG1	2.45	0.49
1:2A:2156:G:H2'	1:2A:2157:G:C5	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:159:ALA:HB1	3:2D:198:ASN:O	2.12	0.49
12:2Q:10:ARG:NH2	55:2x:64:G:H4'	2.26	0.49
26:24:58:ARG:HG3	50:2s:65:ASN:HA	1.94	0.49
57:2a:1176:A:H2'	57:2a:1177:G:O4'	2.11	0.49
57:2a:1179:A:H2'	57:2a:1180:A:O4'	2.12	0.49
33:2b:30:ARG:HH21	33:2b:194:PRO:HB2	1.78	0.49
36:2e:146:ALA:O	36:2e:150:ARG:HG2	2.12	0.49
1:1A:174:U:H2'	1:1A:175:G:C8	2.48	0.49
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.93	0.49
32:1a:679:C:H2'	32:1a:680:C:C6	2.48	0.49
32:1a:933:G:OP2	38:1g:3:ARG:HB2	2.13	0.49
32:1a:1151:A:O2'	32:1a:1152:A:H8	1.94	0.49
32:1a:1530:G:H2'	32:1a:1531:A:C8	2.47	0.49
47:1p:74:LEU:HD23	47:1p:79:VAL:HG21	1.94	0.49
1:2A:832:G:OP1	63:2A:3951:HOH:O	2.18	0.49
7:2H:86:GLU:OE2	7:2H:132:ARG:NH2	2.45	0.49
21:2Z:155:LEU:HB3	21:2Z:157:LEU:HG	1.94	0.49
26:24:33:VAL:HG12	26:24:35:VAL:H	1.77	0.49
29:27:12:ARG:NH2	29:27:44:PRO:HB3	2.26	0.49
33:2b:16:HIS:HB2	33:2b:204:ASN:HD22	1.77	0.49
54:2w:18:G:O2'	54:2w:57:G:N2	2.39	0.49
1:1A:578:U:O2'	1:1A:579:G:N7	2.46	0.49
1:1A:599:U:H2'	1:1A:600:G:C8	2.47	0.49
10:1O:10:VAL:HG21	10:1O:16:ALA:C	2.36	0.49
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.45	0.49
32:1a:461:A:O2'	32:1a:471:G:N7	2.44	0.49
32:1a:1149:C:H2'	32:1a:1150:U:C6	2.47	0.49
32:1a:1305:G:H5''	52:1u:4:GLY:HA3	1.94	0.49
32:1a:1343:G:H1'	40:1i:121:ARG:NH1	2.27	0.49
1:2A:2156:G:H2'	1:2A:2157:G:C4	2.48	0.49
1:2A:2819:G:N7	63:2A:4032:HOH:O	2.35	0.49
57:2a:547:A:H4'	57:2a:548:G:O5'	2.12	0.49
57:2a:1305:G:O2'	57:2a:1331:G:N2	2.45	0.49
34:2c:20:SER:HB3	34:2c:22:TRP:HE1	1.78	0.49
48:2q:22:LEU:HD13	48:2q:41:LYS:HG2	1.93	0.49
48:2q:70:ARG:C	48:2q:71:PHE:HD1	2.20	0.49
1:1A:709:G:H5''	11:1P:16:ARG:HG2	1.93	0.49
1:1A:2155:G:H21	1:1A:2156:A:H62	1.61	0.49
1:1A:2699:U:H2'	1:1A:2700:U:O4'	2.13	0.49
1:1A:2800:C:H1'	4:1E:62:PRO:HG3	1.93	0.49
5:1F:70:THR:CG2	5:1F:72:ARG:H	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:136:PHE:O	21:1Z:137:ILE:HG13	2.13	0.49
32:1a:649:G:H2'	32:1a:650:G:C8	2.47	0.49
32:1a:864:A:H2'	32:1a:865:A:C8	2.48	0.49
33:1b:16:HIS:HB2	33:1b:204:ASN:CB	2.43	0.49
33:1b:93:VAL:HG21	33:1b:97:TRP:CD1	2.46	0.49
1:2A:857:C:H1'	22:20:26:TYR:CE1	2.48	0.49
1:2A:2165:G:H2'	1:2A:2166:G:O4'	2.13	0.49
1:2A:2572:A:N7	4:2E:145:LYS:HB2	2.28	0.49
1:2A:2815:C:H2'	1:2A:2816:C:H6	1.77	0.49
57:2a:391:G:N7	63:2a:3331:HOH:O	2.35	0.49
39:2h:51:VAL:HG12	39:2h:52:ASP:H	1.78	0.49
50:2s:66:MET:HB2	50:2s:74:PHE:CZ	2.48	0.49
1:1A:561:A:H2'	1:1A:562:C:C6	2.47	0.49
7:1H:24:VAL:HG22	7:1H:35:VAL:HB	1.95	0.49
8:1I:31:LEU:HD21	8:1I:38:LEU:HG	1.94	0.49
11:1P:106:LEU:HD22	11:1P:112:LEU:HG	1.94	0.49
15:1T:51:ARG:HG3	15:1T:98:LYS:HD2	1.95	0.49
26:14:17:GLY:C	26:14:19:GLY:H	2.20	0.49
43:1I:53:ARG:HB3	43:1I:69:TYR:HE1	1.77	0.49
1:2A:1589:C:H2'	1:2A:1590:U:C6	2.48	0.49
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.78	0.49
1:2A:2025:C:H2'	1:2A:2026:C:C6	2.48	0.49
1:2A:2298:A:N6	1:2A:2318:G:C8	2.80	0.49
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.48	0.49
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.45	0.49
14:2S:15:ARG:HB3	14:2S:19:LYS:NZ	2.28	0.49
57:2a:130:A:O2'	57:2a:131:C:O5'	2.26	0.49
57:2a:442:C:H42	57:2a:492:G:H1	1.60	0.49
57:2a:865:A:H5'	57:2a:1078:U:C5	2.47	0.49
33:2b:55:PHE:HE1	33:2b:218:ALA:HA	1.77	0.49
36:2e:6:PHE:HB3	36:2e:34:VAL:HG22	1.93	0.49
47:2p:51:VAL:HG12	47:2p:53:VAL:N	2.27	0.49
50:2s:64:GLU:CD	50:2s:64:GLU:H	2.20	0.49
1:1A:1370:G:N7	63:1A:4417:HOH:O	2.34	0.49
1:1A:2143:G:H1	1:1A:2199:C:N4	2.10	0.49
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.93	0.49
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.93	0.49
32:1a:1136:U:H5''	32:1a:1137:C:C4	2.48	0.49
39:1h:81:HIS:N	39:1h:138:TRP:O	2.45	0.49
57:2a:142:G:H2'	57:2a:143:A:C8	2.48	0.49
57:2a:187:C:H2'	57:2a:188:C:H6	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2a:1360:A:H8	57:2a:1360:A:OP1	1.95	0.49
33:2b:73:THR:HB	33:2b:95:GLN:O	2.12	0.49
1:1A:1150:C:H2'	1:1A:1151:U:C6	2.48	0.49
1:1A:1834:A:O2'	3:1D:259:THR:HG21	2.13	0.49
32:1a:711:G:OP1	37:1f:54:LYS:NZ	2.34	0.49
32:1a:715:A:H2'	32:1a:716:A:C8	2.48	0.49
32:1a:1030(A):G:H1'	32:1a:1031:G:H1	1.77	0.49
34:1c:150:LYS:HG3	34:1c:169:ALA:HB2	1.94	0.49
40:1i:43:ALA:C	40:1i:45:ALA:H	2.21	0.49
41:1j:38:ILE:HG12	41:1j:71:LEU:O	2.12	0.49
47:1p:51:VAL:HG12	47:1p:53:VAL:H	1.78	0.49
56:1y:7:A:O2'	56:1y:49:C:OP2	2.20	0.49
1:2A:27:G:N2	1:2A:512:G:H1'	2.28	0.49
1:2A:500:G:N1	1:2A:503:A:OP2	2.46	0.49
1:2A:1213:A:N3	1:2A:1238:G:O2'	2.42	0.49
4:2E:14:ILE:HG13	4:2E:21:VAL:HG13	1.94	0.49
8:2I:110:ASP:H	8:2I:130:TYR:HH	1.56	0.49
12:2Q:10:ARG:NH1	55:2x:64:G:H4'	2.27	0.49
21:2Z:130:PRO:HA	21:2Z:133:ILE:HG13	1.95	0.49
57:2a:735:C:H2'	57:2a:736:C:H6	1.78	0.49
33:2b:29:ALA:HA	33:2b:32:ILE:HD12	1.94	0.49
33:2b:219:VAL:HA	33:2b:222:ILE:HD12	1.95	0.49
1:1A:1177:G:H21	9:1N:73:THR:CG2	2.26	0.48
1:1A:2579:G:H2'	1:1A:2580:C:C6	2.48	0.48
6:1G:122:PRO:HB3	6:1G:170:ARG:HH12	1.77	0.48
7:1H:41:MET:HE2	7:1H:65:HIS:HA	1.95	0.48
8:1I:77:LEU:HD21	8:1I:79:ILE:HD11	1.95	0.48
32:1a:265:G:O2'	48:1q:67:LYS:N	2.46	0.48
32:1a:277:C:OP1	48:1q:68:ARG:NH2	2.44	0.48
41:1j:5:ARG:NH1	41:1j:71:LEU:HD21	2.28	0.48
1:2A:646:A:H2'	1:2A:647:G:O4'	2.13	0.48
1:2A:1359:A:H2'	1:2A:1360:A:H5'	1.95	0.48
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.48	0.48
1:2A:2250:G:OP1	12:2Q:85:LYS:NZ	2.41	0.48
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.48	0.48
10:2O:86:ILE:HG22	10:2O:94:ARG:HD3	1.94	0.48
57:2a:1513:A:H2'	57:2a:1514:C:C6	2.48	0.48
37:2f:70:ASP:OD1	37:2f:70:ASP:N	2.46	0.48
44:2m:23:TYR:CE2	44:2m:71:ARG:HG3	2.48	0.48
1:1A:308:U:H2'	1:1A:309:C:C6	2.48	0.48
1:1A:2193:A:O2'	1:1A:2194:U:H5''	2.13	0.48

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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	0.48
12:1Q:135:ASP:N	12:1Q:138:ASP:OD2	2.43	0.48
15:1T:36:GLU:OE1	15:1T:41:ARG:HD3	2.13	0.48
32:1a:973:G:H3'	32:1a:974:A:H5''	1.95	0.48
34:1c:73:PRO:HB3	34:1c:103:VAL:HG11	1.95	0.48
1:2A:111:A:O2'	24:22:65:ASN:ND2	2.43	0.48
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.13	0.48
18:2W:4:LYS:HE3	18:2W:6:ILE:HD11	1.94	0.48
57:2a:148:G:H2'	57:2a:149:A:H8	1.78	0.48
57:2a:377:G:OP1	47:2p:3:LYS:HD3	2.13	0.48
35:2d:173:TRP:CE3	35:2d:189:PRO:HG3	2.48	0.48
40:2i:4:TYR:HD1	40:2i:87:GLN:HG3	1.78	0.48
16:1U:85:LYS:HD3	16:1U:116:ALA:O	2.13	0.48
26:14:58:ARG:O	26:14:61:ARG:HB3	2.12	0.48
30:18:23:VAL:CG1	30:18:47:LYS:HD3	2.43	0.48
32:1a:165:C:H2'	32:1a:166:G:C8	2.48	0.48
32:1a:814:A:H2'	32:1a:816:A:H5''	1.95	0.48
32:1a:1126:U:O2	32:1a:1280:A:H2'	2.14	0.48
33:1b:63:MET:HG3	33:1b:225:ALA:HB1	1.95	0.48
34:1c:68:VAL:HG12	34:1c:70:VAL:HG23	1.94	0.48
1:2A:300:A:H2'	1:2A:334:C:H1'	1.96	0.48
1:2A:597:U:H2'	1:2A:598:G:C8	2.49	0.48
1:2A:811:U:H2'	11:2P:21:ARG:HA	1.95	0.48
1:2A:1837:C:O2'	1:2A:1927:A:N3	2.42	0.48
25:23:23:LEU:HD13	25:23:50:VAL:HG11	1.96	0.48
57:2a:160:A:H1'	57:2a:344:A:C5	2.49	0.48
57:2a:399:G:H2'	57:2a:400:C:C6	2.48	0.48
34:2c:52:LEU:HD21	34:2c:55:VAL:HG23	1.95	0.48
38:2g:22:LEU:HG	38:2g:62:PHE:CE2	2.49	0.48
39:2h:51:VAL:HG21	39:2h:60:ARG:HB2	1.94	0.48
1:1A:54:G:O2'	1:1A:125:A:N1	2.43	0.48
1:1A:2444:A:C4	23:11:33:LYS:HG2	2.48	0.48
1:1A:2705:A:H2'	1:1A:2706:G:H8	1.78	0.48
8:1I:27:ARG:HG2	23:11:71:TYR:CZ	2.47	0.48
26:14:63:TYR:N	26:14:63:TYR:CD1	2.81	0.48
32:1a:8:A:N6	35:1d:205:GLU:O	2.47	0.48
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.11	0.48
32:1a:175:C:H2'	32:1a:176:C:H6	1.76	0.48
51:1t:56:MET:HE3	51:1t:85:MET:HG2	1.94	0.48
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.12	0.48
1:2A:1791:A:H5'	3:2D:206:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:93:ASP:CB	21:2Z:131:ARG:HH22	2.27	0.48
25:23:46:ASN:O	25:23:50:VAL:HG22	2.13	0.48
26:24:57:GLU:CB	26:24:58:ARG:HD2	2.43	0.48
33:2b:12:GLU:O	33:2b:15:VAL:HG22	2.12	0.48
1:1A:605:G:H2'	1:1A:606:G:C8	2.48	0.48
1:1A:883:G:N7	63:1A:4426:HOH:O	2.35	0.48
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.13	0.48
32:1a:179:A:H2'	32:1a:180:U:C6	2.47	0.48
32:1a:653:A:OP1	39:1h:56:LYS:NZ	2.46	0.48
32:1a:1260:C:O5'	32:1a:1284:C:H4'	2.14	0.48
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.30	0.48
40:1i:53:VAL:O	40:1i:55:ALA:N	2.46	0.48
2:2B:4:C:H42	2:2B:117:G:H1	1.60	0.48
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.95	0.48
9:2N:42:TRP:HA	9:2N:48:MET:SD	2.54	0.48
12:2Q:30:GLY:HA2	12:2Q:107:ALA:HB2	1.95	0.48
57:2a:187:C:H2'	57:2a:188:C:C6	2.48	0.48
57:2a:328:C:H4'	57:2a:329:A:H5'	1.96	0.48
57:2a:1120:G:C6	57:2a:1121:U:C4	3.02	0.48
42:2k:122:LYS:O	42:2k:126:ARG:HG3	2.13	0.48
1:1A:731:G:OP1	29:17:16:HIS:ND1	2.41	0.48
1:1A:1993:A:OP2	3:1D:242:ARG:NH2	2.47	0.48
8:1I:81:VAL:HG21	8:1I:88:ILE:HD13	1.94	0.48
32:1a:501:C:H2'	32:1a:502:G:C8	2.49	0.48
32:1a:1030:C:N4	32:1a:1031:G:H1	2.07	0.48
1:2A:851:U:H5'	25:23:49:LYS:HD2	1.95	0.48
1:2A:910:A:N1	1:2A:2277:G:H1'	2.27	0.48
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.14	0.48
1:2A:2169:A:H1'	56:2y:56:C:C5	2.48	0.48
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.32	0.48
57:2a:815:A:N7	57:2a:1509:C:O2'	2.43	0.48
57:2a:1329:A:OP2	52:2u:7:ARG:NH1	2.35	0.48
34:2c:111:LEU:HD11	34:2c:144:SER:O	2.14	0.48
50:2s:30:LEU:HD11	50:2s:50:ALA:HB2	1.94	0.48
1:1A:1121:C:H2'	1:1A:1122:C:H5'	1.95	0.48
1:1A:1201:A:OP1	16:1U:55:ARG:HD3	2.14	0.48
1:1A:2227:G:OP2	1:1A:2227:G:H4'	2.14	0.48
1:1A:2603:C:H2'	1:1A:2604:G:C8	2.48	0.48
32:1a:1349:A:OP2	40:1i:118:LYS:HE2	2.13	0.48
32:1a:1376:U:H2'	32:1a:1377:A:H8	1.78	0.48
41:1j:81:THR:C	41:1j:83:GLU:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:25:40:LYS:NZ	27:25:44:THR:O	2.44	0.48
57:2a:114:U:H2'	57:2a:115:G:C8	2.48	0.48
57:2a:719:C:O2'	49:2r:49:LYS:HB3	2.13	0.48
57:2a:737:A:H1'	37:2f:73:ASN:HD21	1.78	0.48
57:2a:1074:G:O2'	57:2a:1101:A:N1	2.46	0.48
57:2a:1239:A:H62	57:2a:1299:A:N6	2.11	0.48
33:2b:50:GLU:HB3	33:2b:200:ILE:O	2.13	0.48
41:2j:16:LEU:HD23	41:2j:70:ARG:HG2	1.96	0.48
56:2y:44:G:H3'	56:2y:45:U:C6	2.48	0.48
1:1A:821:A:H2'	1:1A:821:A:N3	2.28	0.48
1:1A:2225:U:O4'	3:1D:151:LYS:HE2	2.13	0.48
1:1A:2288:G:N7	63:1A:4423:HOH:O	2.35	0.48
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.48	0.48
40:1i:128:ARG:NH1	55:1x:35:A:OP2	2.46	0.48
45:1n:48:ALA:HB2	45:1n:53:LEU:HD12	1.95	0.48
1:2A:71:A:N7	19:2X:31:HIS:HE1	2.11	0.48
1:2A:277:C:H4'	1:2A:278:A:C8	2.49	0.48
1:2A:1354:A:H5''	3:2D:38:LYS:HD3	1.96	0.48
1:2A:1843:C:H5'	3:2D:253:GLN:OE1	2.14	0.48
1:2A:2065:C:H2'	1:2A:2066:C:C6	2.48	0.48
1:2A:2366:A:H2'	1:2A:2367:G:O4'	2.13	0.48
1:2A:2674:G:H2'	1:2A:2675:A:C8	2.49	0.48
2:2B:66:A:H61	2:2B:109:C:H5''	1.78	0.48
4:2E:9:VAL:HG13	4:2E:25:VAL:O	2.14	0.48
4:2E:111:ARG:HD3	4:2E:160:TYR:CD2	2.48	0.48
5:2F:31:HIS:NE2	5:2F:35:GLU:OE2	2.47	0.48
8:2I:140:LEU:HD22	8:2I:142:VAL:HG22	1.96	0.48
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.57	0.48
20:2Y:38:ILE:HD11	20:2Y:66:PRO:HG3	1.96	0.48
57:2a:1256:A:H5'	57:2a:1258:G:O4'	2.14	0.48
34:2c:134:ILE:HG22	34:2c:168:ALA:HB3	1.96	0.48
35:2d:22:LYS:HG3	61:2d:501:SF4:S4	2.53	0.48
44:2m:23:TYR:HB3	44:2m:67:GLU:HA	1.95	0.48
45:2n:27:CYS:SG	45:2n:28:GLY:N	2.86	0.48
48:2q:13:ASP:OD1	48:2q:13:ASP:N	2.44	0.48
54:2w:68:C:H2'	54:2w:69:G:H8	1.78	0.48
1:1A:1121:C:H42	1:1A:1123:A:H62	1.62	0.48
32:1a:453:A:H4'	47:1p:72:ARG:HG3	1.96	0.48
1:2A:588:U:H2'	1:2A:589:C:C6	2.49	0.48
1:2A:1753:G:H5''	15:2T:95:ARG:HD2	1.96	0.48
1:2A:1853:A:N3	1:2A:2233:U:O2'	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2206:G:H5''	1:2A:2207:G:C8	2.48	0.48
1:2A:2224:G:OP1	3:2D:268:ARG:NE	2.47	0.48
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.14	0.48
57:2a:1010:G:H2'	57:2a:1011:G:C8	2.47	0.48
57:2a:1080:A:OP1	36:2e:47:LYS:HD3	2.13	0.48
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.82	0.48
1:1A:925:A:N6	1:1A:945:A:O2'	2.47	0.48
1:1A:1627:A:OP2	1:1A:1627:A:H8	1.97	0.48
15:1T:33:LYS:O	15:1T:82:LEU:HD23	2.14	0.48
32:1a:148:G:H2'	32:1a:149:A:H8	1.79	0.48
32:1a:160:A:H1'	32:1a:344:A:C5	2.49	0.48
32:1a:262:A:H2'	32:1a:263:A:C8	2.49	0.48
33:1b:163:PHE:CD1	33:1b:185:ILE:HG13	2.48	0.48
33:1b:189:ASP:OD1	33:1b:189:ASP:N	2.44	0.48
35:1d:205:GLU:OE2	36:1e:107:ARG:NH1	2.47	0.48
39:1h:44:PHE:HB3	39:1h:80:ILE:HG12	1.96	0.48
40:1i:4:TYR:CE1	40:1i:88:TYR:HA	2.49	0.48
1:2A:800:A:H8	1:2A:800:A:OP1	1.97	0.48
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.48	0.48
1:2A:2144:U:H1'	1:2A:2148:G:H22	1.79	0.48
1:2A:2315:G:H2'	1:2A:2316:C:H6	1.79	0.48
1:2A:2609:U:H2'	58:B:5:ASN:HD21	1.79	0.48
2:2B:3:C:H2'	2:2B:4:C:C6	2.48	0.48
4:2E:143:ASN:HD22	4:2E:147:PRO:HD3	1.79	0.48
12:2Q:134:ARG:CZ	21:2Z:122:ARG:HH21	2.27	0.48
57:2a:501:C:H2'	57:2a:502:G:C8	2.49	0.48
57:2a:1118:C:H1'	57:2a:1179:A:C5	2.48	0.48
57:2a:1137:C:H5''	57:2a:1138:G:OP1	2.13	0.48
57:2a:1138:G:C6	57:2a:1140:C:H1'	2.49	0.48
57:2a:1286:A:H8	57:2a:1287:A:H4'	1.79	0.48
38:2g:111:ARG:HB2	38:2g:119:ARG:HD2	1.95	0.48
39:2h:6:ILE:O	39:2h:10:LEU:HG	2.14	0.48
43:2l:56:ALA:HB2	43:2l:70:ILE:HD11	1.96	0.48
44:2m:29:ARG:HD3	44:2m:64:TRP:CE2	2.49	0.48
50:2s:27:GLU:CB	50:2s:28:LYS:HA	2.44	0.48
1:1A:312:C:H2'	1:1A:313:A:H8	1.77	0.47
1:1A:929:G:H4'	54:1w:19:G:O6	2.14	0.47
1:1A:2178:G:H2'	1:1A:2179:G:C2	2.48	0.47
1:1A:2705:A:H2'	1:1A:2706:G:C8	2.49	0.47
4:1E:11:MET:HG2	4:1E:24:THR:HB	1.96	0.47
26:14:49:PHE:HB3	26:14:50:VAL:H	1.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1032:G:H2'	32:1a:1033:G:C8	2.49	0.47
33:1b:132:LYS:O	33:1b:136:VAL:HG23	2.14	0.47
41:1j:54:PHE:O	41:1j:56:HIS:N	2.36	0.47
1:2A:131:G:OP1	63:2A:3954:HOH:O	2.19	0.47
5:2F:187:VAL:HG12	11:2P:3:LEU:HD12	1.96	0.47
57:2a:157:G:N2	57:2a:164:U:O2	2.29	0.47
57:2a:1310:G:H5'	44:2m:77:ASN:ND2	2.29	0.47
57:2a:1499:A:H1'	57:2a:1520:G:H5'	1.95	0.47
33:2b:16:HIS:CD2	33:2b:204:ASN:H	2.32	0.47
38:2g:79:ARG:NH2	38:2g:80:VAL:HA	2.29	0.47
47:2p:48:TRP:HH2	47:2p:76:GLN:NE2	2.12	0.47
55:2x:55:PSU:O2'	55:2x:57:A:N7	2.45	0.47
56:2y:37:A:H2'	56:2y:38:A:O4'	2.14	0.47
1:1A:236:G:H4'	1:1A:413:G:C5	2.49	0.47
1:1A:2133:C:N4	1:1A:2166:U:O2'	2.46	0.47
1:1A:2175:G:H2'	1:1A:2176:G:H8	1.78	0.47
1:1A:2190:G:N1	1:1A:2193:A:C8	2.81	0.47
32:1a:90:U:O2'	32:1a:91:C:OP1	2.22	0.47
32:1a:1166:G:N2	32:1a:1170:A:OP2	2.47	0.47
32:1a:1220:G:N2	50:1s:54:GLY:O	2.41	0.47
34:1c:69:HIS:CD2	34:1c:104:GLN:HG2	2.49	0.47
56:1y:67:C:H2'	56:1y:68:C:C6	2.49	0.47
1:2A:287:C:H2'	1:2A:288:C:C6	2.49	0.47
1:2A:947:G:H2'	1:2A:948:G:H8	1.77	0.47
1:2A:1147:C:H2'	1:2A:1148:A:H8	1.79	0.47
1:2A:1754:C:OP1	15:2T:96:ARG:NH1	2.47	0.47
1:2A:2609:U:H2'	58:B:5:ASN:ND2	2.29	0.47
13:2R:92:GLY:HA2	13:2R:94:TYR:CZ	2.49	0.47
57:2a:560:U:H5'	57:2a:566:G:N2	2.29	0.47
57:2a:1518:MA6:N6	57:2a:1519:MA6:H103	2.29	0.47
43:2l:57:LYS:HA	43:2l:67:THR:HA	1.96	0.47
49:2r:45:SER:HB3	49:2r:51:LEU:HD21	1.96	0.47
28:16:14:THR:HG21	28:16:48:VAL:HG13	1.96	0.47
32:1a:110:C:O2'	47:1p:25:ARG:O	2.31	0.47
32:1a:236:G:H5''	48:1q:42:TYR:OH	2.14	0.47
38:1g:27:ILE:HD13	38:1g:40:ALA:HA	1.96	0.47
1:2A:829:A:N7	1:2A:2248:C:H5'	2.29	0.47
1:2A:1019:U:OP1	1:2A:1035:U:O2'	2.21	0.47
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.14	0.47
23:21:52:ARG:HH21	23:21:57:GLU:HB2	1.78	0.47
25:23:18:ASP:OD1	25:23:18:ASP:N	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2a:885:G:O2'	57:2a:914:A:N1	2.44	0.47
57:2a:1356:G:H2'	57:2a:1357:A:C8	2.49	0.47
41:2j:35:SER:HB3	41:2j:73:ASP:H	1.79	0.47
44:2m:101:GLN:OE1	44:2m:101:GLN:N	2.42	0.47
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	1.96	0.47
55:2x:15:G:H21	55:2x:21:A:H1'	1.80	0.47
1:1A:928:G:C2	1:1A:929:G:H1'	2.50	0.47
1:1A:1312:G:O5'	18:1W:15:ARG:NH2	2.48	0.47
32:1a:45:U:H2'	32:1a:46:G:C8	2.49	0.47
32:1a:179:A:H2'	32:1a:180:U:H6	1.79	0.47
32:1a:848:C:H2'	32:1a:849:C:C6	2.49	0.47
33:1b:36:ARG:C	33:1b:38:GLY:H	2.23	0.47
48:1q:66:SER:OG	48:1q:69:LYS:HB2	2.13	0.47
55:1x:75:C:H5''	55:1x:76:A:OP2	2.14	0.47
1:2A:821:A:N1	63:2A:4036:HOH:O	2.35	0.47
5:2F:108:LYS:HG2	5:2F:112:MET:HE2	1.97	0.47
8:2I:123:LEU:HD21	8:2I:145:VAL:HA	1.96	0.47
17:2V:1:MET:CE	17:2V:44:LYS:H	2.27	0.47
23:21:4:VAL:HG11	23:21:11:ARG:NH2	2.28	0.47
57:2a:324:G:OP1	51:2t:22:ARG:HD3	2.15	0.47
55:2x:8:4SU:O2	55:2x:21:A:H2	1.96	0.47
9:1N:96:GLU:H	9:1N:96:GLU:CD	2.23	0.47
13:1R:28:LEU:HD22	13:1R:44:LEU:HD13	1.94	0.47
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.48	0.47
34:1c:58:GLU:H	34:1c:65:ALA:HB3	1.79	0.47
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.95	0.47
56:1y:36:A:H2'	56:1y:37:A:O4'	2.14	0.47
1:2A:212:G:H2'	1:2A:213:A:O4'	2.14	0.47
1:2A:1695:G:N7	3:2D:14:ARG:NH2	2.62	0.47
1:2A:2180:U:H2'	1:2A:2181:G:O4'	2.13	0.47
1:2A:2506:U:O2'	54:2w:76:A:H4'	2.14	0.47
1:2A:2732:G:H3'	1:2A:2733:A:O4'	2.15	0.47
6:2G:120:LEU:HD12	6:2G:178:PHE:HB3	1.95	0.47
57:2a:160:A:H1'	57:2a:344:A:N7	2.29	0.47
34:2c:9:GLY:HA3	45:2n:49:HIS:HA	1.97	0.47
37:2f:61:LEU:HB3	37:2f:63:TYR:HE2	1.78	0.47
42:2k:48:ILE:C	42:2k:50:TYR:H	2.22	0.47
1:1A:347:G:C8	5:1F:171:PRO:HG3	2.49	0.47
1:1A:660:C:O2'	1:1A:664:U:OP1	2.25	0.47
1:1A:768:C:H2'	1:1A:769:A:C8	2.50	0.47
1:1A:1470:G:H2'	1:1A:1471:G:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	1.96	0.47
13:1R:38:VAL:HG22	13:1R:112:ALA:HB2	1.96	0.47
17:1V:49:THR:HG22	17:1V:49:THR:O	2.15	0.47
32:1a:134:A:H61	47:1p:25:ARG:HH12	1.62	0.47
1:2A:288:C:H2'	1:2A:289:A:H8	1.80	0.47
1:2A:2438:U:O2'	1:2A:2440:C:OP1	2.26	0.47
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	1.97	0.47
57:2a:1006:C:H2'	57:2a:1007:C:C6	2.49	0.47
57:2a:1272:G:N2	57:2a:1273:G:C4	2.82	0.47
57:2a:1347:G:O2'	57:2a:1373:G:N1	2.45	0.47
33:2b:189:ASP:O	33:2b:192:SER:OG	2.31	0.47
47:2p:15:PRO:HD2	47:2p:42:ARG:HD2	1.97	0.47
1:1A:1074:A:N6	1:1A:1171:G:H2'	2.30	0.47
5:1F:28:ILE:O	5:1F:30:PRO:HD3	2.15	0.47
7:1H:97:ARG:NE	7:1H:104:GLU:OE1	2.47	0.47
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.48	0.47
11:1P:101:VAL:HG21	11:1P:108:LYS:HG2	1.96	0.47
28:16:38:LYS:HE3	28:16:38:LYS:HB3	1.51	0.47
32:1a:184:G:H2'	32:1a:185:A:C8	2.49	0.47
32:1a:266:G:H2'	32:1a:266:G:N3	2.28	0.47
32:1a:1004:A:C5'	32:1a:1024:G:H1	2.27	0.47
32:1a:1236:A:H4'	32:1a:1304:G:H4'	1.97	0.47
32:1a:1279:A:H5''	32:1a:1280:A:OP1	2.15	0.47
37:1f:89:MET:HG2	37:1f:91:VAL:HG23	1.95	0.47
39:1h:91:ARG:HD3	48:1q:32:TYR:O	2.14	0.47
48:1q:83:ASP:N	48:1q:83:ASP:OD1	2.48	0.47
55:1x:67:C:H2'	55:1x:68:C:H6	1.79	0.47
1:2A:265:A:C8	1:2A:266:G:H1'	2.49	0.47
1:2A:323:G:O2'	1:2A:1205:U:N3	2.33	0.47
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.49	0.47
1:2A:1754:C:H5	15:2T:96:ARG:NH2	2.12	0.47
1:2A:1833:U:OP1	63:2A:3956:HOH:O	2.20	0.47
1:2A:2473:U:O2	1:2A:2473:U:H2'	2.14	0.47
2:2B:105:A:H5'	2:2B:106:G:OP2	2.15	0.47
4:2E:9:VAL:HG22	4:2E:25:VAL:HB	1.95	0.47
4:2E:111:ARG:HD3	4:2E:160:TYR:CE2	2.49	0.47
5:2F:9:ILE:HG21	5:2F:125:LEU:HD13	1.97	0.47
7:2H:3:ARG:HH11	7:2H:4:ILE:H	1.61	0.47
12:2Q:26:TYR:O	12:2Q:67:ARG:NH1	2.40	0.47
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.15	0.47
21:2Z:73:GLN:HB3	21:2Z:87:ASP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2a:1062:U:H2'	57:2a:1063:C:C6	2.49	0.47
57:2a:1068:G:H8	57:2a:1068:G:OP2	1.97	0.47
57:2a:1358:U:H5'	45:2n:34:TYR:CD1	2.49	0.47
34:2c:6:HIS:HB3	45:2n:49:HIS:ND1	2.30	0.47
34:2c:20:SER:HB3	34:2c:22:TRP:NE1	2.30	0.47
36:2e:20:GLN:NE2	36:2e:21:ALA:O	2.48	0.47
38:2g:79:ARG:HH21	38:2g:80:VAL:HA	1.80	0.47
41:2j:13:HIS:HB3	41:2j:68:HIS:CE1	2.50	0.47
48:2q:45:HIS:CD2	48:2q:47:PRO:HD3	2.49	0.47
54:2w:29:G:H2'	54:2w:30:G:C8	2.50	0.47
56:2y:28:G:H2'	56:2y:29:G:H8	1.80	0.47
56:2y:57:G:H2'	56:2y:58:A:H5'	1.97	0.47
1:1A:1136:U:C2	1:1A:1148:C:H1'	2.50	0.47
7:1H:84:SER:OG	7:1H:132:ARG:NH1	2.48	0.47
32:1a:946:A:H2'	32:1a:947:G:C8	2.50	0.47
40:1i:117:HIS:HB2	40:1i:121:ARG:HG2	1.96	0.47
1:2A:643:A:N1	1:2A:2369:A:O2'	2.38	0.47
31:29:7:VAL:HG12	31:29:34:GLN:HB3	1.97	0.47
57:2a:336:C:H2'	57:2a:337:C:C6	2.49	0.47
57:2a:1130:A:HO2'	40:2i:3:GLN:HE22	1.58	0.47
57:2a:1241:G:H2'	57:2a:1242:C:C6	2.50	0.47
40:2i:18:PHE:HD2	40:2i:62:TYR:HD2	1.61	0.47
54:2w:19:G:N2	54:2w:57:G:H1'	2.30	0.47
1:1A:886:U:H2'	1:1A:887:C:C6	2.50	0.47
1:1A:956:A:N1	1:1A:2289:G:H1'	2.29	0.47
1:1A:2157:A:H5'	1:1A:2182:G:H4'	1.97	0.47
1:1A:2318:C:O2	63:1G:5001:HOH:O	2.15	0.47
6:1G:15:VAL:HG22	6:1G:175:LEU:HB3	1.96	0.47
11:1P:90:ARG:NH1	11:1P:105:LEU:HD11	2.30	0.47
24:12:32:LEU:HD22	24:12:36:ARG:NH1	2.30	0.47
25:13:18:ASP:OD1	25:13:18:ASP:N	2.48	0.47
26:14:48:ARG:HD3	26:14:48:ARG:HA	1.66	0.47
32:1a:1060:C:OP1	45:1n:45:ARG:NH2	2.42	0.47
46:1o:18:PHE:CE2	46:1o:21:ASP:HB2	2.50	0.47
1:2A:328:U:H4'	20:2Y:68:HIS:CD2	2.50	0.47
4:2E:5:LEU:HD22	4:2E:197:ILE:HG12	1.96	0.47
6:2G:123:ASN:O	6:2G:125:PHE:N	2.48	0.47
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.97	0.47
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.50	0.47
10:2O:120:GLU:HG2	10:2O:122:LEU:HG	1.97	0.47
21:2Z:73:GLN:O	21:2Z:87:ASP:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2a:662:G:H2'	57:2a:663:A:C8	2.49	0.47
57:2a:828:A:H2'	57:2a:829:G:O4'	2.14	0.47
53:2v:12:A:N3	53:2v:12:A:H2'	2.30	0.47
56:2y:15:G:N1	56:2y:48:C:N3	2.54	0.47
1:1A:1091:A:OP1	1:1A:1092:A:H3'	2.15	0.47
1:1A:2053:A:C6	1:1A:2510:C:H1'	2.50	0.47
5:1F:133:ASN:N	5:1F:138:GLU:OE1	2.31	0.47
7:1H:41:MET:HE1	7:1H:54:ARG:HB3	1.96	0.47
12:1Q:60:ARG:HH11	12:1Q:60:ARG:HB2	1.78	0.47
32:1a:56:U:H2'	32:1a:57:G:C8	2.50	0.47
48:1q:15:MET:HE1	48:1q:43:LEU:HD22	1.97	0.47
1:2A:652(B):A:N6	1:2A:655:A:H1'	2.30	0.47
1:2A:1005:C:O2'	9:2N:28:THR:HG21	2.15	0.47
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.49	0.47
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.14	0.47
1:2A:2112:G:H2'	1:2A:2113:U:O4'	2.15	0.47
1:2A:2184:G:H2'	1:2A:2185:C:C6	2.50	0.47
3:2D:73:VAL:HG13	3:2D:120:GLY:HA3	1.97	0.47
7:2H:18:GLU:HG3	7:2H:25:LYS:HB3	1.96	0.47
57:2a:1054:C:C5	54:2w:34:G:H1'	2.50	0.47
57:2a:1132:C:H2'	57:2a:1133:G:H8	1.79	0.47
57:2a:1345:U:H2'	63:2a:3410:HOH:O	2.16	0.47
41:2j:38:ILE:HG12	41:2j:71:LEU:O	2.15	0.47
56:2y:2:C:H2'	56:2y:3:C:H6	1.80	0.47
1:1A:646:A:OP2	11:1P:108:LYS:NZ	2.48	0.46
1:1A:1410:G:P	23:11:3:LYS:HG3	2.55	0.46
1:1A:1451:U:H2'	1:1A:1452:U:C6	2.51	0.46
1:1A:1639:G:H2'	1:1A:1640:G:C8	2.50	0.46
32:1a:739:C:O2'	46:1o:42:HIS:ND1	2.44	0.46
32:1a:1429:C:H2'	32:1a:1430:C:C6	2.50	0.46
46:1o:56:LEU:O	46:1o:60:VAL:HG23	2.15	0.46
48:1q:6:LEU:HD13	48:1q:71:PHE:HE2	1.79	0.46
1:2A:1639:U:H2'	1:2A:1640:C:H5''	1.96	0.46
1:2A:2134:A:H2'	1:2A:2134:A:N3	2.29	0.46
57:2a:434:U:H2'	57:2a:435:C:C6	2.50	0.46
57:2a:1109:C:H2'	57:2a:1110:A:O4'	2.14	0.46
57:2a:1381:U:H1'	38:2g:79:ARG:HG2	1.96	0.46
37:2f:35:ALA:HA	37:2f:67:MET:HB3	1.97	0.46
1:1A:1132:A:H5'	1:1A:1133:G:OP1	2.15	0.46
18:1W:4:LYS:HD2	18:1W:6:ILE:HD11	1.97	0.46
34:1c:11:ARG:NH2	34:1c:177:THR:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:60:GLU:HG3	35:1d:202:LEU:HD12	1.98	0.46
55:1x:67:C:H2'	55:1x:68:C:C6	2.50	0.46
1:2A:445:C:OP1	16:2U:2:PRO:HA	2.14	0.46
1:2A:1169:G:N2	1:2A:1181:C:N3	2.62	0.46
8:2I:122:GLU:O	8:2I:126:TYR:OH	2.31	0.46
21:2Z:97:GLU:HA	21:2Z:126:VAL:O	2.15	0.46
57:2a:955:U:O2'	50:2s:83:HIS:HD2	1.97	0.46
44:2m:82:MET:O	44:2m:93:ARG:NH2	2.44	0.46
1:1A:360:C:OP1	20:1Y:84:ARG:HG2	2.15	0.46
1:1A:1314:A:C2	1:1A:2035:A:C4	3.04	0.46
1:1A:1473:A:H4'	1:1A:1474:C:O4'	2.16	0.46
1:1A:1495:G:H4'	1:1A:1589:A:OP1	2.16	0.46
1:1A:2091:G:OP2	63:1A:4358:HOH:O	2.21	0.46
9:1N:108:PRO:O	9:1N:113:GLY:HA3	2.15	0.46
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.95	0.46
32:1a:376:G:H5''	47:1p:5:ARG:HB2	1.98	0.46
33:1b:60:ASP:O	33:1b:64:ARG:HG2	2.16	0.46
56:1y:57:G:H2'	56:1y:58:A:H5'	1.97	0.46
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.51	0.46
14:2S:14:VAL:HG21	14:2S:90:GLY:O	2.15	0.46
57:2a:1020:U:H2'	57:2a:1021:G:H8	1.79	0.46
39:2h:7:ALA:O	39:2h:11:THR:OG1	2.25	0.46
43:2l:117:ARG:HG2	43:2l:122:THR:HB	1.97	0.46
46:2o:15:PHE:CE1	46:2o:84:LYS:HD3	2.50	0.46
1:1A:555:G:N1	1:1A:2045:G:OP1	2.33	0.46
1:1A:605:G:OP2	63:1A:4357:HOH:O	2.20	0.46
1:1A:1101:G:H1	1:1A:1150:C:N4	2.10	0.46
1:1A:1405:A:C2	1:1A:1418:U:O4	2.65	0.46
1:1A:2130:C:H2'	1:1A:2131:U:H6	1.81	0.46
1:1A:2203:G:O2'	1:1A:2204:G:OP1	2.33	0.46
1:1A:2298:A:H4'	1:1A:2299:A:O4'	2.15	0.46
25:13:7:LYS:HE3	25:13:32:GLN:NE2	2.31	0.46
32:1a:69:G:H2'	32:1a:70:G:C8	2.50	0.46
47:1p:43:LYS:HG2	47:1p:48:TRP:CE2	2.50	0.46
56:1y:48:C:C2	56:1y:59:U:H1'	2.50	0.46
1:2A:582:G:H2'	1:2A:583:G:C8	2.51	0.46
5:2F:178:PRO:HB2	5:2F:201:VAL:HG21	1.96	0.46
14:2S:3:ARG:HD3	14:2S:4:LEU:H	1.80	0.46
57:2a:12:U:H4'	57:2a:526:C:O2'	2.16	0.46
57:2a:109:A:C6	57:2a:326:G:C6	3.03	0.46
57:2a:376:G:H5''	47:2p:5:ARG:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:31:TYR:CE2	33:2b:200:ILE:HG21	2.51	0.46
38:2g:74:GLU:HG2	38:2g:91:VAL:HG22	1.98	0.46
54:2w:7:A:H5'	54:2w:8:4SU:H5	1.97	0.46
1:1A:2623:U:H6	1:1A:2623:U:H5'	1.80	0.46
32:1a:435:C:H2'	32:1a:436:C:H6	1.80	0.46
32:1a:685:G:O2'	32:1a:686:U:H5'	2.16	0.46
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.50	0.46
33:1b:74:LYS:HD2	33:1b:166:ASP:HB2	1.97	0.46
35:1d:155:LEU:HB2	35:1d:158:ILE:HG12	1.97	0.46
1:2A:242:G:C8	30:28:5:LYS:HG2	2.50	0.46
1:2A:274:G:H2'	1:2A:275:G:C8	2.50	0.46
1:2A:302:C:OP2	20:2Y:73:ARG:NH1	2.47	0.46
1:2A:2558:C:H2'	1:2A:2559:C:O4'	2.16	0.46
57:2a:54:C:N4	57:2a:353:A:OP2	2.45	0.46
57:2a:97:G:H2'	57:2a:98:G:O4'	2.15	0.46
57:2a:457:C:H2'	57:2a:458:C:H6	1.80	0.46
57:2a:792:A:H4'	57:2a:793:U:H5''	1.97	0.46
57:2a:876:G:O5'	39:2h:14:ARG:NH1	2.49	0.46
57:2a:937:A:H1'	57:2a:1379:G:N2	2.30	0.46
57:2a:1259:C:C4	57:2a:1260:C:H1'	2.51	0.46
47:2p:22:THR:HA	47:2p:33:ILE:HG13	1.98	0.46
1:1A:2143:G:H2'	1:1A:2144:U:C6	2.51	0.46
3:1D:127:VAL:HA	3:1D:193:VAL:HG22	1.97	0.46
5:1F:74:ARG:H	5:1F:74:ARG:HG3	1.35	0.46
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.51	0.46
30:18:8:LYS:O	30:18:12:LYS:HG3	2.16	0.46
32:1a:767:A:H2'	32:1a:768:A:O4'	2.15	0.46
32:1a:1531:A:H8	32:1a:1531:A:O5'	1.98	0.46
33:1b:88:ALA:HB2	33:1b:219:VAL:HG13	1.96	0.46
33:1b:91:PRO:HG2	33:1b:155:LEU:HD13	1.98	0.46
41:1j:11:PHE:CE1	41:1j:67:THR:HG22	2.50	0.46
49:1r:47:THR:HG23	49:1r:49:LYS:HG3	1.96	0.46
50:1s:12:ASP:OD2	50:1s:35:SER:OG	2.20	0.46
54:1w:51:U:H2'	54:1w:52:G:H8	1.80	0.46
56:1y:8:4SU:H4'	56:1y:48:C:H4'	1.98	0.46
1:2A:274:G:H2'	1:2A:275:G:H8	1.80	0.46
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.27	0.46
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	1.98	0.46
1:2A:2115:G:H4'	1:2A:2167:U:C4	2.51	0.46
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.31	0.46
1:2A:2376:A:N3	14:2S:106:ARG:NH2	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:1:U:H2'	2:2B:2:C:C6	2.50	0.46
6:2G:131:TYR:HB3	6:2G:159:VAL:HG13	1.96	0.46
15:2T:109:GLU:HG2	15:2T:112:ARG:NH2	2.31	0.46
57:2a:309:G:O2'	57:2a:607:A:N1	2.48	0.46
57:2a:405:U:O4	35:2d:2:GLY:N	2.49	0.46
33:2b:162:ILE:HD11	33:2b:184:VAL:HG22	1.97	0.46
33:2b:212:GLN:NE2	33:2b:235:SER:HA	2.31	0.46
35:2d:148:VAL:HG12	35:2d:153:ARG:HG2	1.97	0.46
1:1A:927:G:H1	1:1A:944:C:N4	2.12	0.46
1:1A:1735:U:O2'	1:1A:1747:A:N7	2.43	0.46
1:1A:2142:G:C2'	1:1A:2143:G:H5'	2.46	0.46
1:1A:2178:G:OP2	1:1A:2178:G:H8	1.98	0.46
1:1A:2494:G:O3'	54:1w:64:A:H4'	2.16	0.46
1:1A:2764:G:C4	7:1H:2:SER:HA	2.51	0.46
9:1N:48:MET:HE3	9:1N:48:MET:HB3	1.64	0.46
12:1Q:134:ARG:NH2	21:1Z:122:ARG:HE	2.14	0.46
32:1a:407:G:H2'	32:1a:408:A:C8	2.51	0.46
46:1o:8:LYS:HE3	46:1o:31:LEU:HD22	1.98	0.46
1:2A:581:C:H2'	1:2A:582:G:C8	2.51	0.46
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.15	0.46
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.46	0.46
57:2a:524:G:H2'	57:2a:525:C:C6	2.50	0.46
57:2a:1245:A:H2'	57:2a:1246:C:O4'	2.16	0.46
40:2i:55:ALA:HA	40:2i:58:HIS:HD2	1.81	0.46
42:2k:73:MET:HG2	42:2k:103:LEU:HD21	1.96	0.46
1:1A:1221:G:N2	1:1A:1223:C:OP2	2.48	0.46
1:1A:1554:A:O2'	1:1A:1555:C:H5''	2.15	0.46
4:1E:12:THR:HG22	15:1T:58:ASN:OD1	2.15	0.46
6:1G:114:ILE:HB	6:1G:117:PHE:HB2	1.98	0.46
8:1I:124:GLY:H	8:1I:144:VAL:HG23	1.81	0.46
16:1U:46:ALA:O	16:1U:50:ARG:HG2	2.16	0.46
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.66	0.46
32:1a:254:G:O2'	48:1q:16:GLN:O	2.34	0.46
51:1t:43:LEU:O	51:1t:47:GLY:N	2.37	0.46
1:2A:35:G:H2'	1:2A:36:G:O4'	2.16	0.46
1:2A:492:A:H2'	1:2A:493:G:O4'	2.16	0.46
1:2A:2129:C:H5'	1:2A:2130:U:OP2	2.16	0.46
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.97	0.46
21:2Z:93:ASP:HB3	21:2Z:131:ARG:HH22	1.81	0.46
57:2a:999:C:N3	57:2a:1042:G:N2	2.55	0.46
49:2r:53:ARG:HH21	49:2r:59:SER:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1324:A:OP1	13:1R:36:THR:HG23	2.16	0.46
1:1A:1476:C:H2'	1:1A:1477:U:C6	2.50	0.46
1:1A:2658:C:H2'	1:1A:2659:U:O4'	2.15	0.46
1:1A:2863:C:H2'	1:1A:2864:G:C8	2.51	0.46
5:1F:64:ILE:HG21	5:1F:78:ILE:HG23	1.98	0.46
11:1P:97:PRO:HD3	11:1P:126:VAL:O	2.15	0.46
16:1U:104:GLN:NE2	16:1U:105:VAL:HG23	2.31	0.46
32:1a:78:G:O2'	32:1a:79:G:H5'	2.16	0.46
32:1a:1028:C:H2'	32:1a:1029:C:O4'	2.16	0.46
44:1m:123:ALA:HB2	54:1w:39:PSU:H1'	1.97	0.46
1:2A:639:U:H2'	1:2A:640:C:C6	2.51	0.46
1:2A:1924:C:H4'	55:2x:13:C:O2'	2.16	0.46
1:2A:2059:A:O2'	5:2F:69:HIS:HD2	1.98	0.46
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.33	0.46
2:2B:55:U:H1'	6:2G:29:TRP:CD1	2.51	0.46
7:2H:4:ILE:O	7:2H:69:ARG:HD2	2.15	0.46
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	1.96	0.46
9:2N:99:LEU:HD22	9:2N:103:VAL:HG23	1.98	0.46
15:2T:18:ASP:OD1	15:2T:18:ASP:N	2.36	0.46
21:2Z:75:ASN:O	21:2Z:84:GLU:HG3	2.16	0.46
25:23:7:LYS:HE3	25:23:32:GLN:NE2	2.31	0.46
57:2a:1054:C:C4	54:2w:34:G:H1'	2.50	0.46
57:2a:1142:G:H2'	57:2a:1143:G:O4'	2.15	0.46
57:2a:1219:U:OP1	45:2n:19:ARG:NH1	2.40	0.46
57:2a:1304:G:C6	57:2a:1305:G:N1	2.84	0.46
34:2c:34:LEU:HD11	34:2c:38:ARG:NH2	2.31	0.46
1:1A:602:G:H2'	1:1A:603:C:C6	2.51	0.46
1:1A:1051:C:H5''	63:1A:4773:HOH:O	2.16	0.46
1:1A:1093:G:HO2'	1:1A:1094:A:P	2.39	0.46
1:1A:2418:U:H2'	1:1A:2418:U:OP2	2.17	0.46
25:13:8:LEU:HG	25:13:31:LEU:HD23	1.98	0.46
26:14:33:VAL:HG12	26:14:35:VAL:H	1.81	0.46
27:15:48:GLU:O	27:15:60:VAL:HG11	2.15	0.46
32:1a:222:U:H2'	32:1a:223:U:C6	2.51	0.46
32:1a:737:A:H2'	32:1a:738:C:C6	2.51	0.46
32:1a:1030(D):A:H2'	32:1a:1031:G:H4'	1.97	0.46
32:1a:1469:G:H2'	32:1a:1470:G:H8	1.79	0.46
35:1d:18:LYS:HD2	35:1d:20:TYR:CZ	2.51	0.46
35:1d:101:LEU:HB2	35:1d:138:TYR:HB3	1.97	0.46
1:2A:839:U:H2'	1:2A:840:C:C6	2.51	0.46
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.81	0.46
4:2E:2:LYS:HB2	4:2E:95:ILE:HD12	1.98	0.46
57:2a:7:G:H21	36:2e:121:LYS:HG2	1.80	0.46
57:2a:1328:C:O2'	44:2m:29:ARG:NH2	2.47	0.46
39:2h:91:ARG:HD3	48:2q:33:GLY:HA3	1.96	0.46
1:1A:44:G:H5''	1:1A:45:C:OP1	2.15	0.45
1:1A:1091:A:O2'	1:1A:1093:G:C4	2.68	0.45
1:1A:1103:A:N6	1:1A:1133:G:OP2	2.49	0.45
1:1A:1845:G:H4'	3:1D:51:VAL:HG21	1.98	0.45
1:1A:2148:A:N1	1:1A:2184:G:O2'	2.35	0.45
1:1A:2285:A:H2'	1:1A:2286:A:C8	2.51	0.45
1:1A:2291:G:O6	22:10:14:ARG:HG3	2.15	0.45
1:1A:2638:C:H2'	1:1A:2639:G:O4'	2.15	0.45
35:1d:194:LEU:HD23	35:1d:194:LEU:HA	1.69	0.45
37:1f:75:LEU:O	37:1f:79:LEU:HG	2.16	0.45
46:1o:29:VAL:HG11	46:1o:67:LEU:HD21	1.97	0.45
1:2A:271(X):G:C2	1:2A:271(Y):U:O4	2.68	0.45
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.15	0.45
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.51	0.45
8:2I:93:THR:N	8:2I:96:ASP:HB2	2.31	0.45
10:2O:15:GLY:O	10:2O:47:ILE:HG12	2.17	0.45
13:2R:63:ARG:O	13:2R:67:LEU:HB2	2.16	0.45
13:2R:72:ASP:O	13:2R:76:VAL:HG23	2.16	0.45
17:2V:1:MET:HE3	17:2V:43:GLU:H	1.80	0.45
57:2a:129(A):G:C6	57:2a:189(E):U:H4'	2.51	0.45
57:2a:189(A):C:H2'	57:2a:189(B):C:H6	1.81	0.45
57:2a:411:A:H2'	57:2a:412:A:H4'	1.98	0.45
57:2a:1023:G:H3'	57:2a:1024:G:H8	1.80	0.45
57:2a:1201:A:H4'	57:2a:1202:G:O5'	2.16	0.45
57:2a:1261:A:H5'	57:2a:1284:C:OP1	2.16	0.45
1:1A:2660:C:H2'	1:1A:2661:U:C6	2.52	0.45
1:1A:2801:C:P	4:1E:61:ARG:HH21	2.38	0.45
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.51	0.45
32:1a:300:A:H1'	32:1a:565:U:O2	2.16	0.45
1:2A:686:G:N2	1:2A:788:A:H61	2.13	0.45
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.51	0.45
26:24:47:GLN:C	26:24:49:PHE:H	2.24	0.45
57:2a:1077:G:N1	57:2a:1080:A:OP2	2.48	0.45
57:2a:1176:A:H2'	57:2a:1177:G:C8	2.52	0.45
57:2a:1264:C:N3	57:2a:1271:G:N2	2.54	0.45
35:2d:5:ILE:HA	35:2d:115:ARG:HH22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:64:LEU:HB2	35:2d:198:VAL:HG11	1.98	0.45
40:2i:105:ASP:HB2	40:2i:107:ARG:HG3	1.97	0.45
1:1A:310:C:H2'	1:1A:311:C:H6	1.81	0.45
1:1A:927:G:H2'	1:1A:928:G:C8	2.41	0.45
1:1A:1081:U:H2'	1:1A:1082:G:C8	2.51	0.45
1:1A:1766:G:H1'	1:1A:1770:A:H61	1.81	0.45
3:1D:242:ARG:N	3:1D:242:ARG:HD3	2.31	0.45
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	1.98	0.45
23:11:56:GLN:HE21	23:11:87:PRO:HG3	1.80	0.45
25:13:29:ARG:HD2	63:13:3104:HOH:O	2.17	0.45
32:1a:977:A:H1'	32:1a:982:U:O4	2.17	0.45
32:1a:1064:G:H4'	32:1a:1065:U:OP1	2.16	0.45
32:1a:1066:C:O2'	32:1a:1067:A:H5'	2.17	0.45
33:1b:59:GLU:HB3	33:1b:221:LEU:HD11	1.98	0.45
40:1i:8:GLY:HA3	40:1i:76:ALA:O	2.17	0.45
41:1j:64:GLU:OE2	41:1j:66:ARG:NE	2.45	0.45
43:1l:113:ARG:HA	43:1l:113:ARG:HD2	1.64	0.45
44:1m:37:THR:O	44:1m:55:ARG:NH1	2.29	0.45
1:2A:902:C:H2'	1:2A:903:C:C6	2.51	0.45
1:2A:1042:G:C5	1:2A:1043:C:H5	2.35	0.45
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.51	0.45
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.99	0.45
1:2A:2467:C:H4'	12:2Q:123:HIS:CD2	2.51	0.45
1:2A:2815:C:H2'	1:2A:2816:C:C6	2.51	0.45
8:2I:50:ARG:NH2	63:2I:5001:HOH:O	2.45	0.45
8:2I:134:PRO:C	8:2I:136:VAL:H	2.24	0.45
21:2Z:28:MET:HE2	21:2Z:35:ARG:HB2	1.99	0.45
57:2a:44:G:C2	57:2a:45:U:H1'	2.52	0.45
57:2a:299:G:H8	57:2a:299:G:O5'	1.99	0.45
57:2a:1442:G:O2'	57:2a:1442(A):G:H5'	2.17	0.45
33:2b:24:TRP:CZ3	33:2b:26:PRO:HA	2.51	0.45
38:2g:27:ILE:HD13	38:2g:40:ALA:HA	1.98	0.45
38:2g:69:VAL:HG22	38:2g:135:VAL:HG22	1.97	0.45
1:1A:2255:U:H2'	1:1A:2256:U:C6	2.51	0.45
5:1F:95:ARG:HD3	5:1F:97:TYR:CZ	2.52	0.45
32:1a:262:A:C6	32:1a:263:A:C6	3.04	0.45
32:1a:1159:U:OP1	33:1b:133:LYS:NZ	2.49	0.45
1:2A:1805:U:O2	3:2D:50:THR:HB	2.17	0.45
1:2A:2067:G:O2'	1:2A:2069:G:H5'	2.15	0.45
1:2A:2184:G:O2'	1:2A:2185:C:H5'	2.16	0.45
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:33:G:H5'	6:2G:2:PRO:HD3	1.97	0.45
14:2S:77:ALA:HB1	14:2S:82:ILE:HB	1.98	0.45
16:2U:49:HIS:HA	16:2U:52:ARG:HB2	1.97	0.45
23:21:81:LYS:HE2	23:21:81:LYS:HB3	1.78	0.45
57:2a:714:G:H2'	57:2a:715:A:C8	2.51	0.45
57:2a:1271:G:N1	57:2a:1272:G:O6	2.49	0.45
36:2e:12:LEU:O	36:2e:30:ALA:HA	2.16	0.45
38:2g:113:GLU:HB2	38:2g:119:ARG:HG2	1.98	0.45
1:1A:1116:A:N7	1:1A:1142:A:O2'	2.44	0.45
1:1A:1140:U:H2'	1:1A:1141:A:C8	2.51	0.45
1:1A:1821:C:H2'	1:1A:1822:A:C5	2.51	0.45
1:1A:2218:C:O2'	1:1A:2219:U:H5'	2.15	0.45
10:1O:48:PRO:CB	32:1a:1422:G:H5''	2.47	0.45
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.50	0.45
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.51	0.45
32:1a:1027:C:C4	32:1a:1034:G:N1	2.85	0.45
54:1w:18:G:H4'	54:1w:60:U:C6	2.51	0.45
54:1w:37:MIA:H162	54:1w:37:MIA:H121	1.68	0.45
1:2A:621:A:OP2	11:2P:108:LYS:NZ	2.45	0.45
2:2B:94:C:H2'	2:2B:95:C:C6	2.52	0.45
3:2D:274:ARG:O	3:2D:275:LYS:HD2	2.16	0.45
6:2G:150:ASP:OD1	6:2G:150:ASP:N	2.48	0.45
8:2I:116:LEU:HD11	8:2I:120:ILE:HG13	1.99	0.45
19:2X:5:TYR:CE2	24:22:30:ARG:HB2	2.51	0.45
20:2Y:19:LYS:HE2	20:2Y:20:TYR:CE2	2.52	0.45
26:24:1:MET:HE2	26:24:6:HIS:CD2	2.52	0.45
57:2a:576:G:O6	57:2a:880:C:O2'	2.29	0.45
57:2a:1306:A:H2'	57:2a:1307:U:O4'	2.16	0.45
57:2a:1402:4OC:CM2	57:2a:1403:C:H5'	2.46	0.45
33:2b:27:LYS:HD2	33:2b:193:ASP:OD1	2.16	0.45
42:2k:33:THR:HG22	42:2k:39:PRO:HA	1.98	0.45
44:2m:60:VAL:HG12	44:2m:66:LEU:HD11	1.98	0.45
1:1A:704:U:H2'	1:1A:705:C:H6	1.82	0.45
1:1A:1403:U:H2'	1:1A:1404:G:O4'	2.16	0.45
1:1A:1686:U:O2'	1:1A:1687:C:H5'	2.17	0.45
6:1G:82:LEU:HD21	6:1G:88:ILE:HG21	1.98	0.45
21:1Z:8:TYR:HB2	21:1Z:38:TYR:CE2	2.51	0.45
32:1a:193:C:H2'	32:1a:194:C:H6	1.82	0.45
32:1a:1370:G:N7	63:1a:3643:HOH:O	2.36	0.45
35:1d:108:LEU:HD23	35:1d:110:PHE:CZ	2.52	0.45
1:2A:920:G:H2'	1:2A:921:G:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.52	0.45
1:2A:2747:G:O6	1:2A:2755:C:H5''	2.17	0.45
2:2B:13:A:O2'	2:2B:14:U:H3'	2.17	0.45
3:2D:242:ARG:N	3:2D:242:ARG:HD3	2.32	0.45
7:2H:149:ARG:HG3	7:2H:162:ILE:O	2.16	0.45
9:2N:58:ASP:OD1	9:2N:58:ASP:N	2.47	0.45
16:2U:16:LYS:HE2	16:2U:16:LYS:HB3	1.64	0.45
57:2a:202:U:H3'	57:2a:203:U:C5	2.51	0.45
57:2a:340:U:H2'	57:2a:341:C:C6	2.52	0.45
57:2a:458:C:H2'	57:2a:460:G:O4'	2.16	0.45
57:2a:542:G:OP1	35:2d:10:ARG:NH2	2.35	0.45
57:2a:921:U:H2'	57:2a:922:G:O4'	2.16	0.45
57:2a:1005:A:OP1	57:2a:1006:C:N4	2.49	0.45
57:2a:1240:U:OP2	38:2g:115:ARG:HA	2.17	0.45
33:2b:73:THR:HA	33:2b:94:ASN:O	2.16	0.45
34:2c:87:LEU:O	34:2c:91:LEU:N	2.44	0.45
43:2l:24:VAL:HB	43:2l:27:LEU:HD22	1.99	0.45
56:2y:26:A:N6	56:2y:44:G:C6	2.85	0.45
1:1A:1067:A:H3'	1:1A:1067:A:N3	2.32	0.45
1:1A:1604:C:H5''	1:1A:1605:A:OP2	2.16	0.45
1:1A:1733:C:H2'	1:1A:1734:G:O4'	2.16	0.45
1:1A:1952:G:O2'	1:1A:1990:G:O6	2.23	0.45
1:1A:2331:G:N2	14:1S:3:ARG:HA	2.32	0.45
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.81	0.45
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.98	0.45
32:1a:232:G:H1'	32:1a:262:A:N1	2.31	0.45
32:1a:584:G:H2'	32:1a:585:G:C8	2.52	0.45
32:1a:619:U:N3	35:1d:134:ASP:OD1	2.46	0.45
32:1a:1272:G:H2'	32:1a:1273:G:O4'	2.17	0.45
1:2A:644:A:H4'	1:2A:645:C:C4	2.52	0.45
1:2A:1374:G:H2'	1:2A:1375:C:C6	2.52	0.45
1:2A:2408:U:H2'	1:2A:2409:G:C8	2.51	0.45
3:2D:275:LYS:HA	3:2D:276:LYS:C	2.42	0.45
13:2R:33:ARG:NH1	13:2R:115:GLU:OE1	2.43	0.45
57:2a:509:A:O2'	57:2a:510:A:OP1	2.28	0.45
57:2a:892:A:O2'	57:2a:1415:G:H4'	2.17	0.45
57:2a:1134:G:H1	57:2a:1140:C:N4	2.12	0.45
57:2a:1328:C:O2'	44:2m:29:ARG:NE	2.45	0.45
33:2b:31:TYR:HE2	33:2b:200:ILE:HG21	1.82	0.45
40:2i:32:ASP:HB3	40:2i:35:GLU:HB2	1.98	0.45
40:2i:82:ALA:HA	40:2i:85:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:2x:44:A:H2'	55:2x:45:G:C8	2.51	0.45
1:1A:273:G:O2'	1:1A:274:U:H5''	2.17	0.45
1:1A:945:A:H2'	1:1A:945:A:N3	2.32	0.45
1:1A:1140:U:N3	1:1A:1142:A:H5'	2.31	0.45
3:1D:8:PRO:HB3	3:1D:14:ARG:HG2	1.98	0.45
19:1X:12:VAL:HG21	19:1X:27:THR:HG22	1.99	0.45
23:11:56:GLN:HB2	23:11:90:ILE:HD12	1.99	0.45
36:1e:116:THR:HG23	36:1e:117:ASP:OD2	2.17	0.45
37:1f:76:ALA:O	37:1f:80:ARG:HG3	2.16	0.45
1:2A:191:A:H2'	1:2A:192:C:C6	2.51	0.45
1:2A:1300:U:H4'	1:2A:1301:A:H5''	1.98	0.45
1:2A:1837:C:OP1	57:2a:784:C:H4'	2.17	0.45
1:2A:2029:G:H2'	1:2A:2031:A:OP1	2.15	0.45
1:2A:2137:C:N3	1:2A:2155:G:N1	2.65	0.45
1:2A:2512:C:H2'	1:2A:2513:G:O4'	2.16	0.45
11:2P:121:LYS:HD3	11:2P:123:LEU:HD11	1.99	0.45
12:2Q:111:GLU:OE1	12:2Q:133:ARG:NH2	2.49	0.45
16:2U:8:VAL:O	16:2U:12:ARG:HG3	2.17	0.45
57:2a:594:G:H2'	57:2a:595:G:O4'	2.16	0.45
57:2a:1064:G:OP1	57:2a:1386:G:H4'	2.17	0.45
38:2g:150:ALA:HA	42:2k:59:TYR:HB3	1.99	0.45
46:2o:43:LEU:HD12	46:2o:56:LEU:HD13	1.99	0.45
54:2w:34:G:H2'	54:2w:35:A:C8	2.52	0.45
1:1A:2148:A:N3	1:1A:2149:G:H1'	2.32	0.45
1:1A:2159:C:H2'	1:1A:2160:C:C6	2.52	0.45
1:1A:2661:U:H2'	1:1A:2662:U:C6	2.51	0.45
21:1Z:121:HIS:HB3	21:1Z:123:ASP:O	2.17	0.45
32:1a:38:G:O2'	32:1a:39:G:H5''	2.17	0.45
32:1a:393:A:OP1	47:1p:13:HIS:HE1	2.00	0.45
32:1a:1084:G:C5	32:1a:1085:U:C4	3.05	0.45
32:1a:1176:A:H2'	32:1a:1177:G:C8	2.51	0.45
33:1b:162:ILE:O	33:1b:185:ILE:HG12	2.17	0.45
46:1o:18:PHE:C	46:1o:20:GLY:H	2.24	0.45
1:2A:320:A:H4'	1:2A:322:A:N7	2.32	0.45
1:2A:521:G:H2'	1:2A:522:G:H8	1.82	0.45
1:2A:709:U:H2'	1:2A:710:G:C8	2.52	0.45
1:2A:882:G:H1	1:2A:894:C:N4	2.08	0.45
1:2A:2405:G:H5'	11:2P:75:ILE:HD13	1.99	0.45
1:2A:2657:A:O3'	7:2H:160:LYS:NZ	2.38	0.45
1:2A:2769:C:H2'	1:2A:2770:G:O4'	2.17	0.45
2:2B:57:A:N3	6:2G:29:TRP:HB3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:46:GLU:O	7:2H:48:GLY:N	2.50	0.45
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.98	0.45
9:2N:123:TYR:CZ	9:2N:129:PRO:HD2	2.52	0.45
10:2O:63:VAL:HG23	10:2O:64:ARG:HG3	1.98	0.45
57:2a:840:C:H4'	57:2a:841:U:OP1	2.15	0.45
57:2a:954:G:H2'	57:2a:955:U:O4'	2.17	0.45
57:2a:1177:G:H3'	57:2a:1178:G:H8	1.82	0.45
34:2c:3:ASN:OD1	34:2c:3:ASN:N	2.49	0.45
35:2d:73:ARG:HD2	35:2d:73:ARG:HA	1.77	0.45
36:2e:99:GLY:O	36:2e:117:ASP:HA	2.17	0.45
47:2p:48:TRP:CE3	47:2p:49:LEU:HB2	2.52	0.45
1:1A:353:G:OP2	20:1Y:71:LYS:HD2	2.17	0.45
1:1A:756:U:H2'	1:1A:757:G:C8	2.52	0.45
1:1A:1104:G:N1	1:1A:1126:C:N4	2.36	0.45
1:1A:1128:U:C4	1:1A:1132:A:N1	2.76	0.45
1:1A:1882:U:H2'	1:1A:1883:C:O4'	2.17	0.45
8:1I:5:LEU:HD11	8:1I:19:VAL:HG22	1.98	0.45
14:1S:34:HIS:O	14:1S:97:ARG:NH2	2.50	0.45
16:1U:58:ARG:HA	16:1U:61:TRP:CE3	2.52	0.45
32:1a:189(B):C:H2'	32:1a:189(C):C:C6	2.52	0.45
32:1a:510:A:OP2	35:1d:49:ARG:NH1	2.50	0.45
32:1a:664:G:N2	32:1a:741:G:H1	2.05	0.45
32:1a:909:A:H2'	32:1a:910:C:O4'	2.16	0.45
33:1b:97:TRP:CZ2	33:1b:102:LEU:HD13	2.51	0.45
54:1w:66:U:H1'	63:1w:3103:HOH:O	2.17	0.45
1:2A:108:U:H2'	1:2A:109:G:C8	2.52	0.45
1:2A:455:C:N3	1:2A:472:A:H2'	2.32	0.45
1:2A:1024:G:HO2'	1:2A:1144:G:HO2'	1.64	0.45
1:2A:1991:U:H2'	1:2A:1992:G:H5''	1.99	0.45
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.51	0.45
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.99	0.45
4:2E:30:PRO:HB3	4:2E:92:THR:HG22	1.99	0.45
13:2R:54:LEU:HB3	13:2R:62:ALA:HB1	1.98	0.45
57:2a:973:G:H3'	57:2a:974:A:H5''	1.98	0.45
57:2a:977:A:O2'	57:2a:979:C:OP2	2.35	0.45
57:2a:1435:G:H2'	57:2a:1436:U:C6	2.51	0.45
34:2c:156:ARG:H	34:2c:196:LEU:HD22	1.82	0.45
41:2j:74:ILE:HG22	63:2j:8101:HOH:O	2.17	0.45
44:2m:92:HIS:CE1	44:2m:98:VAL:HG21	2.52	0.45
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.42	0.45
55:2x:66:C:H2'	55:2x:67:C:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B:4:GLY:HA2	58:B:13:ALA:HB2	1.98	0.45
1:1A:645:G:H5'	1:1A:645:G:N3	2.31	0.44
1:1A:1715:A:H4'	1:1A:1716:A:O5'	2.17	0.44
1:1A:2087:C:H2'	1:1A:2088:C:C6	2.52	0.44
1:1A:2102:G:OP1	23:11:35:THR:HG21	2.17	0.44
1:1A:2315:G:O6	63:1A:4359:HOH:O	2.21	0.44
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.51	0.44
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.52	0.44
8:1I:60:GLU:HG3	8:1I:61:ARG:NH1	2.32	0.44
13:1R:117:VAL:HG12	13:1R:118:GLU:H	1.82	0.44
14:1S:110:LEU:HD12	14:1S:110:LEU:HA	1.77	0.44
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.98	0.44
32:1a:881:G:H2'	32:1a:882:C:O4'	2.18	0.44
1:2A:236:C:H2'	1:2A:237:C:C6	2.51	0.44
1:2A:857:C:H1'	22:20:26:TYR:HE1	1.81	0.44
1:2A:1851:U:H2'	1:2A:1852:C:O4'	2.17	0.44
1:2A:2238:G:H2'	1:2A:2238:G:N3	2.32	0.44
3:2D:77:ALA:HB2	3:2D:97:TYR:CD1	2.51	0.44
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	1.99	0.44
5:2F:106:ARG:H	5:2F:106:ARG:HG2	1.50	0.44
57:2a:72:C:H2'	57:2a:73:G:C8	2.51	0.44
57:2a:148:G:H2'	57:2a:149:A:C8	2.51	0.44
57:2a:841:U:C5	57:2a:848:C:H1'	2.52	0.44
57:2a:1012:U:H2'	57:2a:1013:G:C8	2.52	0.44
57:2a:1343:G:H1'	40:2i:121:ARG:HH12	1.82	0.44
33:2b:134:GLU:HA	33:2b:137:ARG:NE	2.29	0.44
1:1A:672:G:H2'	1:1A:673:G:O4'	2.17	0.44
1:1A:1552:C:H2'	1:1A:1553:A:C8	2.52	0.44
3:1D:34:VAL:HG12	3:1D:63:ARG:HG3	1.99	0.44
24:12:32:LEU:HD12	24:12:57:ILE:HD12	1.98	0.44
32:1a:539:A:H2'	32:1a:540:G:C8	2.52	0.44
32:1a:620:C:H2'	32:1a:621:A:O4'	2.18	0.44
32:1a:648:A:H2'	32:1a:649:G:H8	1.83	0.44
32:1a:1291:G:OP1	38:1g:37:ASN:ND2	2.50	0.44
1:2A:77:C:OP1	24:22:59:ARG:NE	2.46	0.44
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.18	0.44
1:2A:2168:G:C8	1:2A:2170:A:N7	2.85	0.44
2:2B:27:C:N4	2:2B:56:G:O6	2.51	0.44
3:2D:37:LEU:HD13	3:2D:87:ASN:ND2	2.32	0.44
8:2I:38:LEU:H	8:2I:38:LEU:HG	1.50	0.44
8:2I:110:ASP:N	8:2I:130:TYR:OH	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2R:38:VAL:HG22	13:2R:112:ALA:HB2	1.99	0.44
22:20:53:MET:HG3	22:20:59:LEU:HD23	1.98	0.44
57:2a:1002:G:N3	57:2a:1003:G:H1'	2.33	0.44
57:2a:1157:A:H4'	57:2a:1158:C:O5'	2.17	0.44
57:2a:1255:G:N7	41:2j:43:ARG:NH2	2.65	0.44
39:2h:51:VAL:HG11	39:2h:60:ARG:HH12	1.82	0.44
1:1A:1338:U:H2'	1:1A:1339:C:C6	2.53	0.44
1:1A:2473:C:H2'	1:1A:2474:U:C6	2.52	0.44
2:1B:24:G:N7	2:1B:56:G:H2'	2.32	0.44
2:1B:78:A:C2	2:1B:100:A:C4	3.04	0.44
5:1F:53:THR:HG22	5:1F:56:GLU:HG3	1.99	0.44
16:1U:29:SER:O	16:1U:30:LYS:HD3	2.17	0.44
16:1U:86:ALA:O	17:1V:49:THR:HG23	2.17	0.44
32:1a:815:A:N7	32:1a:1509:C:O2'	2.47	0.44
32:1a:1348:U:H4'	40:1i:120:ARG:HD2	2.00	0.44
32:1a:1350:A:O2'	38:1g:33:ASP:OD1	2.31	0.44
32:1a:1469:G:H2'	32:1a:1470:G:C8	2.53	0.44
40:1i:24:GLY:HA2	40:1i:59:PHE:O	2.17	0.44
42:1k:66:LEU:O	42:1k:70:LYS:HG3	2.17	0.44
45:1n:14:PRO:HG3	45:1n:20:ALA:HB2	1.99	0.44
54:1w:2:C:H42	54:1w:71:G:H1	1.64	0.44
54:1w:11:C:O5'	54:1w:11:C:H6	2.00	0.44
1:2A:375:C:H2'	1:2A:376:C:C6	2.53	0.44
1:2A:2507:C:H5''	1:2A:2573:C:C4	2.52	0.44
8:2I:9:LEU:HD21	8:2I:35:LEU:HD13	2.00	0.44
21:2Z:76:LEU:HA	21:2Z:83:PRO:HA	1.99	0.44
29:27:47:ARG:HA	29:27:47:ARG:HD3	1.60	0.44
57:2a:126:G:H4'	57:2a:634:C:O2	2.17	0.44
57:2a:1456:G:N1	51:2t:51:GLU:OE2	2.48	0.44
38:2g:20:ASP:HB3	38:2g:23:VAL:HG23	1.99	0.44
48:2q:6:LEU:HD23	48:2q:23:VAL:HG11	1.99	0.44
1:1A:34:C:H5''	1:1A:35:G:OP2	2.17	0.44
1:1A:664:U:H2'	1:1A:665:C:C6	2.53	0.44
1:1A:1405:A:H2'	1:1A:1406:A:H5'	1.99	0.44
1:1A:2274:U:OP1	1:1A:2399:U:O2'	2.30	0.44
1:1A:2346:G:H4'	1:1A:2347:A:OP2	2.17	0.44
32:1a:193:C:H2'	32:1a:194:C:C6	2.53	0.44
32:1a:377:G:OP1	47:1p:3:LYS:HD3	2.16	0.44
32:1a:865:A:H2	32:1a:918:A:H4'	1.83	0.44
1:2A:660:G:H5'	5:2F:99:TYR:CE1	2.53	0.44
1:2A:754:C:H2'	1:2A:755:C:C6	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:878:A:H61	1:2A:899:A:H1'	1.82	0.44
1:2A:2484:G:C2	1:2A:2485:G:C8	3.05	0.44
15:2T:118:ARG:HG2	57:2a:1442(A):G:C8	2.52	0.44
16:2U:76:TYR:CE2	16:2U:80:ILE:HG13	2.53	0.44
17:2V:40:LEU:HB2	17:2V:46:VAL:CG1	2.47	0.44
20:2Y:8:LYS:HD3	20:2Y:97:ARG:NH1	2.33	0.44
57:2a:258:G:H2'	57:2a:259:G:H8	1.83	0.44
57:2a:448:A:P	57:2a:485:G:H22	2.39	0.44
44:2m:123:ALA:HB2	54:2w:39:PSU:H1'	1.98	0.44
50:2s:27:GLU:HG2	50:2s:28:LYS:HD3	1.99	0.44
1:1A:1810:U:H2'	63:1A:4705:HOH:O	2.17	0.44
1:1A:2150:C:H42	1:1A:2182:G:H1	1.66	0.44
8:1I:4:ILE:HG12	8:1I:18:VAL:HG22	2.00	0.44
12:1Q:60:ARG:HB2	12:1Q:60:ARG:NH1	2.31	0.44
27:15:16:ARG:HD2	27:15:20:ARG:NH1	2.33	0.44
32:1a:100:C:H2'	32:1a:101:A:C8	2.52	0.44
32:1a:271:C:H2'	32:1a:272:C:H6	1.83	0.44
32:1a:1402:4OC:HM22	32:1a:1403:C:H5'	2.00	0.44
33:1b:16:HIS:HB2	33:1b:204:ASN:HB3	1.98	0.44
35:1d:153:ARG:O	35:1d:158:ILE:HD11	2.17	0.44
47:1p:17:TYR:HE2	47:1p:41:PRO:HG3	1.83	0.44
1:2A:141:A:H8	1:2A:1408:C:HO2'	1.56	0.44
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.52	0.44
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	1.99	0.44
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG11	1.98	0.44
57:2a:983:A:H3'	57:2a:983:A:N3	2.33	0.44
57:2a:1144:G:H21	57:2a:1146:A:H62	1.66	0.44
57:2a:1187:G:H5'	40:2i:113:LYS:HE3	1.99	0.44
34:2c:130:VAL:HG11	34:2c:153:VAL:HG11	2.00	0.44
36:2e:85:GLY:O	36:2e:86:ALA:HB3	2.17	0.44
56:2y:52:G:H1	56:2y:62:C:H42	1.66	0.44
1:1A:541:C:OP1	27:15:13:LYS:NZ	2.38	0.44
1:1A:1827:U:H2'	1:1A:1828:C:H6	1.83	0.44
1:1A:2735:G:H2'	1:1A:2736:C:C6	2.52	0.44
2:1B:66:A:H61	2:1B:109:C:H5'	1.83	0.44
3:1D:77:ALA:HA	3:1D:97:TYR:HA	1.98	0.44
5:1F:52:LYS:HD3	5:1F:56:GLU:O	2.17	0.44
6:1G:7:LEU:HD21	6:1G:176:LEU:HD22	2.00	0.44
21:1Z:15:PRO:O	21:1Z:19:ARG:HG3	2.17	0.44
37:1f:99:ALA:HB1	49:1r:23:LYS:HE3	2.00	0.44
1:2A:251:A:C5	1:2A:252:G:H1'	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:271(T):C:H2'	1:2A:271(U):G:H8	1.82	0.44
1:2A:340:A:H2'	1:2A:341:G:O4'	2.17	0.44
1:2A:1530:C:H1'	1:2A:1531:C:OP1	2.18	0.44
1:2A:2327:A:H2'	1:2A:2328:A:O4'	2.18	0.44
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.14	0.44
4:2E:170:LEU:HB3	4:2E:184:VAL:HG22	2.00	0.44
11:2P:90:ARG:NH1	11:2P:105:LEU:HD11	2.33	0.44
23:21:67:ILE:N	23:21:68:PRO:HD2	2.32	0.44
57:2a:37:U:O2'	57:2a:500:G:H4'	2.18	0.44
57:2a:302:G:N3	57:2a:556:C:H4'	2.32	0.44
57:2a:814:A:N7	57:2a:816:A:C4	2.85	0.44
57:2a:819:A:N1	63:2a:3333:HOH:O	2.36	0.44
33:2b:178:ARG:HH22	39:2h:74:PRO:HB3	1.82	0.44
49:2r:32:ARG:NE	63:2r:5001:HOH:O	2.48	0.44
55:2x:21:A:N6	55:2x:46:G:H2'	2.32	0.44
1:1A:928:G:H3'	1:1A:929:G:H8	1.81	0.44
1:1A:2018:C:H4'	1:1A:2019:G:OP1	2.18	0.44
1:1A:2140:U:OP1	1:1A:2170:G:H4'	2.17	0.44
11:1P:101:VAL:HG23	11:1P:106:LEU:O	2.18	0.44
33:1b:54:THR:O	33:1b:58:ILE:HG13	2.18	0.44
34:1c:13:GLY:HA3	45:1n:57:ARG:HH21	1.83	0.44
38:1g:108:ALA:HA	38:1g:111:ARG:HG3	1.99	0.44
1:2A:277:C:H4'	1:2A:278:A:H8	1.82	0.44
1:2A:1263:U:C4	1:2A:1264:G:C6	3.06	0.44
1:2A:2540:C:H2'	1:2A:2541:A:O4'	2.18	0.44
2:2B:94:C:H2'	2:2B:95:C:H6	1.82	0.44
6:2G:12:TYR:HA	6:2G:16:ARG:HG3	2.00	0.44
6:2G:106:LEU:O	6:2G:111:LEU:HG	2.18	0.44
6:2G:122:PRO:HG3	6:2G:182:LYS:H	1.83	0.44
7:2H:127:GLU:HB3	7:2H:129:THR:HG22	2.00	0.44
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.98	0.44
28:26:35:GLU:OE2	28:26:50:ARG:NH1	2.45	0.44
57:2a:429:U:H1'	57:2a:430:A:H5''	1.99	0.44
57:2a:1148:U:H2'	57:2a:1149:C:O4'	2.18	0.44
34:2c:131:ARG:NE	34:2c:135:LYS:HE3	2.32	0.44
36:2e:78:HIS:CD2	39:2h:104:ARG:HD2	2.38	0.44
37:2f:44:GLY:HA2	37:2f:59:TYR:CE1	2.52	0.44
40:2i:26:VAL:HG13	40:2i:61:ALA:HB3	1.98	0.44
49:2r:35:ARG:O	49:2r:37:VAL:N	2.51	0.44
1:1A:1108:G:N2	1:1A:1134:A:C6	2.85	0.44
1:1A:2724:U:O2'	1:1A:2726:A:H5'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2761:A:H5'	7:1H:4:ILE:HD12	1.99	0.44
32:1a:1026:G:C8	32:1a:1027:C:O2	2.67	0.44
35:1d:88:VAL:HG12	35:1d:90:GLY:H	1.83	0.44
54:1w:24:G:H5'	54:1w:25:C:OP2	2.18	0.44
1:2A:184:C:H2'	1:2A:185:U:C6	2.53	0.44
1:2A:673:C:H5''	5:2F:81:PRO:HD2	1.99	0.44
1:2A:952:G:OP1	12:2Q:16:ARG:NH2	2.51	0.44
1:2A:1777:U:H2'	1:2A:1778:U:C6	2.52	0.44
2:2B:96:U:OP1	21:2Z:14:LYS:NZ	2.50	0.44
11:2P:59:LEU:HD12	30:28:58:ILE:HG12	2.00	0.44
11:2P:126:VAL:HG12	11:2P:148:LEU:HD22	2.00	0.44
12:2Q:118:LEU:HD12	12:2Q:131:ILE:HG23	1.99	0.44
15:2T:93:ARG:HH22	15:2T:95:ARG:HH21	1.65	0.44
18:2W:45:TYR:CZ	18:2W:49:LYS:HE2	2.53	0.44
28:26:23:THR:OG1	28:26:24:GLU:N	2.46	0.44
57:2a:509:A:H5''	35:2d:55:ALA:HB2	2.00	0.44
57:2a:1371:G:O3'	40:2i:69:GLY:HA3	2.18	0.44
33:2b:60:ASP:OD1	33:2b:64:ARG:NH1	2.50	0.44
1:1A:459:A:N6	63:1A:4551:HOH:O	2.47	0.44
1:1A:1653:C:H4'	1:1A:1654:A:O5'	2.18	0.44
2:1B:2:C:H2'	2:1B:3:C:H6	1.83	0.44
4:1E:97:LYS:HE2	4:1E:97:LYS:HB3	1.68	0.44
10:1O:64:ARG:HD2	10:1O:79:PHE:CD1	2.53	0.44
12:1Q:59:ARG:C	12:1Q:61:GLY:H	2.26	0.44
14:1S:5:THR:OG1	14:1S:8:GLU:HG2	2.18	0.44
21:1Z:65:GLN:OE1	21:1Z:67:LEU:HD21	2.18	0.44
32:1a:828:A:H2'	32:1a:829:G:O4'	2.17	0.44
32:1a:1328:C:H2'	32:1a:1329:A:O4'	2.18	0.44
33:1b:24:TRP:H	33:1b:24:TRP:HD1	1.65	0.44
35:1d:122:ARG:HA	35:1d:122:ARG:HD2	1.86	0.44
40:1i:49:PRO:HD3	40:1i:78:LYS:HG3	1.99	0.44
41:1j:81:THR:C	41:1j:83:GLU:N	2.76	0.44
56:1y:38:A:H2'	56:1y:39:PSU:O4'	2.17	0.44
1:2A:579:G:H2'	1:2A:580:C:C6	2.53	0.44
1:2A:740:U:H2'	1:2A:741:G:C8	2.53	0.44
2:2B:19:G:H2'	2:2B:20:C:O4'	2.18	0.44
3:2D:71:ASP:CB	3:2D:103:ARG:HH12	2.30	0.44
4:2E:181:LEU:HD12	4:2E:181:LEU:HA	1.68	0.44
6:2G:96:ARG:H	6:2G:99:MET:HE2	1.82	0.44
6:2G:138:GLN:C	6:2G:140:ILE:H	2.26	0.44
10:2O:71:ARG:HH22	10:2O:122:LEU:C	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2X:94:GLY:H	19:2X:95:LEU:HA	1.83	0.44
57:2a:189(K):U:H2'	57:2a:189(L):G:C8	2.53	0.44
57:2a:583:A:H2'	57:2a:584:G:O4'	2.18	0.44
57:2a:921:U:O2	36:2e:19:MET:HB2	2.18	0.44
33:2b:109:SER:O	33:2b:112:VAL:HG22	2.17	0.44
45:2n:27:CYS:SG	45:2n:29:ARG:HB2	2.57	0.44
49:2r:26:LEU:HD11	49:2r:42:ARG:HD3	2.00	0.44
56:2y:46:G7M:H2'	56:2y:46:G7M:H8	1.69	0.44
1:1A:1090:G:H5'	1:1A:1091:A:OP2	2.17	0.43
1:1A:1248:G:H5'	11:1P:3:LEU:HD23	1.99	0.43
1:1A:1535:U:O3'	1:1A:1536:A:H8	2.01	0.43
1:1A:2193:A:O2'	1:1A:2194:U:H6	2.01	0.43
1:1A:2210:C:H2'	1:1A:2211:U:O4'	2.18	0.43
1:1A:2697:G:H5'	10:1O:68:GLU:OE2	2.18	0.43
8:1I:62:LYS:O	8:1I:66:GLU:HG2	2.18	0.43
13:1R:44:LEU:HD23	13:1R:44:LEU:HA	1.80	0.43
32:1a:267:C:OP1	48:1q:67:LYS:HB2	2.18	0.43
32:1a:975:A:H5'	32:1a:975:A:H8	1.83	0.43
32:1a:1021:G:HO2'	32:1a:1022:G:P	2.40	0.43
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.52	0.43
37:1f:19:LEU:HD11	37:1f:59:TYR:CZ	2.52	0.43
51:1t:47:GLY:N	51:1t:48:LYS:HB2	2.32	0.43
1:2A:42:G:H2'	1:2A:43:A:O4'	2.18	0.43
1:2A:108:U:H2'	1:2A:109:G:H8	1.82	0.43
1:2A:2031:A:C6	1:2A:2498:C:H1'	2.53	0.43
2:2B:83:G:N2	2:2B:94:C:O2	2.33	0.43
14:2S:15:ARG:HB3	14:2S:19:LYS:HZ2	1.81	0.43
19:2X:94:GLY:N	19:2X:95:LEU:HA	2.33	0.43
30:28:62:LEU:HB3	30:28:65:GLU:HG2	2.00	0.43
57:2a:539:A:OP2	43:2l:115:LYS:NZ	2.50	0.43
57:2a:1004:A:H1'	57:2a:1038:C:O2	2.18	0.43
57:2a:1013:G:H2'	57:2a:1015:A:OP2	2.17	0.43
47:2p:3:LYS:O	47:2p:21:VAL:HA	2.18	0.43
58:B:2:SER:HA	58:B:3:PRO:HD3	1.74	0.43
1:1A:925:A:N6	1:1A:946:A:C8	2.86	0.43
1:1A:933:C:N3	1:1A:934:A:H8	2.15	0.43
1:1A:943:C:H4'	54:1w:56:C:P	2.58	0.43
1:1A:977:G:OP2	25:13:29:ARG:NH2	2.51	0.43
1:1A:2327:G:H2'	1:1A:2328:C:C6	2.52	0.43
4:1E:47:VAL:O	4:1E:80:GLU:HA	2.19	0.43
32:1a:1057:G:H2'	32:1a:1058:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1381:U:H1'	38:1g:79:ARG:HG2	2.00	0.43
33:1b:201:ILE:HG21	33:1b:214:ILE:HG21	1.99	0.43
34:1c:131:ARG:HE	34:1c:135:LYS:HE3	1.83	0.43
35:1d:178:VAL:HG12	35:1d:179:GLU:H	1.83	0.43
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.53	0.43
1:2A:932:G:H4'	1:2A:933:A:O5'	2.18	0.43
1:2A:1935:G:H1'	1:2A:1964:G:N2	2.33	0.43
1:2A:2033:A:O2'	1:2A:2035:G:OP2	2.33	0.43
1:2A:2432:A:C6	1:2A:2433:A:C6	3.06	0.43
7:2H:35:VAL:HG13	7:2H:71:LEU:HD23	2.00	0.43
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.18	0.43
13:2R:36:THR:HG22	13:2R:37:THR:H	1.83	0.43
57:2a:836:G:C6	57:2a:851:G:C6	3.06	0.43
33:2b:192:SER:O	33:2b:194:PRO:HD3	2.19	0.43
43:2l:84:LEU:HB2	43:2l:105:TYR:CE2	2.53	0.43
1:1A:320:C:H2'	1:1A:321:C:C6	2.54	0.43
1:1A:455:A:OP2	1:1A:455:A:H8	2.01	0.43
1:1A:831:A:C5	3:1D:229:VAL:HG21	2.54	0.43
2:1B:13:A:N1	2:1B:69:G:O2'	2.45	0.43
15:1T:127:ALA:C	15:1T:129:ARG:N	2.76	0.43
21:1Z:105:VAL:O	21:1Z:141:VAL:HG22	2.18	0.43
29:17:12:ARG:NH2	29:17:44:PRO:HB3	2.33	0.43
32:1a:452:A:O2'	32:1a:453:A:OP2	2.30	0.43
32:1a:841:U:OP2	32:1a:841:U:H6	2.00	0.43
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.86	0.43
36:1e:105:VAL:HG21	36:1e:128:PRO:HB3	2.00	0.43
38:1g:26:PHE:O	38:1g:30:ILE:HD12	2.17	0.43
40:1i:28:VAL:HG22	40:1i:63:ILE:HB	1.99	0.43
1:2A:18:C:O2'	1:2A:554:U:OP1	2.32	0.43
1:2A:1779:U:H2'	63:2A:4223:HOH:O	2.18	0.43
1:2A:2161:C:H2'	1:2A:2162:G:O4'	2.18	0.43
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.19	0.43
1:2A:2812:G:H2'	1:2A:2813:A:C8	2.53	0.43
1:2A:2819:G:H2'	1:2A:2821:A:N7	2.33	0.43
6:2G:111:LEU:HB3	6:2G:117:PHE:CE1	2.53	0.43
7:2H:25:LYS:HB2	7:2H:25:LYS:HE3	1.69	0.43
57:2a:1252:A:H61	57:2a:1285:A:H61	1.66	0.43
33:2b:98:LEU:HG	33:2b:101:MET:HE3	1.99	0.43
38:2g:89:MET:SD	38:2g:155:ARG:HB2	2.58	0.43
40:2i:53:VAL:O	40:2i:55:ALA:N	2.51	0.43
1:1A:196:A:H2'	1:1A:197:C:O4'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:386:U:H6	1:1A:386:U:H2'	1.63	0.43
1:1A:390:G:H2'	1:1A:391:G:C8	2.52	0.43
1:1A:1049:G:O2'	1:1A:1056:A:N1	2.49	0.43
1:1A:1091:A:OP1	1:1A:1091:A:H4'	2.17	0.43
1:1A:2455:C:OP1	5:1F:68:LYS:HD3	2.19	0.43
32:1a:265:G:H5'	48:1q:64:PRO:O	2.18	0.43
32:1a:1225:A:OP2	44:1m:104:ARG:HG3	2.18	0.43
32:1a:1370:G:C2	32:1a:1371:G:C8	3.07	0.43
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	2.00	0.43
1:2A:686:G:H8	29:27:6:GLN:O	2.02	0.43
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.53	0.43
1:2A:1359:A:C2	1:2A:1372:U:O4	2.71	0.43
10:2O:105:GLU:OE1	10:2O:105:GLU:N	2.50	0.43
13:2R:87:TYR:OH	13:2R:117:VAL:O	2.35	0.43
57:2a:300:A:H1'	57:2a:565:U:O2	2.18	0.43
57:2a:1054:C:H4'	57:2a:1055:A:O5'	2.19	0.43
36:2e:148:VAL:HG21	39:2h:107:LEU:HD22	1.99	0.43
1:1A:2177:G:H3'	1:1A:2178:G:C8	2.53	0.43
1:1A:2331:G:H22	14:1S:3:ARG:NE	2.17	0.43
32:1a:690:G:C6	32:1a:691:G:C6	3.07	0.43
32:1a:1530:G:H4'	32:1a:1530:G:OP1	2.19	0.43
36:1e:78:HIS:CD2	39:1h:104:ARG:HD2	2.54	0.43
44:1m:16:ASP:OD1	44:1m:16:ASP:N	2.50	0.43
50:1s:80:TYR:CZ	50:1s:82:GLY:HA2	2.54	0.43
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.44	0.43
1:2A:2336:A:H61	22:20:43:THR:HG22	1.83	0.43
9:2N:21:LYS:NZ	9:2N:140:VAL:OXT	2.45	0.43
15:2T:51:ARG:HG2	15:2T:62:THR:HB	2.01	0.43
21:2Z:54:HIS:HB3	21:2Z:101:PRO:HD3	2.00	0.43
57:2a:1057:G:H2'	57:2a:1058:G:O4'	2.18	0.43
57:2a:1113:C:H2'	57:2a:1114:C:H6	1.84	0.43
37:2f:99:ALA:HB1	49:2r:23:LYS:HE3	2.01	0.43
1:1A:540:A:H1'	1:1A:604:C:H1'	2.00	0.43
1:1A:649:C:O2'	1:1A:704:U:OP1	2.35	0.43
1:1A:1566:U:H2'	1:1A:1567:G:O4'	2.18	0.43
1:1A:1961:5MU:OP1	1:1A:2616:U:O2'	2.29	0.43
7:1H:62:LYS:HB3	7:1H:62:LYS:HE2	1.84	0.43
32:1a:184:G:N2	32:1a:194:C:C2	2.87	0.43
32:1a:598:U:H2'	32:1a:599:C:H6	1.84	0.43
32:1a:1026:G:H3'	32:1a:1027:C:O2	2.18	0.43
32:1a:1127:G:H5'	32:1a:1280:A:O2'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1318:A:H5''	50:1s:3:ARG:NH1	2.33	0.43
34:1c:109:PRO:HA	34:1c:115:LEU:HD23	2.00	0.43
40:1i:29:ASN:ND2	40:1i:65:VAL:O	2.25	0.43
41:1j:78:ASN:C	41:1j:80:LYS:H	2.26	0.43
55:1x:6:G:O6	55:1x:67:C:N3	2.50	0.43
56:1y:26:A:N6	56:1y:44:G:N1	2.62	0.43
1:2A:686:G:H21	1:2A:788:A:H61	1.65	0.43
1:2A:783:A:OP2	63:2A:3959:HOH:O	2.21	0.43
7:2H:11:VAL:HG21	7:2H:50:VAL:HG23	2.01	0.43
7:2H:28:GLY:HA3	7:2H:79:VAL:HB	2.00	0.43
57:2a:736:C:OP1	49:2r:72:ARG:NH2	2.47	0.43
57:2a:999:C:C4	57:2a:1000:U:C4	3.07	0.43
57:2a:1118:C:H1'	57:2a:1179:A:C4	2.53	0.43
33:2b:163:PHE:HD1	33:2b:185:ILE:HG13	1.80	0.43
34:2c:120:VAL:HG13	34:2c:133:ALA:HB1	2.01	0.43
47:2p:20:VAL:HG21	47:2p:32:TYR:CG	2.53	0.43
55:2x:15:G:H2'	55:2x:59:A:N1	2.33	0.43
1:1A:1273:G:OP1	16:1U:13:LYS:HG2	2.18	0.43
1:1A:2519:C:H2'	1:1A:2520:G:O4'	2.19	0.43
1:1A:2647:C:H4'	4:1E:48:GLN:HE21	1.83	0.43
11:1P:63:PRO:HD3	30:18:27:THR:HG22	2.00	0.43
32:1a:163:C:H2'	32:1a:164:U:C6	2.53	0.43
32:1a:501:C:H2'	32:1a:502:G:H8	1.83	0.43
1:2A:493:G:H2'	1:2A:494:G:O4'	2.18	0.43
1:2A:570:G:H2'	1:2A:2030:A:C5	2.53	0.43
1:2A:571:A:O2'	17:2V:78:LYS:HE2	2.19	0.43
1:2A:826:U:H4'	11:2P:55:ARG:HB3	2.00	0.43
1:2A:2191:G:H2'	1:2A:2192:G:O4'	2.18	0.43
1:2A:2547:U:O2	10:2O:23:ARG:NH2	2.46	0.43
2:2B:11:C:H3'	2:2B:12:C:C6	2.53	0.43
9:2N:20:GLY:HA2	9:2N:61:ARG:HG3	2.00	0.43
9:2N:28:THR:HG22	9:2N:29:LYS:N	2.33	0.43
20:2Y:97:ARG:H	20:2Y:97:ARG:HG2	1.62	0.43
28:26:25:LYS:NZ	28:26:30:THR:O	2.48	0.43
30:28:6:THR:HG22	30:28:63:PRO:HD2	2.01	0.43
34:2c:150:LYS:HG3	34:2c:169:ALA:HB2	2.00	0.43
36:2e:71:LEU:HD11	36:2e:113:ALA:O	2.18	0.43
40:2i:42:ARG:NH1	40:2i:71:SER:OG	2.52	0.43
54:2w:53:G:H1	54:2w:61:C:H42	1.66	0.43
56:2y:58:A:H1'	56:2y:60:U:C5	2.54	0.43
1:1A:202:A:H2'	1:1A:203:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:271:U:H1'	8:1I:50:ARG:NH1	2.33	0.43
1:1A:515:G:N7	18:1W:49:LYS:NZ	2.67	0.43
1:1A:1410:G:OP2	23:11:3:LYS:HG3	2.19	0.43
1:1A:2158:C:N3	1:1A:2177:G:C2	2.84	0.43
19:1X:44:GLU:HG2	19:1X:49:VAL:O	2.18	0.43
32:1a:1368:G:OP1	40:1i:111:ARG:NH2	2.51	0.43
35:1d:155:LEU:O	35:1d:158:ILE:HG13	2.19	0.43
43:1l:28:LYS:HE2	43:1l:64:TYR:CE2	2.54	0.43
44:1m:23:TYR:HB3	44:1m:67:GLU:HA	2.00	0.43
46:1o:70:LEU:HD11	46:1o:77:ARG:HB3	2.01	0.43
51:1t:29:LYS:O	51:1t:33:ILE:HG13	2.19	0.43
1:2A:253:C:O2'	63:2A:3957:HOH:O	2.21	0.43
1:2A:748:G:C8	18:2W:89:ALA:HB1	2.54	0.43
1:2A:2037:G:H2'	1:2A:2038:G:C8	2.54	0.43
1:2A:2103:C:H2'	1:2A:2104:G:C8	2.54	0.43
6:2G:17:PRO:HA	6:2G:20:ILE:HD12	2.00	0.43
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	2.01	0.43
6:2G:111:LEU:HA	6:2G:114:ILE:HD12	2.01	0.43
10:2O:68:GLU:HB3	10:2O:78:ARG:HB2	2.01	0.43
15:2T:26:ASP:O	15:2T:49:VAL:HG22	2.19	0.43
19:2X:41:ASN:O	19:2X:45:THR:HG23	2.19	0.43
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.18	0.43
57:2a:8:A:C5	35:2d:209:ARG:HA	2.54	0.43
57:2a:108:G:N1	51:2t:15:ARG:HG2	2.34	0.43
57:2a:472:A:HO2'	47:2p:82:GLN:H	1.64	0.43
57:2a:1286:A:H2	52:2u:18:TYR:OH	2.02	0.43
33:2b:74:LYS:HD2	33:2b:166:ASP:HB2	2.01	0.43
35:2d:178:VAL:HG12	35:2d:179:GLU:H	1.83	0.43
37:2f:100:ASN:ND2	49:2r:23:LYS:HE2	2.34	0.43
3:1D:182:LEU:HD23	3:1D:182:LEU:HA	1.86	0.43
6:1G:138:GLN:CD	6:1G:138:GLN:H	2.27	0.43
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.17	0.43
7:1H:25:LYS:HE3	7:1H:25:LYS:HB2	1.86	0.43
8:1I:61:ARG:HA	8:1I:61:ARG:HD3	1.78	0.43
20:1Y:14:LEU:HB2	20:1Y:75:ILE:HD11	2.00	0.43
21:1Z:138:GLU:H	21:1Z:156:LYS:HE2	1.84	0.43
32:1a:719:C:O2'	49:1r:49:LYS:HB3	2.19	0.43
32:1a:1016:A:H2'	32:1a:1017:G:O4'	2.18	0.43
32:1a:1202:G:O4'	45:1n:29:ARG:NH1	2.47	0.43
35:1d:196:LEU:C	35:1d:198:VAL:H	2.27	0.43
39:1h:110:ALA:HB3	39:1h:121:ASP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1m:23:TYR:CE2	44:1m:71:ARG:HG3	2.54	0.43
1:2A:107:C:H2'	1:2A:108:U:H6	1.84	0.43
1:2A:1231:G:H2'	1:2A:1232:G:C8	2.54	0.43
1:2A:2023:G:H5'	1:2A:2617:C:H4'	2.01	0.43
1:2A:2065:C:H4'	1:2A:2251:OMG:HM22	2.01	0.43
2:2B:68:C:H2'	2:2B:69:G:H8	1.83	0.43
6:2G:114:ILE:HG13	6:2G:140:ILE:HG12	2.01	0.43
7:2H:16:SER:OG	7:2H:27:LYS:HB2	2.19	0.43
22:20:6:GLY:O	22:20:7:LEU:HD23	2.18	0.43
57:2a:540:G:C6	57:2a:541:G:C5	3.07	0.43
57:2a:642:A:N3	39:2h:113:SER:OG	2.52	0.43
57:2a:1161:C:H2'	57:2a:1162:C:C6	2.54	0.43
57:2a:1296:C:OP1	44:2m:44:ARG:NH2	2.52	0.43
38:2g:26:PHE:O	38:2g:30:ILE:HD12	2.19	0.43
41:2j:78:ASN:O	41:2j:80:LYS:N	2.52	0.43
56:2y:43:C:H2'	56:2y:44:G:H1'	2.01	0.43
1:1A:559:U:H2'	1:1A:560:C:C6	2.54	0.43
1:1A:891:C:C2'	1:1A:892:G:H5'	2.49	0.43
1:1A:1785:C:OP1	15:1T:96:ARG:NH1	2.48	0.43
1:1A:1817:A:H8	63:1A:4619:HOH:O	2.02	0.43
8:1I:62:LYS:HE3	8:1I:62:LYS:HB2	1.67	0.43
32:1a:600:C:H2'	32:1a:601:C:H6	1.84	0.43
32:1a:976:G:OP2	32:1a:1358:U:O2'	2.31	0.43
33:1b:12:GLU:O	33:1b:15:VAL:HG22	2.18	0.43
35:1d:19:LEU:HB3	35:1d:21:LEU:HD21	2.00	0.43
38:1g:76:ARG:HD3	38:1g:89:MET:HB2	2.01	0.43
47:1p:37:GLY:HA3	47:1p:50:LYS:O	2.19	0.43
1:2A:143:G:H2'	1:2A:143(A):C:H6	1.82	0.43
1:2A:197:A:N6	1:2A:2430:A:H2'	2.34	0.43
1:2A:311:A:C6	1:2A:328:U:C4	3.06	0.43
1:2A:415:A:H2'	1:2A:416:C:O4'	2.19	0.43
1:2A:612:C:C2	1:2A:616:G:N2	2.87	0.43
1:2A:862:G:H2'	1:2A:863:A:O4'	2.19	0.43
1:2A:1493:C:N4	1:2A:2206:G:O2'	2.49	0.43
1:2A:2318:G:H21	14:2S:3:ARG:HE	1.67	0.43
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.48	0.43
2:2B:28:C:H2'	2:2B:29:A:O4'	2.19	0.43
21:2Z:70:LEU:HD23	21:2Z:70:LEU:HA	1.75	0.43
26:24:59:PHE:C	26:24:61:ARG:H	2.26	0.43
57:2a:643:C:H2'	57:2a:644:G:H8	1.84	0.43
57:2a:909:A:H2'	57:2a:910:C:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2a:959:A:O2'	57:2a:984:C:O2'	2.24	0.43
57:2a:1004:A:N6	57:2a:1037:C:H1'	2.34	0.43
57:2a:1256:A:N1	57:2a:1278:U:H1'	2.34	0.43
57:2a:1288:A:N3	57:2a:1352:C:O2'	2.42	0.43
45:2n:59:ALA:HB1	45:2n:61:TRP:HZ3	1.83	0.43
46:2o:8:LYS:O	46:2o:12:ILE:HG13	2.19	0.43
51:2t:98:PRO:O	51:2t:99:LEU:HB2	2.19	0.43
1:1A:388:A:H2'	1:1A:389:G:C8	2.53	0.42
1:1A:2331:G:C2	14:1S:3:ARG:HA	2.53	0.42
1:1A:2430:A:H2'	1:1A:2431:U:C6	2.54	0.42
3:1D:70:TRP:HB3	3:1D:190:TYR:CE2	2.53	0.42
7:1H:104:GLU:HG3	7:1H:114:VAL:HG22	2.01	0.42
7:1H:113:VAL:HG11	7:1H:151:ILE:HG21	2.00	0.42
13:1R:50:HIS:ND1	63:1R:301:HOH:O	2.22	0.42
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.54	0.42
32:1a:1136:U:H5''	32:1a:1137:C:N3	2.34	0.42
33:1b:52:GLU:HG2	33:1b:56:ARG:HH21	1.83	0.42
1:2A:848:G:C4	1:2A:933:A:H8	2.37	0.42
1:2A:1188:U:C4'	17:2V:79:VAL:HG22	2.48	0.42
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.53	0.42
1:2A:1799:G:O2'	3:2D:181:GLU:OE2	2.28	0.42
1:2A:2145:C:O2'	1:2A:2147:G:N7	2.50	0.42
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.54	0.42
3:2D:26:LYS:NZ	3:2D:28:GLU:O	2.51	0.42
3:2D:77:ALA:HA	3:2D:97:TYR:HA	2.01	0.42
57:2a:255:G:C6	57:2a:256:U:C4	3.07	0.42
57:2a:993:G:N3	57:2a:993:G:H2'	2.33	0.42
57:2a:1051:C:H2'	57:2a:1052:U:H6	1.84	0.42
57:2a:1212:U:H5'	57:2a:1213:A:C8	2.54	0.42
57:2a:1323:G:H2'	57:2a:1324:A:C8	2.54	0.42
33:2b:115:LEU:O	33:2b:119:GLU:HG2	2.19	0.42
38:2g:115:ARG:HH11	38:2g:118:VAL:HG21	1.84	0.42
1:1A:449:A:H2'	1:1A:450:A:C8	2.54	0.42
1:1A:484:G:O2'	29:17:39:ARG:HD2	2.18	0.42
1:1A:572:A:H1'	1:1A:573:G:OP1	2.20	0.42
1:1A:662:A:OP1	11:1P:133:SER:OG	2.34	0.42
1:1A:964:A:H5''	2:1B:98:G:O2'	2.18	0.42
1:1A:1016:C:H2'	1:1A:1017:G:O4'	2.18	0.42
1:1A:1343:C:O2'	1:1A:1348:A:N1	2.46	0.42
1:1A:2164:C:N3	1:1A:2171:G:O6	2.52	0.42
3:1D:2:ALA:O	3:1D:20:ASP:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:86:THR:O	8:1I:123:LEU:HB2	2.19	0.42
32:1a:67:C:H2'	32:1a:68:G:H8	1.77	0.42
32:1a:627:G:O2'	32:1a:628:G:H5'	2.19	0.42
32:1a:646:U:H2'	32:1a:647:C:C6	2.54	0.42
32:1a:1001(A):G:C2	32:1a:1002:G:H1'	2.54	0.42
35:1d:173:TRP:CE3	35:1d:174:LEU:HG	2.54	0.42
40:1i:43:ALA:O	40:1i:45:ALA:N	2.52	0.42
1:2A:524:U:H2'	1:2A:525:U:C6	2.54	0.42
1:2A:586:A:H5'	5:2F:89:VAL:HG21	2.01	0.42
1:2A:652(T):C:H2'	1:2A:652(U):G:C8	2.54	0.42
1:2A:1628:G:H2'	1:2A:1629:U:C6	2.54	0.42
2:2B:119:G:H5'	2:2B:120:A:OP2	2.19	0.42
3:2D:26:LYS:HB3	3:2D:83:GLU:HG2	2.01	0.42
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	2.00	0.42
31:29:33:LYS:HB2	31:29:33:LYS:HE3	1.86	0.42
57:2a:67:C:H2'	57:2a:68:G:H8	1.84	0.42
57:2a:539:A:H2'	57:2a:540:G:C8	2.54	0.42
57:2a:946:A:H2'	57:2a:947:G:C8	2.54	0.42
34:2c:68:VAL:HG12	34:2c:70:VAL:HG23	2.01	0.42
37:2f:82:ARG:HB2	37:2f:85:VAL:HG23	2.00	0.42
39:2h:23:SER:HA	39:2h:63:LEU:HD13	2.00	0.42
41:2j:63:PHE:HE2	45:2n:45:ARG:HA	1.84	0.42
1:1A:119:G:H4'	1:1A:149:A:H5'	2.00	0.42
1:1A:1834:A:H4'	3:1D:259:THR:HG23	2.01	0.42
1:1A:2149:G:N2	1:1A:2183:C:N3	2.56	0.42
2:1B:8:U:O3'	14:1S:25:ARG:NH2	2.52	0.42
13:1R:94:TYR:C	13:1R:117:VAL:HG23	2.44	0.42
30:18:6:THR:HG22	30:18:64:TYR:HD2	1.84	0.42
32:1a:833:U:H2'	32:1a:834:C:H6	1.83	0.42
32:1a:1053:G:O6	32:1a:1199:U:H2'	2.19	0.42
1:2A:271(S):G:C6	1:2A:271(T):C:C4	3.08	0.42
1:2A:412:A:N6	1:2A:2412:A:O4'	2.52	0.42
1:2A:478:A:N1	1:2A:500:G:H4'	2.35	0.42
1:2A:2140:C:H2'	1:2A:2141:G:H5'	2.01	0.42
9:2N:103:VAL:HG11	9:2N:120:LEU:HD22	2.01	0.42
15:2T:41:ARG:NH2	57:2a:346:G:OP1	2.51	0.42
19:2X:44:GLU:HG2	19:2X:49:VAL:O	2.20	0.42
30:28:63:PRO:HG2	30:28:64:TYR:CE2	2.54	0.42
57:2a:620:C:H2'	57:2a:621:A:O4'	2.19	0.42
57:2a:751:U:H4'	46:2o:24:SER:HA	2.02	0.42
57:2a:974:A:P	45:2n:29:ARG:HH21	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.54	0.42
48:2q:66:SER:OG	48:2q:69:LYS:HB2	2.19	0.42
50:2s:80:TYR:C	50:2s:82:GLY:H	2.27	0.42
58:A:2:SER:HA	58:A:3:PRO:HD3	1.63	0.42
1:1A:70:A:N7	19:1X:31:HIS:HE1	2.17	0.42
1:1A:174:U:H4'	1:1A:207:A:H4'	2.02	0.42
1:1A:1314:A:H2'	1:1A:1315:A:O4'	2.19	0.42
1:1A:2429:C:OP1	11:1P:65:ARG:NH2	2.51	0.42
6:1G:43:LEU:HB3	6:1G:44:GLY:H	1.61	0.42
8:1I:84:GLY:O	8:1I:86:THR:N	2.51	0.42
32:1a:228:A:H4'	47:1p:62:VAL:HG11	2.01	0.42
54:1w:29:G:H1	54:1w:41:C:H42	1.68	0.42
56:1y:19:G:N1	56:1y:56:C:N4	2.66	0.42
1:2A:244:A:C2	1:2A:255:A:C4	3.08	0.42
1:2A:1342:A:O2'	1:2A:1344:G:OP2	2.36	0.42
1:2A:2061:G:H5''	1:2A:2503:2MA:C2	2.49	0.42
9:2N:38:HIS:NE2	9:2N:50:ASP:OD2	2.53	0.42
11:2P:135:LEU:HD23	11:2P:135:LEU:HA	1.80	0.42
14:2S:87:PHE:CE1	14:2S:102:ALA:HB2	2.54	0.42
15:2T:127:ALA:C	15:2T:129:ARG:N	2.76	0.42
57:2a:107:G:H2'	57:2a:108:G:O4'	2.19	0.42
57:2a:600:C:H2'	57:2a:601:C:C6	2.54	0.42
57:2a:736:C:H2'	57:2a:737:A:C8	2.54	0.42
33:2b:218:ALA:O	33:2b:222:ILE:HG13	2.19	0.42
41:2j:11:PHE:CE1	41:2j:67:THR:HG22	2.55	0.42
42:2k:92:GLU:HB3	42:2k:96:ARG:NH1	2.32	0.42
58:B:3:PRO:HG2	58:B:12:SER:HB2	2.01	0.42
1:1A:116:A:C8	1:1A:117:A:C8	3.07	0.42
1:1A:467:U:O2	5:1F:46:ARG:NH2	2.40	0.42
1:1A:1110:C:N3	1:1A:1120:G:O6	2.53	0.42
1:1A:1941:A:OP2	1:1A:1942:4OC:H5	2.19	0.42
6:1G:7:LEU:HD12	6:1G:104:GLU:HA	2.01	0.42
9:1N:68:GLU:HG3	9:1N:88:GLU:OE2	2.19	0.42
9:1N:73:THR:HG23	9:1N:82:LEU:HD11	2.02	0.42
13:1R:111:LEU:HD12	13:1R:111:LEU:HA	1.86	0.42
25:13:31:LEU:HD23	25:13:31:LEU:HA	1.90	0.42
32:1a:21:G:H2'	32:1a:22:G:C8	2.55	0.42
32:1a:109:A:C6	32:1a:326:G:C6	3.08	0.42
32:1a:840:C:H4'	32:1a:841:U:OP1	2.18	0.42
32:1a:1003:G:N3	32:1a:1004:A:H2	2.18	0.42
33:1b:33:TYR:HB2	33:1b:43:ASP:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:105:PHE:C	33:1b:107:THR:N	2.78	0.42
34:1c:79:ARG:C	34:1c:81:GLY:H	2.28	0.42
35:1d:19:LEU:O	35:1d:21:LEU:HG	2.18	0.42
38:1g:70:LYS:O	38:1g:138:LYS:HD2	2.19	0.42
38:1g:76:ARG:HE	38:1g:156:TRP:HZ2	1.67	0.42
49:1r:45:SER:OG	49:1r:47:THR:HG22	2.18	0.42
56:1y:6:G:O6	56:1y:7:A:N6	2.53	0.42
1:2A:288:C:H2'	1:2A:289:A:C8	2.54	0.42
1:2A:956:G:H2'	1:2A:957:A:H2'	2.01	0.42
1:2A:1006:C:C2	1:2A:1138:G:N2	2.87	0.42
1:2A:1507:A:O2'	1:2A:1508:A:C8	2.72	0.42
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.19	0.42
1:2A:2070:G:C2	1:2A:2442:C:C2	3.08	0.42
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.55	0.42
6:2G:173:LEU:O	6:2G:178:PHE:N	2.43	0.42
7:2H:56:SER:OG	7:2H:61:HIS:ND1	2.48	0.42
14:2S:5:THR:OG1	14:2S:8:GLU:HG2	2.20	0.42
26:24:24:THR:OG1	26:24:25:TYR:N	2.30	0.42
57:2a:730:G:C5	57:2a:731:G:H1'	2.55	0.42
57:2a:1057:G:C4	57:2a:1204:A:C2	3.08	0.42
57:2a:1399:C:H4'	57:2a:1400:5MC:H3'	2.01	0.42
38:2g:78:ARG:O	38:2g:84:ASN:HA	2.19	0.42
41:2j:54:PHE:O	41:2j:55:LYS:HG2	2.20	0.42
48:2q:59:ILE:HG13	48:2q:71:PHE:HD2	1.85	0.42
1:1A:794:U:O2	1:1A:2036:A:H1'	2.20	0.42
1:1A:795:G:C8	18:1W:89:ALA:HB1	2.55	0.42
1:1A:956:A:N3	1:1A:2276:C:O2'	2.45	0.42
1:1A:1093:G:O2'	1:1A:1094:A:O5'	2.31	0.42
1:1A:1387:U:O4'	19:1X:57:LEU:HD23	2.19	0.42
1:1A:1452:U:H2'	1:1A:1453:C:H6	1.82	0.42
1:1A:1692:G:H5''	1:1A:1693:C:H5'	2.01	0.42
1:1A:1766:G:H1'	1:1A:1770:A:N6	2.35	0.42
5:1F:161:GLU:O	5:1F:165:ARG:HB2	2.19	0.42
9:1N:61:ARG:HD3	9:1N:61:ARG:HA	1.82	0.42
25:13:7:LYS:HB2	25:13:34:GLU:HG2	2.02	0.42
32:1a:79:G:C6	32:1a:90:U:C2	3.07	0.42
32:1a:1136:U:H5''	32:1a:1137:C:C2	2.54	0.42
32:1a:1309:G:OP1	44:1m:88:ARG:NH2	2.53	0.42
36:1e:84:PHE:CE2	36:1e:133:TYR:HD2	2.37	0.42
44:1m:118:ALA:HB2	55:1x:28:C:H4'	2.02	0.42
1:2A:300:A:P	20:2Y:86:ARG:NH2	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:11:TYR:OH	6:2G:16:ARG:HD3	2.18	0.42
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.55	0.42
16:2U:58:ARG:HA	16:2U:61:TRP:CE3	2.55	0.42
57:2a:402:G:N7	63:2a:3334:HOH:O	2.37	0.42
57:2a:861:G:O6	57:2a:869:G:N2	2.52	0.42
57:2a:1121:U:C2'	57:2a:1122:U:H5'	2.50	0.42
39:2h:13:ILE:O	39:2h:17:THR:HG23	2.19	0.42
45:2n:33:VAL:HA	45:2n:40:CYS:HA	2.01	0.42
46:2o:3:ILE:HD11	46:2o:38:ARG:HG3	2.00	0.42
1:1A:32:C:O2'	1:1A:33:U:H5'	2.20	0.42
1:1A:320:C:H2'	1:1A:321:C:H6	1.85	0.42
1:1A:848:G:O6	5:1F:53:THR:OG1	2.36	0.42
1:1A:2023:A:OP1	13:1R:9:LYS:NZ	2.51	0.42
1:1A:2897:U:H2'	1:1A:2898:C:C6	2.55	0.42
10:1O:23:ARG:HD2	10:1O:23:ARG:HA	1.85	0.42
32:1a:435:C:H2'	32:1a:436:C:C6	2.55	0.42
32:1a:458:C:H2'	32:1a:460:G:O4'	2.19	0.42
32:1a:544:G:P	35:1d:59:ARG:HH22	2.41	0.42
32:1a:993:G:H2'	32:1a:993:G:N3	2.34	0.42
33:1b:15:VAL:HG21	33:1b:213:LEU:HD13	2.00	0.42
37:1f:11:ASN:HB3	37:1f:14:LEU:HG	2.01	0.42
38:1g:28:ASN:HD22	38:1g:31:MET:HE2	1.85	0.42
48:1q:4:LYS:HG3	48:1q:6:LEU:HD11	2.02	0.42
54:1w:11:C:H2'	54:1w:12:U:C6	2.55	0.42
1:2A:208:C:H2'	1:2A:209:C:C6	2.55	0.42
1:2A:717:G:H2'	1:2A:718:A:O4'	2.20	0.42
1:2A:921:G:C6	1:2A:922:U:C4	3.08	0.42
1:2A:2136:C:O2'	1:2A:2137:C:H6	2.03	0.42
4:2E:35:GLN:OE1	4:2E:66:HIS:HE1	2.03	0.42
6:2G:3:LEU:O	6:2G:8:LYS:NZ	2.33	0.42
7:2H:156:ALA:O	7:2H:172:LYS:HG2	2.19	0.42
8:2I:124:GLY:N	8:2I:144:VAL:HG23	2.35	0.42
10:2O:49:ARG:NH2	57:2a:1423:G:OP1	2.37	0.42
14:2S:24:LEU:HB2	14:2S:85:VAL:HG23	2.02	0.42
30:28:55:ALA:O	30:28:59:LYS:HG3	2.19	0.42
57:2a:396:G:O2'	57:2a:398:C:OP1	2.29	0.42
57:2a:397:A:H5'	57:2a:398:C:OP1	2.20	0.42
57:2a:616:G:P	35:2d:141:ARG:HH22	2.41	0.42
57:2a:765:G:N1	57:2a:812:C:O2'	2.46	0.42
57:2a:890:G:O2'	57:2a:906:G:O6	2.30	0.42
57:2a:1011:G:H1	57:2a:1018:C:N4	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2a:1073:U:O2'	33:2b:104:ASN:OD1	2.37	0.42
57:2a:1291:G:C6	57:2a:1292:U:C4	3.08	0.42
57:2a:1305:G:H22	57:2a:1331:G:H1'	1.83	0.42
57:2a:1517:G:N7	57:2a:1518:MA6:H103	2.35	0.42
36:2e:53:LEU:HA	36:2e:56:GLN:HG2	2.00	0.42
43:2l:41:ARG:HH22	43:2l:57:LYS:HZ1	1.67	0.42
49:2r:22:VAL:HG23	49:2r:55:ARG:O	2.20	0.42
1:1A:105:C:H2'	1:1A:106:U:H6	1.83	0.42
1:1A:866:A:C4	1:1A:1234:A:C2	3.08	0.42
1:1A:977:G:H4'	1:1A:978:A:O5'	2.20	0.42
1:1A:1463:C:H2'	1:1A:1464:G:O4'	2.19	0.42
1:1A:1897:C:H2'	1:1A:1898:A:O4'	2.19	0.42
9:1N:58:ASP:OD1	9:1N:58:ASP:N	2.52	0.42
22:10:4:LYS:NZ	63:10:202:HOH:O	2.46	0.42
24:12:52:ASP:O	24:12:56:GLN:HG3	2.20	0.42
32:1a:78:G:O6	32:1a:92:C:N4	2.53	0.42
32:1a:870:U:H4'	32:1a:871:U:H5''	2.02	0.42
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.19	0.42
32:1a:1286:A:H2'	32:1a:1287:A:H4'	2.01	0.42
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	2.01	0.42
1:2A:884:C:H3'	1:2A:885:C:C6	2.55	0.42
1:2A:1791:A:H8	1:2A:1791:A:OP2	2.03	0.42
2:2B:17:C:H2'	2:2B:18:G:O4'	2.20	0.42
5:2F:178:PRO:HB3	5:2F:198:ALA:HA	2.02	0.42
7:2H:3:ARG:CZ	7:2H:5:GLY:H	2.32	0.42
21:2Z:8:TYR:HB2	21:2Z:38:TYR:CE2	2.55	0.42
31:29:10:ILE:HD12	31:29:32:HIS:HA	2.00	0.42
57:2a:407:G:H2'	57:2a:408:A:C8	2.55	0.42
57:2a:562:C:H4'	57:2a:563:A:O5'	2.20	0.42
57:2a:997:U:H2'	57:2a:998:G:C8	2.55	0.42
57:2a:1240:U:OP2	38:2g:116:ALA:N	2.52	0.42
57:2a:1358:U:OP1	45:2n:35:ARG:HG2	2.19	0.42
48:2q:84:LEU:HA	48:2q:87:LYS:HZ2	1.84	0.42
1:1A:733:G:H8	29:17:6:GLN:O	2.03	0.42
1:1A:1140:U:H3	1:1A:1142:A:H5'	1.85	0.42
1:1A:2044:U:OP1	63:1A:4361:HOH:O	2.22	0.42
1:1A:2190:G:C6	1:1A:2193:A:C8	3.08	0.42
3:1D:68:LYS:HB2	3:1D:70:TRP:CE2	2.55	0.42
4:1E:103:ASP:OD2	4:1E:168:MET:HE2	2.20	0.42
6:1G:125:PHE:HB2	63:1G:5005:HOH:O	2.19	0.42
32:1a:160:A:H2'	32:1a:161:A:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1f:91:VAL:HG11	49:1r:72:ARG:NH1	2.35	0.42
39:1h:17:THR:HB	39:1h:78:GLN:OE1	2.20	0.42
39:1h:49:GLU:HG2	39:1h:62:TYR:HE2	1.84	0.42
42:1k:40:ILE:HD13	42:1k:40:ILE:HA	1.86	0.42
44:1m:82:MET:O	44:1m:93:ARG:NH2	2.52	0.42
54:1w:63:G:H2'	54:1w:64:A:C8	2.55	0.42
56:1y:36:A:C6	56:1y:37:A:C5	3.08	0.42
1:2A:271(K):U:H4'	1:2A:271(L):U:OP2	2.20	0.42
1:2A:606:U:H4'	1:2A:658:C:H4'	2.00	0.42
1:2A:747:U:O2	1:2A:2014:A:H1'	2.19	0.42
1:2A:2375:G:O2'	1:2A:2377:A:N7	2.36	0.42
1:2A:2419:U:H2'	1:2A:2420:C:C6	2.55	0.42
7:2H:154:PRO:HB3	7:2H:163:TYR:CZ	2.55	0.42
8:2I:53:ALA:O	8:2I:57:ARG:HG2	2.20	0.42
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HE2	2.02	0.42
23:21:23:LYS:HB3	23:21:29:GLY:HA3	2.02	0.42
31:29:17:ILE:HD12	31:29:17:ILE:HA	1.78	0.42
57:2a:404:U:H2'	57:2a:405:U:C6	2.55	0.42
57:2a:1132:C:H42	57:2a:1142:G:H1	1.66	0.42
35:2d:200:GLU:OE1	35:2d:200:GLU:N	2.53	0.42
54:2w:4:C:N4	54:2w:69:G:N1	2.35	0.42
1:1A:74:G:H4'	24:12:55:ARG:NH1	2.34	0.42
1:1A:1810:U:OP2	63:1A:4360:HOH:O	2.22	0.42
1:1A:2874:G:OP1	15:1T:119:LYS:HD2	2.20	0.42
3:1D:38:LYS:HA	3:1D:38:LYS:HD2	1.82	0.42
6:1G:28:VAL:O	6:1G:31:VAL:HG13	2.20	0.42
15:1T:108:ARG:HG3	15:1T:109:GLU:N	2.34	0.42
30:18:26:LYS:HG2	30:18:46:ARG:O	2.20	0.42
32:1a:26:A:H1'	35:1d:209:ARG:HH21	1.85	0.42
32:1a:1036:G:H5''	32:1a:1037:C:C5	2.55	0.42
32:1a:1402:4OC:O5'	32:1a:1402:4OC:H6	2.20	0.42
35:1d:173:TRP:CD2	35:1d:189:PRO:HG3	2.55	0.42
40:1i:17:VAL:HG23	40:1i:63:ILE:HG12	2.02	0.42
41:1j:38:ILE:HG12	41:1j:38:ILE:H	1.61	0.42
49:1r:24:ALA:C	49:1r:26:LEU:H	2.28	0.42
1:2A:234:C:H2'	1:2A:235:U:C6	2.55	0.42
1:2A:910:A:H2'	1:2A:911:A:C8	2.55	0.42
1:2A:1169:G:C2	1:2A:1170:G:N7	2.88	0.42
1:2A:1495:A:H2'	1:2A:1496:A:H8	1.83	0.42
1:2A:1592:C:H2'	1:2A:1593:G:H8	1.85	0.42
1:2A:2377:A:H2'	1:2A:2378:A:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.79	0.42
11:2P:59:LEU:HD11	30:28:10:ALA:CB	2.45	0.42
57:2a:20:U:H2'	57:2a:21:G:O4'	2.19	0.42
57:2a:376:G:OP2	47:2p:67:THR:HG21	2.20	0.42
57:2a:664:G:P	49:2r:64:ARG:HH21	2.42	0.42
34:2c:180:ALA:HB1	34:2c:203:PHE:CE1	2.55	0.42
37:2f:76:ALA:O	37:2f:80:ARG:HG3	2.20	0.42
56:2y:28:G:H2'	56:2y:29:G:C8	2.55	0.42
1:1A:7:G:H2'	1:1A:8:A:O4'	2.21	0.41
1:1A:253:C:O2'	1:1A:254:A:H2'	2.20	0.41
1:1A:1120:G:N1	1:1A:1121:C:H1'	2.35	0.41
1:1A:1132:A:H5''	1:1A:1132:A:N3	2.35	0.41
1:1A:1821:C:H5''	1:1A:1822:A:OP1	2.20	0.41
3:1D:132:PRO:HD3	3:1D:190:TYR:CZ	2.55	0.41
10:1O:106:LEU:HD23	10:1O:106:LEU:HA	1.90	0.41
32:1a:93:G:H2'	32:1a:96:U:O4'	2.21	0.41
32:1a:117:G:H2'	32:1a:118:U:O4'	2.20	0.41
32:1a:189:G:C6	32:1a:189(L):G:N1	2.88	0.41
51:1t:36:LEU:HD12	51:1t:62:LEU:HD12	2.02	0.41
1:2A:68:G:H2'	1:2A:69:C:O4'	2.19	0.41
1:2A:383:U:H2'	1:2A:385:C:H5	1.85	0.41
1:2A:956:G:N2	1:2A:959:A:H3'	2.35	0.41
1:2A:988:A:N7	63:2A:4041:HOH:O	2.37	0.41
1:2A:1545:A:H2'	1:2A:1546:C:O4'	2.20	0.41
10:2O:9:GLU:H	10:2O:9:GLU:HG2	1.67	0.41
15:2T:28:VAL:HG13	15:2T:86:ILE:HG23	2.01	0.41
57:2a:1198:G:H2'	57:2a:1199:U:C6	2.56	0.41
57:2a:1323:G:H4'	57:2a:1363:C:N3	2.35	0.41
34:2c:125:GLU:HG2	34:2c:190:ARG:O	2.20	0.41
36:2e:123:LEU:HD23	36:2e:123:LEU:HA	1.84	0.41
38:2g:23:VAL:O	38:2g:27:ILE:HG13	2.20	0.41
56:2y:23:A:H2'	56:2y:24:G:C8	2.55	0.41
58:B:2:SER:C	58:B:4:GLY:HA3	2.45	0.41
1:1A:385:G:N1	1:1A:386:U:O4	2.53	0.41
1:1A:655:G:OP2	30:18:15:LYS:NZ	2.38	0.41
1:1A:1320:A:N3	1:1A:1343:C:H1'	2.35	0.41
1:1A:1617:A:H2'	1:1A:1618:A:C8	2.56	0.41
7:1H:20:ALA:HB3	7:1H:23:ARG:HG3	2.02	0.41
32:1a:141:A:H1'	32:1a:182:U:O2	2.19	0.41
32:1a:1107:C:OP1	34:1c:172:ARG:HG3	2.20	0.41
32:1a:1304:G:C6	32:1a:1305:G:N1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1g:79:ARG:HD2	38:1g:80:VAL:H	1.85	0.41
47:1p:22:THR:HA	47:1p:33:ILE:HG13	2.02	0.41
54:1w:46:G7M:H8	54:1w:46:G7M:H2'	1.90	0.41
1:2A:315:G:H2'	1:2A:316:C:C6	2.55	0.41
1:2A:598:G:C6	1:2A:599:G:C5	3.08	0.41
1:2A:637:A:H2'	11:2P:117:GLU:OE1	2.19	0.41
1:2A:652(A):A:H2'	1:2A:652(A):A:N3	2.34	0.41
1:2A:676:A:H1'	1:2A:2443:C:H1'	2.02	0.41
1:2A:684:G:OP1	29:27:16:HIS:ND1	2.52	0.41
1:2A:852:G:H2'	1:2A:853:G:C8	2.44	0.41
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.31	0.41
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.55	0.41
1:2A:1866:C:H2'	1:2A:1876:A:O4'	2.20	0.41
1:2A:2137:C:N3	1:2A:2155:G:C6	2.88	0.41
1:2A:2315:G:H1'	6:2G:126:ASP:OD2	2.19	0.41
1:2A:2518:A:OP2	63:2A:3961:HOH:O	2.22	0.41
4:2E:12:THR:HG21	15:2T:11:GLU:OE2	2.19	0.41
8:2I:87:LYS:HE3	8:2I:87:LYS:HB2	1.73	0.41
15:2T:27:THR:HB	15:2T:89:VAL:HG23	2.02	0.41
23:21:50:ARG:HD2	23:21:57:GLU:OE2	2.18	0.41
27:25:49:CYS:SG	27:25:51:TYR:HB2	2.61	0.41
57:2a:271:C:H2'	57:2a:272:C:C6	2.55	0.41
57:2a:580:U:H2'	57:2a:581:G:O4'	2.20	0.41
57:2a:1026:G:N3	57:2a:1026:G:H2'	2.35	0.41
57:2a:1330:U:H4'	44:2m:23:TYR:CE1	2.54	0.41
36:2e:107:ARG:O	36:2e:111:GLU:N	2.47	0.41
54:2w:14:A:H61	54:2w:21:A:H2	1.67	0.41
1:1A:502:G:H4'	1:1A:527:A:N1	2.35	0.41
1:1A:1093:G:H2'	1:1A:1156:G:N2	2.35	0.41
1:1A:2081:A:O3'	5:1F:69:HIS:HA	2.21	0.41
1:1A:2155:G:N2	1:1A:2156:A:H62	2.19	0.41
1:1A:2205:C:H2'	1:1A:2206:G:H8	1.85	0.41
1:1A:2246:G:N7	63:1A:4443:HOH:O	2.37	0.41
12:1Q:111:GLU:O	12:1Q:115:MET:HG2	2.20	0.41
15:1T:127:ALA:O	15:1T:128:GLU:HG2	2.20	0.41
18:1W:92:ARG:NH1	63:1W:303:HOH:O	2.52	0.41
21:1Z:99:TYR:HB3	21:1Z:123:ASP:OD2	2.19	0.41
32:1a:1152:A:OP1	41:1j:68:HIS:ND1	2.53	0.41
32:1a:1289:A:N1	32:1a:1371:G:O2'	2.52	0.41
32:1a:1401:G:C2	32:1a:1402:4OC:H1'	2.55	0.41
33:1b:109:SER:O	33:1b:112:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:61:LYS:HD2	35:1d:207:TYR:OH	2.21	0.41
38:1g:104:LEU:HD12	38:1g:104:LEU:HA	1.88	0.41
40:1i:17:VAL:HG11	40:1i:80:GLY:C	2.46	0.41
1:2A:1480:G:C6	1:2A:1481:U:C4	3.08	0.41
1:2A:1550:C:H2'	1:2A:1551:C:C6	2.55	0.41
1:2A:2165:G:O5'	1:2A:2165:G:H8	2.03	0.41
1:2A:2321:G:N3	1:2A:2321:G:H2'	2.35	0.41
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.35	0.41
1:2A:2745:C:H2'	1:2A:2746:U:O4'	2.21	0.41
2:2B:43:C:O4'	6:2G:66:GLN:NE2	2.54	0.41
29:27:12:ARG:HB3	29:27:46:VAL:HG21	2.03	0.41
57:2a:7:G:H5'	57:2a:298:A:O4'	2.20	0.41
57:2a:8:A:N6	35:2d:209:ARG:HB2	2.34	0.41
57:2a:577:G:H2'	57:2a:578:C:H6	1.85	0.41
57:2a:1151:A:O2'	57:2a:1152:A:H8	2.03	0.41
57:2a:1465:C:H2'	57:2a:1466:C:O4'	2.20	0.41
57:2a:1518:MA6:C6	57:2a:1519:MA6:H103	2.51	0.41
35:2d:78:LEU:HD22	35:2d:96:LEU:HB3	2.01	0.41
47:2p:20:VAL:HG21	47:2p:32:TYR:CD2	2.55	0.41
54:2w:46:G7M:O2'	54:2w:47:U:H4'	2.19	0.41
1:1A:908:A:C2	1:1A:963:A:C4	3.09	0.41
1:1A:1400:A:H2'	1:1A:1401:G:O4'	2.20	0.41
1:1A:1864:U:O2'	1:1A:1991:A:N1	2.48	0.41
1:1A:2250:G:N3	1:1A:2250:G:H2'	2.34	0.41
4:1E:143:ASN:HD22	4:1E:147:PRO:HD3	1.85	0.41
18:1W:7:ALA:HB2	18:1W:50:VAL:HG22	2.01	0.41
24:12:53:LEU:HD23	24:12:53:LEU:HA	1.80	0.41
32:1a:836:G:OP1	49:1r:61:LYS:NZ	2.41	0.41
32:1a:1034:G:N2	32:1a:1035:A:N3	2.68	0.41
46:1o:57:LEU:HD23	46:1o:57:LEU:HA	1.92	0.41
48:1q:4:LYS:HG3	48:1q:6:LEU:CD1	2.50	0.41
1:2A:839:U:H2'	1:2A:840:C:H6	1.85	0.41
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.20	0.41
1:2A:1589:C:H2'	1:2A:1590:U:H6	1.85	0.41
1:2A:1630:G:H2'	1:2A:1631:C:C6	2.56	0.41
1:2A:1652:A:C2'	1:2A:1653:G:H5'	2.50	0.41
1:2A:1697:G:OP2	1:2A:1698:A:O2'	2.27	0.41
1:2A:2103:C:O2'	1:2A:2104:G:H5'	2.20	0.41
1:2A:2802:G:H2'	1:2A:2803:C:O4'	2.20	0.41
2:2B:8:U:O3'	14:2S:25:ARG:NH2	2.53	0.41
2:2B:11:C:OP2	2:2B:12:C:N4	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:80:U:H2'	2:2B:81:G:C8	2.55	0.41
4:2E:109:LYS:O	4:2E:111:ARG:NH1	2.53	0.41
5:2F:132:VAL:HG21	5:2F:163:VAL:HG22	2.03	0.41
5:2F:133:ASN:O	5:2F:162:LEU:HD23	2.19	0.41
8:2I:59:ALA:HA	8:2I:62:LYS:HB3	2.00	0.41
11:2P:77:ARG:HG3	11:2P:78:PRO:HD2	2.02	0.41
57:2a:779:C:H2'	57:2a:780:A:O4'	2.20	0.41
57:2a:1319:A:H61	57:2a:1361:G:H21	1.67	0.41
34:2c:142:MET:HG3	34:2c:170:GLN:HB3	2.02	0.41
39:2h:87:SER:HB2	39:2h:93:VAL:HB	2.03	0.41
40:2i:79:LEU:O	40:2i:83:ARG:HB2	2.20	0.41
44:2m:94:ARG:NH2	50:2s:81:ARG:HA	2.35	0.41
55:2x:3:C:H42	55:2x:70:G:H1	1.68	0.41
1:1A:943:C:C2	1:1A:944:C:C4	3.08	0.41
1:1A:1108:G:C5	1:1A:1134:A:H2'	2.56	0.41
4:1E:47:VAL:HG22	4:1E:84:PHE:O	2.21	0.41
10:1O:98:VAL:HG22	10:1O:118:ALA:HA	2.03	0.41
11:1P:135:LEU:HD23	11:1P:135:LEU:HA	1.77	0.41
13:1R:12:ARG:HG2	13:1R:16:HIS:CE1	2.55	0.41
14:1S:65:VAL:O	14:1S:69:VAL:HG12	2.20	0.41
18:1W:23:LEU:HD12	18:1W:23:LEU:HA	1.93	0.41
32:1a:313:A:H2'	32:1a:314:C:C6	2.55	0.41
32:1a:1265:G:H2'	32:1a:1266:G:O4'	2.21	0.41
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.55	0.41
54:1w:63:G:H2'	54:1w:64:A:H8	1.86	0.41
1:2A:93:G:H2'	1:2A:94:C:C6	2.54	0.41
1:2A:407:G:H2'	1:2A:408:G:H8	1.85	0.41
1:2A:536:A:H2'	1:2A:537:C:C6	2.55	0.41
1:2A:569:U:C4	1:2A:570:G:C6	3.09	0.41
1:2A:1372:U:H2'	1:2A:1373:A:O4'	2.21	0.41
1:2A:1473:G:C6	1:2A:1474:C:C4	3.09	0.41
1:2A:2284:C:OP2	28:26:2:ALA:N	2.54	0.41
2:2B:90:A:N7	2:2B:91:C:H1'	2.36	0.41
2:2B:115:G:H2'	2:2B:116:G:O4'	2.20	0.41
5:2F:154:VAL:HG22	5:2F:191:ARG:HB2	2.02	0.41
7:2H:3:ARG:HG2	7:2H:6:ARG:HE	1.84	0.41
7:2H:7:LEU:HD23	7:2H:69:ARG:NH2	2.35	0.41
12:2Q:17:LEU:HB3	12:2Q:39:PRO:HB2	2.02	0.41
17:2V:31:ALA:O	17:2V:61:VAL:HG12	2.19	0.41
23:21:8:SER:HB3	23:21:66:HIS:CD2	2.56	0.41
57:2a:139:G:H2'	57:2a:140:A:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2a:1098:C:H2'	57:2a:1099:G:O4'	2.20	0.41
57:2a:1319:A:N6	57:2a:1361:G:H21	2.18	0.41
34:2c:151:VAL:HA	34:2c:199:LYS:O	2.21	0.41
39:2h:39:LEU:HB3	39:2h:45:ILE:HG12	2.01	0.41
47:2p:43:LYS:HG2	47:2p:48:TRP:CG	2.55	0.41
54:2w:8:4SU:S4	54:2w:14:A:N7	2.94	0.41
1:1A:173:C:H2'	1:1A:174:U:H6	1.84	0.41
1:1A:233:A:C2	1:1A:244:A:C4	3.09	0.41
1:1A:645:G:N3	1:1A:645:G:H2'	2.35	0.41
1:1A:670:C:O5'	1:1A:670:C:H6	2.03	0.41
1:1A:873:U:H4'	11:1P:55:ARG:HB3	2.03	0.41
1:1A:1162:C:H5'	1:1A:1163:G:OP2	2.20	0.41
1:1A:2177:G:H3'	1:1A:2178:G:H8	1.86	0.41
1:1A:2205:C:HO2'	1:1A:2206:G:P	2.42	0.41
2:1B:88:C:H2'	2:1B:89:G:O4'	2.20	0.41
6:1G:72:ARG:HH12	6:1G:87:PRO:HG3	1.85	0.41
12:1Q:60:ARG:HH22	54:1w:53:G:P	2.44	0.41
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.56	0.41
24:12:32:LEU:HD11	24:12:54:LYS:HG2	2.02	0.41
32:1a:189(F):U:C2	48:1q:72:ARG:NH2	2.88	0.41
32:1a:270:A:H2'	32:1a:271:C:C6	2.55	0.41
33:1b:196:LEU:HD12	33:1b:196:LEU:HA	1.76	0.41
34:1c:120:VAL:O	34:1c:124:ILE:HG23	2.21	0.41
1:2A:460:A:C2	1:2A:470:A:C4	3.09	0.41
1:2A:764:A:H5'	3:2D:210:GLY:HA2	2.03	0.41
1:2A:855:G:C6	1:2A:856:C:C4	3.09	0.41
1:2A:1773:A:H5''	63:2A:4614:HOH:O	2.19	0.41
1:2A:2095:C:H2'	1:2A:2096:U:O4'	2.20	0.41
1:2A:2792:G:H2'	1:2A:2792:G:N3	2.36	0.41
19:2X:1:MET:HE1	24:22:26:ARG:HH21	1.85	0.41
57:2a:254:G:OP1	48:2q:66:SER:OG	2.34	0.41
57:2a:351:G:H4'	57:2a:352:C:OP1	2.20	0.41
57:2a:1318:A:H4'	50:2s:10:PHE:CD2	2.55	0.41
36:2e:105:VAL:HB	36:2e:106:PRO:HD3	2.02	0.41
37:2f:61:LEU:HB3	37:2f:63:TYR:CE2	2.55	0.41
37:2f:69:GLU:O	37:2f:72:VAL:HG22	2.20	0.41
50:2s:52:TYR:HA	50:2s:57:HIS:HA	2.01	0.41
54:2w:36:A:H2'	54:2w:37:MIA:H8	2.01	0.41
1:1A:327:U:H2'	1:1A:328:G:H8	1.86	0.41
1:1A:397:G:H4'	1:1A:398:A:OP2	2.20	0.41
1:1A:505:A:N3	1:1A:507:G:H5''	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:929:G:H1	1:1A:940:C:N4	2.03	0.41
1:1A:1053:C:OP1	9:1N:37:LYS:NZ	2.54	0.41
1:1A:1255:A:H5''	1:1A:1257:G:O4'	2.20	0.41
1:1A:2096:U:H2'	1:1A:2097:U:C6	2.55	0.41
1:1A:2621:U:H5'	58:A:5:ASN:HD21	1.85	0.41
2:1B:1:U:HO2'	2:1B:2:C:P	2.43	0.41
20:1Y:6:HIS:CD2	20:1Y:6:HIS:H	2.37	0.41
31:19:27:CYS:SG	31:19:28:GLU:N	2.94	0.41
35:1d:3:ARG:HG3	35:1d:5:ILE:HG23	2.02	0.41
37:1f:35:ALA:HA	37:1f:67:MET:HB3	2.03	0.41
47:1p:50:LYS:HA	47:1p:50:LYS:HD2	1.90	0.41
56:1y:65:G:N3	56:1y:65:G:H2'	2.35	0.41
1:2A:11:G:C2'	1:2A:12:U:H5'	2.51	0.41
1:2A:531:C:H4'	1:2A:532:A:H5''	2.03	0.41
1:2A:784:A:N6	3:2D:229:VAL:HG11	2.35	0.41
1:2A:848:G:N9	1:2A:933:A:H8	2.19	0.41
1:2A:1192:G:OP2	11:2P:17:LYS:NZ	2.50	0.41
1:2A:1702:G:H2'	1:2A:1703:G:O4'	2.21	0.41
1:2A:2130:U:O2'	1:2A:2133:G:H4'	2.21	0.41
1:2A:2197:U:H1'	1:2A:2198:A:C8	2.56	0.41
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.21	0.41
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	2.03	0.41
57:2a:1085:U:H3'	57:2a:1086:U:C5	2.55	0.41
57:2a:1272:G:N2	57:2a:1273:G:N9	2.68	0.41
57:2a:1366:C:H2'	57:2a:1367:C:C6	2.56	0.41
57:2a:1376:U:P	38:2g:94:ARG:HH22	2.43	0.41
33:2b:167:PRO:HD3	33:2b:187:LEU:O	2.20	0.41
35:2d:110:PHE:CE2	35:2d:148:VAL:HG23	2.56	0.41
40:2i:4:TYR:HB2	40:2i:19:LEU:HB2	2.03	0.41
48:2q:5:VAL:O	48:2q:6:LEU:HD12	2.21	0.41
1:1A:670:C:H5''	1:1A:671:A:OP2	2.20	0.41
1:1A:847:A:H8	1:1A:847:A:OP1	2.03	0.41
1:1A:1014:U:O5'	1:1A:1014:U:H6	2.04	0.41
1:1A:2128:G:H2'	1:1A:2129:C:C6	2.55	0.41
18:1W:25:ARG:NH2	18:1W:74:ALA:O	2.48	0.41
26:14:18:CYS:SG	26:14:20:ASN:HB2	2.61	0.41
32:1a:552:U:H4'	43:1l:86:ARG:HD2	2.02	0.41
32:1a:580:U:H2'	32:1a:581:G:O4'	2.20	0.41
32:1a:667:G:H4'	46:1o:51:HIS:CE1	2.56	0.41
32:1a:1070:U:H2'	32:1a:1071:C:C6	2.56	0.41
32:1a:1251:A:H2'	32:1a:1252:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1258:G:H2'	32:1a:1259:C:H6	1.86	0.41
35:1d:8:VAL:O	35:1d:11:LEU:HB2	2.20	0.41
1:2A:127:A:H5''	1:2A:128:C:C6	2.55	0.41
1:2A:1539:G:H2'	1:2A:1540:U:O4'	2.20	0.41
1:2A:1557:C:H5''	1:2A:1558:A:OP2	2.21	0.41
1:2A:2250:G:O2'	1:2A:2496:C:OP1	2.35	0.41
1:2A:2678:C:H2'	1:2A:2679:A:O4'	2.21	0.41
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.56	0.41
10:2O:24:VAL:HG12	10:2O:33:ALA:HB2	2.03	0.41
11:2P:59:LEU:HD22	11:2P:60:MET:HE2	2.03	0.41
30:28:23:VAL:HG13	30:28:47:LYS:HB3	2.02	0.41
57:2a:678:U:H2'	57:2a:679:C:C6	2.56	0.41
57:2a:745:C:H2'	57:2a:746:A:C8	2.56	0.41
57:2a:973:G:N3	41:2j:54:PHE:HE1	2.19	0.41
57:2a:1190:G:H5'	34:2c:176:HIS:CE1	2.55	0.41
35:2d:11:LEU:O	35:2d:15:GLU:HG2	2.20	0.41
40:2i:83:ARG:O	40:2i:86:VAL:HG22	2.21	0.41
44:2m:60:VAL:HG13	44:2m:64:TRP:CE3	2.56	0.41
1:1A:63:A:C5	19:1X:66:LEU:HD13	2.56	0.41
1:1A:492:A:N3	1:1A:730:C:H1'	2.35	0.41
1:1A:1899:A:H5''	1:1A:1900:G:OP2	2.21	0.41
1:1A:2153:G:H5''	1:1A:2154:U:H3'	2.02	0.41
1:1A:2171:G:N1	1:1A:2172:U:O2	2.54	0.41
1:1A:2364:A:N6	1:1A:2377:G:O2'	2.53	0.41
1:1A:2724:U:H1'	1:1A:2725:A:C8	2.56	0.41
2:1B:43:C:H4'	6:1G:98:ARG:HH21	1.86	0.41
3:1D:26:LYS:HD3	3:1D:83:GLU:OE2	2.21	0.41
3:1D:35:LYS:HB2	3:1D:36:PRO:HD2	2.02	0.41
5:1F:135:LYS:HB2	5:1F:138:GLU:HG3	2.03	0.41
6:1G:116:ASP:OD2	44:1m:68:GLY:HA3	2.21	0.41
7:1H:154:PRO:HB3	7:1H:163:TYR:CE1	2.56	0.41
9:1N:120:LEU:HG	9:1N:122:VAL:HG23	2.01	0.41
12:1Q:17:LEU:HB3	12:1Q:39:PRO:HB2	2.02	0.41
17:1V:1:MET:HE2	17:1V:41:GLY:O	2.20	0.41
26:14:61:ARG:HH21	50:1s:42:PRO:CD	2.34	0.41
32:1a:502:G:H2'	32:1a:503:C:O4'	2.20	0.41
32:1a:576:G:O6	32:1a:880:C:O2'	2.32	0.41
32:1a:942:G:H21	40:1i:124:GLN:NE2	2.18	0.41
35:1d:88:VAL:HG22	36:1e:97:GLY:HA2	2.03	0.41
39:1h:86:ILE:HG13	39:1h:133:LEU:HD22	2.03	0.41
43:1l:40:VAL:HG11	43:1l:77:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1t:56:MET:HE3	51:1t:85:MET:HE2	2.03	0.41
1:2A:27:G:C2	1:2A:512:G:N3	2.89	0.41
1:2A:218:A:C2	1:2A:235:U:H4'	2.56	0.41
1:2A:322:A:H5'	1:2A:340:A:H1'	2.03	0.41
1:2A:1653:G:H3'	13:2R:2:ARG:HD3	2.02	0.41
1:2A:1919:A:O2'	57:2a:1517:G:N3	2.52	0.41
1:2A:1926:U:O2'	1:2A:1928:A:N7	2.46	0.41
1:2A:2489:G:C2'	1:2A:2490:G:H5'	2.51	0.41
1:2A:2552:2MU:H2'	1:2A:2554:U:OP2	2.21	0.41
1:2A:2626:C:H2'	1:2A:2627:G:O4'	2.21	0.41
1:2A:2689:U:H4'	1:2A:2690:C:H5'	2.03	0.41
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.53	0.41
3:2D:4:LYS:HB3	3:2D:18:VAL:HG23	2.02	0.41
3:2D:232:PRO:HB3	3:2D:244:ARG:CZ	2.51	0.41
4:2E:97:LYS:HB3	4:2E:97:LYS:HE2	1.80	0.41
6:2G:138:GLN:OE1	6:2G:138:GLN:N	2.49	0.41
7:2H:8:PRO:O	7:2H:10:PRO:HD3	2.20	0.41
7:2H:127:GLU:C	7:2H:129:THR:H	2.28	0.41
7:2H:170:ARG:O	7:2H:171:LEU:HD23	2.20	0.41
14:2S:26:LEU:HD22	14:2S:87:PHE:HD1	1.86	0.41
15:2T:60:THR:HG22	15:2T:77:PRO:HA	2.02	0.41
18:2W:78:GLU:OE2	18:2W:99:ARG:HD3	2.21	0.41
28:26:9:LEU:HD13	28:26:51:GLU:HB2	2.02	0.41
57:2a:677:U:H1'	42:2k:119:CYS:SG	2.61	0.41
57:2a:1070:U:H2'	57:2a:1071:C:C6	2.55	0.41
57:2a:1206:G:O2'	34:2c:193:TYR:HA	2.21	0.41
57:2a:1324:A:H4'	57:2a:1362:C:O3'	2.21	0.41
33:2b:24:TRP:H	33:2b:24:TRP:HD1	1.67	0.41
33:2b:36:ARG:C	33:2b:38:GLY:H	2.29	0.41
33:2b:163:PHE:HA	33:2b:185:ILE:HG12	2.03	0.41
35:2d:61:LYS:HD2	35:2d:207:TYR:OH	2.21	0.41
36:2e:91:LEU:HG	36:2e:118:ILE:HD11	2.03	0.41
37:2f:25:ILE:HD13	37:2f:82:ARG:HD3	2.02	0.41
38:2g:71:PRO:HG3	38:2g:103:TRP:CH2	2.56	0.41
38:2g:111:ARG:HD3	38:2g:123:GLU:OE1	2.20	0.41
43:2l:53:ARG:HB3	43:2l:69:TYR:HE1	1.86	0.41
44:2m:14:ARG:NE	44:2m:42:ALA:HA	2.36	0.41
44:2m:27:LYS:HD2	44:2m:27:LYS:HA	1.82	0.41
54:2w:44:G:C2'	54:2w:45:U:H5'	2.51	0.41
1:1A:662:A:H2'	11:1P:117:GLU:OE1	2.21	0.41
1:1A:1640:G:H2'	1:1A:1641:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2387:G:O2'	1:1A:2389:A:N7	2.45	0.41
4:1E:2:LYS:HG3	4:1E:200:GLU:HB2	2.02	0.41
6:1G:41:GLN:HG2	6:1G:154:GLY:O	2.21	0.41
6:1G:66:GLN:HG3	26:14:1:MET:HE1	2.03	0.41
32:1a:7:G:H21	36:1e:121:LYS:HG2	1.86	0.41
32:1a:343:U:O2'	32:1a:344:A:H2'	2.21	0.41
32:1a:613:C:H2'	32:1a:614:A:C8	2.54	0.41
32:1a:731:G:H5'	32:1a:766:A:H4'	2.02	0.41
33:1b:100:GLY:O	33:1b:104:ASN:N	2.45	0.41
41:1j:38:ILE:CG1	41:1j:71:LEU:HB3	2.51	0.41
42:1k:34:ASP:OD1	42:1k:38:ASN:N	2.51	0.41
44:1m:20:THR:HA	44:1m:25:ILE:O	2.21	0.41
56:1y:34:G:H2'	56:1y:35:A:C8	2.55	0.41
1:2A:866:A:C6	1:2A:914:C:C5	3.09	0.41
1:2A:2274:A:C5	1:2A:2276:G:C8	3.09	0.41
1:2A:2667:C:H2'	1:2A:2668:G:O4'	2.21	0.41
4:2E:11:MET:HG2	4:2E:24:THR:HB	2.03	0.41
5:2F:23:ASP:O	5:2F:24:LEU:HD12	2.21	0.41
5:2F:156:LEU:HD21	5:2F:163:VAL:HG12	2.02	0.41
12:2Q:137:TYR:CE1	21:2Z:83:PRO:HG3	2.56	0.41
24:22:1:MET:SD	24:22:56:GLN:NE2	2.94	0.41
57:2a:316:G:OP2	57:2a:351:G:O2'	2.35	0.41
57:2a:580:U:H5''	46:2o:58:MET:HG2	2.01	0.41
57:2a:967:5MC:H2'	57:2a:968:A:N7	2.35	0.41
57:2a:1133:G:C4	57:2a:1134:G:C8	3.09	0.41
57:2a:1305:G:H5'	52:2u:4:GLY:HA3	2.03	0.41
35:2d:173:TRP:CD1	35:2d:173:TRP:H	2.38	0.41
35:2d:192:GLU:C	35:2d:194:LEU:H	2.29	0.41
36:2e:110:LEU:HD13	36:2e:118:ILE:HG21	2.03	0.41
45:2n:37:PHE:C	45:2n:39:LEU:H	2.28	0.41
48:2q:81:ARG:HB3	48:2q:84:LEU:HD12	2.03	0.41
55:2x:40:C:H2'	55:2x:41:C:H6	1.86	0.41
56:2y:52:G:H1'	56:2y:63:G:N2	2.35	0.41
1:1A:346:A:H5'	1:1A:364:A:H1'	2.01	0.40
1:1A:1102:G:H5''	1:1A:1103:A:O4'	2.21	0.40
1:1A:1478:C:H2'	1:1A:1479:U:O4'	2.22	0.40
1:1A:2177:G:H2'	1:1A:2177:G:N3	2.37	0.40
4:1E:98:PRO:HD3	4:1E:175:VAL:HG13	2.03	0.40
7:1H:87:LEU:HD23	7:1H:164:TYR:HA	2.02	0.40
7:1H:101:ARG:NH1	7:1H:117:PRO:HG2	2.36	0.40
12:1Q:30:GLY:HA2	12:1Q:107:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1R:12:ARG:HG2	13:1R:16:HIS:ND1	2.36	0.40
16:1U:16:LYS:HB3	16:1U:16:LYS:HE2	1.77	0.40
20:1Y:13:VAL:HG12	20:1Y:74:PRO:HA	2.03	0.40
23:11:8:SER:HB3	23:11:66:HIS:CD2	2.57	0.40
32:1a:353:A:H8	32:1a:353:A:H5'	1.86	0.40
32:1a:672:U:O2'	32:1a:673:G:O5'	2.35	0.40
32:1a:892:A:O2'	32:1a:1415:G:H4'	2.21	0.40
32:1a:1237:C:O2'	32:1a:1300:G:N2	2.45	0.40
32:1a:1355:G:H2'	32:1a:1356:G:C8	2.56	0.40
36:1e:90:VAL:O	36:1e:120:THR:HA	2.21	0.40
39:1h:124:ALA:O	39:1h:128:GLY:N	2.50	0.40
44:1m:108:ARG:HA	44:1m:108:ARG:HD3	1.81	0.40
48:1q:45:HIS:H	48:1q:72:ARG:HA	1.86	0.40
56:1y:19:G:H1	56:1y:56:C:N4	2.18	0.40
1:2A:551:G:O2'	1:2A:1220:A:N3	2.51	0.40
1:2A:656:G:H2'	1:2A:657:U:O4'	2.21	0.40
1:2A:1777:U:H2'	1:2A:1778:U:H6	1.84	0.40
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.56	0.40
1:2A:2126:A:N3	1:2A:2127:G:H1'	2.36	0.40
1:2A:2461:C:H2'	1:2A:2462:U:C6	2.56	0.40
3:2D:39:LYS:HB3	3:2D:39:LYS:HE2	1.86	0.40
3:2D:68:LYS:HB2	3:2D:70:TRP:CE2	2.56	0.40
4:2E:56:PRO:C	4:2E:58:ARG:H	2.28	0.40
4:2E:170:LEU:HB3	4:2E:184:VAL:CG2	2.51	0.40
11:2P:88:LEU:HD11	11:2P:114:ILE:HD12	2.03	0.40
15:2T:94:ALA:HB1	15:2T:99:LEU:HD21	2.03	0.40
21:2Z:75:ASN:HB2	21:2Z:85:HIS:HB3	2.03	0.40
57:2a:114:U:O2'	57:2a:115:G:H5'	2.22	0.40
57:2a:977:A:C2	57:2a:1224:G:C5	3.09	0.40
57:2a:1111:A:H2	34:2c:179:ARG:HH12	1.70	0.40
57:2a:1236:A:O2'	57:2a:1304:G:H4'	2.21	0.40
57:2a:1388:C:H2'	57:2a:1389:C:C6	2.56	0.40
34:2c:25:GLY:O	34:2c:29:TYR:HB2	2.22	0.40
35:2d:145:GLU:HA	35:2d:183:GLY:O	2.21	0.40
40:2i:18:PHE:O	40:2i:61:ALA:HA	2.21	0.40
55:2x:19:G:C4	55:2x:57:A:C2	3.09	0.40
1:1A:327:U:H2'	1:1A:328:G:C8	2.56	0.40
1:1A:1312:G:O2'	1:1A:2034:G:O6	2.21	0.40
1:1A:1992:A:H4'	1:1A:1993:A:OP1	2.21	0.40
1:1A:2119:C:H2'	1:1A:2120:U:O4'	2.21	0.40
1:1A:2283:G:OP1	22:10:18:ALA:HB1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2672:A:N7	7:1H:175:LYS:NZ	2.70	0.40
1:1A:2864:G:H2'	1:1A:2865:C:C6	2.56	0.40
4:1E:1:MET:HE3	4:1E:199:ARG:HD2	2.02	0.40
18:1W:65:LEU:HD23	18:1W:65:LEU:HA	1.85	0.40
25:13:23:LEU:HD13	25:13:50:VAL:HG11	2.03	0.40
26:14:61:ARG:HH12	50:1s:9:VAL:HG11	1.86	0.40
32:1a:109:A:H2'	32:1a:326:G:N2	2.36	0.40
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.56	0.40
32:1a:1427:U:H2'	32:1a:1428:A:C8	2.56	0.40
45:1n:23:ARG:NH1	45:1n:30:ALA:HB2	2.36	0.40
1:2A:196:A:N3	1:2A:196:A:H2'	2.36	0.40
1:2A:265:A:H1'	1:2A:266:G:O4'	2.22	0.40
1:2A:573:G:O2'	1:2A:574:C:H3'	2.21	0.40
1:2A:1198:U:H2'	1:2A:1199:U:C6	2.57	0.40
1:2A:1754:C:H2'	1:2A:1755:A:O4'	2.21	0.40
4:2E:127:ASP:OD2	63:2E:401:HOH:O	2.22	0.40
20:2Y:8:LYS:HD3	20:2Y:97:ARG:HH11	1.86	0.40
25:23:12:PRO:HB2	25:23:20:LYS:HG2	2.02	0.40
57:2a:8:A:C6	35:2d:209:ARG:HB2	2.57	0.40
57:2a:9:G:H2'	57:2a:10:A:C8	2.56	0.40
57:2a:338:A:H2'	57:2a:339:C:O4'	2.21	0.40
57:2a:418:C:H2'	57:2a:419:C:H6	1.86	0.40
57:2a:532:A:C2	57:2a:1055:A:H1'	2.56	0.40
57:2a:719:C:N4	49:2r:71:LYS:HE2	2.36	0.40
57:2a:767:A:H2'	57:2a:768:A:O4'	2.21	0.40
57:2a:1051:C:H2'	57:2a:1052:U:C6	2.56	0.40
57:2a:1434:A:H2'	57:2a:1435:G:O4'	2.21	0.40
33:2b:10:LEU:HD23	33:2b:10:LEU:HA	1.90	0.40
33:2b:212:GLN:O	33:2b:216:SER:OG	2.29	0.40
1:1A:297:C:H2'	1:1A:298:G:C8	2.53	0.40
1:1A:312:C:H2'	1:1A:313:A:C8	2.56	0.40
1:1A:440:C:OP2	63:1A:4362:HOH:O	2.22	0.40
1:1A:2331:G:N1	14:1S:3:ARG:HA	2.36	0.40
8:1I:27:ARG:HD3	23:11:71:TYR:CE2	2.56	0.40
25:13:59:VAL:O	25:13:60:GLU:HG3	2.21	0.40
32:1a:107:G:N7	51:1t:15:ARG:NH2	2.68	0.40
32:1a:110:C:H2'	32:1a:111:G:O4'	2.21	0.40
32:1a:657:G:O4'	46:1o:28:GLN:NE2	2.46	0.40
32:1a:1317:C:OP1	45:1n:17:LYS:HG2	2.20	0.40
33:1b:41:ILE:HD13	33:1b:41:ILE:HA	1.96	0.40
35:1d:79:PHE:CE1	35:1d:204:ILE:HD13	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1f:46:ARG:NH2	49:1r:37:VAL:HG11	2.33	0.40
41:1j:5:ARG:HH11	41:1j:71:LEU:HD21	1.85	0.40
42:1k:33:THR:OG1	42:1k:34:ASP:O	2.38	0.40
1:2A:56:A:H2'	1:2A:57:C:O4'	2.21	0.40
1:2A:94(A):G:H2'	1:2A:95:G:O4'	2.22	0.40
1:2A:517:C:OP1	27:25:16:ARG:NH2	2.54	0.40
24:22:53:LEU:HD23	24:22:53:LEU:HA	1.95	0.40
26:24:68:ARG:HD3	26:24:69:LYS:H	1.86	0.40
30:28:34:TRP:CG	30:28:35:GLN:N	2.90	0.40
57:2a:371:G:O2'	57:2a:373:A:N7	2.53	0.40
57:2a:457:C:H2'	57:2a:458:C:C6	2.56	0.40
57:2a:554:C:H2'	57:2a:555:C:C6	2.57	0.40
57:2a:942:G:C2	57:2a:1342:C:C2	3.09	0.40
57:2a:1276:G:C2'	57:2a:1277:C:H5'	2.51	0.40
57:2a:1333:A:H2'	57:2a:1334:G:O4'	2.21	0.40
35:2d:140:VAL:HG11	35:2d:146:ILE:HD11	2.03	0.40
36:2e:78:HIS:CE1	36:2e:142:LEU:HD23	2.56	0.40
36:2e:89:ILE:HD12	36:2e:89:ILE:HA	1.92	0.40
39:2h:2:LEU:HD11	39:2h:8:ASP:HB2	2.03	0.40
39:2h:3:THR:O	39:2h:5:PRO:HD3	2.21	0.40
56:2y:4:C:H2'	56:2y:5:G:O4'	2.21	0.40
56:2y:43:C:H2'	56:2y:44:G:C1'	2.51	0.40
1:1A:831:A:C6	3:1D:229:VAL:HG11	2.56	0.40
1:1A:1154:U:H2'	1:1A:1155:C:O4'	2.22	0.40
1:1A:1410:G:OP1	23:11:2:SER:HA	2.21	0.40
1:1A:2453:C:OP2	1:1A:2598:C:O2'	2.38	0.40
1:1A:2769:U:H1'	1:1A:2770:A:H5''	2.04	0.40
5:1F:123:LEU:HD13	5:1F:192:LEU:HD13	2.04	0.40
13:1R:9:LYS:O	13:1R:17:ARG:HD3	2.21	0.40
21:1Z:72:ARG:HA	21:1Z:72:ARG:HD3	1.95	0.40
32:1a:96:U:H2'	32:1a:97:G:H8	1.86	0.40
35:1d:178:VAL:O	35:1d:180:GLY:N	2.55	0.40
36:1e:105:VAL:HB	36:1e:106:PRO:HD3	2.03	0.40
39:1h:28:ALA:HA	39:1h:59:LEU:HG	2.02	0.40
42:1k:82:VAL:HB	42:1k:108:ILE:HG12	2.04	0.40
1:2A:262:A:H2'	1:2A:263:C:O4'	2.21	0.40
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.57	0.40
1:2A:463:G:N2	1:2A:466:A:OP2	2.50	0.40
1:2A:647:G:H8	1:2A:647:G:O5'	2.03	0.40
1:2A:864:G:OP2	12:2Q:22:LYS:HE3	2.21	0.40
1:2A:900:A:H2'	1:2A:901:A:H8	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1221(A):C:C2	1:2A:1229:G:C2	3.10	0.40
1:2A:1507:A:O2'	1:2A:1508:A:H8	2.03	0.40
1:2A:1547:C:H2'	1:2A:1548:C:H6	1.85	0.40
7:2H:126:PRO:HB2	7:2H:127:GLU:H	1.65	0.40
14:2S:8:GLU:HG2	14:2S:8:GLU:H	1.65	0.40
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.56	0.40
29:27:26:GLY:O	29:27:30:VAL:HG23	2.21	0.40
57:2a:418:C:H2'	57:2a:419:C:C6	2.57	0.40
57:2a:447:G:O6	57:2a:485:G:O2'	2.19	0.40
57:2a:1144:G:N2	57:2a:1146:A:H62	2.18	0.40
57:2a:1353:G:C2	57:2a:1370:G:C2	3.09	0.40
33:2b:16:HIS:CB	33:2b:204:ASN:HB3	2.45	0.40
33:2b:77:ALA:HA	33:2b:80:ILE:HG22	2.03	0.40
33:2b:114:ARG:HH11	33:2b:117:GLU:CD	2.29	0.40
33:2b:178:ARG:HE	33:2b:178:ARG:HB3	1.54	0.40
35:2d:31:CYS:HB2	61:2d:501:SF4:S3	2.61	0.40
35:2d:155:LEU:HD23	35:2d:155:LEU:HA	1.90	0.40
37:2f:84:ASN:O	37:2f:86:ARG:HG3	2.20	0.40
1:1A:213:G:H2'	1:1A:214:A:O4'	2.21	0.40
1:1A:950:C:O2'	21:1Z:169:GLU:OE2	2.29	0.40
1:1A:1100:A:N6	1:1A:1101:G:C6	2.89	0.40
1:1A:1756:U:H2'	1:1A:1757:C:C6	2.56	0.40
1:1A:2021:C:H4'	1:1A:2736:C:O2	2.22	0.40
1:1A:2158:C:N4	1:1A:2177:G:C6	2.84	0.40
8:1I:6:LEU:HD11	8:1I:37:VAL:HG23	2.04	0.40
32:1a:60:A:N1	32:1a:107:G:O2'	2.43	0.40
32:1a:260:G:H2'	32:1a:261:U:C6	2.56	0.40
32:1a:557:G:N1	32:1a:558:G:C2	2.90	0.40
32:1a:756:C:H2'	32:1a:757:U:O4'	2.21	0.40
32:1a:911:U:OP1	43:1I:95:GLY:HA2	2.21	0.40
32:1a:935:A:O2'	32:1a:1383:C:N3	2.52	0.40
32:1a:1183:A:O2'	32:1a:1184:G:OP1	2.34	0.40
32:1a:1457:G:H5''	51:1t:35:THR:HG21	2.02	0.40
33:1b:185:ILE:HG22	33:1b:199:TYR:HD2	1.86	0.40
42:1k:77:MET:HE2	42:1k:77:MET:HB2	1.97	0.40
1:2A:1232:G:H2'	1:2A:1233:C:C6	2.56	0.40
1:2A:1426:G:OP2	1:2A:1427:A:O2'	2.34	0.40
1:2A:1720:U:H2'	1:2A:1721:G:O4'	2.21	0.40
1:2A:2270:G:H2'	1:2A:2271:G:O4'	2.20	0.40
1:2A:2375:G:N2	1:2A:2378:A:OP2	2.49	0.40
1:2A:2788:C:H5''	4:2E:61:ARG:HH21	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:88:C:H2'	2:2B:89:G:O4'	2.21	0.40
5:2F:126:VAL:HG21	5:2F:129:PHE:CZ	2.57	0.40
14:2S:3:ARG:HD3	14:2S:4:LEU:N	2.36	0.40
15:2T:13:ARG:HB2	15:2T:14:TYR:CD2	2.57	0.40
15:2T:74:ARG:HG2	15:2T:76:PHE:CZ	2.57	0.40
17:2V:18:LEU:HD12	17:2V:19:LYS:N	2.37	0.40
57:2a:336:C:H2'	57:2a:337:C:H6	1.86	0.40
57:2a:473:G:C2	57:2a:474:G:C5	3.10	0.40
57:2a:1001:A:H2'	57:2a:1001(A):G:H8	1.87	0.40
57:2a:1246:C:H2'	57:2a:1247:U:H6	1.87	0.40
57:2a:1274:G:N2	57:2a:1275:A:H62	2.20	0.40
57:2a:1356:G:N2	57:2a:1367:C:O2	2.55	0.40
34:2c:6:HIS:HA	34:2c:7:PRO:HD3	1.96	0.40
34:2c:121:ALA:HB2	34:2c:198:VAL:HG21	2.03	0.40
36:2e:75:THR:OG1	36:2e:117:ASP:O	2.27	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%)	261 (96%)	12 (4%)	0	100	100
3	2D	273/276 (99%)	259 (95%)	14 (5%)	0	100	100
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	48
4	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	24	48
5	1F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24	48
5	2F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	24	48
6	1G	179/182 (98%)	168 (94%)	8 (4%)	3 (2%)	7	19
6	2G	179/182 (98%)	162 (90%)	13 (7%)	4 (2%)	5	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	1H	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	21	44
7	2H	172/180 (96%)	156 (91%)	13 (8%)	3 (2%)	7	19
8	1I	144/148 (97%)	130 (90%)	13 (9%)	1 (1%)	18	41
8	2I	144/148 (97%)	129 (90%)	13 (9%)	2 (1%)	9	23
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
10	1O	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
10	2O	120/122 (98%)	112 (93%)	6 (5%)	2 (2%)	7	19
11	1P	147/150 (98%)	134 (91%)	12 (8%)	1 (1%)	18	41
11	2P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	18	41
12	1Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
12	2Q	139/141 (99%)	130 (94%)	6 (4%)	3 (2%)	5	14
13	1R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
13	2R	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
14	2S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	14	35
15	1T	129/146 (88%)	123 (95%)	5 (4%)	1 (1%)	16	37
15	2T	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	12	32
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12	32
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	110 (100%)	0	0	100	100
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	11	29
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	12	32
20	2Y	105/110 (96%)	100 (95%)	4 (4%)	1 (1%)	12	32
21	1Z	148/206 (72%)	134 (90%)	12 (8%)	2 (1%)	9	23
21	2Z	156/206 (76%)	138 (88%)	15 (10%)	3 (2%)	6	17
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	20	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	29
23	21	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	57 (100%)	0	0	100	100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	1
26	24	67/71 (94%)	53 (79%)	13 (19%)	1 (2%)	8	22
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	194 (85%)	26 (11%)	9 (4%)	2	5
33	2b	229/256 (90%)	201 (88%)	21 (9%)	7 (3%)	3	8
34	1c	204/239 (85%)	188 (92%)	13 (6%)	3 (2%)	8	22
34	2c	204/239 (85%)	178 (87%)	24 (12%)	2 (1%)	12	32
35	1d	206/209 (99%)	193 (94%)	11 (5%)	2 (1%)	12	32
35	2d	206/209 (99%)	189 (92%)	14 (7%)	3 (2%)	8	22
36	1e	146/162 (90%)	135 (92%)	8 (6%)	3 (2%)	5	15
36	2e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	9	23
37	1f	98/101 (97%)	94 (96%)	3 (3%)	1 (1%)	12	32
37	2f	98/101 (97%)	94 (96%)	3 (3%)	1 (1%)	12	32
38	1g	153/156 (98%)	142 (93%)	10 (6%)	1 (1%)	18	41
38	2g	153/156 (98%)	140 (92%)	9 (6%)	4 (3%)	4	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	1h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
39	2h	135/138 (98%)	118 (87%)	17 (13%)	0	100	100
40	1i	125/128 (98%)	109 (87%)	14 (11%)	2 (2%)	7	20
40	2i	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
41	1j	95/105 (90%)	84 (88%)	6 (6%)	5 (5%)	1	3
41	2j	94/105 (90%)	79 (84%)	10 (11%)	5 (5%)	1	3
42	1k	112/129 (87%)	105 (94%)	6 (5%)	1 (1%)	14	35
42	2k	112/129 (87%)	105 (94%)	5 (4%)	2 (2%)	6	18
43	1l	119/132 (90%)	114 (96%)	5 (4%)	0	100	100
43	2l	119/132 (90%)	110 (92%)	9 (8%)	0	100	100
44	1m	121/126 (96%)	111 (92%)	9 (7%)	1 (1%)	16	37
44	2m	120/126 (95%)	108 (90%)	12 (10%)	0	100	100
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	51 (88%)	5 (9%)	2 (3%)	3	7
46	1o	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	10	27
46	2o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
47	1p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	9	25
47	2p	80/88 (91%)	70 (88%)	9 (11%)	1 (1%)	9	25
48	1q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
48	2q	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
49	1r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	2 (3%)	1 (2%)	8	22
50	1s	81/93 (87%)	72 (89%)	8 (10%)	1 (1%)	10	27
50	2s	81/93 (87%)	68 (84%)	10 (12%)	3 (4%)	2	6
51	1t	94/106 (89%)	85 (90%)	5 (5%)	4 (4%)	2	4
51	2t	94/106 (89%)	85 (90%)	4 (4%)	5 (5%)	1	3
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	15 (71%)	6 (29%)	0	100	100
58	A	12/18 (67%)	5 (42%)	5 (42%)	2 (17%)	0	0
58	B	12/18 (67%)	6 (50%)	4 (33%)	2 (17%)	0	0
All	All	11394/12164 (94%)	10597 (93%)	676 (6%)	121 (1%)	11	29

All (121) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	47	LYS
7	1H	126	PRO
8	1I	10	GLU
20	1Y	55	TYR
23	1I	3	LYS
33	1b	10	LEU
33	1b	17	PHE
40	1i	54	ASP
41	1j	79	ARG
51	1t	100	ILE
5	2F	130	ALA
6	2G	47	LYS
7	2H	47	GLU
7	2H	126	PRO
20	2Y	55	TYR
38	2g	6	ARG
50	2s	81	ARG
51	2t	10	LEU
51	2t	47	GLY
58	A	12	SER
5	1F	130	ALA
15	1T	37	GLY
19	1X	93	GLU
21	1Z	156	LYS
33	1b	22	LYS
33	1b	126	GLU
36	1e	85	GLY
41	1j	55	LYS
44	1m	67	GLU
51	1t	47	GLY
6	2G	49	ASP
6	2G	124	SER
8	2I	10	GLU
10	2O	5	GLN
12	2Q	17	LEU
17	2V	79	VAL
21	2Z	172	ALA
33	2b	17	PHE
34	2c	95	THR
41	2j	29	ARG
41	2j	75	ILE
42	2k	49	GLY

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Mol	Chain	Res	Type
49	2r	36	ASN
51	2t	100	ILE
58	A	16	ASN
58	B	12	SER
58	B	16	ASN
26	14	18	CYS
33	1b	8	LYS
37	1f	40	VAL
41	1j	77	PRO
46	1o	19	PRO
51	1t	10	LEU
7	2H	12	PRO
8	2I	85	GLU
14	2S	96	GLY
21	2Z	142	SER
33	2b	8	LYS
33	2b	20	GLU
35	2d	178	VAL
35	2d	179	GLU
38	2g	4	ARG
41	2j	78	ASN
50	2s	27	GLU
51	2t	99	LEU
4	1E	52	LEU
6	1G	49	ASP
26	14	55	ARG
26	14	57	GLU
26	14	64	GLY
34	1c	65	ALA
36	1e	86	ALA
38	1g	80	VAL
41	1j	29	ARG
41	1j	78	ASN
50	1s	27	GLU
4	2E	52	LEU
33	2b	16	HIS
33	2b	74	LYS
33	2b	125	PRO
36	2e	85	GLY
38	2g	80	VAL
45	2n	19	ARG
50	2s	9	VAL

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Mol	Chain	Res	Type
6	1G	43	LEU
11	1P	29	LYS
17	1V	79	VAL
21	1Z	147	GLY
33	1b	9	GLU
33	1b	16	HIS
33	1b	231	GLU
35	1d	178	VAL
35	1d	179	GLU
10	2O	29	ASN
12	2Q	16	ARG
26	24	64	GLY
36	2e	112	LEU
41	2j	79	ARG
6	2G	52	ILE
11	2P	122	PRO
21	2Z	146	ILE
34	2c	66	VAL
45	2n	60	SER
34	1c	66	VAL
42	1k	105	VAL
47	1p	53	VAL
12	2Q	15	GLY
33	2b	127	ILE
42	2k	105	VAL
35	2d	171	GLY
51	2t	102	GLY
51	1t	102	GLY
38	2g	17	VAL
41	2j	91	PRO
47	2p	53	VAL
26	14	29	PRO
33	1b	234	PRO
36	1e	69	VAL
40	1i	44	VAL
37	2f	40	VAL
34	1c	81	GLY

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	199 (93%)	16 (7%)	13	32
3	2D	215/218 (99%)	202 (94%)	13 (6%)	17	41
4	1E	164/166 (99%)	147 (90%)	17 (10%)	7	17
4	2E	164/166 (99%)	147 (90%)	17 (10%)	7	17
5	1F	160/166 (96%)	147 (92%)	13 (8%)	11	27
5	2F	159/166 (96%)	145 (91%)	14 (9%)	9	23
6	1G	143/156 (92%)	133 (93%)	10 (7%)	14	34
6	2G	143/156 (92%)	137 (96%)	6 (4%)	26	55
7	1H	144/148 (97%)	134 (93%)	10 (7%)	14	34
7	2H	144/148 (97%)	137 (95%)	7 (5%)	22	49
8	1I	113/124 (91%)	102 (90%)	11 (10%)	8	20
8	2I	105/124 (85%)	94 (90%)	11 (10%)	6	17
9	1N	118/119 (99%)	109 (92%)	9 (8%)	12	30
9	2N	118/119 (99%)	111 (94%)	7 (6%)	18	42
10	1O	100/100 (100%)	95 (95%)	5 (5%)	22	48
10	2O	100/100 (100%)	94 (94%)	6 (6%)	17	41
11	1P	115/116 (99%)	105 (91%)	10 (9%)	9	24
11	2P	115/116 (99%)	111 (96%)	4 (4%)	32	61
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	16	39
12	2Q	111/111 (100%)	103 (93%)	8 (7%)	13	32
13	1R	101/101 (100%)	88 (87%)	13 (13%)	4	10
13	2R	101/101 (100%)	90 (89%)	11 (11%)	6	16
14	1S	86/88 (98%)	79 (92%)	7 (8%)	11	27
14	2S	85/88 (97%)	75 (88%)	10 (12%)	5	13
15	1T	115/127 (91%)	110 (96%)	5 (4%)	26	54
15	2T	113/127 (89%)	110 (97%)	3 (3%)	39	69
16	1U	93/94 (99%)	86 (92%)	7 (8%)	12	31
16	2U	93/94 (99%)	91 (98%)	2 (2%)	45	74
17	1V	80/82 (98%)	70 (88%)	10 (12%)	4	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	19
18	1W	90/92 (98%)	83 (92%)	7 (8%)	11	29
18	2W	90/92 (98%)	84 (93%)	6 (7%)	15	36
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28	57
19	2X	77/78 (99%)	76 (99%)	1 (1%)	61	83
20	1Y	85/91 (93%)	77 (91%)	8 (9%)	8	21
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	13	33
21	1Z	135/179 (75%)	121 (90%)	14 (10%)	7	17
21	2Z	137/179 (76%)	122 (89%)	15 (11%)	6	16
22	10	65/67 (97%)	63 (97%)	2 (3%)	35	65
22	20	65/67 (97%)	59 (91%)	6 (9%)	8	22
23	11	80/83 (96%)	78 (98%)	2 (2%)	42	71
23	21	80/83 (96%)	78 (98%)	2 (2%)	42	71
24	12	65/67 (97%)	64 (98%)	1 (2%)	57	81
24	22	65/67 (97%)	63 (97%)	2 (3%)	35	65
25	13	51/52 (98%)	49 (96%)	2 (4%)	28	57
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	28
26	14	59/63 (94%)	55 (93%)	4 (7%)	14	35
26	24	53/63 (84%)	50 (94%)	3 (6%)	18	43
27	15	50/52 (96%)	46 (92%)	4 (8%)	11	28
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	28
28	16	51/52 (98%)	43 (84%)	8 (16%)	2	7
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	19
29	17	41/42 (98%)	37 (90%)	4 (10%)	7	19
29	27	41/42 (98%)	38 (93%)	3 (7%)	13	32
30	18	54/55 (98%)	49 (91%)	5 (9%)	8	21
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	44
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	32 (94%)	2 (6%)	18	42
33	1b	192/220 (87%)	183 (95%)	9 (5%)	23	51
33	2b	187/220 (85%)	172 (92%)	15 (8%)	11	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	1c	142/188 (76%)	134 (94%)	8 (6%)	19	44
34	2c	140/188 (74%)	136 (97%)	4 (3%)	37	67
35	1d	169/181 (93%)	157 (93%)	12 (7%)	13	33
35	2d	173/181 (96%)	162 (94%)	11 (6%)	16	38
36	1e	113/123 (92%)	107 (95%)	6 (5%)	20	46
36	2e	114/123 (93%)	107 (94%)	7 (6%)	17	40
37	1f	84/90 (93%)	82 (98%)	2 (2%)	43	72
37	2f	85/90 (94%)	79 (93%)	6 (7%)	13	33
38	1g	119/127 (94%)	113 (95%)	6 (5%)	22	48
38	2g	120/127 (94%)	115 (96%)	5 (4%)	26	55
39	1h	114/119 (96%)	107 (94%)	7 (6%)	17	40
39	2h	114/119 (96%)	109 (96%)	5 (4%)	25	53
40	1i	90/99 (91%)	85 (94%)	5 (6%)	19	44
40	2i	89/99 (90%)	80 (90%)	9 (10%)	7	18
41	1j	66/92 (72%)	63 (96%)	3 (4%)	24	52
41	2j	69/92 (75%)	67 (97%)	2 (3%)	37	67
42	1k	82/99 (83%)	77 (94%)	5 (6%)	17	40
42	2k	83/99 (84%)	78 (94%)	5 (6%)	17	41
43	1l	96/108 (89%)	92 (96%)	4 (4%)	26	55
43	2l	96/108 (89%)	92 (96%)	4 (4%)	26	55
44	1m	93/101 (92%)	83 (89%)	10 (11%)	6	16
44	2m	92/101 (91%)	85 (92%)	7 (8%)	12	30
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	12
45	2n	49/50 (98%)	45 (92%)	4 (8%)	10	27
46	1o	78/80 (98%)	75 (96%)	3 (4%)	29	58
46	2o	78/80 (98%)	74 (95%)	4 (5%)	21	48
47	1p	69/74 (93%)	64 (93%)	5 (7%)	13	32
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5	13
48	1q	94/97 (97%)	90 (96%)	4 (4%)	26	54
48	2q	94/97 (97%)	88 (94%)	6 (6%)	16	38
49	1r	59/77 (77%)	56 (95%)	3 (5%)	21	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	2r	59/77 (77%)	57 (97%)	2 (3%)	32	62
50	1s	69/80 (86%)	65 (94%)	4 (6%)	18	42
50	2s	67/80 (84%)	66 (98%)	1 (2%)	57	81
51	1t	70/82 (85%)	67 (96%)	3 (4%)	26	54
51	2t	70/82 (85%)	69 (99%)	1 (1%)	59	82
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	44
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19	44
58	A	9/9 (100%)	7 (78%)	2 (22%)	1	3
58	B	9/9 (100%)	7 (78%)	2 (22%)	1	3
All	All	9321/10082 (92%)	8701 (93%)	620 (7%)	15	36

All (620) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	14	ARG
3	1D	32	SER
3	1D	37	LEU
3	1D	39	LYS
3	1D	61	LEU
3	1D	99	ASP
3	1D	106	ILE
3	1D	113	VAL
3	1D	141	VAL
3	1D	155	LEU
3	1D	173	VAL
3	1D	193	VAL
3	1D	211	ARG
3	1D	221	VAL
3	1D	229	VAL
4	1E	9	VAL
4	1E	12	THR
4	1E	21	VAL
4	1E	24	THR
4	1E	33	VAL
4	1E	34	VAL
4	1E	47	VAL
4	1E	49	LEU
4	1E	73	GLU

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Mol	Chain	Res	Type
4	1E	75	VAL
4	1E	116	VAL
4	1E	167	VAL
4	1E	170	LEU
4	1E	175	VAL
4	1E	181	LEU
4	1E	184	VAL
4	1E	195	LEU
5	1F	12	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	70	THR
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	125	LEU
5	1F	170	LEU
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	3	LEU
6	1G	5	VAL
6	1G	31	VAL
6	1G	43	LEU
6	1G	82	LEU
6	1G	133	LEU
6	1G	135	LEU
6	1G	140	ILE
6	1G	159	VAL
6	1G	175	LEU
7	1H	15	VAL
7	1H	23	ARG
7	1H	44	VAL
7	1H	71	LEU
7	1H	81	GLU
7	1H	98	LEU
7	1H	122	THR
7	1H	124	GLU
7	1H	134	SER
7	1H	139	GLN
8	1I	9	LEU

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Mol	Chain	Res	Type
8	1I	27	ARG
8	1I	38	LEU
8	1I	47	LEU
8	1I	77	LEU
8	1I	78	THR
8	1I	92	VAL
8	1I	101	LEU
8	1I	109	ILE
8	1I	123	LEU
8	1I	140	LEU
9	1N	14	VAL
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	48	MET
9	1N	62	VAL
9	1N	73	THR
9	1N	87	LEU
9	1N	99	LEU
10	1O	10	VAL
10	1O	23	ARG
10	1O	24	VAL
10	1O	69	ILE
10	1O	98	VAL
11	1P	1	MET
11	1P	3	LEU
11	1P	59	LEU
11	1P	75	ILE
11	1P	77	ARG
11	1P	83	VAL
11	1P	95	VAL
11	1P	112	LEU
11	1P	125	VAL
11	1P	126	VAL
12	1Q	7	MET
12	1Q	22	LYS
12	1Q	35	VAL
12	1Q	75	THR
12	1Q	101	ARG
12	1Q	109	VAL
12	1Q	110	THR
13	1R	6	SER

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Mol	Chain	Res	Type
13	1R	8	ARG
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	100	LEU
13	1R	111	LEU
13	1R	114	VAL
13	1R	117	VAL
14	1S	14	VAL
14	1S	36	TYR
14	1S	46	VAL
14	1S	69	VAL
14	1S	73	LEU
14	1S	85	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	30	VAL
15	1T	49	VAL
15	1T	95	ARG
15	1T	96	ARG
16	1U	8	VAL
16	1U	31	SER
16	1U	74	LEU
16	1U	77	SER
16	1U	83	LEU
16	1U	85	LYS
16	1U	95	LEU
17	1V	1	MET
17	1V	35	LEU
17	1V	46	VAL
17	1V	51	VAL
17	1V	52	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	73	SER
17	1V	79	VAL
18	1W	11	ARG

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Mol	Chain	Res	Type
18	1W	15	ARG
18	1W	17	VAL
18	1W	19	LEU
18	1W	23	LEU
18	1W	92	ARG
18	1W	107	LEU
19	1X	35	THR
19	1X	52	VAL
19	1X	81	VAL
20	1Y	7	VAL
20	1Y	50	ARG
20	1Y	64	GLU
20	1Y	72	VAL
20	1Y	90	LEU
20	1Y	97	ARG
20	1Y	99	CYS
20	1Y	107	ASP
21	1Z	18	LEU
21	1Z	33	LEU
21	1Z	61	LEU
21	1Z	71	VAL
21	1Z	76	LEU
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	126	VAL
21	1Z	129	SER
21	1Z	146	ILE
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	170	THR
21	1Z	171	ILE
22	10	10	THR
22	10	39	ARG
23	11	30	VAL
23	11	95	LEU
24	12	53	LEU
25	13	23	LEU
25	13	54	VAL
26	14	49	PHE
26	14	50	VAL
26	14	56	VAL
26	14	61	ARG

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Mol	Chain	Res	Type
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
27	15	58	LEU
28	16	6	ARG
28	16	9	LEU
28	16	19	ARG
28	16	24	GLU
28	16	38	LYS
28	16	44	ARG
28	16	47	THR
28	16	48	VAL
29	17	39	ARG
29	17	41	ARG
29	17	43	THR
29	17	46	VAL
30	18	6	THR
30	18	14	VAL
30	18	23	VAL
30	18	29	LYS
30	18	32	LEU
33	1b	54	THR
33	1b	56	ARG
33	1b	94	ASN
33	1b	111	ARG
33	1b	112	VAL
33	1b	127	ILE
33	1b	178	ARG
33	1b	185	ILE
33	1b	196	LEU
34	1c	3	ASN
34	1c	8	ILE
34	1c	57	ILE
34	1c	112	SER
34	1c	115	LEU
34	1c	138	VAL
34	1c	195	VAL
34	1c	206	GLU
35	1d	5	ILE
35	1d	19	LEU
35	1d	31	CYS
35	1d	70	ILE

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Mol	Chain	Res	Type
35	1d	107	ARG
35	1d	112	VAL
35	1d	135	LEU
35	1d	144	ASP
35	1d	158	ILE
35	1d	170	VAL
35	1d	178	VAL
35	1d	196	LEU
36	1e	16	THR
36	1e	20	GLN
36	1e	41	VAL
36	1e	67	VAL
36	1e	91	LEU
36	1e	131	ILE
37	1f	21	LEU
37	1f	45	LEU
38	1g	16	LEU
38	1g	59	LEU
38	1g	79	ARG
38	1g	104	LEU
38	1g	111	ARG
38	1g	114	ARG
39	1h	25	ASP
39	1h	26	VAL
39	1h	51	VAL
39	1h	63	LEU
39	1h	82	HIS
39	1h	83	ILE
39	1h	112	LEU
40	1i	54	ASP
40	1i	64	THR
40	1i	103	THR
40	1i	121	ARG
40	1i	128	ARG
41	1j	38	ILE
41	1j	81	THR
41	1j	92	THR
42	1k	33	THR
42	1k	48	ILE
42	1k	87	THR
42	1k	109	VAL
42	1k	114	VAL

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Mol	Chain	Res	Type
43	1l	27	LEU
43	1l	33	ARG
43	1l	83	VAL
43	1l	113	ARG
44	1m	14	ARG
44	1m	19	LEU
44	1m	43	THR
44	1m	49	THR
44	1m	70	LEU
44	1m	78	ILE
44	1m	102	ARG
44	1m	104	ARG
44	1m	105	THR
44	1m	117	VAL
45	1n	6	LEU
45	1n	7	ILE
45	1n	18	VAL
45	1n	22	THR
45	1n	32	SER
45	1n	33	VAL
46	1o	5	LYS
46	1o	39	LEU
46	1o	87	ILE
47	1p	2	VAL
47	1p	20	VAL
47	1p	21	VAL
47	1p	62	VAL
47	1p	67	THR
48	1q	9	VAL
48	1q	63	ARG
48	1q	70	ARG
48	1q	72	ARG
49	1r	26	LEU
49	1r	37	VAL
49	1r	54	ARG
50	1s	41	VAL
50	1s	70	LYS
50	1s	77	THR
50	1s	79	THR
51	1t	8	ARG
51	1t	10	LEU
51	1t	22	ARG

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Mol	Chain	Res	Type
52	1u	24	ARG
3	2D	3	VAL
3	2D	61	LEU
3	2D	75	ILE
3	2D	111	LEU
3	2D	113	VAL
3	2D	138	VAL
3	2D	142	VAL
3	2D	171	ASP
3	2D	173	VAL
3	2D	193	VAL
3	2D	211	ARG
3	2D	257	LEU
3	2D	259	THR
4	2E	9	VAL
4	2E	12	THR
4	2E	14	ILE
4	2E	21	VAL
4	2E	24	THR
4	2E	27	LEU
4	2E	34	VAL
4	2E	38	THR
4	2E	75	VAL
4	2E	97	LYS
4	2E	107	THR
4	2E	116	VAL
4	2E	134	ILE
4	2E	170	LEU
4	2E	175	VAL
4	2E	181	LEU
4	2E	183	LEU
5	2F	28	ILE
5	2F	33	LEU
5	2F	53	THR
5	2F	70	THR
5	2F	74	ARG
5	2F	88	VAL
5	2F	106	ARG
5	2F	108	LYS
5	2F	157	VAL
5	2F	158	THR
5	2F	183	VAL

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Mol	Chain	Res	Type
5	2F	192	LEU
5	2F	195	ASP
5	2F	201	VAL
6	2G	3	LEU
6	2G	5	VAL
6	2G	43	LEU
6	2G	140	ILE
6	2G	159	VAL
6	2G	161	THR
7	2H	15	VAL
7	2H	67	LEU
7	2H	70	THR
7	2H	71	LEU
7	2H	95	ARG
7	2H	103	LEU
7	2H	134	SER
8	2I	15	VAL
8	2I	38	LEU
8	2I	44	LEU
8	2I	47	LEU
8	2I	92	VAL
8	2I	101	LEU
8	2I	102	SER
8	2I	123	LEU
8	2I	127	VAL
8	2I	142	VAL
8	2I	144	VAL
9	2N	14	VAL
9	2N	28	THR
9	2N	34	LEU
9	2N	46	VAL
9	2N	62	VAL
9	2N	99	LEU
9	2N	140	VAL
10	2O	9	GLU
10	2O	23	ARG
10	2O	52	VAL
10	2O	63	VAL
10	2O	66	LYS
10	2O	116	SER
11	2P	58	THR
11	2P	95	VAL

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Mol	Chain	Res	Type
11	2P	125	VAL
11	2P	148	LEU
12	2Q	1	MET
12	2Q	2	LEU
12	2Q	35	VAL
12	2Q	38	GLU
12	2Q	60	ARG
12	2Q	75	THR
12	2Q	109	VAL
12	2Q	110	THR
13	2R	6	SER
13	2R	24	GLN
13	2R	29	LEU
13	2R	36	THR
13	2R	44	LEU
13	2R	54	LEU
13	2R	65	LEU
13	2R	96	ARG
13	2R	100	LEU
13	2R	111	LEU
13	2R	114	VAL
14	2S	8	GLU
14	2S	23	ARG
14	2S	25	ARG
14	2S	36	TYR
14	2S	48	LEU
14	2S	52	SER
14	2S	65	VAL
14	2S	71	ARG
14	2S	80	LEU
14	2S	110	LEU
15	2T	74	ARG
15	2T	104	ASN
15	2T	115	ARG
16	2U	8	VAL
16	2U	95	LEU
17	2V	7	THR
17	2V	12	TYR
17	2V	46	VAL
17	2V	61	VAL
17	2V	62	LEU
17	2V	66	ARG

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Mol	Chain	Res	Type
17	2V	72	VAL
17	2V	79	VAL
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	19	LEU
18	2W	23	LEU
18	2W	107	LEU
19	2X	35	THR
20	2Y	7	VAL
20	2Y	42	VAL
20	2Y	49	VAL
20	2Y	72	VAL
20	2Y	98	VAL
20	2Y	106	LEU
21	2Z	18	LEU
21	2Z	24	LEU
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	53	ILE
21	2Z	71	VAL
21	2Z	72	ARG
21	2Z	84	GLU
21	2Z	91	LEU
21	2Z	126	VAL
21	2Z	141	VAL
21	2Z	144	LEU
21	2Z	154	ASP
21	2Z	170	THR
21	2Z	174	VAL
22	20	9	SER
22	20	14	ARG
22	20	27	GLU
22	20	39	ARG
22	20	63	VAL
22	20	74	ARG
23	21	35	THR
23	21	95	LEU
24	22	28	LYS
24	22	59	ARG
25	23	23	LEU
25	23	31	LEU

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Mol	Chain	Res	Type
25	23	54	VAL
25	23	56	VAL
26	24	49	PHE
26	24	50	VAL
26	24	53	GLU
27	25	6	VAL
27	25	29	THR
27	25	40	LYS
27	25	58	LEU
28	26	9	LEU
28	26	14	THR
28	26	19	ARG
28	26	44	ARG
28	26	48	VAL
29	27	39	ARG
29	27	41	ARG
29	27	43	THR
30	28	14	VAL
30	28	32	LEU
30	28	37	SER
31	29	7	VAL
31	29	17	ILE
33	2b	7	VAL
33	2b	23	ARG
33	2b	93	VAL
33	2b	94	ASN
33	2b	111	ARG
33	2b	124	SER
33	2b	126	GLU
33	2b	127	ILE
33	2b	154	LEU
33	2b	176	GLU
33	2b	185	ILE
33	2b	189	ASP
33	2b	192	SER
33	2b	196	LEU
33	2b	230	VAL
34	2c	44	GLU
34	2c	57	ILE
34	2c	128	PHE
34	2c	166	GLU
35	2d	31	CYS

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Mol	Chain	Res	Type
35	2d	49	ARG
35	2d	83	SER
35	2d	108	LEU
35	2d	135	LEU
35	2d	150	GLU
35	2d	170	VAL
35	2d	175	SER
35	2d	178	VAL
35	2d	194	LEU
35	2d	208	SER
36	2e	41	VAL
36	2e	68	GLU
36	2e	75	THR
36	2e	80	ILE
36	2e	83	GLU
36	2e	111	GLU
36	2e	120	THR
37	2f	37	VAL
37	2f	40	VAL
37	2f	43	LEU
37	2f	72	VAL
37	2f	81	ILE
37	2f	93	SER
38	2g	13	GLN
38	2g	16	LEU
38	2g	50	ILE
38	2g	78	ARG
38	2g	79	ARG
39	2h	3	THR
39	2h	11	THR
39	2h	14	ARG
39	2h	51	VAL
39	2h	112	LEU
40	2i	14	VAL
40	2i	50	LEU
40	2i	53	VAL
40	2i	54	ASP
40	2i	64	THR
40	2i	81	ILE
40	2i	102	LEU
40	2i	108	VAL
40	2i	128	ARG

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Mol	Chain	Res	Type
41	2j	81	THR
41	2j	97	GLU
42	2k	14	VAL
42	2k	48	ILE
42	2k	82	VAL
42	2k	84	VAL
42	2k	114	VAL
43	2l	62	SER
43	2l	83	VAL
43	2l	113	ARG
43	2l	117	ARG
44	2m	4	ILE
44	2m	19	LEU
44	2m	48	LEU
44	2m	49	THR
44	2m	81	LEU
44	2m	90	LEU
44	2m	108	ARG
45	2n	6	LEU
45	2n	18	VAL
45	2n	33	VAL
45	2n	56	VAL
46	2o	31	LEU
46	2o	39	LEU
46	2o	65	ARG
46	2o	87	ILE
47	2p	1	MET
47	2p	2	VAL
47	2p	21	VAL
47	2p	29	ASP
47	2p	60	LEU
47	2p	62	VAL
47	2p	67	THR
47	2p	69	THR
48	2q	14	LYS
48	2q	36	ILE
48	2q	58	GLU
48	2q	60	ILE
48	2q	83	ASP
48	2q	87	LYS
49	2r	37	VAL
49	2r	76	LEU

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Mol	Chain	Res	Type
50	2s	5	LEU
51	2t	33	ILE
52	2u	10	ARG
58	A	12	SER
58	A	14	SER
58	B	12	SER
58	B	14	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	126	GLN
5	1F	203	GLN
6	1G	26	GLN
8	1I	11	ASN
10	1O	3	GLN
10	1O	89	ASN
12	1Q	57	HIS
13	1R	71	GLN
14	1S	61	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
20	1Y	43	ASN
21	1Z	73	GLN
21	1Z	151	HIS
22	10	50	ASN
23	11	56	GLN
24	12	46	GLN
25	13	32	GLN
31	19	20	HIS
33	1b	212	GLN
34	1c	6	HIS
34	1c	98	ASN
34	1c	102	ASN
34	1c	162	GLN
34	1c	170	GLN
35	1d	77	ASN
35	1d	119	GLN
35	1d	125	HIS
35	1d	161	ASN
36	1e	78	HIS

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Mol	Chain	Res	Type
37	1f	13	ASN
37	1f	73	ASN
37	1f	100	ASN
38	1g	28	ASN
38	1g	97	GLN
38	1g	148	ASN
40	1i	31	GLN
40	1i	58	HIS
40	1i	87	GLN
40	1i	124	GLN
43	1l	99	HIS
45	1n	49	HIS
46	1o	46	HIS
46	1o	50	HIS
47	1p	13	HIS
50	1s	23	ASN
50	1s	69	HIS
50	1s	83	HIS
51	1t	16	HIS
51	1t	73	HIS
3	2D	87	ASN
3	2D	164	GLN
3	2D	166	GLN
4	2E	48	GLN
4	2E	169	ASN
5	2F	69	HIS
5	2F	75	HIS
6	2G	26	GLN
6	2G	66	GLN
9	2N	94	HIS
9	2N	131	GLN
12	2Q	123	HIS
13	2R	50	HIS
13	2R	71	GLN
14	2S	68	GLN
16	2U	72	HIS
16	2U	94	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	55	HIS
21	2Z	73	GLN
21	2Z	75	ASN

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Mol	Chain	Res	Type
22	20	50	ASN
24	22	56	GLN
25	23	32	GLN
26	24	46	GLN
30	28	35	GLN
33	2b	40	HIS
33	2b	78	GLN
33	2b	94	ASN
33	2b	212	GLN
34	2c	6	HIS
34	2c	102	ASN
34	2c	162	GLN
34	2c	170	GLN
34	2c	181	ASN
35	2d	77	ASN
35	2d	125	HIS
35	2d	201	GLN
36	2e	38	GLN
36	2e	78	HIS
37	2f	73	ASN
37	2f	100	ASN
38	2g	28	ASN
38	2g	148	ASN
40	2i	3	GLN
40	2i	58	HIS
40	2i	87	GLN
40	2i	124	GLN
41	2j	56	HIS
42	2k	22	HIS
44	2m	62	ASN
44	2m	77	ASN
49	2r	63	GLN
50	2s	69	HIS
50	2s	83	HIS
51	2t	75	ASN
58	A	5	ASN
58	B	5	ASN

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	410 (14%)	38 (1%)
1	2A	2791/2915 (95%)	459 (16%)	25 (0%)
2	1B	120/121 (99%)	10 (8%)	1 (0%)
2	2B	118/121 (97%)	27 (22%)	0
32	1a	1497/1521 (98%)	228 (15%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	1 (8%)	0
54	1w	72/76 (94%)	23 (31%)	0
54	2w	69/76 (90%)	22 (31%)	0
55	1x	75/77 (97%)	10 (13%)	0
55	2x	75/77 (97%)	14 (18%)	0
56	1y	72/76 (94%)	19 (26%)	0
56	2y	70/76 (92%)	18 (25%)	0
57	2a	1501/1521 (98%)	261 (17%)	0
All	All	9348/9620 (97%)	1504 (16%)	64 (0%)

All (1504) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	54	G
1	1A	70	A
1	1A	71	U
1	1A	73	A
1	1A	74	G
1	1A	77	A
1	1A	83	A
1	1A	94	G
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	137	G
1	1A	170	A
1	1A	171	A
1	1A	185	A
1	1A	186	A
1	1A	188	A
1	1A	194	G
1	1A	203	G

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Mol	Chain	Res	Type
1	1A	204	G
1	1A	205	A
1	1A	211	A
1	1A	217	A
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	271	U
1	1A	272	U
1	1A	273	G
1	1A	275	C
1	1A	276	C
1	1A	289	G
1	1A	296	U
1	1A	299	G
1	1A	303	C
1	1A	335	A
1	1A	353	G
1	1A	354	A
1	1A	376	G
1	1A	387	G
1	1A	388	A
1	1A	389	G
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	448	U
1	1A	455	A
1	1A	470	C
1	1A	474	U
1	1A	480	A
1	1A	482	C
1	1A	483	A
1	1A	507	G
1	1A	529	U
1	1A	530	A
1	1A	533	G
1	1A	534	C
1	1A	537	G

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Mol	Chain	Res	Type
1	1A	553	A
1	1A	554	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	597	C
1	1A	598	A
1	1A	609	A
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	639	G
1	1A	641	G
1	1A	642	G
1	1A	652	A
1	1A	662	A
1	1A	670	C
1	1A	671	A
1	1A	678	A
1	1A	697	C
1	1A	699	C
1	1A	716	G
1	1A	733	G
1	1A	764	G
1	1A	777	C
1	1A	811	A
1	1A	812	G
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	830	A
1	1A	831	A
1	1A	832	G
1	1A	837	C
1	1A	839	G
1	1A	852	G
1	1A	859	C

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Mol	Chain	Res	Type
1	1A	866	A
1	1A	874	U
1	1A	875	U
1	1A	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	936	C
1	1A	937	A
1	1A	940	C
1	1A	942	A
1	1A	943	C
1	1A	944	C
1	1A	946	A
1	1A	956	A
1	1A	977	G
1	1A	990	A
1	1A	991	G
1	1A	1003	U
1	1A	1004	A
1	1A	1006	C
1	1A	1008	U
1	1A	1019	G
1	1A	1020	C
1	1A	1029	A
1	1A	1042	A
1	1A	1051	C
1	1A	1058	U
1	1A	1059	C
1	1A	1068	G
1	1A	1072	U
1	1A	1073	A
1	1A	1079	U
1	1A	1084	C
1	1A	1087	C
1	1A	1091	A

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Mol	Chain	Res	Type
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1097	G
1	1A	1100	A
1	1A	1101	G
1	1A	1104	G
1	1A	1109	G
1	1A	1113	A
1	1A	1114	G
1	1A	1116	A
1	1A	1117	G
1	1A	1119	A
1	1A	1120	G
1	1A	1121	C
1	1A	1122	C
1	1A	1124	U
1	1A	1125	C
1	1A	1134	A
1	1A	1135	G
1	1A	1136	U
1	1A	1137	G
1	1A	1139	G
1	1A	1140	U
1	1A	1142	A
1	1A	1147	U
1	1A	1157	A
1	1A	1158	G
1	1A	1161	G
1	1A	1162	C
1	1A	1174	A
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	1256	U
1	1A	1290	G

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Mol	Chain	Res	Type
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1346	U
1	1A	1347	A
1	1A	1349	G
1	1A	1366	C
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1418	U
1	1A	1426	G
1	1A	1430	A
1	1A	1431	G
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1491	A
1	1A	1497	G
1	1A	1502	G
1	1A	1514	C
1	1A	1529	G
1	1A	1536	A
1	1A	1539	C
1	1A	1542	A
1	1A	1554	A
1	1A	1555	C
1	1A	1556	A
1	1A	1586	G
1	1A	1589	A
1	1A	1590	C
1	1A	1605	A
1	1A	1606	G
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1628	G
1	1A	1631	C

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Mol	Chain	Res	Type
1	1A	1632	A
1	1A	1654	A
1	1A	1655	A
1	1A	1656	A
1	1A	1695	C
1	1A	1700	G
1	1A	1701	A
1	1A	1721	G
1	1A	1743	G
1	1A	1747	A
1	1A	1750	G
1	1A	1767	A
1	1A	1776	G
1	1A	1787	G
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1811	A
1	1A	1813	C
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1847	G
1	1A	1860	A
1	1A	1878	A
1	1A	1889	G
1	1A	1899	A
1	1A	1900	G
1	1A	1911	A
1	1A	1922	A
1	1A	1928	G
1	1A	1941	A
1	1A	1951	G
1	1A	1952	G
1	1A	1959	A
1	1A	1960	A
1	1A	1977	U
1	1A	1985	U
1	1A	1987	C
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A

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Mol	Chain	Res	Type
1	1A	1994	A
1	1A	2014	G
1	1A	2015	U
1	1A	2019	G
1	1A	2042	A
1	1A	2045	G
1	1A	2053	A
1	1A	2054	G
1	1A	2055	A
1	1A	2061	C
1	1A	2065	C
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2091	G
1	1A	2132	G
1	1A	2135	U
1	1A	2137	G
1	1A	2138	G
1	1A	2143	G
1	1A	2149	G
1	1A	2151	C
1	1A	2152	U
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2157	A
1	1A	2158	C
1	1A	2163	G
1	1A	2164	C
1	1A	2165	C
1	1A	2166	U
1	1A	2168	C
1	1A	2169	G
1	1A	2172	U
1	1A	2173	G
1	1A	2178	G
1	1A	2179	G
1	1A	2180	A
1	1A	2181	G

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Mol	Chain	Res	Type
1	1A	2187	G
1	1A	2188	G
1	1A	2189	U
1	1A	2190	G
1	1A	2191	A
1	1A	2193	A
1	1A	2194	U
1	1A	2196	C
1	1A	2200	C
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	2229	A
1	1A	2237	A
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2292	G
1	1A	2295	C
1	1A	2299	A
1	1A	2301	G
1	1A	2317	A
1	1A	2320	G
1	1A	2325	C
1	1A	2332	A
1	1A	2337	G
1	1A	2346	G
1	1A	2348	A
1	1A	2359	C
1	1A	2362	C
1	1A	2373	A
1	1A	2395	G
1	1A	2397	C
1	1A	2411	G
1	1A	2418	U
1	1A	2419	G
1	1A	2437	A
1	1A	2441	G

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Mol	Chain	Res	Type
1	1A	2442	A
1	1A	2443	U
1	1A	2447	A
1	1A	2451	A
1	1A	2452	C
1	1A	2453	C
1	1A	2460	A
1	1A	2488	A
1	1A	2490	A
1	1A	2514	G
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2541	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2585	C
1	1A	2598	C
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	2666	A
1	1A	2701	U
1	1A	2702	C
1	1A	2714	U
1	1A	2715	C
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2746	A
1	1A	2770	A
1	1A	2778	A
1	1A	2779	G
1	1A	2782	C
1	1A	2791	A
1	1A	2803	A
1	1A	2804	C

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Mol	Chain	Res	Type
1	1A	2806	G
1	1A	2813	G
1	1A	2814	C
1	1A	2830	A
1	1A	2831	A
1	1A	2845	A
1	1A	2882	G
1	1A	2890	C
1	1A	2901	A
1	1A	2903	G
2	1B	2	C
2	1B	15	A
2	1B	45	A
2	1B	50	G
2	1B	52	A
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	51	A
32	1a	54	C
32	1a	61	G
32	1a	69	G
32	1a	79	G
32	1a	91	C
32	1a	96	U
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	115	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	145	G
32	1a	162	A

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Mol	Chain	Res	Type
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	218	C
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	342	C
32	1a	348	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	392	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	421	U
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C

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Mol	Chain	Res	Type
32	1a	452	A
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	524	G
32	1a	527	G7M
32	1a	531	U
32	1a	532	A
32	1a	533	A
32	1a	547	A
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	562	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	630	G
32	1a	653	A
32	1a	659	U
32	1a	665	A
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	752	G
32	1a	755	G
32	1a	774	G

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Mol	Chain	Res	Type
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	870	U
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	1000	U
32	1a	1001(A)	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G

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Mol	Chain	Res	Type
32	1a	1027	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1030(D)	A
32	1a	1031	G
32	1a	1033	G
32	1a	1039	C
32	1a	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	1125	U
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1141	C
32	1a	1152	A
32	1a	1157	A
32	1a	1159	U
32	1a	1160	G
32	1a	1168	A
32	1a	1172	C
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A

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Mol	Chain	Res	Type
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
32	1a	1273	G
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	C
32	1a	1338	G
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1381	U
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	24	A
54	1w	2	C
54	1w	6	G

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Mol	Chain	Res	Type
54	1w	7	A
54	1w	8	4SU
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	45	U
54	1w	46	G7M
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	62	C
54	1w	67	C
54	1w	68	C
54	1w	69	G
54	1w	70	G
54	1w	72	C
54	1w	73	A
54	1w	74	C
55	1x	9	G
55	1x	14	A
55	1x	18	G
55	1x	19	G
55	1x	21	A
55	1x	47	U
55	1x	61	C
55	1x	63	G
55	1x	69	C
55	1x	76	A
56	1y	6	G
56	1y	8	4SU
56	1y	13	C
56	1y	19	G
56	1y	20	U
56	1y	21	A
56	1y	35	A
56	1y	36	A
56	1y	44	G
56	1y	45	U
56	1y	46	G7M

Continued on next page...

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Mol	Chain	Res	Type
56	1y	48	C
56	1y	49	C
56	1y	53	G
56	1y	54	5MU
56	1y	59	U
56	1y	65	G
56	1y	69	G
56	1y	70	G
1	2A	11	G
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	141	A
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
1	2A	248	G
1	2A	249	C

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Mol	Chain	Res	Type
1	2A	250	G
1	2A	266	G
1	2A	267	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	279	C
1	2A	283	A
1	2A	294	A
1	2A	311	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	352	G
1	2A	354	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	363(D)	G
1	2A	386	G
1	2A	396	G
1	2A	405	U
1	2A	406	G
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	422	A
1	2A	435	C
1	2A	444	C
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	494	G
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	528	A

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Mol	Chain	Res	Type
1	2A	529	A
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	592	G
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	651	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	771	G
1	2A	774	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A

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Mol	Chain	Res	Type
1	2A	827	U
1	2A	828	U
1	2A	852	G
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	870	A
1	2A	874	G
1	2A	875	G
1	2A	877	U
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	883	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	914	C
1	2A	917	A
1	2A	923	C
1	2A	932	G
1	2A	933	A
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A

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Mol	Chain	Res	Type
1	2A	996	A
1	2A	997	G
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1020	A
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1037	G
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1116	C
1	2A	1135	C
1	2A	1136	G
1	2A	1137	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1144	G
1	2A	1155	A
1	2A	1171	G
1	2A	1188	U
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1248	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1284	A
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1308	A
1	2A	1314	C
1	2A	1345	C
1	2A	1352	U

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Mol	Chain	Res	Type
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	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1460	A
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1543	C
1	2A	1545	A
1	2A	1547	C
1	2A	1558	A
1	2A	1559	G
1	2A	1569	A
1	2A	1578	U
1	2A	1583	A

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Mol	Chain	Res	Type
1	2A	1584	C
1	2A	1586	A
1	2A	1603	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C
1	2A	1647	G
1	2A	1648	C
1	2A	1653	G
1	2A	1654	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1746	G
1	2A	1747	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1811	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G

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Mol	Chain	Res	Type
1	2A	1889	A
1	2A	1900	A
1	2A	1906	G
1	2A	1912	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1931	U
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2096	U
1	2A	2097	C
1	2A	2104	G
1	2A	2105	C
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2126	A
1	2A	2127	G

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Mol	Chain	Res	Type
1	2A	2129	C
1	2A	2130	U
1	2A	2131	G
1	2A	2132	U
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2146	C
1	2A	2150	U
1	2A	2153	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
1	2A	2161	C
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2174	C
1	2A	2182	G
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2219	G
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C

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Mol	Chain	Res	Type
1	2A	2287	A
1	2A	2288	A
1	2A	2294	C
1	2A	2305	A
1	2A	2308	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2372	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2402	C
1	2A	2403	C
1	2A	2406	U
1	2A	2419	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2434	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2468	G
1	2A	2469	A
1	2A	2476	A
1	2A	2487	G
1	2A	2490	G
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2536	G

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Mol	Chain	Res	Type
1	2A	2554	U
1	2A	2562	U
1	2A	2564	A
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2574	G
1	2A	2586	C
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2758	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2780	G
1	2A	2789	C
1	2A	2793	G
1	2A	2802	G
1	2A	2803	C
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2872	G

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Mol	Chain	Res	Type
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	13	A
2	2B	19	G
2	2B	25	A
2	2B	30	C
2	2B	32	C
2	2B	34	U
2	2B	42	C
2	2B	53	A
2	2B	56	G
2	2B	63	G
2	2B	65	C
2	2B	67	G
2	2B	72	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	90	A
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	111	G
2	2B	114	C
2	2B	116	G
2	2B	120	A
57	2a	9	G
57	2a	22	G
57	2a	31	G
57	2a	32	A
57	2a	39	G
57	2a	47	C
57	2a	48	C
57	2a	50	A
57	2a	51	A
57	2a	66	G

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Mol	Chain	Res	Type
57	2a	73	G
57	2a	79	G
57	2a	89	C
57	2a	98	G
57	2a	101	A
57	2a	115	G
57	2a	116	A
57	2a	121	C
57	2a	131	C
57	2a	144	G
57	2a	163	C
57	2a	174	C
57	2a	182	U
57	2a	189(F)	U
57	2a	195	A
57	2a	197	A
57	2a	201	C
57	2a	202	U
57	2a	203	U
57	2a	204	U
57	2a	216	G
57	2a	247	G
57	2a	251	G
57	2a	258	G
57	2a	266	G
57	2a	267	C
57	2a	281	G
57	2a	289	G
57	2a	300	A
57	2a	321	A
57	2a	328	C
57	2a	332	G
57	2a	342	C
57	2a	351	G
57	2a	352	C
57	2a	353	A
57	2a	354	G
57	2a	367	U
57	2a	372	C
57	2a	384	G
57	2a	397	A
57	2a	398	C

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Mol	Chain	Res	Type
57	2a	406	G
57	2a	412	A
57	2a	423	G
57	2a	429	U
57	2a	430	A
57	2a	439	A
57	2a	442	C
57	2a	452	A
57	2a	461	A
57	2a	470	C
57	2a	477	A
57	2a	482	A
57	2a	484	G
57	2a	485	G
57	2a	496	A
57	2a	498	U
57	2a	499	A
57	2a	505	G
57	2a	510	A
57	2a	511	C
57	2a	518	C
57	2a	521	G
57	2a	531	U
57	2a	532	A
57	2a	533	A
57	2a	547	A
57	2a	559	A
57	2a	564	C
57	2a	568	G
57	2a	572	A
57	2a	573	A
57	2a	576	G
57	2a	577	G
57	2a	596	C
57	2a	630	G
57	2a	653	A
57	2a	665	A
57	2a	666	G
57	2a	687	A
57	2a	688	G
57	2a	695	A
57	2a	721	G

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Mol	Chain	Res	Type
57	2a	723	U
57	2a	724	G
57	2a	731	G
57	2a	749	C
57	2a	755	G
57	2a	777	A
57	2a	792	A
57	2a	793	U
57	2a	794	A
57	2a	816	A
57	2a	817	C
57	2a	821	G
57	2a	828	A
57	2a	840	C
57	2a	841	U
57	2a	853	G
57	2a	859	A
57	2a	874	G
57	2a	885	G
57	2a	902	G
57	2a	914	A
57	2a	926	G
57	2a	927	G
57	2a	934	C
57	2a	935	A
57	2a	942	G
57	2a	960	U
57	2a	961	U
57	2a	968	A
57	2a	969	A
57	2a	971	G
57	2a	972	C
57	2a	974	A
57	2a	975	A
57	2a	976	G
57	2a	977	A
57	2a	982	U
57	2a	984	C
57	2a	989	C
57	2a	992	U
57	2a	993	G
57	2a	997	U

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Mol	Chain	Res	Type
57	2a	998	G
57	2a	999	C
57	2a	1001	A
57	2a	1001(A)	G
57	2a	1002	G
57	2a	1003	G
57	2a	1004	A
57	2a	1005	A
57	2a	1006	C
57	2a	1009	G
57	2a	1011	G
57	2a	1016	A
57	2a	1020	U
57	2a	1021	G
57	2a	1022	G
57	2a	1025	U
57	2a	1026	G
57	2a	1027	C
57	2a	1029	C
57	2a	1030	C
57	2a	1030(A)	G
57	2a	1031	G
57	2a	1032	G
57	2a	1035	A
57	2a	1038	C
57	2a	1039	C
57	2a	1040	U
57	2a	1045	C
57	2a	1046	A
57	2a	1051	C
57	2a	1053	G
57	2a	1054	C
57	2a	1055	A
57	2a	1065	U
57	2a	1066	C
57	2a	1068	G
57	2a	1077	G
57	2a	1078	U
57	2a	1079	G
57	2a	1081	G
57	2a	1086	U
57	2a	1094	G

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Mol	Chain	Res	Type
57	2a	1095	U
57	2a	1101	A
57	2a	1108	G
57	2a	1113	C
57	2a	1117	G
57	2a	1122	U
57	2a	1125	U
57	2a	1129	C
57	2a	1130	A
57	2a	1132	C
57	2a	1136	U
57	2a	1137	C
57	2a	1138	G
57	2a	1139	G
57	2a	1146	A
57	2a	1147	C
57	2a	1152	A
57	2a	1157	A
57	2a	1158	C
57	2a	1159	U
57	2a	1160	G
57	2a	1182	G
57	2a	1183	A
57	2a	1184	G
57	2a	1193	G
57	2a	1196	U
57	2a	1197	G
57	2a	1202	G
57	2a	1211	U
57	2a	1213	A
57	2a	1227	A
57	2a	1236	A
57	2a	1238	A
57	2a	1240	U
57	2a	1241	G
57	2a	1256	A
57	2a	1257	U
57	2a	1258	G
57	2a	1260	C
57	2a	1261	A
57	2a	1264	C
57	2a	1267	C

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Mol	Chain	Res	Type
57	2a	1268	A
57	2a	1270	C
57	2a	1272	G
57	2a	1273	G
57	2a	1276	G
57	2a	1277	C
57	2a	1278	U
57	2a	1279	A
57	2a	1280	A
57	2a	1286	A
57	2a	1287	A
57	2a	1302	U
57	2a	1303	C
57	2a	1305	G
57	2a	1323	G
57	2a	1338	G
57	2a	1340	A
57	2a	1346	A
57	2a	1347	G
57	2a	1358	U
57	2a	1359	C
57	2a	1363	C
57	2a	1368	G
57	2a	1370	G
57	2a	1378	C
57	2a	1419	G
57	2a	1442	G
57	2a	1442(A)	G
57	2a	1447	A
57	2a	1452	C
57	2a	1456	G
57	2a	1492	A
57	2a	1497	G
57	2a	1504	G
57	2a	1506	U
57	2a	1517	G
57	2a	1520	G
57	2a	1529	G
57	2a	1530	G
57	2a	1531	A
57	2a	1532	U
53	2v	13	A

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Mol	Chain	Res	Type
54	2w	3	C
54	2w	4	C
54	2w	5	G
54	2w	6	G
54	2w	8	4SU
54	2w	11	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	27	G
54	2w	46	G7M
54	2w	47	U
54	2w	48	C
54	2w	50	U
54	2w	62	C
54	2w	64	A
54	2w	65	G
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	73	A
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	21	A
55	2x	22	G
55	2x	46	G
55	2x	47	U
55	2x	48	C
55	2x	51	C
55	2x	52	G
55	2x	53	G
55	2x	67	C
55	2x	68	C
55	2x	76	A
56	2y	5	G
56	2y	8	4SU
56	2y	13	C
56	2y	19	G
56	2y	35	A
56	2y	37	A

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Mol	Chain	Res	Type
56	2y	44	G
56	2y	45	U
56	2y	46	G7M
56	2y	48	C
56	2y	49	C
56	2y	53	G
56	2y	54	5MU
56	2y	59	U
56	2y	65	G
56	2y	66	U
56	2y	69	G
56	2y	70	G

All (64) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	115	G
1	1A	185	A
1	1A	271	U
1	1A	302	A
1	1A	509	A
1	1A	572	A
1	1A	596	G
1	1A	716	G
1	1A	732	A
1	1A	793	A
1	1A	811	A
1	1A	821	A
1	1A	913	A
1	1A	941	U
1	1A	1003	U
1	1A	1019	G
1	1A	1065	U
1	1A	1067	A
1	1A	1093	G
1	1A	1201	A
1	1A	1219	A
1	1A	1221	G
1	1A	1255	A
1	1A	1425	A
1	1A	1554	A
1	1A	1654	A

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Mol	Chain	Res	Type
1	1A	1700	G
1	1A	1793	A
1	1A	2014	G
1	1A	2156	A
1	1A	2203	G
1	1A	2205	C
1	1A	2418	U
1	1A	2442	A
1	1A	2451	A
1	1A	2641	A
1	1A	2701	U
1	1A	2769	U
2	1B	1	U
1	2A	34	C
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	752	A
1	2A	774	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	958	U
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1608	A
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2689	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
54	G7M	2w	46	54	23,26,27	2.38	4 (17%)	34,39,42	2.99	11 (32%)
57	5MC	2a	1407	57	19,22,23	1.50	3 (15%)	26,32,35	1.22	3 (11%)
54	PSU	2w	55	54	18,21,22	1.40	2 (11%)	21,30,33	2.05	3 (14%)
54	PSU	1w	39	54	18,21,22	1.36	2 (11%)	21,30,33	1.92	3 (14%)
1	5MU	2A	1939	59,1	19,22,23	1.43	5 (26%)	27,32,35	2.38	6 (22%)
56	PSU	1y	39	56	18,21,22	1.34	2 (11%)	21,30,33	2.00	4 (19%)
1	PSU	2A	1917	1	18,21,22	1.38	2 (11%)	21,30,33	2.04	3 (14%)
54	MIA	2w	37	54	24,27,32	2.15	5 (20%)	32,39,47	2.44	10 (31%)
55	4SU	2x	8	55,59	18,21,22	2.08	4 (22%)	25,30,33	1.47	6 (24%)
57	4OC	2a	1402	57	20,23,24	0.77	0	25,32,35	1.06	2 (8%)
56	4SU	2y	8	56,59	18,21,22	1.75	4 (22%)	25,30,33	2.11	4 (16%)
32	UR3	1a	1498	32	19,22,23	1.07	1 (5%)	26,32,35	1.79	4 (15%)
43	0TD	1l	92	43	8,9,10	4.50	1 (12%)	6,11,13	2.36	2 (33%)
56	G7M	1y	46	56	23,26,27	2.40	5 (21%)	34,39,42	3.04	10 (29%)
56	PSU	2y	39	56	18,21,22	1.29	2 (11%)	21,30,33	2.00	3 (14%)
1	5MU	2A	1915	1	19,22,23	1.45	6 (31%)	27,32,35	2.20	5 (18%)
56	5MU	1y	54	56	19,22,23	1.49	5 (26%)	27,32,35	1.81	5 (18%)
43	0TD	2l	92	43	8,9,10	4.58	1 (12%)	6,11,13	3.35	3 (50%)
57	5MC	2a	1404	57	19,22,23	1.70	3 (15%)	26,32,35	1.22	3 (11%)
1	PSU	1A	1939	1	18,21,22	1.35	2 (11%)	21,30,33	2.07	3 (14%)
1	5MC	2A	1942	1	19,22,23	1.64	3 (15%)	26,32,35	1.16	2 (7%)
32	5MC	1a	1407	32	19,22,23	1.48	3 (15%)	26,32,35	1.13	2 (7%)
54	4SU	2w	8	54	18,21,22	1.68	4 (22%)	25,30,33	2.49	5 (20%)
54	G7M	1w	46	54	23,26,27	2.46	5 (21%)	34,39,42	2.87	10 (29%)
56	PSU	2y	55	56	18,21,22	1.36	2 (11%)	21,30,33	2.04	3 (14%)
1	2MA	1A	2515	59,1	22,25,26	1.40	4 (18%)	32,37,40	2.23	9 (28%)
1	OMG	2A	2251	55,59,1	23,26,27	1.24	3 (13%)	32,38,41	2.03	6 (18%)
56	4SU	1y	8	56	18,21,22	1.75	5 (27%)	25,30,33	1.99	5 (20%)
55	5MC	2x	32	55	19,22,23	1.64	2 (10%)	26,32,35	1.19	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	BB9	B	6	58	2,5,6	4.08	1 (50%)	1,5,7	2.75	1 (100%)
57	PSU	2a	516	57	18,21,22	1.31	2 (11%)	21,30,33	2.05	4 (19%)
57	5MC	2a	967	57	19,22,23	1.74	3 (15%)	26,32,35	1.09	2 (7%)
32	5MC	1a	1404	32	19,22,23	1.73	3 (15%)	26,32,35	1.20	4 (15%)
1	2MA	2A	2503	59,1	22,25,26	1.47	5 (22%)	32,37,40	2.28	9 (28%)
1	2MU	1A	2564	59,1	19,22,24	1.22	2 (10%)	25,31,36	2.05	6 (24%)
56	5MU	2y	54	56	19,22,23	1.52	5 (26%)	27,32,35	2.02	9 (33%)
57	MA6	2a	1519	57	23,26,27	1.59	4 (17%)	33,38,41	2.31	12 (36%)
32	MA6	1a	1518	32	23,26,27	1.56	5 (21%)	33,38,41	2.19	12 (36%)
56	PSU	1y	32	56	18,21,22	1.40	2 (11%)	21,30,33	1.96	3 (14%)
1	PSU	2A	2605	1	18,21,22	1.35	2 (11%)	21,30,33	2.10	5 (23%)
57	5MC	2a	1400	57	19,22,23	1.71	3 (15%)	26,32,35	1.25	3 (11%)
32	G7M	1a	527	32,59	23,26,27	2.45	5 (21%)	34,39,42	2.89	10 (29%)
55	5MC	1x	32	55	19,22,23	1.63	3 (15%)	26,32,35	1.22	2 (7%)
57	UR3	2a	1498	57	19,22,23	1.02	1 (5%)	26,32,35	1.79	3 (11%)
32	M2G	1a	966	32	24,27,28	1.30	4 (16%)	33,40,43	1.82	6 (18%)
32	MA6	1a	1519	32	23,26,27	1.52	4 (17%)	33,38,41	2.36	14 (42%)
55	PSU	1x	55	55,59	18,21,22	1.31	2 (11%)	21,30,33	2.04	4 (19%)
1	5MU	1A	1961	1	19,22,23	1.41	5 (26%)	27,32,35	2.38	6 (22%)
54	PSU	1w	32	54,59	18,21,22	1.35	2 (11%)	21,30,33	1.93	3 (14%)
32	5MC	1a	967	32	19,22,23	1.58	2 (10%)	26,32,35	1.05	2 (7%)
1	2MU	2A	2552	59,1	19,22,24	1.29	2 (10%)	25,31,36	2.02	6 (24%)
55	4SU	1x	8	55	18,21,22	2.12	5 (27%)	25,30,33	1.66	6 (24%)
1	OMG	1A	2263	55,59,1	23,26,27	1.21	3 (13%)	32,38,41	1.99	6 (18%)
54	MIA	1w	37	54	28,31,32	2.36	6 (21%)	38,44,47	2.69	11 (28%)
54	5MU	2w	54	54	19,22,23	1.38	5 (26%)	27,32,35	1.72	6 (22%)
54	PSU	2w	39	54	18,21,22	1.40	2 (11%)	21,30,33	1.76	3 (14%)
56	PSU	1y	55	56	18,21,22	1.41	2 (11%)	21,30,33	2.07	3 (14%)
57	MA6	2a	1518	57	23,26,27	1.60	4 (17%)	33,38,41	2.29	12 (36%)
54	4SU	1w	8	54	18,21,22	1.76	5 (27%)	25,30,33	1.89	4 (16%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	1.06	1 (4%)
57	M2G	2a	966	57	24,27,28	1.31	4 (16%)	33,40,43	1.92	6 (18%)
1	5MC	1A	1984	59,1	19,22,23	1.61	3 (15%)	26,32,35	1.10	2 (7%)
54	5MU	1w	54	54	19,22,23	1.36	5 (26%)	27,32,35	2.11	7 (25%)
55	PSU	2x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.02	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	G7M	2y	46	56	23,26,27	2.43	5 (21%)	34,39,42	3.07	10 (29%)
1	5MU	1A	1937	1	19,22,23	1.39	4 (21%)	27,32,35	2.28	6 (22%)
1	PSU	1A	2617	59,1	18,21,22	1.39	3 (16%)	21,30,33	2.12	4 (19%)
32	2MG	1a	1207	32	23,26,27	1.22	3 (13%)	33,38,41	2.28	9 (27%)
57	G7M	2a	527	57,59	23,26,27	2.36	5 (21%)	34,39,42	3.02	10 (29%)
1	5MC	1A	1964	59,1	19,22,23	1.46	3 (15%)	26,32,35	1.12	2 (7%)
58	BB9	A	17	58	2,5,6	4.59	1 (50%)	1,5,7	4.29	1 (100%)
55	5MU	1x	54	55,59	19,22,23	1.44	6 (31%)	27,32,35	2.00	7 (25%)
56	PSU	2y	32	56	18,21,22	1.37	2 (11%)	21,30,33	1.92	4 (19%)
54	PSU	2w	32	54	18,21,22	1.32	2 (11%)	21,30,33	1.95	4 (19%)
1	4OC	2A	1920	1	19,22,24	0.76	0	25,31,35	0.88	1 (4%)
1	PSU	1A	1933	1	18,21,22	1.43	2 (11%)	21,30,33	2.06	3 (14%)
1	5MC	2A	1962	59,1	19,22,23	1.70	3 (15%)	26,32,35	1.18	3 (11%)
58	BB9	A	6	58	2,5,6	4.24	1 (50%)	1,5,7	2.55	1 (100%)
58	BB9	A	9	58	2,5,6	4.61	1 (50%)	1,5,7	2.56	1 (100%)
57	2MG	2a	1207	57	23,26,27	1.25	3 (13%)	33,38,41	2.16	7 (21%)
58	BB9	B	9	58	2,5,6	4.94	1 (50%)	1,5,7	2.89	1 (100%)
32	PSU	1a	516	32,59	18,21,22	1.35	3 (16%)	21,30,33	1.97	5 (23%)
54	PSU	1w	55	54	18,21,22	1.43	2 (11%)	21,30,33	2.01	4 (19%)
55	5MU	2x	54	55	19,22,23	1.42	5 (26%)	27,32,35	2.18	6 (22%)
1	PSU	2A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	1.98	4 (19%)
1	4OC	1A	1942	1	19,22,24	0.78	0	25,31,35	0.95	1 (4%)
32	5MC	1a	1400	32	19,22,23	1.61	3 (15%)	26,32,35	1.15	3 (11%)
58	BB9	B	17	58	2,5,6	4.30	1 (50%)	1,5,7	4.14	1 (100%)

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
54	G7M	2w	46	54	-	3/7/25/26	0/3/3/3
57	5MC	2a	1407	57	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	59,1	-	0/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
55	4SU	2x	8	55,59	-	1/7/25/26	0/2/2/2
57	4OC	2a	1402	57	-	2/9/29/30	0/2/2/2
56	4SU	2y	8	56,59	-	2/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
56	G7M	1y	46	56	-	1/7/25/26	0/3/3/3
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	2/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
57	5MC	2a	1404	57	-	0/7/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	3/7/25/26	0/3/3/3
56	PSU	2y	55	56	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	59,1	-	1/7/25/26	0/3/3/3
1	OMG	2A	2251	55,59,1	-	0/9/27/28	0/3/3/3
56	4SU	1y	8	56	-	2/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
58	BB9	B	6	58	-	0/0/4/6	-
57	PSU	2a	516	57	-	0/7/25/26	0/2/2/2
57	5MC	2a	967	57	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	59,1	-	1/7/25/26	0/3/3/3
1	2MU	1A	2564	59,1	-	0/9/27/28	0/2/2/2
56	5MU	2y	54	56	-	3/7/25/26	0/2/2/2
57	MA6	2a	1519	57	-	6/11/29/30	0/3/3/3
32	MA6	1a	1518	32	-	1/11/29/30	0/3/3/3
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
57	5MC	2a	1400	57	-	4/7/25/26	0/2/2/2
32	G7M	1a	527	32,59	-	3/7/25/26	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
57	UR3	2a	1498	57	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	1a	1519	32	-	4/11/29/30	0/3/3/3
55	PSU	1x	55	55,59	-	0/7/25/26	0/2/2/2
1	5MU	1A	1961	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54,59	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	59,1	-	0/9/27/28	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	OMG	1A	2263	55,59,1	-	0/9/27/28	0/3/3/3
54	MIA	1w	37	54	-	2/15/33/34	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
57	MA6	2a	1518	57	-	2/11/29/30	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
57	M2G	2a	966	57	-	0/11/29/30	0/3/3/3
1	5MC	1A	1984	59,1	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
56	G7M	2y	46	56	-	1/7/25/26	0/3/3/3
1	5MU	1A	1937	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	59,1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
57	G7M	2a	527	57,59	-	3/7/25/26	0/3/3/3
1	5MC	1A	1964	59,1	-	0/7/25/26	0/2/2/2
58	BB9	A	17	58	-	0/0/4/6	-
55	5MU	1x	54	55,59	-	0/7/25/26	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	59,1	-	0/7/25/26	0/2/2/2
58	BB9	A	6	58	-	0/0/4/6	-
58	BB9	A	9	58	-	0/0/4/6	-
57	2MG	2a	1207	57	-	2/9/27/28	0/3/3/3
58	BB9	B	9	58	-	0/0/4/6	-
32	PSU	1a	516	32,59	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	4OC	1A	1942	1	-	1/9/27/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
58	BB9	B	17	58	-	0/0/4/6	-

All (264) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.66	1.69	1.82
43	1l	92	0TD	CB-SB	-12.29	1.69	1.82
54	2w	46	G7M	C8-N7	8.11	1.46	1.33
32	1a	527	G7M	C8-N7	7.91	1.46	1.33
57	2a	527	G7M	C8-N7	7.78	1.46	1.33
54	1w	46	G7M	C8-N7	7.74	1.46	1.33
56	1y	46	G7M	C8-N7	7.66	1.46	1.33
56	2y	46	G7M	C8-N7	7.63	1.46	1.33
54	2w	37	MIA	C2-S10	-7.24	1.69	1.75
54	1w	37	MIA	C13-C14	6.96	1.53	1.32
58	B	9	BB9	C-CA	-6.95	1.33	1.45
54	1w	37	MIA	C2-S10	-6.94	1.70	1.75
58	A	9	BB9	C-CA	-6.48	1.34	1.45
57	2a	967	5MC	C5-C4	6.43	1.49	1.44
58	A	17	BB9	C-CA	-6.42	1.34	1.45
57	2a	1400	5MC	C5-C4	6.31	1.48	1.44
1	2A	1962	5MC	C5-C4	6.29	1.48	1.44
57	2a	1404	5MC	C5-C4	6.22	1.48	1.44
32	1a	1404	5MC	C5-C4	6.12	1.48	1.44
58	B	17	BB9	C-CA	-6.01	1.35	1.45
58	A	6	BB9	C-CA	-5.96	1.35	1.45
1	2A	1942	5MC	C5-C4	5.88	1.48	1.44
55	1x	32	5MC	C5-C4	5.81	1.48	1.44
1	1A	1984	5MC	C5-C4	5.81	1.48	1.44
55	2x	32	5MC	C5-C4	5.80	1.48	1.44
32	1a	1400	5MC	C5-C4	5.78	1.48	1.44
58	B	6	BB9	C-CA	-5.74	1.35	1.45
32	1a	967	5MC	C5-C4	5.62	1.48	1.44
32	1a	1407	5MC	C5-C4	5.29	1.48	1.44
57	2a	1407	5MC	C5-C4	5.10	1.48	1.44
57	2a	1518	MA6	C5-C4	5.03	1.48	1.39
1	1A	1964	5MC	C5-C4	4.99	1.47	1.44
54	2w	37	MIA	C5-C4	4.98	1.48	1.39
55	2x	8	4SU	C4-N3	-4.94	1.32	1.37
54	1w	46	G7M	C5-N7	-4.87	1.33	1.39
57	2a	1519	MA6	C5-C4	4.86	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C5-C4	4.84	1.47	1.39
54	2w	8	4SU	C4-S4	-4.79	1.60	1.68
55	1x	8	4SU	C4-N3	-4.78	1.32	1.37
56	2y	8	4SU	C4-S4	-4.74	1.60	1.68
32	1a	1518	MA6	C5-C4	4.71	1.47	1.39
54	1w	8	4SU	C4-S4	-4.66	1.60	1.68
32	1a	527	G7M	C5-N7	-4.56	1.33	1.39
32	1a	527	G7M	C8-N9	4.46	1.47	1.35
55	1x	8	4SU	C4-S4	-4.45	1.60	1.68
32	1a	1519	MA6	C5-C4	4.45	1.47	1.39
55	2x	8	4SU	C4-S4	-4.42	1.60	1.68
56	1y	8	4SU	C4-S4	-4.42	1.60	1.68
56	1y	46	G7M	C5-N7	-4.38	1.34	1.39
56	2y	46	G7M	C8-N9	4.34	1.47	1.35
56	2y	46	G7M	C5-N7	-4.34	1.34	1.39
54	1w	46	G7M	C8-N9	4.34	1.47	1.35
56	1y	46	G7M	C8-N9	4.28	1.47	1.35
57	2a	527	G7M	C8-N9	4.28	1.47	1.35
1	2A	2503	2MA	C5-C4	4.25	1.46	1.39
56	2y	46	G7M	C5-C4	4.24	1.48	1.38
54	2w	46	G7M	C8-N9	4.23	1.47	1.35
54	1w	55	PSU	C6-C5	4.17	1.39	1.35
56	1y	46	G7M	C5-C4	4.12	1.48	1.38
32	1a	527	G7M	C5-C4	4.10	1.48	1.38
1	1A	2515	2MA	C5-C4	4.10	1.46	1.39
57	2a	527	G7M	C5-N7	-4.08	1.34	1.39
54	1w	46	G7M	C5-C4	4.05	1.48	1.38
56	1y	32	PSU	C6-C5	4.03	1.39	1.35
56	2y	55	PSU	C6-C5	3.96	1.39	1.35
56	2y	32	PSU	C6-C5	3.95	1.39	1.35
54	2w	46	G7M	C5-N7	-3.90	1.34	1.39
54	2w	55	PSU	C6-C5	3.89	1.39	1.35
56	1y	55	PSU	C6-C5	3.86	1.39	1.35
55	1x	8	4SU	C2-N3	-3.81	1.31	1.38
54	2w	46	G7M	C5-C4	3.81	1.47	1.38
57	2a	527	G7M	C5-C4	3.78	1.47	1.38
56	1y	39	PSU	C6-C5	3.68	1.39	1.35
54	2w	39	PSU	C6-C5	3.63	1.39	1.35
1	1A	1933	PSU	C6-C5	3.62	1.39	1.35
55	2x	55	PSU	C6-C5	3.62	1.39	1.35
56	2y	39	PSU	C6-C5	3.58	1.39	1.35
54	1w	32	PSU	C6-C5	3.55	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1911	PSU	C6-C5	3.52	1.39	1.35
1	1A	1939	PSU	C6-C5	3.50	1.39	1.35
54	1w	39	PSU	C6-C5	3.48	1.39	1.35
1	2A	2605	PSU	C6-C5	3.45	1.39	1.35
55	2x	8	4SU	C2-N3	-3.44	1.32	1.38
1	2A	1917	PSU	C6-C5	3.41	1.39	1.35
57	2a	516	PSU	C6-C5	3.39	1.39	1.35
54	2w	32	PSU	C6-C5	3.36	1.39	1.35
57	2a	966	M2G	C5-C4	3.28	1.47	1.38
56	2y	54	5MU	C2-N1	3.28	1.43	1.38
55	1x	8	4SU	C5-C4	-3.28	1.38	1.42
56	1y	8	4SU	C4-N3	-3.25	1.34	1.37
32	1a	516	PSU	C6-C5	3.23	1.38	1.35
1	1A	2263	OMG	C5-C4	3.22	1.47	1.38
57	2a	1519	MA6	C5-C6	3.21	1.49	1.41
57	2a	1207	2MG	C5-C4	3.20	1.47	1.38
1	2A	2251	OMG	C5-C4	3.17	1.47	1.38
57	2a	1518	MA6	C5-C6	3.16	1.49	1.41
54	1w	8	4SU	C4-N3	-3.16	1.34	1.37
56	1y	54	5MU	C6-C5	3.13	1.39	1.34
32	1a	966	M2G	C2-N2	3.12	1.40	1.35
55	1x	55	PSU	C6-C5	3.12	1.38	1.35
32	1a	1207	2MG	C5-C4	3.04	1.47	1.38
1	1A	1961	5MU	C4-N3	-3.03	1.33	1.38
32	1a	966	M2G	C5-C4	3.02	1.47	1.38
32	1a	1518	MA6	C5-C6	2.98	1.49	1.41
55	2x	54	5MU	C6-C5	2.97	1.39	1.34
1	1A	2564	2MU	C4-N3	-2.95	1.33	1.38
54	2w	37	MIA	C5-C6	2.93	1.49	1.41
55	1x	32	5MC	C6-C5	2.91	1.39	1.34
1	2A	1939	5MU	C4-N3	-2.90	1.33	1.38
56	2y	8	4SU	C4-N3	-2.88	1.34	1.37
55	2x	32	5MC	C6-C5	2.87	1.39	1.34
57	2a	1407	5MC	C6-C5	2.87	1.39	1.34
32	1a	1400	5MC	C6-C5	2.87	1.39	1.34
32	1a	967	5MC	C6-C5	2.86	1.39	1.34
55	2x	8	4SU	C5-C4	-2.86	1.39	1.42
54	1w	37	MIA	C5-C6	2.82	1.48	1.41
1	2A	1915	5MU	C6-C5	2.82	1.39	1.34
56	2y	54	5MU	C6-C5	2.81	1.39	1.34
1	2A	2552	2MU	C4-N3	-2.81	1.33	1.38
57	2a	966	M2G	C2-N2	2.80	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2a	967	5MC	C6-C5	2.78	1.39	1.34
55	1x	54	5MU	C6-C5	2.78	1.39	1.34
1	2A	1939	5MU	C6-C5	2.78	1.39	1.34
54	2w	54	5MU	C6-C5	2.78	1.39	1.34
57	2a	1404	5MC	C6-C5	2.76	1.39	1.34
32	1a	1519	MA6	C5-C6	2.71	1.48	1.41
1	2A	1911	PSU	C4-N3	-2.70	1.33	1.38
55	1x	54	5MU	C4-N3	-2.69	1.33	1.38
1	1A	1961	5MU	C2-N3	-2.69	1.33	1.38
1	1A	1937	5MU	C4-N3	-2.68	1.33	1.38
32	1a	516	PSU	C4-N3	-2.68	1.33	1.38
1	1A	2617	PSU	C4-N3	-2.67	1.33	1.38
57	2a	1400	5MC	C6-C5	2.67	1.39	1.34
54	1w	39	PSU	C4-N3	-2.67	1.33	1.38
1	2A	1915	5MU	C2-N1	2.66	1.42	1.38
1	1A	2515	2MA	C5-C6	2.66	1.48	1.41
54	2w	54	5MU	C4-N3	-2.65	1.33	1.38
1	2A	1942	5MC	C6-C5	2.65	1.38	1.34
54	2w	39	PSU	C4-N3	-2.64	1.33	1.38
32	1a	1404	5MC	C6-C5	2.63	1.38	1.34
1	1A	1933	PSU	C4-N3	-2.63	1.33	1.38
1	2A	1915	5MU	C4-N3	-2.60	1.34	1.38
56	1y	54	5MU	C4-N3	-2.60	1.34	1.38
54	1w	54	5MU	C6-C5	2.60	1.38	1.34
1	1A	2617	PSU	C6-C5	2.59	1.38	1.35
54	2w	8	4SU	C4-N3	-2.58	1.34	1.37
56	1y	54	5MU	C4-C5	2.58	1.49	1.44
1	1A	1937	5MU	C2-N1	2.58	1.42	1.38
1	1A	1937	5MU	C6-C5	2.58	1.38	1.34
54	1w	46	G7M	C6-N1	-2.57	1.34	1.38
1	1A	1961	5MU	C6-C5	2.57	1.38	1.34
56	2y	46	G7M	C6-N1	-2.57	1.34	1.38
55	2x	54	5MU	C4-N3	-2.54	1.34	1.38
1	1A	2617	PSU	C2-N1	-2.54	1.33	1.36
1	1A	1961	5MU	C6-N1	-2.53	1.33	1.38
54	1w	37	MIA	C5-N7	-2.53	1.34	1.39
32	1a	1498	UR3	C2-N1	2.53	1.42	1.38
1	2A	1939	5MU	C6-N1	-2.52	1.33	1.38
1	2A	2251	OMG	C6-N1	-2.52	1.34	1.38
54	2w	55	PSU	C4-N3	-2.52	1.34	1.38
1	1A	1964	5MC	C6-C5	2.52	1.38	1.34
1	2A	1939	5MU	C2-N3	-2.51	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1962	5MC	C6-C5	2.51	1.38	1.34
32	1a	1404	5MC	C6-N1	-2.50	1.33	1.38
1	2A	1915	5MU	C4-C5	2.50	1.48	1.44
1	2A	2605	PSU	C4-N3	-2.50	1.34	1.38
32	1a	1519	MA6	C5-N7	-2.50	1.34	1.39
54	1w	32	PSU	C4-N3	-2.49	1.34	1.38
56	2y	54	5MU	C4-N3	-2.49	1.34	1.38
54	1w	54	5MU	C4-C5	2.48	1.48	1.44
55	1x	54	5MU	C4-C5	2.48	1.48	1.44
56	1y	8	4SU	C2-N1	2.48	1.42	1.38
1	1A	1984	5MC	C6-N1	-2.48	1.33	1.38
56	2y	8	4SU	C5-C4	-2.48	1.39	1.42
1	2A	1917	PSU	C4-N3	-2.48	1.34	1.38
57	2a	527	G7M	C6-N1	-2.48	1.34	1.38
56	2y	54	5MU	C4-C5	2.48	1.48	1.44
32	1a	1207	2MG	C6-N1	-2.48	1.34	1.38
32	1a	1407	5MC	C6-C5	2.47	1.38	1.34
54	2w	8	4SU	C5-C4	-2.47	1.39	1.42
55	2x	54	5MU	C4-C5	2.47	1.48	1.44
1	1A	1964	5MC	C6-N1	-2.46	1.33	1.38
1	1A	1984	5MC	C6-C5	2.46	1.38	1.34
54	1w	8	4SU	C5-C4	-2.45	1.39	1.42
55	1x	55	PSU	C4-N3	-2.44	1.34	1.38
56	1y	39	PSU	C4-N3	-2.44	1.34	1.38
54	2w	32	PSU	C4-N3	-2.44	1.34	1.38
56	2y	55	PSU	C4-N3	-2.43	1.34	1.38
54	2w	37	MIA	C8-N7	2.42	1.36	1.31
54	1w	54	5MU	C4-N3	-2.40	1.34	1.38
57	2a	1207	2MG	C6-N1	-2.40	1.34	1.38
56	1y	55	PSU	C4-N3	-2.40	1.34	1.38
1	2A	2503	2MA	C5-C6	2.39	1.47	1.41
1	2A	2552	2MU	C5-C4	2.39	1.48	1.43
57	2a	1519	MA6	C8-N7	2.38	1.36	1.31
1	1A	2564	2MU	C2-N3	-2.38	1.33	1.38
56	1y	54	5MU	C2-N1	2.37	1.42	1.38
1	2A	2503	2MA	C4-N9	-2.37	1.32	1.37
56	2y	8	4SU	C2-N1	2.37	1.42	1.38
54	1w	37	MIA	C8-N7	2.36	1.36	1.31
1	2A	2503	2MA	C5-N7	-2.36	1.34	1.39
55	2x	55	PSU	C4-N3	-2.36	1.34	1.38
56	1y	32	PSU	C4-N3	-2.36	1.34	1.38
1	2A	2251	OMG	C5-N7	-2.35	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2263	OMG	C6-N1	-2.34	1.34	1.38
57	2a	966	M2G	C6-N1	-2.33	1.34	1.38
56	1y	8	4SU	C5-C4	-2.32	1.39	1.42
55	1x	32	5MC	C6-N1	-2.32	1.34	1.38
55	2x	54	5MU	C2-N1	2.32	1.42	1.38
1	1A	1961	5MU	C4-C5	2.32	1.48	1.44
1	2A	1962	5MC	C6-N1	-2.31	1.34	1.38
1	1A	1937	5MU	C6-N1	-2.29	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.29	1.34	1.38
1	1A	2515	2MA	C8-N7	2.28	1.36	1.31
56	1y	54	5MU	C2-N3	-2.28	1.34	1.38
57	2a	1518	MA6	C8-N7	2.28	1.36	1.31
32	1a	1518	MA6	C8-N7	2.27	1.36	1.31
54	2w	8	4SU	C2-N1	2.27	1.42	1.38
56	2y	32	PSU	C4-N3	-2.26	1.34	1.38
57	2a	1498	UR3	C2-N1	2.26	1.41	1.38
32	1a	1518	MA6	C5-N7	-2.26	1.35	1.39
57	2a	1400	5MC	C6-N1	-2.26	1.34	1.38
32	1a	1518	MA6	C4-N9	-2.25	1.33	1.37
1	2A	2503	2MA	C8-N7	2.24	1.36	1.31
1	1A	1939	PSU	C4-N3	-2.24	1.34	1.38
55	1x	54	5MU	C2-N1	2.23	1.42	1.38
56	1y	46	G7M	C6-N1	-2.22	1.34	1.38
54	1w	55	PSU	C4-N3	-2.22	1.34	1.38
32	1a	1519	MA6	C8-N7	2.22	1.35	1.31
54	2w	54	5MU	C4-C5	2.21	1.48	1.44
1	1A	2263	OMG	C5-N7	-2.21	1.34	1.39
57	2a	516	PSU	C4-N3	-2.20	1.34	1.38
54	2w	37	MIA	C5-N7	-2.20	1.35	1.39
32	1a	966	M2G	C6-N1	-2.19	1.34	1.38
57	2a	1407	5MC	C6-N1	-2.19	1.34	1.38
57	2a	966	M2G	C5-N7	-2.18	1.34	1.39
56	2y	39	PSU	C4-N3	-2.18	1.34	1.38
1	2A	1939	5MU	C4-C5	2.17	1.48	1.44
57	2a	1404	5MC	C6-N1	-2.16	1.34	1.38
32	1a	527	G7M	C6-N1	-2.16	1.34	1.38
57	2a	1519	MA6	C5-N7	-2.16	1.35	1.39
54	1w	8	4SU	C2-N1	2.15	1.41	1.38
1	1A	2515	2MA	C4-N9	-2.14	1.33	1.37
32	1a	1407	5MC	C6-N1	-2.14	1.34	1.38
55	1x	8	4SU	O2-C2	2.13	1.26	1.23
56	2y	54	5MU	C2-N3	-2.13	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1915	5MU	C6-N1	-2.12	1.34	1.38
57	2a	1518	MA6	C5-N7	-2.07	1.35	1.39
32	1a	516	PSU	C2-N3	-2.07	1.34	1.37
55	1x	54	5MU	C2-N3	-2.07	1.34	1.38
55	1x	54	5MU	C6-N1	-2.06	1.34	1.38
54	1w	54	5MU	C6-N1	-2.06	1.34	1.38
57	2a	1207	2MG	C5-N7	-2.06	1.34	1.39
32	1a	966	M2G	C4-N9	-2.06	1.32	1.38
56	1y	8	4SU	C6-C5	2.06	1.39	1.35
54	1w	8	4SU	C2-N3	-2.05	1.34	1.38
57	2a	967	5MC	C6-N1	-2.05	1.34	1.38
54	1w	54	5MU	C2-N1	2.05	1.41	1.38
1	2A	1915	5MU	C2-N3	-2.04	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.03	1.34	1.38
54	2w	54	5MU	C2-N3	-2.03	1.34	1.38
55	2x	54	5MU	C6-N1	-2.03	1.34	1.38
32	1a	1207	2MG	C5-N7	-2.02	1.35	1.39
54	2w	54	5MU	C2-N1	2.01	1.41	1.38

All (433) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	37	MIA	C12-C13-C14	-9.00	110.85	127.01
57	2a	527	G7M	CN7-N7-C8	-8.27	112.27	124.79
54	1w	37	MIA	C5-C4-N3	-8.12	118.62	127.18
54	2w	46	G7M	CN7-N7-C8	-8.11	112.50	124.79
54	2w	37	MIA	C5-C4-N3	-8.11	118.64	127.18
56	1y	46	G7M	CN7-N7-C8	-7.96	112.73	124.79
56	2y	46	G7M	CN7-N7-C8	-7.85	112.91	124.79
32	1a	527	G7M	CN7-N7-C8	-7.82	112.95	124.79
1	2A	2503	2MA	C5-C4-N3	-7.80	118.97	127.18
54	2w	8	4SU	C4-N3-C2	-7.73	119.90	127.31
1	1A	2515	2MA	C5-C4-N3	-7.52	119.25	127.18
54	1w	46	G7M	CN7-N7-C8	-7.17	113.93	124.79
57	2a	1498	UR3	C4-N3-C2	-7.14	118.83	124.58
56	2y	46	G7M	N9-C4-N3	7.12	140.19	125.95
54	2w	46	G7M	N9-C8-N7	-7.11	95.23	112.48
43	2l	92	0TD	CSB-SB-CB	-7.10	89.59	102.36
32	1a	1207	2MG	C2-N3-C4	7.04	120.80	112.00
57	2a	527	G7M	N9-C8-N7	-6.92	95.68	112.48
54	1w	46	G7M	N9-C8-N7	-6.87	95.81	112.48
57	2a	1207	2MG	C2-N3-C4	6.82	120.53	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1498	UR3	C4-N3-C2	-6.76	119.14	124.58
56	1y	46	G7M	N9-C8-N7	-6.73	96.14	112.48
57	2a	527	G7M	C8-N7-C5	6.71	116.17	107.78
32	1a	527	G7M	N9-C8-N7	-6.67	96.29	112.48
56	1y	46	G7M	N9-C4-N3	6.65	139.25	125.95
56	1y	55	PSU	N1-C2-N3	6.60	122.13	115.17
54	2w	46	G7M	C8-N7-C5	6.55	115.97	107.78
56	2y	46	G7M	N9-C8-N7	-6.53	96.63	112.48
56	1y	46	G7M	C8-N7-C5	6.44	115.83	107.78
1	2A	1917	PSU	N1-C2-N3	6.43	121.95	115.17
32	1a	527	G7M	C8-N7-C5	6.42	115.81	107.78
1	2A	2251	OMG	C5-C4-N3	-6.41	118.18	128.39
57	2a	966	M2G	C5-C4-N3	-6.40	118.20	128.39
54	1w	46	G7M	N9-C4-N3	6.39	138.73	125.95
1	1A	1933	PSU	N1-C2-N3	6.34	121.86	115.17
55	2x	55	PSU	N1-C2-N3	6.34	121.85	115.17
56	2y	55	PSU	N1-C2-N3	6.32	121.83	115.17
54	2w	55	PSU	N1-C2-N3	6.27	121.79	115.17
54	2w	37	MIA	N3-C4-N9	6.27	134.94	126.99
57	2a	516	PSU	N1-C2-N3	6.23	121.74	115.17
56	1y	32	PSU	N1-C2-N3	6.22	121.73	115.17
1	1A	2263	OMG	C5-C4-N3	-6.22	118.49	128.39
56	2y	46	G7M	C8-N7-C5	6.22	115.55	107.78
56	1y	39	PSU	N1-C2-N3	6.21	121.72	115.17
1	2A	2503	2MA	N3-C4-N9	6.21	134.87	126.99
1	2A	2605	PSU	N1-C2-N3	6.19	121.70	115.17
1	2A	1911	PSU	N1-C2-N3	6.19	121.70	115.17
1	1A	2617	PSU	N1-C2-N3	6.18	121.69	115.17
55	1x	55	PSU	N1-C2-N3	6.12	121.62	115.17
54	2w	8	4SU	C5-C4-N3	6.09	120.41	114.75
57	2a	527	G7M	N9-C4-N3	6.08	138.12	125.95
56	2y	8	4SU	C4-N3-C2	-6.08	121.48	127.31
1	1A	1939	PSU	N1-C2-N3	6.07	121.57	115.17
54	2w	32	PSU	N1-C2-N3	6.04	121.54	115.17
56	2y	39	PSU	N1-C2-N3	6.02	121.52	115.17
32	1a	527	G7M	N9-C4-N3	5.97	137.88	125.95
1	1A	2564	2MU	N3-C2-N1	5.95	122.63	114.89
32	1a	1519	MA6	C5-C4-N3	-5.94	118.54	126.72
1	2A	1939	5MU	C4-N3-C2	-5.92	119.58	127.34
54	1w	55	PSU	N1-C2-N3	5.91	121.40	115.17
54	1w	46	G7M	C8-N7-C5	5.91	115.17	107.78
32	1a	516	PSU	N1-C2-N3	5.90	121.39	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	32	PSU	N1-C2-N3	5.90	121.39	115.17
56	2y	32	PSU	N1-C2-N3	5.86	121.35	115.17
56	1y	8	4SU	C4-N3-C2	-5.85	121.70	127.31
32	1a	1207	2MG	C5-C4-N3	-5.84	119.09	128.39
54	1w	39	PSU	N1-C2-N3	5.83	121.31	115.17
57	2a	1519	MA6	C5-C4-N3	-5.82	118.71	126.72
56	2y	46	G7M	C5-C4-N3	-5.78	117.23	128.15
57	2a	1207	2MG	C5-C4-N3	-5.77	119.21	128.39
54	1w	37	MIA	N3-C4-N9	5.76	134.31	126.99
1	1A	1961	5MU	C4-N3-C2	-5.76	119.79	127.34
32	1a	966	M2G	C5-C4-N3	-5.65	119.39	128.39
1	1A	2515	2MA	N3-C4-N9	5.64	134.14	126.99
1	1A	1961	5MU	C5-C4-N3	5.63	120.21	115.32
56	2y	8	4SU	C5-C4-N3	5.61	119.97	114.75
55	2x	54	5MU	N3-C2-N1	5.53	122.09	114.89
1	2A	2552	2MU	N3-C2-N1	5.53	122.09	114.89
1	1A	1937	5MU	C4-N3-C2	-5.53	120.09	127.34
57	2a	1518	MA6	C5-C4-N3	-5.49	119.15	126.72
54	2w	39	PSU	N1-C2-N3	5.46	120.93	115.17
54	2w	46	G7M	N9-C4-N3	5.44	136.83	125.95
54	1w	8	4SU	C4-N3-C2	-5.42	122.11	127.31
56	1y	46	G7M	C5-C4-N3	-5.39	117.96	128.15
1	2A	1915	5MU	C4-N3-C2	-5.37	120.29	127.34
1	2A	1939	5MU	C5-C4-N3	5.34	119.97	115.32
55	2x	54	5MU	C4-N3-C2	-5.33	120.36	127.34
1	2A	2552	2MU	C4-N3-C2	-5.28	120.06	126.61
57	2a	527	G7M	C5-C4-N3	-5.27	118.18	128.15
1	1A	1937	5MU	C5-C4-N3	5.26	119.90	115.32
32	1a	527	G7M	C5-C4-N3	-5.26	118.22	128.15
1	2A	1915	5MU	N3-C2-N1	5.20	121.66	114.89
1	2A	1939	5MU	N3-C2-N1	5.18	121.63	114.89
1	1A	2263	OMG	C2-N3-C4	5.11	121.10	112.30
54	1w	54	5MU	C4-N3-C2	-5.10	120.65	127.34
1	1A	1937	5MU	O4-C4-C5	-5.10	119.08	124.92
1	2A	2251	OMG	N9-C4-N3	5.08	136.10	125.95
32	1a	1518	MA6	C5-C4-N3	-5.02	119.80	126.72
1	2A	1939	5MU	C5-C6-N1	-5.01	117.87	123.31
1	1A	1937	5MU	N3-C2-N1	5.01	121.41	114.89
54	1w	8	4SU	C5-C4-N3	4.97	119.38	114.75
57	2a	966	M2G	N9-C4-N3	4.94	135.84	125.95
1	1A	1961	5MU	N3-C2-N1	4.93	121.31	114.89
54	1w	54	5MU	N3-C2-N1	4.87	121.23	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2251	OMG	C2-N3-C4	4.86	120.68	112.30
1	2A	1915	5MU	C5-C4-N3	4.82	119.52	115.32
55	1x	54	5MU	N3-C2-N1	4.82	121.16	114.89
55	1x	54	5MU	C4-N3-C2	-4.80	121.05	127.34
54	1w	46	G7M	C5-C4-N3	-4.76	119.15	128.15
1	1A	2564	2MU	C4-N3-C2	-4.76	120.70	126.61
54	1w	46	G7M	C8-N9-C4	4.73	118.81	107.09
54	2w	46	G7M	C8-N9-C4	4.71	118.76	107.09
57	2a	1518	MA6	C9-N6-C6	-4.71	108.55	120.52
1	1A	2263	OMG	N9-C4-N3	4.70	135.35	125.95
56	2y	46	G7M	C1'-N9-C8	-4.68	110.92	126.74
56	1y	54	5MU	N3-C2-N1	4.67	120.97	114.89
1	1A	1961	5MU	C5-C6-N1	-4.67	118.24	123.31
56	2y	46	G7M	C2-N3-C4	4.67	120.34	112.30
56	1y	8	4SU	C5-C4-N3	4.66	119.08	114.75
32	1a	1519	MA6	N3-C4-N9	4.60	134.99	127.17
56	1y	46	G7M	C1'-N9-C8	-4.56	111.33	126.74
57	2a	1519	MA6	C9-N6-C6	-4.56	108.92	120.52
54	2w	46	G7M	C5-C4-N3	-4.52	119.62	128.15
57	2a	1518	MA6	C2-N1-C6	4.52	122.86	111.83
1	2A	2605	PSU	C4-N3-C2	-4.51	120.15	126.37
54	1w	46	G7M	C1'-N9-C8	-4.48	111.60	126.74
57	2a	966	M2G	C2-N3-C4	4.48	120.80	112.51
56	2y	54	5MU	C5-C4-N3	4.46	119.20	115.32
32	1a	966	M2G	C2-N3-C4	4.45	120.73	112.51
54	2w	8	4SU	C5-C4-S4	-4.44	119.23	124.31
1	1A	2617	PSU	O2-C2-N1	-4.43	118.22	122.79
1	2A	1939	5MU	O4-C4-C5	-4.43	119.85	124.92
56	1y	46	G7M	C2-N3-C4	4.42	119.91	112.30
32	1a	1518	MA6	C2-N1-C6	4.41	122.61	111.83
32	1a	1519	MA6	C9-N6-C6	-4.41	109.29	120.52
54	2w	37	MIA	C12-N6-C6	-4.41	118.76	122.85
54	2w	8	4SU	N3-C2-N1	4.41	120.63	114.89
56	1y	46	G7M	C8-N9-C4	4.40	117.98	107.09
54	1w	54	5MU	C5-C4-N3	4.40	119.14	115.32
57	2a	527	G7M	C8-N9-C4	4.38	117.95	107.09
57	2a	527	G7M	C2-N3-C4	4.38	119.85	112.30
57	2a	1519	MA6	N3-C4-N9	4.36	134.59	127.17
1	1A	2564	2MU	O2-C2-N1	-4.34	117.14	122.80
1	1A	1939	PSU	O2-C2-N1	-4.34	118.31	122.79
56	2y	54	5MU	C4-N3-C2	-4.31	121.69	127.34
57	2a	1518	MA6	C4-C5-N7	-4.29	105.67	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	A	17	BB9	O-C-CA	-4.29	120.01	125.39
57	2a	1519	MA6	C4-C5-N7	-4.25	105.72	110.58
55	2x	54	5MU	C5-C4-N3	4.25	119.02	115.32
56	2y	46	G7M	C8-N9-C4	4.24	117.60	107.09
56	1y	54	5MU	C4-N3-C2	-4.23	121.79	127.34
57	2a	516	PSU	C4-N3-C2	-4.23	120.55	126.37
55	1x	55	PSU	C4-N3-C2	-4.21	120.56	126.37
1	1A	1961	5MU	O4-C4-C5	-4.21	120.10	124.92
32	1a	966	M2G	N9-C4-N3	4.20	134.35	125.95
54	2w	54	5MU	N3-C2-N1	4.19	120.35	114.89
55	1x	54	5MU	C5-C4-N3	4.18	118.96	115.32
56	1y	39	PSU	C4-N3-C2	-4.16	120.64	126.37
56	1y	8	4SU	N3-C2-N1	4.16	120.31	114.89
55	2x	54	5MU	O4-C4-C5	-4.14	120.18	124.92
32	1a	516	PSU	C4-N3-C2	-4.14	120.67	126.37
55	2x	55	PSU	C4-N3-C2	-4.14	120.67	126.37
58	B	17	BB9	O-C-CA	-4.14	120.20	125.39
54	2w	55	PSU	C4-N3-C2	-4.13	120.68	126.37
1	2A	1915	5MU	O4-C4-C5	-4.13	120.19	124.92
1	1A	2617	PSU	C4-N3-C2	-4.13	120.68	126.37
56	2y	39	PSU	C4-N3-C2	-4.12	120.70	126.37
32	1a	527	G7M	C8-N9-C4	4.11	117.28	107.09
56	2y	54	5MU	N3-C2-N1	4.10	120.22	114.89
54	1w	54	5MU	O4-C4-C5	-4.10	120.23	124.92
57	2a	1519	MA6	C2-N1-C6	4.08	121.81	111.83
32	1a	1518	MA6	C4-C5-N7	-4.07	105.92	110.58
43	1l	92	0TD	CSB-SB-CB	-4.07	95.05	102.36
1	1A	1939	PSU	C4-N3-C2	-4.06	120.77	126.37
54	2w	46	G7M	C2-N3-C4	4.06	119.29	112.30
54	2w	32	PSU	C4-N3-C2	-4.05	120.79	126.37
32	1a	1518	MA6	C9-N6-C6	-4.05	110.23	120.52
56	1y	55	PSU	O2-C2-N1	-4.04	118.62	122.79
56	2y	55	PSU	C4-N3-C2	-4.03	120.82	126.37
32	1a	527	G7M	C2-N3-C4	4.02	119.23	112.30
55	1x	8	4SU	C6-C5-C4	-4.01	116.48	119.95
57	2a	1518	MA6	N3-C4-N9	4.00	133.98	127.17
54	1w	37	MIA	C15-C14-C13	-4.00	110.66	122.66
1	1A	1933	PSU	C4-N3-C2	-4.00	120.87	126.37
1	1A	1933	PSU	O2-C2-N1	-4.00	118.67	122.79
1	2A	1917	PSU	O2-C2-N1	-3.96	118.71	122.79
1	2A	1911	PSU	C4-N3-C2	-3.96	120.92	126.37
56	2y	8	4SU	C5-C4-S4	-3.94	119.81	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2a	1400	5MC	C5-C6-N1	-3.88	119.09	123.31
32	1a	1519	MA6	C4-C5-N7	-3.87	106.16	110.58
32	1a	1207	2MG	C6-C5-N7	3.85	137.30	130.29
57	2a	527	G7M	CN7-N7-C5	3.82	131.56	126.80
1	2A	1917	PSU	C4-N3-C2	-3.82	121.11	126.37
32	1a	1519	MA6	C2-N1-C6	3.82	121.16	111.83
54	2w	54	5MU	C4-N3-C2	-3.81	122.34	127.34
56	2y	46	G7M	CN7-N7-C5	3.80	131.54	126.80
54	2w	46	G7M	CN7-N7-C5	3.80	131.53	126.80
54	1w	32	PSU	C4-N3-C2	-3.78	121.17	126.37
56	1y	32	PSU	C4-N3-C2	-3.77	121.18	126.37
54	1w	46	G7M	C2-N3-C4	3.76	118.77	112.30
54	1w	39	PSU	C4-N3-C2	-3.75	121.21	126.37
55	1x	32	5MC	C5-C6-N1	-3.74	119.25	123.31
54	1w	55	PSU	O2-C2-N1	-3.74	118.93	122.79
57	2a	516	PSU	O2-C2-N1	-3.73	118.94	122.79
56	2y	54	5MU	O4-C4-C5	-3.73	120.65	124.92
57	2a	1207	2MG	N9-C4-N3	3.72	133.40	125.95
56	1y	46	G7M	CN7-N7-C5	3.72	131.44	126.80
55	1x	8	4SU	O2-C2-N1	3.72	127.64	122.80
56	2y	55	PSU	O2-C2-N1	-3.71	118.96	122.79
32	1a	1207	2MG	N9-C4-N3	3.71	133.38	125.95
56	1y	55	PSU	C4-N3-C2	-3.71	121.27	126.37
57	2a	1519	MA6	C2-N3-C4	3.71	120.88	111.83
32	1a	1519	MA6	C2-N3-C4	3.70	120.87	111.83
54	1w	32	PSU	O2-C2-N1	-3.69	118.98	122.79
56	2y	8	4SU	N3-C2-N1	3.69	119.69	114.89
55	1x	55	PSU	O2-C2-N1	-3.69	118.98	122.79
1	2A	1962	5MC	C5-C6-N1	-3.67	119.33	123.31
57	2a	1518	MA6	C2-N3-C4	3.66	120.78	111.83
56	2y	39	PSU	O2-C2-N1	-3.66	119.02	122.79
57	2a	1207	2MG	C6-C5-N7	3.66	136.95	130.29
56	1y	54	5MU	C5-C4-N3	3.62	118.47	115.32
1	1A	1961	5MU	O2-C2-N1	-3.60	118.11	122.80
54	1w	8	4SU	N3-C2-N1	3.60	119.58	114.89
32	1a	1207	2MG	N1-C2-N2	3.59	120.23	116.56
56	2y	32	PSU	C4-N3-C2	-3.59	121.43	126.37
32	1a	527	G7M	CN7-N7-C5	3.57	131.24	126.80
54	1w	37	MIA	C2-N3-C4	3.56	121.62	112.29
54	2w	37	MIA	C4-C5-N7	-3.56	106.52	110.58
55	2x	54	5MU	C5-C6-N1	-3.54	119.47	123.31
32	1a	1518	MA6	N3-C4-N9	3.54	133.18	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	54	5MU	C5-C6-N1	-3.53	119.48	123.31
1	1A	2515	2MA	C4-C5-N7	-3.52	106.56	110.58
54	1w	37	MIA	C4-C5-N7	-3.51	106.57	110.58
55	2x	32	5MC	C5-C6-N1	-3.50	119.51	123.31
54	1w	37	MIA	C16-C14-C13	-3.48	112.21	122.66
55	1x	54	5MU	O4-C4-C5	-3.48	120.94	124.92
54	1w	55	PSU	C4-N3-C2	-3.46	121.60	126.37
56	2y	32	PSU	O2-C2-N1	-3.46	119.22	122.79
55	2x	8	4SU	C5-C4-N3	3.45	117.96	114.75
32	1a	1518	MA6	C2-N3-C4	3.45	120.26	111.83
1	2A	1915	5MU	C5-C6-N1	-3.45	119.57	123.31
1	1A	1964	5MC	C5-C6-N1	-3.44	119.58	123.31
54	2w	54	5MU	O4-C4-C5	-3.44	120.98	124.92
57	2a	527	G7M	C1'-N9-C8	-3.43	115.14	126.74
57	2a	1518	MA6	N1-C2-N3	-3.43	123.39	128.58
54	2w	54	5MU	C5-C4-N3	3.42	118.30	115.32
1	2A	1939	5MU	O2-C2-N1	-3.42	118.34	122.80
1	1A	1984	5MC	C5-C6-N1	-3.42	119.60	123.31
54	1w	39	PSU	O2-C2-N1	-3.42	119.27	122.79
57	2a	1407	5MC	C5-C4-N3	-3.40	118.27	121.75
55	1x	8	4SU	C5-C4-N3	3.40	117.91	114.75
54	1w	54	5MU	C5-C6-N1	-3.40	119.62	123.31
57	2a	967	5MC	C5-C6-N1	-3.39	119.63	123.31
54	2w	39	PSU	C4-N3-C2	-3.38	121.71	126.37
56	1y	54	5MU	C5-C6-N1	-3.37	119.65	123.31
1	2A	2503	2MA	C4-C5-N7	-3.37	106.73	110.58
32	1a	527	G7M	C1'-N9-C8	-3.37	115.36	126.74
57	2a	1407	5MC	C5-C6-N1	-3.37	119.65	123.31
57	2a	1404	5MC	C5-C6-N1	-3.35	119.67	123.31
56	1y	32	PSU	O2-C2-N1	-3.33	119.36	122.79
54	2w	37	MIA	C2-N3-C4	3.32	120.99	112.29
1	2A	2552	2MU	O2-C2-N1	-3.31	118.48	122.80
57	2a	1498	UR3	C5-C4-N3	3.31	119.40	115.04
54	1w	37	MIA	C6-C5-N7	3.30	136.02	132.43
54	1w	46	G7M	CN7-N7-C5	3.29	130.90	126.80
54	2w	32	PSU	O2-C2-N1	-3.29	119.40	122.79
54	2w	55	PSU	O2-C2-N1	-3.27	119.41	122.79
32	1a	966	M2G	C6-C5-N7	3.27	136.24	130.29
32	1a	1207	2MG	C4-C5-N7	-3.27	105.49	110.67
32	1a	1407	5MC	C5-C6-N1	-3.27	119.77	123.31
32	1a	1498	UR3	C5-C4-N3	3.26	119.34	115.04
54	2w	46	G7M	C1'-N9-C8	-3.25	115.75	126.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2503	2MA	C4-N9-C8	3.25	109.15	105.74
54	1w	8	4SU	C5-C4-S4	-3.25	120.60	124.31
32	1a	1518	MA6	N1-C2-N3	-3.24	123.67	128.58
1	2A	1942	5MC	C5-C4-N3	-3.21	118.46	121.75
43	1l	92	0TD	OD2-CG-CB	3.20	120.06	113.15
54	2w	37	MIA	C6-C5-N7	3.20	135.92	132.43
56	1y	54	5MU	O4-C4-C5	-3.19	121.26	124.92
32	1a	967	5MC	C5-C6-N1	-3.18	119.86	123.31
1	1A	1937	5MU	C5-C6-N1	-3.14	119.91	123.31
56	1y	8	4SU	C5-C4-S4	-3.11	120.75	124.31
32	1a	1400	5MC	C5-C6-N1	-3.10	119.94	123.31
1	1A	2263	OMG	C6-C5-N7	3.10	135.93	130.29
1	2A	2552	2MU	C5-C4-N3	3.09	119.13	114.80
43	2l	92	0TD	OD2-CG-CB	3.08	119.80	113.15
32	1a	1519	MA6	N1-C2-N3	-3.06	123.95	128.58
57	2a	1519	MA6	N1-C2-N3	-3.05	123.96	128.58
1	2A	2503	2MA	N6-C6-N1	3.05	121.14	117.03
55	1x	32	5MC	C5-C4-N3	-3.05	118.63	121.75
56	2y	54	5MU	C5-C6-N1	-3.04	120.01	123.31
32	1a	1404	5MC	C5-C4-N3	-3.04	118.64	121.75
54	1w	54	5MU	O2-C2-N1	-3.04	118.84	122.80
1	2A	1911	PSU	O2-C2-N1	-3.04	119.66	122.79
32	1a	1207	2MG	N2-C2-N3	-3.03	116.65	120.51
57	2a	1519	MA6	C5-N7-C8	3.03	108.22	103.45
55	2x	55	PSU	O2-C2-N1	-3.00	119.70	122.79
1	2A	2605	PSU	O2-C2-N1	-2.99	119.70	122.79
55	2x	54	5MU	O2-C2-N1	-2.98	118.92	122.80
56	1y	39	PSU	O2-C2-N1	-2.97	119.72	122.79
55	2x	8	4SU	C1'-N1-C2	2.97	122.92	117.59
1	1A	2515	2MA	C2-N1-C6	2.96	122.66	118.10
57	2a	1207	2MG	C4-C5-N7	-2.94	106.01	110.67
58	B	9	BB9	O-C-CA	-2.89	121.76	125.39
32	1a	1519	MA6	C5-N7-C8	2.88	107.98	103.45
1	1A	2564	2MU	C2'-C1'-N1	-2.86	108.81	114.24
32	1a	1400	5MC	C5-C4-N3	-2.86	118.83	121.75
55	1x	8	4SU	C1'-N1-C2	2.85	122.72	117.59
56	2y	54	5MU	C1'-N1-C2	2.84	122.70	117.59
32	1a	516	PSU	O2-C2-N1	-2.84	119.86	122.79
1	1A	2515	2MA	C4-N9-C8	2.84	108.72	105.74
1	2A	2251	OMG	C6-C5-N7	2.83	135.45	130.29
57	2a	1518	MA6	C5-N7-C8	2.83	107.90	103.45
32	1a	1404	5MC	C5-C6-N1	-2.81	120.26	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1518	MA6	C10-N6-C6	-2.81	113.37	120.52
57	2a	966	M2G	C6-C5-N7	2.80	135.38	130.29
56	2y	54	5MU	C1'-N1-C6	-2.79	116.55	121.15
57	2a	1404	5MC	C5-C4-N3	-2.79	118.89	121.75
54	2w	46	G7M	O6-C6-C5	-2.77	121.82	128.01
32	1a	1519	MA6	N1-C6-N6	2.76	120.22	116.86
54	2w	54	5MU	C5-C6-N1	-2.76	120.32	123.31
32	1a	1519	MA6	C4-N9-C8	2.75	108.62	105.74
58	B	6	BB9	O-C-CA	-2.75	121.95	125.39
32	1a	1407	5MC	C5-C4-N3	-2.74	118.95	121.75
32	1a	1518	MA6	C5-N7-C8	2.74	107.75	103.45
1	1A	1964	5MC	C5-C4-N3	-2.73	118.96	121.75
1	2A	2552	2MU	C2'-C1'-N1	-2.73	109.07	114.24
32	1a	1498	UR3	C3U-N3-C4	2.71	121.62	117.87
57	2a	1519	MA6	C4-N9-C8	2.69	108.56	105.74
1	1A	2515	2MA	N6-C6-N1	2.64	120.59	117.03
55	2x	32	5MC	O2-C2-N3	-2.64	118.17	122.33
54	1w	55	PSU	C6-C5-C4	-2.61	116.42	118.17
1	2A	1962	5MC	C5-C4-N3	-2.60	119.09	121.75
57	2a	1207	2MG	N1-C2-N2	2.60	119.21	116.56
55	2x	8	4SU	O2-C2-N1	2.59	126.17	122.80
1	2A	1942	5MC	C5-C6-N1	-2.59	120.50	123.31
58	A	9	BB9	O-C-CA	-2.56	122.18	125.39
54	2w	8	4SU	C1'-N1-C2	2.56	122.19	117.59
54	1w	37	MIA	N3-C2-N1	-2.56	122.33	127.00
32	1a	1402	4OC	C6-C5-C4	2.56	120.08	117.00
57	2a	967	5MC	C5-C4-N3	-2.55	119.14	121.75
58	A	6	BB9	O-C-CA	-2.55	122.19	125.39
1	1A	1937	5MU	O2-C2-N1	-2.55	119.48	122.80
1	2A	2605	PSU	C5-C6-N1	-2.55	118.61	122.14
1	1A	2263	OMG	C4-C5-N7	-2.54	106.64	110.67
54	2w	37	MIA	C5-N7-C8	2.53	107.43	103.45
56	2y	54	5MU	O2-C2-N3	-2.53	116.82	121.49
55	2x	8	4SU	C6-C5-C4	-2.53	117.76	119.95
1	1A	2564	2MU	C5-C4-N3	2.52	118.33	114.80
32	1a	966	M2G	C4-C5-N7	-2.52	106.67	110.67
1	1A	2515	2MA	C6-C5-N7	2.52	136.95	132.09
1	2A	2552	2MU	O4-C4-C5	-2.51	120.83	125.16
54	1w	37	MIA	C2-N1-C6	2.51	122.31	117.54
1	2A	2503	2MA	C5-N7-C8	2.51	107.40	103.45
57	2a	1518	MA6	C10-N6-C9	-2.50	108.14	116.18
55	2x	32	5MC	C5-C4-N3	-2.50	119.19	121.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1518	MA6	C6-C5-N7	2.47	137.38	133.43
1	1A	2515	2MA	C5-N7-C8	2.47	107.33	103.45
54	2w	39	PSU	O2-C2-N1	-2.45	120.26	122.79
32	1a	967	5MC	C5-C4-N3	-2.45	119.24	121.75
55	1x	8	4SU	O2-C2-N3	-2.45	116.98	121.49
1	2A	2251	OMG	C4-C5-N7	-2.44	106.81	110.67
55	1x	8	4SU	S4-C4-N3	-2.44	117.66	120.20
57	2a	1404	5MC	O2-C2-N3	-2.44	118.49	122.33
1	1A	1942	4OC	O2-C2-N3	-2.43	118.50	122.33
57	2a	1402	4OC	C6-C5-C4	2.43	119.92	117.00
57	2a	1207	2MG	N2-C2-N3	-2.42	117.42	120.51
32	1a	1519	MA6	C10-N6-C6	-2.42	114.36	120.52
32	1a	1518	MA6	C4-N9-C8	2.42	108.28	105.74
55	2x	8	4SU	O2-C2-N3	-2.42	117.03	121.49
57	2a	966	M2G	C4-C5-N7	-2.42	106.84	110.67
55	1x	54	5MU	O2-C2-N1	-2.41	119.66	122.80
57	2a	1518	MA6	C4-N9-C8	2.41	108.27	105.74
1	2A	2503	2MA	N9-C8-N7	-2.39	110.55	113.94
1	2A	2503	2MA	C2-N1-C6	2.38	121.75	118.10
1	1A	1984	5MC	C5-C4-N3	-2.37	119.33	121.75
54	2w	37	MIA	C4-N9-C8	2.36	108.22	105.74
57	2a	1518	MA6	C6-C5-N7	2.36	137.19	133.43
57	2a	1400	5MC	C5-C4-N3	-2.35	119.35	121.75
57	2a	1519	MA6	C6-C5-N7	2.34	137.17	133.43
32	1a	966	M2G	O6-C6-C5	-2.34	120.35	126.53
54	2w	37	MIA	C2-N1-C6	2.34	121.98	117.54
55	2x	55	PSU	C5-C6-N1	-2.33	118.91	122.14
32	1a	1404	5MC	CM5-C5-C6	-2.32	119.71	122.85
57	2a	966	M2G	O6-C6-C5	-2.29	120.49	126.53
1	1A	2564	2MU	O4-C4-C5	-2.29	121.22	125.16
32	1a	1519	MA6	C5-C6-N6	-2.28	121.72	125.33
43	2l	92	0TD	OD1-CG-CB	-2.28	117.67	122.44
56	1y	46	G7M	O6-C6-C5	-2.28	122.93	128.01
1	2A	2251	OMG	O6-C6-C5	-2.27	120.53	126.53
57	2a	1400	5MC	O2-C2-N3	-2.27	118.75	122.33
57	2a	1498	UR3	C3U-N3-C4	2.27	121.01	117.87
54	1w	37	MIA	C5-N7-C8	2.26	107.01	103.45
55	2x	8	4SU	S4-C4-N3	-2.26	117.84	120.20
54	1w	46	G7M	O6-C6-C5	-2.26	122.97	128.01
32	1a	1519	MA6	N9-C8-N7	-2.25	110.75	113.94
57	2a	1519	MA6	C10-N6-C6	-2.25	114.81	120.52
54	1w	54	5MU	C5M-C5-C4	2.24	121.17	118.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2263	OMG	O6-C6-C5	-2.24	120.63	126.53
54	2w	32	PSU	C5-C6-N1	-2.24	119.04	122.14
32	1a	527	G7M	O6-C6-C5	-2.23	123.03	128.01
32	1a	1400	5MC	O2-C2-N3	-2.23	118.82	122.33
1	1A	2515	2MA	N9-C8-N7	-2.22	110.78	113.94
57	2a	1519	MA6	N9-C8-N7	-2.22	110.78	113.94
32	1a	1404	5MC	O2-C2-N3	-2.21	118.84	122.33
54	2w	54	5MU	O2-C2-N1	-2.20	119.94	122.80
54	2w	37	MIA	N3-C2-N1	-2.19	123.01	127.00
32	1a	516	PSU	C5-C6-N1	-2.18	119.12	122.14
32	1a	1207	2MG	C8-N7-C5	2.18	108.14	104.26
32	1a	1498	UR3	C1'-N1-C2	2.17	120.60	117.04
56	2y	46	G7M	O6-C6-C5	-2.17	123.16	128.01
1	2A	2503	2MA	C6-C5-N7	2.15	136.24	132.09
57	2a	1518	MA6	C10-N6-C6	-2.15	115.06	120.52
56	1y	39	PSU	C5-C6-N1	-2.15	119.16	122.14
56	2y	32	PSU	C6-C5-C4	-2.14	116.73	118.17
56	2y	54	5MU	C5M-C5-C4	2.14	121.06	118.78
57	2a	527	G7M	O6-C6-C5	-2.13	123.26	128.01
55	1x	55	PSU	C5-C6-N1	-2.12	119.20	122.14
57	2a	516	PSU	O4'-C1'-C2'	2.11	108.07	105.15
1	2A	1911	PSU	O4'-C1'-C2'	2.10	108.06	105.15
1	2A	1920	4OC	O2-C2-N3	-2.10	119.03	122.33
32	1a	516	PSU	O4'-C1'-C2'	2.09	108.05	105.15
1	2A	1962	5MC	CM5-C5-C6	-2.08	120.04	122.85
57	2a	1407	5MC	O2-C2-N3	-2.07	119.06	122.33
57	2a	1402	4OC	O2-C2-N3	-2.07	119.06	122.33
32	1a	1519	MA6	C2'-C1'-N9	-2.07	108.17	113.30
56	1y	8	4SU	C1'-N1-C2	2.06	121.29	117.59
32	1a	1518	MA6	N9-C8-N7	-2.05	111.03	113.94
1	1A	2617	PSU	C5-C6-N1	-2.04	119.31	122.14
32	1a	1207	2MG	CM2-N2-C2	-2.03	119.28	123.65
54	2w	46	G7M	C6-C5-N7	2.02	134.71	132.17
55	1x	54	5MU	C5M-C5-C4	2.01	120.93	118.78
1	2A	2605	PSU	O4-C4-C5	-2.01	119.02	124.01

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB

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Mol	Chain	Res	Type	Atoms
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16
56	1y	8	4SU	O4'-C4'-C5'-O5'
56	1y	46	G7M	C4'-C5'-O5'-P
56	1y	54	5MU	O4'-C4'-C5'-O5'
56	2y	54	5MU	C3'-C4'-C5'-O5'
56	2y	54	5MU	O4'-C4'-C5'-O5'
57	2a	1207	2MG	N1-C2-N2-CM2
57	2a	1207	2MG	N3-C2-N2-CM2
57	2a	1518	MA6	C5-C6-N6-C9
57	2a	1519	MA6	O4'-C4'-C5'-O5'
56	2y	8	4SU	C3'-C4'-C5'-O5'
56	2y	8	4SU	O4'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
54	2w	46	G7M	O4'-C4'-C5'-O5'
54	2w	46	G7M	C3'-C4'-C5'-O5'
56	1y	8	4SU	C3'-C4'-C5'-O5'
57	2a	1402	4OC	O4'-C4'-C5'-O5'
57	2a	1518	MA6	N1-C6-N6-C9
32	1a	1402	4OC	O4'-C4'-C5'-O5'
56	1y	54	5MU	C3'-C4'-C5'-O5'
57	2a	1519	MA6	C3'-C4'-C5'-O5'
57	2a	1519	MA6	C5-C6-N6-C9
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
57	2a	527	G7M	C3'-C4'-C5'-O5'
54	1w	46	G7M	C4'-C5'-O5'-P
56	2y	46	G7M	C4'-C5'-O5'-P
57	2a	1402	4OC	C3'-C4'-C5'-O5'
54	1w	46	G7M	C3'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C10
32	1a	1519	MA6	C5-C6-N6-C10
43	2l	92	0TD	CG-CB-SB-CSB
57	2a	1400	5MC	C2'-C1'-N1-C6
1	2A	1917	PSU	O4'-C4'-C5'-O5'
54	1w	46	G7M	O4'-C4'-C5'-O5'
56	1y	55	PSU	O4'-C1'-C5-C4
57	2a	1519	MA6	C5-C6-N6-C10
57	2a	527	G7M	O4'-C4'-C5'-O5'
54	2w	46	G7M	C4'-C5'-O5'-P
57	2a	1519	MA6	C4'-C5'-O5'-P
57	2a	1400	5MC	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
32	1a	527	G7M	C4'-C5'-O5'-P
57	2a	527	G7M	C4'-C5'-O5'-P
32	1a	1519	MA6	C4'-C5'-O5'-P
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
57	2a	1519	MA6	N1-C6-N6-C9
1	2A	2503	2MA	O4'-C4'-C5'-O5'
54	2w	37	MIA	N1-C6-N6-C12
57	2a	1400	5MC	O4'-C1'-N1-C2
54	2w	37	MIA	C5-C6-N6-C12
1	1A	2515	2MA	C4'-C5'-O5'-P
1	1A	1942	4OC	C2'-C1'-N1-C2
55	2x	8	4SU	C2'-C1'-N1-C2
56	2y	54	5MU	C2'-C1'-N1-C2
57	2a	1400	5MC	C2'-C1'-N1-C2

There are no ring outliers.

29 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2w	46	G7M	1	0
54	1w	39	PSU	1	0
56	1y	39	PSU	1	0
54	2w	37	MIA	1	0
55	2x	8	4SU	1	0
57	2a	1402	4OC	3	0
43	2l	92	0TD	1	0
54	2w	8	4SU	4	0
54	1w	46	G7M	1	0
1	2A	2251	OMG	1	0
56	1y	8	4SU	1	0
57	2a	516	PSU	1	0
57	2a	967	5MC	2	0
1	2A	2503	2MA	1	0
57	2a	1519	MA6	2	0
32	1a	1518	MA6	2	0
57	2a	1400	5MC	1	0
32	1a	1519	MA6	2	0
1	1A	1961	5MU	1	0
1	2A	2552	2MU	1	0
55	1x	8	4SU	2	0
54	1w	37	MIA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2w	39	PSU	1	0
57	2a	1518	MA6	3	0
32	1a	1402	4OC	3	0
55	2x	55	PSU	1	0
56	2y	46	G7M	2	0
57	2a	1207	2MG	2	0
1	1A	1942	4OC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2940 ligands modelled in this entry, 2938 are monoatomic - leaving 2 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	$\# Z > 2$
61	SF4	1d	501	35	0,12,12	-	-	-		
61	SF4	2d	501	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	SF4	1d	501	35	-	-	0/6/5/5
61	SF4	2d	501	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	2d	501	SF4	2	0

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%)	-0.61	121 (4%)	40	37	13, 29, 85, 99	0
1	2A	2789/2915 (95%)	-0.03	124 (4%)	39	35	25, 51, 87, 102	0
2	1B	120/121 (99%)	-0.51	0	100	100	23, 41, 55, 80	0
2	2B	120/121 (99%)	0.91	2 (1%)	69	67	55, 72, 80, 89	0
3	1D	275/276 (99%)	-0.24	3 (1%)	78	76	14, 29, 45, 72	0
3	2D	275/276 (99%)	0.18	6 (2%)	62	59	25, 43, 57, 71	0
4	1E	204/206 (99%)	-0.27	0	100	100	14, 32, 53, 71	0
4	2E	204/206 (99%)	0.37	6 (2%)	53	50	28, 53, 65, 73	0
5	1F	203/210 (96%)	-0.19	2 (0%)	79	78	15, 35, 60, 77	0
5	2F	203/210 (96%)	0.43	4 (1%)	65	62	30, 61, 75, 83	0
6	1G	181/182 (99%)	0.35	6 (3%)	49	45	33, 50, 66, 81	0
6	2G	181/182 (99%)	1.49	39 (21%)	2	2	62, 73, 81, 89	0
7	1H	174/180 (96%)	0.14	3 (1%)	69	67	31, 45, 59, 63	0
7	2H	174/180 (96%)	1.52	39 (22%)	2	2	65, 78, 84, 88	0
8	1I	146/148 (98%)	0.74	3 (2%)	63	61	37, 66, 76, 80	0
8	2I	146/148 (98%)	0.85	8 (5%)	30	27	48, 65, 75, 81	0
9	1N	140/140 (100%)	-0.21	1 (0%)	84	83	18, 31, 53, 63	0
9	2N	140/140 (100%)	0.67	3 (2%)	63	61	40, 57, 71, 79	0
10	1O	122/122 (100%)	-0.23	0	100	100	21, 32, 48, 54	0
10	2O	122/122 (100%)	0.36	1 (0%)	82	81	41, 53, 63, 68	0
11	1P	149/150 (99%)	-0.06	1 (0%)	84	83	14, 37, 63, 72	0
11	2P	149/150 (99%)	0.49	3 (2%)	65	62	29, 61, 75, 82	0
12	1Q	141/141 (100%)	-0.24	1 (0%)	84	83	21, 32, 50, 67	0
12	2Q	141/141 (100%)	0.94	14 (9%)	13	10	40, 61, 72, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.38	0 100 100	18, 27, 41, 48	0
13	2R	118/118 (100%)	0.12	2 (1%) 69 67	34, 45, 55, 65	0
14	1S	110/112 (98%)	0.02	0 100 100	30, 41, 54, 59	0
14	2S	110/112 (98%)	1.28	17 (15%) 5 4	56, 67, 75, 80	0
15	1T	131/146 (89%)	0.01	2 (1%) 72 70	24, 35, 61, 70	0
15	2T	131/146 (89%)	0.48	3 (2%) 61 58	44, 55, 73, 77	0
16	1U	116/118 (98%)	-0.57	0 100 100	15, 23, 37, 54	0
16	2U	116/118 (98%)	0.47	0 100 100	38, 55, 69, 76	0
17	1V	101/101 (100%)	-0.38	0 100 100	15, 32, 47, 57	0
17	2V	101/101 (100%)	0.86	4 (3%) 42 38	35, 64, 70, 75	0
18	1W	112/113 (99%)	-0.41	1 (0%) 81 80	17, 25, 44, 78	0
18	2W	112/113 (99%)	0.21	3 (2%) 56 53	31, 42, 59, 87	0
19	1X	95/96 (98%)	-0.14	2 (2%) 63 61	17, 31, 52, 73	0
19	2X	95/96 (98%)	0.50	4 (4%) 40 37	38, 53, 65, 76	0
20	1Y	107/110 (97%)	0.10	3 (2%) 55 51	28, 42, 62, 77	0
20	2Y	107/110 (97%)	0.99	7 (6%) 25 22	50, 65, 73, 80	0
21	1Z	154/206 (74%)	0.56	10 (6%) 25 22	33, 56, 77, 85	0
21	2Z	160/206 (77%)	1.61	43 (26%) 1 1	63, 76, 86, 89	0
22	10	83/85 (97%)	0.01	4 (4%) 35 32	22, 29, 51, 60	0
22	20	83/85 (97%)	1.11	10 (12%) 9 7	39, 58, 67, 74	0
23	11	97/98 (98%)	0.08	2 (2%) 63 61	20, 36, 62, 70	0
23	21	97/98 (98%)	0.52	2 (2%) 63 61	33, 49, 69, 73	0
24	12	70/72 (97%)	0.08	1 (1%) 73 72	29, 41, 53, 67	0
24	22	70/72 (97%)	0.52	1 (1%) 73 72	52, 63, 71, 76	0
25	13	59/60 (98%)	-0.26	2 (3%) 48 44	17, 28, 50, 75	0
25	23	59/60 (98%)	0.77	5 (8%) 16 14	46, 58, 75, 84	0
26	14	69/71 (97%)	0.84	10 (14%) 6 5	41, 65, 81, 87	0
26	24	69/71 (97%)	1.86	26 (37%) 1 0	71, 79, 87, 89	0
27	15	59/60 (98%)	-0.44	1 (1%) 69 67	15, 24, 44, 53	0
27	25	59/60 (98%)	0.06	0 100 100	31, 46, 56, 72	0
28	16	53/54 (98%)	-0.32	0 100 100	25, 34, 49, 56	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.54	0 100 100	42, 54, 63, 68	0
29	17	48/49 (97%)	-0.36	1 (2%) 63 61	16, 22, 47, 54	0
29	27	48/49 (97%)	0.00	1 (2%) 63 61	27, 34, 57, 66	0
30	18	64/65 (98%)	-0.40	0 100 100	21, 26, 36, 48	0
30	28	64/65 (98%)	0.42	0 100 100	40, 49, 57, 60	0
31	19	37/37 (100%)	-0.29	0 100 100	22, 31, 48, 53	0
31	29	37/37 (100%)	1.19	3 (8%) 18 15	55, 63, 72, 73	0
32	1a	1488/1521 (97%)	0.16	48 (3%) 50 46	28, 57, 86, 101	0
33	1b	231/256 (90%)	1.19	38 (16%) 4 4	57, 72, 82, 90	0
33	2b	231/256 (90%)	1.61	66 (28%) 1 1	67, 80, 86, 91	0
34	1c	206/239 (86%)	0.83	10 (4%) 35 31	51, 64, 75, 82	0
34	2c	206/239 (86%)	1.75	75 (36%) 1 0	67, 78, 83, 88	0
35	1d	208/209 (99%)	0.94	17 (8%) 17 15	49, 61, 73, 81	0
35	2d	208/209 (99%)	1.15	24 (11%) 9 8	56, 66, 74, 81	0
36	1e	148/162 (91%)	0.56	2 (1%) 73 72	44, 55, 68, 72	0
36	2e	148/162 (91%)	1.50	39 (26%) 1 1	60, 72, 79, 84	0
37	1f	100/101 (99%)	0.62	0 100 100	44, 60, 69, 77	0
37	2f	100/101 (99%)	0.56	1 (1%) 79 78	50, 61, 69, 78	0
38	1g	155/156 (99%)	0.53	9 (5%) 29 25	46, 61, 74, 86	0
38	2g	155/156 (99%)	1.08	17 (10%) 10 9	62, 71, 80, 85	0
39	1h	137/138 (99%)	0.66	3 (2%) 62 59	48, 58, 65, 72	0
39	2h	137/138 (99%)	1.15	12 (8%) 15 13	60, 71, 76, 81	0
40	1i	127/128 (99%)	0.86	8 (6%) 26 23	47, 67, 76, 80	0
40	2i	127/128 (99%)	1.87	50 (39%) 1 0	66, 76, 82, 84	0
41	1j	97/105 (92%)	1.30	18 (18%) 3 3	48, 70, 80, 85	0
41	2j	96/105 (91%)	2.03	42 (43%) 0 0	70, 79, 87, 91	0
42	1k	114/129 (88%)	0.64	6 (5%) 32 28	36, 57, 68, 76	0
42	2k	114/129 (88%)	0.99	12 (10%) 11 9	48, 65, 74, 78	0
43	1l	121/132 (91%)	0.34	3 (2%) 58 55	36, 45, 57, 62	0
43	2l	121/132 (91%)	0.84	7 (5%) 29 25	48, 61, 71, 76	0
44	1m	123/126 (97%)	0.49	4 (3%) 49 45	46, 60, 69, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	2m	122/126 (96%)	1.62	32 (26%) 1 1	65, 75, 80, 82	0
45	1n	60/61 (98%)	0.63	1 (1%) 69 67	50, 57, 66, 69	0
45	2n	60/61 (98%)	2.25	35 (58%) 0 0	70, 77, 81, 83	0
46	1o	88/89 (98%)	0.53	5 (5%) 29 26	42, 56, 67, 74	0
46	2o	88/89 (98%)	0.82	4 (4%) 38 34	53, 67, 75, 77	0
47	1p	82/88 (93%)	0.88	2 (2%) 59 56	48, 59, 69, 71	0
47	2p	82/88 (93%)	0.94	6 (7%) 21 18	55, 63, 70, 73	0
48	1q	99/105 (94%)	0.54	1 (1%) 79 78	47, 58, 70, 72	0
48	2q	99/105 (94%)	0.85	4 (4%) 42 38	56, 65, 74, 79	0
49	1r	68/88 (77%)	0.53	2 (2%) 53 50	49, 58, 70, 72	0
49	2r	68/88 (77%)	0.67	1 (1%) 72 70	53, 64, 74, 79	0
50	1s	83/93 (89%)	0.69	5 (6%) 27 24	52, 62, 70, 77	0
50	2s	83/93 (89%)	2.10	41 (49%) 0 0	71, 79, 85, 86	0
51	1t	96/106 (90%)	0.90	10 (10%) 11 10	49, 60, 71, 77	0
51	2t	96/106 (90%)	0.82	7 (7%) 21 18	54, 64, 75, 77	0
52	1u	23/27 (85%)	0.96	2 (8%) 16 13	53, 57, 63, 66	0
52	2u	23/27 (85%)	2.10	14 (60%) 0 0	68, 73, 77, 79	0
53	1v	13/24 (54%)	0.35	2 (15%) 5 4	41, 47, 71, 95	0
53	2v	13/24 (54%)	1.65	4 (30%) 1 1	59, 72, 89, 91	0
54	1w	67/76 (88%)	1.27	16 (23%) 2 1	34, 80, 94, 98	0
54	2w	65/76 (85%)	1.79	24 (36%) 1 0	52, 89, 95, 101	0
55	1x	72/77 (93%)	0.34	5 (6%) 23 20	28, 59, 75, 84	0
55	2x	72/77 (93%)	0.85	2 (2%) 55 51	43, 72, 83, 85	0
56	1y	68/76 (89%)	1.04	8 (11%) 9 7	28, 84, 91, 95	0
56	2y	67/76 (88%)	1.50	16 (23%) 2 1	46, 90, 94, 97	0
57	2a	1491/1521 (98%)	0.70	118 (7%) 18 16	42, 70, 89, 101	0
58	A	13/18 (72%)	0.17	2 (15%) 5 4	17, 21, 65, 77	0
58	B	13/18 (72%)	1.00	2 (15%) 5 4	32, 35, 69, 80	0
All	All	20903/21784 (95%)	0.34	1442 (6%) 23 20	13, 56, 83, 102	0

All (1442) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	2l	2	SER	7.5
45	1n	2	ALA	7.0
38	1g	80	VAL	6.2
57	2a	1030(B)	C	5.9
1	2A	883	G	5.9
45	2n	2	ALA	5.8
33	2b	237	ALA	5.6
57	2a	1030(A)	G	5.2
21	1Z	141	VAL	5.2
44	2m	104	ARG	5.2
54	2w	71	G	5.0
1	2A	896	A	5.0
6	1G	182	LYS	4.9
50	2s	13	ASP	4.9
1	2A	2155	G	4.9
26	24	65	ASP	4.8
54	1w	70	G	4.7
40	2i	14	VAL	4.7
1	2A	2146	C	4.7
50	2s	79	THR	4.7
57	2a	1033	G	4.7
1	2A	2145	C	4.5
6	2G	48	GLU	4.5
38	2g	80	VAL	4.5
25	23	60	GLU	4.4
32	1a	1447	A	4.4
31	29	37	GLY	4.4
38	2g	82	GLY	4.4
50	2s	29	ARG	4.4
57	2a	1030	C	4.4
3	1D	276	LYS	4.4
34	2c	182	ILE	4.4
44	2m	102	ARG	4.4
54	1w	71	G	4.4
3	2D	38	LYS	4.3
38	1g	82	GLY	4.3
6	2G	28	VAL	4.3
45	2n	39	LEU	4.3
57	2a	1034	G	4.3
3	1D	275	LYS	4.3
40	2i	126	SER	4.3
1	2A	1536	C	4.3
1	2A	2159	G	4.3

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Mol	Chain	Res	Type	RSRZ
15	1T	131	ALA	4.2
57	2a	1036	G	4.2
18	2W	112	GLY	4.2
6	2G	50	ALA	4.2
1	1A	932	C	4.2
41	2j	65	LEU	4.2
1	2A	882	G	4.2
44	2m	123	ALA	4.1
18	2W	60	ASN	4.1
41	2j	47	PHE	4.1
12	2Q	22	LYS	4.1
35	2d	164	ALA	4.1
45	2n	34	TYR	4.1
23	11	2	SER	4.1
41	2j	32	ALA	4.1
32	1a	1531	A	4.1
19	1X	95	LEU	4.1
33	1b	237	ALA	4.0
45	2n	6	LEU	4.0
26	24	59	PHE	4.0
1	1A	2167	C	4.0
7	1H	2	SER	4.0
3	2D	275	LYS	4.0
33	2b	236	TYR	4.0
53	2v	24	A	4.0
38	2g	84	ASN	4.0
1	1A	926	G	3.9
38	2g	81	GLY	3.9
26	14	63	TYR	3.9
1	1A	944	C	3.9
26	24	56	VAL	3.9
1	2A	2133	G	3.9
35	1d	169	LYS	3.9
52	2u	11	GLY	3.9
32	1a	1035	A	3.9
1	1A	931	C	3.9
51	1t	103	GLY	3.9
54	1w	1	G	3.9
32	1a	1503	A	3.9
41	1j	33	GLN	3.9
21	1Z	146	ILE	3.9
32	1a	1030	C	3.9

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Mol	Chain	Res	Type	RSRZ
50	1s	84	GLY	3.9
1	2A	2160	G	3.8
32	1a	1003	G	3.8
21	2Z	146	ILE	3.8
34	2c	188	LEU	3.8
50	2s	71	LEU	3.8
15	1T	130	ALA	3.8
14	2S	3	ARG	3.8
22	20	84	LEU	3.8
1	2A	2156	G	3.8
54	2w	70	G	3.8
34	2c	195	VAL	3.8
45	2n	33	VAL	3.8
34	2c	62	ASP	3.8
26	24	63	TYR	3.8
1	1A	943	C	3.8
22	10	6	GLY	3.8
21	2Z	170	THR	3.7
33	2b	97	TRP	3.7
36	2e	10	MET	3.7
54	1w	72	C	3.7
54	2w	72	C	3.7
45	2n	18	VAL	3.7
21	2Z	144	LEU	3.7
32	1a	204	U	3.7
57	2a	1202	G	3.7
33	2b	165	VAL	3.7
1	2A	884	C	3.7
35	2d	154	ASN	3.7
27	15	60	VAL	3.7
1	2A	2112	G	3.7
32	1a	1030(A)	G	3.7
33	1b	11	LEU	3.7
1	2A	885	C	3.7
20	1Y	1	MET	3.7
32	1a	1257	U	3.6
40	2i	102	LEU	3.6
50	2s	77	THR	3.6
42	2k	54	ARG	3.6
38	2g	83	ALA	3.6
41	1j	32	ALA	3.6
26	24	49	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	3.6
44	2m	5	ALA	3.6
52	2u	2	GLY	3.6
32	1a	1030(C)	G	3.6
57	2a	1038	C	3.6
1	2A	2144	U	3.6
57	2a	1035	A	3.6
54	2w	4	C	3.6
1	2A	2154	G	3.6
32	1a	1023	G	3.6
32	1a	1036	G	3.6
21	2Z	172	ALA	3.6
38	1g	83	ALA	3.6
58	A	15	ALA	3.6
1	1A	1140	U	3.6
38	2g	7	ALA	3.5
41	2j	34	VAL	3.5
32	1a	1025	U	3.5
1	1A	2180	A	3.5
21	2Z	173	ALA	3.5
1	2A	886	C	3.5
54	1w	4	C	3.5
22	10	3	HIS	3.5
32	1a	1034	G	3.5
33	2b	136	VAL	3.5
34	2c	198	VAL	3.5
1	1A	2135	U	3.5
32	1a	1532	U	3.5
34	2c	157	ILE	3.5
58	B	16	ASN	3.5
21	2Z	168	GLU	3.5
50	2s	9	VAL	3.5
31	29	17	ILE	3.5
1	1A	1133	G	3.5
1	2A	2127	G	3.5
1	2A	2147	G	3.5
41	2j	8	LEU	3.5
52	2u	14	TRP	3.5
50	2s	80	TYR	3.4
32	1a	163	C	3.4
1	2A	2113	U	3.4
6	1G	48	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
12	2Q	104	PHE	3.4
36	2e	33	VAL	3.4
7	2H	136	ILE	3.4
33	1b	127	ILE	3.4
1	2A	898	C	3.4
1	2A	2111	C	3.4
21	2Z	167	PRO	3.4
33	2b	234	PRO	3.4
40	2i	10	ARG	3.4
33	2b	7	VAL	3.4
1	2A	2166	G	3.4
45	2n	7	ILE	3.4
42	2k	49	GLY	3.4
41	2j	78	ASN	3.4
45	2n	3	ARG	3.4
1	1A	1127	U	3.4
56	1y	20	U	3.4
42	2k	25	TYR	3.4
1	1A	927	G	3.4
1	1A	1221	G	3.4
1	2A	2149	G	3.4
57	2a	1001(A)	G	3.4
53	2v	14	A	3.4
19	2X	92	LEU	3.4
26	24	64	GLY	3.4
35	1d	194	LEU	3.4
37	2f	21	LEU	3.4
33	2b	230	VAL	3.4
1	2A	897	C	3.3
1	2A	2139	C	3.3
57	2a	1027	C	3.3
26	24	54	GLY	3.3
45	2n	38	GLY	3.3
53	2v	13	A	3.3
1	2A	2802	G	3.3
41	1j	86	MET	3.3
33	1b	22	LYS	3.3
40	2i	81	ILE	3.3
26	24	66	SER	3.3
1	2A	889	C	3.3
54	2w	13	C	3.3
54	2w	67	C	3.3

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Mol	Chain	Res	Type	RSRZ
57	2a	1149	C	3.3
26	24	57	GLU	3.3
40	2i	49	PRO	3.3
3	2D	2	ALA	3.3
32	1a	1030(D)	A	3.3
1	1A	1114	G	3.3
1	1A	2134	G	3.3
1	1A	2181	G	3.3
57	2a	1021	G	3.3
35	2d	73	ARG	3.3
41	2j	59	SER	3.3
45	2n	21	TYR	3.3
36	2e	85	GLY	3.3
50	2s	84	GLY	3.3
29	27	45	ALA	3.3
57	2a	1257	U	3.3
32	1a	1029	C	3.3
35	1d	170	VAL	3.3
40	1i	91	ASP	3.3
1	1A	925	A	3.3
1	2A	652(B)	A	3.3
54	2w	73	A	3.3
57	2a	1447	A	3.3
1	1A	930	G	3.3
1	2A	2115	G	3.3
41	2j	90	LEU	3.3
38	1g	85	TYR	3.3
7	2H	45	VAL	3.3
34	2c	8	ILE	3.3
43	2l	18	VAL	3.3
57	2a	1532	U	3.3
32	1a	1030(B)	C	3.2
21	1Z	149	SER	3.2
40	2i	124	GLN	3.2
21	2Z	21	ALA	3.2
1	1A	929	G	3.2
1	2A	2168	G	3.2
57	2a	1026	G	3.2
21	2Z	174	VAL	3.2
1	1A	935	C	3.2
40	2i	19	LEU	3.2
41	2j	40	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
34	2c	2	GLY	3.2
1	1A	942	A	3.2
1	2A	2158	A	3.2
44	1m	2	ALA	3.2
53	2v	12	A	3.2
6	2G	136	ARG	3.2
32	1a	1001(A)	G	3.2
32	1a	1024	G	3.2
32	1a	1032	G	3.2
33	2b	21	ARG	3.2
57	2a	1030(C)	G	3.2
1	1A	1124	U	3.2
14	2S	59	LYS	3.2
40	2i	11	LYS	3.2
44	2m	122	LYS	3.2
39	2h	2	LEU	3.2
34	2c	9	GLY	3.2
1	1A	696	C	3.2
38	2g	85	TYR	3.2
41	2j	44	VAL	3.2
32	1a	1286	A	3.2
54	1w	73	A	3.2
40	2i	91	ASP	3.2
26	24	53	GLU	3.2
1	2A	2308	G	3.2
32	1a	346	G	3.2
32	1a	1031	G	3.2
32	1a	1033	G	3.2
36	2e	22	GLY	3.2
6	2G	76	SER	3.2
7	2H	52	VAL	3.2
33	2b	15	VAL	3.2
34	2c	193	TYR	3.2
44	2m	87	TYR	3.2
1	1A	1121	C	3.1
32	1a	91	C	3.1
42	2k	117	ASN	3.1
1	2A	887	A	3.1
1	2A	2119	A	3.1
33	1b	126	GLU	3.1
41	2j	100	THR	3.1
19	1X	94	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
36	2e	114	GLY	3.1
58	B	15	ALA	3.1
33	2b	185	ILE	3.1
21	2Z	96	VAL	3.1
54	1w	69	G	3.1
12	2Q	6	ARG	3.1
38	1g	84	ASN	3.1
1	1A	936	C	3.1
1	2A	2896	C	3.1
12	2Q	2	LEU	3.1
21	2Z	157	LEU	3.1
34	2c	32	LEU	3.1
22	20	68	GLU	3.1
35	2d	179	GLU	3.1
1	2A	899	A	3.1
1	2A	2173	A	3.1
53	1v	12	A	3.1
34	2c	129	ALA	3.1
38	1g	2	ALA	3.1
50	2s	49	ILE	3.1
33	2b	152	PHE	3.1
1	1A	271	U	3.1
1	1A	1143	U	3.1
34	2c	201	TYR	3.1
1	1A	1105	G	3.1
50	2s	2	PRO	3.1
1	1A	1110	C	3.1
45	2n	13	THR	3.1
57	2a	1004	A	3.1
33	1b	7	VAL	3.1
34	1c	207	VAL	3.1
40	2i	28	VAL	3.1
1	2A	1026	U	3.1
33	2b	187	LEU	3.1
50	2s	5	LEU	3.1
22	20	43	THR	3.1
56	2y	18	G	3.1
20	2Y	54	LYS	3.1
41	2j	74	ILE	3.1
41	2j	96	ILE	3.1
1	1A	2160	C	3.1
32	1a	1028	C	3.1

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Mol	Chain	Res	Type	RSRZ
1	1A	2141	A	3.0
1	2A	2169	A	3.0
57	2a	1357	A	3.0
6	2G	52	ILE	3.0
6	2G	15	VAL	3.0
26	14	56	VAL	3.0
1	1A	928	G	3.0
1	2A	879	G	3.0
1	2A	880	G	3.0
54	2w	15	G	3.0
50	2s	15	LEU	3.0
43	1l	64	TYR	3.0
1	1A	945	A	3.0
1	2A	2126	A	3.0
21	2Z	171	ILE	3.0
46	1o	88	ARG	3.0
51	2t	103	GLY	3.0
36	2e	21	ALA	3.0
33	1b	17	PHE	3.0
41	2j	63	PHE	3.0
45	2n	25	VAL	3.0
45	2n	44	LEU	3.0
6	2G	146	TYR	3.0
57	2a	1002	G	3.0
1	1A	2164	C	3.0
1	2A	2137	C	3.0
1	2A	2175	C	3.0
1	1A	1141	A	3.0
32	1a	162	A	3.0
46	2o	88	ARG	3.0
57	2a	1531	A	3.0
26	14	54	GLY	3.0
41	2j	10	GLY	3.0
43	1l	63	GLY	3.0
44	2m	6	GLY	3.0
56	2y	33	U	3.0
35	2d	188	LEU	3.0
46	2o	86	GLY	3.0
32	1a	1002	G	3.0
1	2A	888	C	3.0
32	1a	1027	C	3.0
50	2s	24	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
32	1a	1001	A	3.0
34	2c	128	PHE	3.0
56	2y	36	A	3.0
57	2a	1286	A	3.0
57	2a	1446	U	2.9
47	2p	82	GLN	2.9
21	1Z	148	ASP	2.9
26	24	51	ASP	2.9
40	2i	9	ARG	2.9
21	1Z	170	THR	2.9
1	2A	11	G	2.9
1	2A	1171	G	2.9
57	2a	1116	C	2.9
41	2j	37	PRO	2.9
54	2w	45	U	2.9
34	2c	79	ARG	2.9
40	2i	20	ARG	2.9
45	2n	31	ARG	2.9
52	2u	6	ARG	2.9
6	1G	146	TYR	2.9
33	1b	236	TYR	2.9
40	2i	62	TYR	2.9
14	2S	35	ILE	2.9
34	2c	194	GLY	2.9
35	1d	167	GLY	2.9
8	2I	146	ALA	2.9
40	2i	122	ALA	2.9
6	2G	31	VAL	2.9
26	24	50	VAL	2.9
33	1b	229	VAL	2.9
3	1D	38	LYS	2.9
43	2l	126	LYS	2.9
39	2h	67	PRO	2.9
1	1A	2158	C	2.9
44	1m	104	ARG	2.9
54	2w	2	C	2.9
1	1A	2163	G	2.9
1	1A	2178	G	2.9
56	2y	15	G	2.9
43	2l	64	TYR	2.9
33	2b	123	ALA	2.9
34	2c	189	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
7	2H	36	PRO	2.9
40	2i	90	PRO	2.9
33	1b	233	SER	2.9
41	1j	4	ILE	2.9
36	2e	5	ASP	2.9
45	2n	40	CYS	2.9
1	1A	1555	C	2.9
1	1A	2807	C	2.9
1	2A	2132	U	2.9
35	2d	87	GLY	2.9
57	2a	1260	C	2.9
1	2A	881	G	2.9
21	2Z	41	LEU	2.9
40	1i	106	ALA	2.9
21	2Z	141	VAL	2.9
22	20	30	VAL	2.9
33	2b	112	VAL	2.9
34	2c	138	VAL	2.9
51	1t	10	LEU	2.9
57	2a	976	G	2.9
26	24	58	ARG	2.8
34	2c	39	ILE	2.8
50	2s	68	GLY	2.8
40	2i	119	ALA	2.8
1	1A	2154	U	2.8
1	1A	2172	U	2.8
36	2e	51	VAL	2.8
40	1i	59	PHE	2.8
1	2A	2134	A	2.8
1	1A	1122	C	2.8
1	1A	2133	C	2.8
1	1A	2168	C	2.8
1	2A	2803	C	2.8
1	1A	2137	G	2.8
1	2A	2116	G	2.8
6	2G	128	ARG	2.8
54	2w	5	G	2.8
57	2a	630	G	2.8
57	2a	993	G	2.8
57	2a	1031	G	2.8
57	2a	1032	G	2.8
21	2Z	149	SER	2.8

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Mol	Chain	Res	Type	RSRZ
34	2c	124	ILE	2.8
41	2j	85	LEU	2.8
50	1s	71	LEU	2.8
34	2c	137	ALA	2.8
33	2b	71	VAL	2.8
36	2e	115	VAL	2.8
47	2p	9	PHE	2.8
26	24	62	ARG	2.8
34	2c	73	PRO	2.8
35	2d	132	ARG	2.8
57	2a	1150	U	2.8
1	1A	2136	A	2.8
57	2a	1030(D)	A	2.8
1	1A	933	C	2.8
1	2A	894	C	2.8
1	2A	1509	C	2.8
21	2Z	53	ILE	2.8
1	1A	2155	G	2.8
1	2A	1533	G	2.8
26	14	45	GLY	2.8
33	1b	228	GLY	2.8
41	2j	93	GLY	2.8
5	2F	166	ALA	2.8
22	20	3	HIS	2.8
52	2u	8	THR	2.8
26	14	59	PHE	2.8
1	1A	1115	A	2.8
1	2A	2176	A	2.8
32	1a	160	A	2.8
46	1o	87	ILE	2.8
50	2s	31	ILE	2.8
48	2q	99	SER	2.8
14	2S	4	LEU	2.8
36	2e	74	GLY	2.8
34	2c	17	ASP	2.8
40	2i	105	ASP	2.8
7	2H	17	VAL	2.8
33	2b	225	ALA	2.8
34	2c	200	ALA	2.8
34	2c	207	VAL	2.8
35	1d	195	ALA	2.8
36	2e	120	THR	2.8

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Mol	Chain	Res	Type	RSRZ
44	2m	7	VAL	2.8
1	2A	2157	G	2.8
34	2c	190	ARG	2.8
45	2n	14	PRO	2.7
36	2e	12	LEU	2.7
1	1A	572	A	2.7
34	2c	197	GLY	2.7
33	1b	19	HIS	2.7
1	2A	2136	C	2.7
22	20	2	ALA	2.7
7	1H	3	ARG	2.7
22	20	69	PHE	2.7
31	29	16	VAL	2.7
34	2c	68	VAL	2.7
34	2c	92	ALA	2.7
34	2c	99	VAL	2.7
39	2h	53	VAL	2.7
42	2k	14	VAL	2.7
50	1s	9	VAL	2.7
57	2a	1029	C	2.7
25	23	2	PRO	2.7
40	2i	92	TYR	2.7
9	2N	83	LYS	2.7
41	2j	55	LYS	2.7
1	1A	639	G	2.7
1	1A	1108	G	2.7
1	2A	2151	G	2.7
57	2a	1131	G	2.7
34	2c	77	ILE	2.7
8	2I	68	LEU	2.7
14	2S	32	LEU	2.7
34	2c	196	LEU	2.7
33	2b	124	SER	2.7
55	1x	47	U	2.7
7	2H	96	ALA	2.7
34	2c	149	ALA	2.7
38	2g	5	ARG	2.7
44	2m	15	VAL	2.7
45	2n	22	THR	2.7
52	2u	24	ARG	2.7
1	2A	2114	A	2.7
21	2Z	159	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
7	2H	175	LYS	2.7
14	2S	92	TYR	2.7
50	2s	61	TYR	2.7
57	2a	1114	C	2.7
33	2b	208	ILE	2.7
41	2j	23	ILE	2.7
50	2s	30	LEU	2.7
1	1A	2174	G	2.7
32	1a	1026	G	2.7
46	1o	89	GLY	2.7
57	2a	1042	G	2.7
57	2a	1117	G	2.7
5	2F	62	ARG	2.7
36	2e	125	SER	2.7
41	1j	76	ASN	2.7
4	2E	204	ALA	2.7
12	2Q	121	ALA	2.7
50	2s	63	THR	2.7
33	2b	232	PRO	2.7
41	2j	91	PRO	2.7
24	12	70	GLN	2.7
1	2A	1847	A	2.7
6	2G	20	ILE	2.7
34	2c	5	ILE	2.7
7	2H	41	MET	2.7
34	2c	52	LEU	2.7
40	2i	115	GLY	2.7
41	1j	31	GLY	2.7
40	1i	2	GLU	2.7
15	2T	131	ALA	2.7
26	24	69	LYS	2.7
33	1b	230	VAL	2.7
41	1j	34	VAL	2.7
43	2l	32	PHE	2.7
34	2c	36	ASP	2.7
46	1o	19	PRO	2.7
1	1A	1135	G	2.6
1	2A	2165	G	2.6
36	2e	20	GLN	2.6
1	1A	1072	U	2.6
35	1d	158	ILE	2.6
50	2s	62	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
33	2b	11	LEU	2.6
44	2m	70	LEU	2.6
48	2q	98	LEU	2.6
34	2c	4	LYS	2.6
6	1G	80	PHE	2.6
7	2H	19	VAL	2.6
9	2N	9	VAL	2.6
21	2Z	166	SER	2.6
40	2i	17	VAL	2.6
40	2i	86	VAL	2.6
8	2I	137	PRO	2.6
42	1k	36	ASP	2.6
20	2Y	44	ILE	2.6
26	24	25	TYR	2.6
1	2A	2153	G	2.6
1	2A	2167	U	2.6
54	2w	10	G	2.6
55	1x	70	G	2.6
57	2a	1003	G	2.6
33	2b	215	LEU	2.6
40	1i	19	LEU	2.6
26	14	55	ARG	2.6
26	24	55	ARG	2.6
34	2c	158	GLY	2.6
35	2d	23	GLY	2.6
36	1e	85	GLY	2.6
1	1A	1113	A	2.6
1	2A	878	A	2.6
1	2A	2801(A)	A	2.6
32	1a	161	A	2.6
57	2a	1001	A	2.6
7	2H	76	VAL	2.6
46	2o	60	VAL	2.6
8	2I	86	THR	2.6
34	1c	107	GLN	2.6
1	1A	34	C	2.6
54	1w	3	C	2.6
57	2a	979	C	2.6
57	2a	1045	C	2.6
7	2H	88	LEU	2.6
21	2Z	99	TYR	2.6
33	2b	148	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
50	2s	52	TYR	2.6
15	2T	111	ARG	2.6
35	2d	47	ARG	2.6
41	1j	79	ARG	2.6
45	2n	29	ARG	2.6
56	2y	45	U	2.6
1	1A	2179	G	2.6
1	1A	2187	G	2.6
1	2A	892	G	2.6
1	2A	2131	G	2.6
1	2A	2319	G	2.6
54	1w	44	G	2.6
57	2a	631	G	2.6
57	2a	1024	G	2.6
57	2a	1182	G	2.6
57	2a	1224	G	2.6
57	2a	1272	G	2.6
7	2H	29	PRO	2.6
21	2Z	136	PHE	2.6
21	2Z	164	ALA	2.6
33	1b	120	ALA	2.6
34	2c	65	ALA	2.6
36	2e	34	VAL	2.6
41	2j	77	PRO	2.6
41	2j	30	SER	2.6
41	1j	74	ILE	2.6
1	1A	2162	C	2.6
1	2A	1043	C	2.6
1	2A	2297	C	2.6
21	1Z	150	LEU	2.6
34	2c	184	TYR	2.6
36	2e	25	ARG	2.6
44	2m	94	ARG	2.6
3	2D	276	LYS	2.6
50	2s	32	LYS	2.6
33	1b	12	GLU	2.6
45	2n	55	GLY	2.6
7	2H	43	VAL	2.6
21	2Z	71	VAL	2.6
14	2S	29	PHE	2.6
33	1b	188	ALA	2.6
33	2b	91	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
43	1l	18	VAL	2.6
50	2s	76	PRO	2.6
55	2x	47	U	2.6
35	2d	161	ASN	2.6
34	2c	15	THR	2.5
12	2Q	103	MET	2.5
33	2b	83	MET	2.5
54	2w	6	G	2.5
54	2w	18	G	2.5
54	2w	44	G	2.5
56	1y	44	G	2.5
57	2a	1058	G	2.5
6	2G	88	ILE	2.5
33	2b	10	LEU	2.5
41	2j	88	LEU	2.5
57	2a	1503	A	2.5
50	2s	81	ARG	2.5
34	2c	6	HIS	2.5
40	2i	125	TYR	2.5
26	24	30	GLU	2.5
33	1b	129	GLU	2.5
1	1A	2161	C	2.5
1	1A	2186	C	2.5
1	2A	2128	C	2.5
54	1w	2	C	2.5
44	2m	100	GLY	2.5
4	2E	167	VAL	2.5
17	2V	50	PRO	2.5
6	2G	180	PHE	2.5
41	2j	54	PHE	2.5
41	2j	42	THR	2.5
1	2A	614(A)	U	2.5
57	2a	1219	U	2.5
35	1d	173	TRP	2.5
42	2k	36	ASP	2.5
39	1h	80	ILE	2.5
22	20	5	LYS	2.5
33	2b	22	LYS	2.5
34	2c	33	LEU	2.5
38	1g	79	ARG	2.5
51	2t	10	LEU	2.5
1	2A	2162	G	2.5

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Mol	Chain	Res	Type	RSRZ
1	1A	302	A	2.5
1	1A	934	A	2.5
1	1A	2157	A	2.5
20	2Y	55	TYR	2.5
32	1a	1005	A	2.5
21	2Z	106	GLY	2.5
23	21	28	GLY	2.5
43	2l	63	GLY	2.5
52	2u	4	GLY	2.5
52	2u	16	GLY	2.5
33	2b	122	PHE	2.5
1	1A	2159	C	2.5
57	2a	980	C	2.5
33	1b	24	TRP	2.5
40	2i	127	LYS	2.5
1	1A	2906	U	2.5
6	2G	51	ARG	2.5
38	2g	4	ARG	2.5
38	2g	16	LEU	2.5
39	2h	102	ARG	2.5
51	1t	100	ILE	2.5
6	2G	173	LEU	2.5
6	2G	175	LEU	2.5
21	2Z	150	LEU	2.5
12	2Q	30	GLY	2.5
33	1b	18	GLY	2.5
41	1j	93	GLY	2.5
44	2m	112	GLY	2.5
50	2s	54	GLY	2.5
51	2t	98	PRO	2.5
1	1A	218	A	2.5
1	1A	1116	A	2.5
1	1A	2212	G	2.5
1	2A	2117	A	2.5
7	2H	79	VAL	2.5
12	2Q	1	MET	2.5
21	1Z	105	VAL	2.5
32	1a	78	G	2.5
50	2s	11	VAL	2.5
57	2a	1053	G	2.5
57	2a	1356	G	2.5
12	2Q	136	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
33	2b	17	PHE	2.5
34	2c	187	ALA	2.5
35	2d	160	GLN	2.5
38	2g	152	ALA	2.5
40	2i	7	THR	2.5
35	2d	166	LYS	2.5
40	2i	95	LYS	2.5
26	24	61	ARG	2.5
33	1b	214	ILE	2.5
36	2e	13	ILE	2.5
35	2d	173	TRP	2.5
35	2d	194	LEU	2.5
39	1h	112	LEU	2.5
40	2i	99	LEU	2.5
40	2i	104	ARG	2.5
1	2A	2138	C	2.5
32	1a	1037	C	2.5
54	2w	3	C	2.5
57	2a	1019	C	2.5
57	2a	1115	C	2.5
1	2A	895	U	2.5
54	2w	66	U	2.5
7	2H	48	GLY	2.5
7	2H	174	GLY	2.5
14	2S	7	TYR	2.5
40	2i	5	TYR	2.5
44	1m	124	PRO	2.5
50	2s	42	PRO	2.5
7	2H	169	VAL	2.5
40	2i	113	LYS	2.4
26	24	52	THR	2.4
50	2s	48	THR	2.4
21	2Z	122	ARG	2.4
14	2S	58	LEU	2.4
34	2c	47	LEU	2.4
1	1A	938	G	2.4
1	1A	2184	G	2.4
1	2A	614(B)	G	2.4
1	2A	1114	G	2.4
1	2A	2125	G	2.4
1	2A	2893	G	2.4
6	2G	29	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
21	2Z	121	HIS	2.4
33	1b	97	TRP	2.4
41	2j	58	ASP	2.4
50	1s	13	ASP	2.4
35	1d	180	GLY	2.4
35	2d	167	GLY	2.4
39	2h	106	GLY	2.4
56	1y	45	U	2.4
57	2a	1020	U	2.4
45	2n	54	PRO	2.4
42	1k	25	TYR	2.4
9	1N	140	VAL	2.4
21	2Z	139	VAL	2.4
33	2b	229	VAL	2.4
42	1k	14	VAL	2.4
7	2H	75	ALA	2.4
25	23	29	ARG	2.4
14	2S	61	ASN	2.4
33	1b	187	LEU	2.4
33	2b	200	ILE	2.4
34	1c	87	LEU	2.4
36	2e	109	ILE	2.4
40	2i	79	LEU	2.4
48	1q	98	LEU	2.4
58	A	16	ASN	2.4
7	2H	61	HIS	2.4
44	2m	92	HIS	2.4
1	1A	2156	A	2.4
1	2A	229	A	2.4
1	2A	890	A	2.4
57	2a	1256	A	2.4
33	1b	128	GLU	2.4
1	2A	2805	G	2.4
32	1a	1021	G	2.4
57	2a	1023	G	2.4
6	2G	17	PRO	2.4
6	2G	42	GLY	2.4
18	1W	112	GLY	2.4
1	2A	2143	C	2.4
5	2F	89	VAL	2.4
1	1A	1112	U	2.4
34	1c	193	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
57	2a	1054	C	2.4
18	2W	90	ARG	2.4
21	2Z	103	ARG	2.4
33	2b	161	ALA	2.4
34	2c	53	ALA	2.4
35	1d	110	PHE	2.4
45	2n	20	ALA	2.4
51	2t	97	ALA	2.4
57	2a	1148	U	2.4
38	2g	3	ARG	2.4
38	2g	79	ARG	2.4
42	1k	48	ILE	2.4
33	1b	134	GLU	2.4
1	1A	1123	A	2.4
1	1A	1142	A	2.4
1	1A	1222	A	2.4
1	2A	901	A	2.4
1	2A	2170	A	2.4
7	1H	13	LYS	2.4
56	1y	35	A	2.4
56	1y	36	A	2.4
21	2Z	147	GLY	2.4
33	2b	99	GLY	2.4
25	23	59	VAL	2.4
34	2c	116	VAL	2.4
36	2e	100	VAL	2.4
1	1A	2173	G	2.4
1	1A	2228	G	2.4
33	2b	31	TYR	2.4
40	2i	114	TYR	2.4
43	2l	41	ARG	2.4
52	1u	24	ARG	2.4
54	2w	19	G	2.4
57	2a	1253	G	2.4
6	2G	53	LEU	2.4
36	2e	31	LEU	2.4
1	1A	1128	U	2.4
1	2A	645	C	2.4
1	2A	2161	C	2.4
1	2A	2897	U	2.4
49	2r	47	THR	2.4
54	2w	11	C	2.4

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Mol	Chain	Res	Type	RSRZ
57	2a	1018	C	2.4
57	2a	1025	U	2.4
57	2a	1358	U	2.4
33	2b	19	HIS	2.4
41	2j	62	HIS	2.4
23	1l	75	GLU	2.4
25	13	60	GLU	2.4
33	2b	166	ASP	2.4
42	2k	124	LYS	2.4
52	2u	23	PRO	2.4
33	2b	89	GLY	2.4
45	2n	51	GLY	2.4
33	2b	95	GLN	2.4
33	1b	165	VAL	2.4
34	2c	130	VAL	2.4
35	1d	168	ARG	2.4
1	1A	937	A	2.4
1	1A	1103	A	2.4
33	2b	57	PHE	2.4
36	2e	119	LEU	2.3
40	2i	4	TYR	2.3
44	2m	19	LEU	2.3
44	2m	34	LEU	2.3
46	1o	69	TYR	2.3
34	2c	152	ILE	2.3
36	1e	13	ILE	2.3
41	1j	75	ILE	2.3
14	2S	34	HIS	2.3
38	1g	153	HIS	2.3
20	1Y	92	ASN	2.3
1	1A	2132	G	2.3
1	1A	2177	G	2.3
1	1A	2816	G	2.3
1	2A	2148	G	2.3
1	2A	2207	G	2.3
1	2A	2793	G	2.3
56	2y	5	G	2.3
40	2i	2	GLU	2.3
57	2a	1205	U	2.3
33	2b	101	MET	2.3
1	1A	670	C	2.3
1	1A	2183	C	2.3

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Mol	Chain	Res	Type	RSRZ
22	10	5	LYS	2.3
29	17	48	LYS	2.3
45	2n	15	LYS	2.3
57	2a	999	C	2.3
7	2H	82	GLY	2.3
38	1g	81	GLY	2.3
51	2t	101	GLY	2.3
14	2S	14	VAL	2.3
21	2Z	48	PHE	2.3
26	14	49	PHE	2.3
36	2e	54	ALA	2.3
40	2i	13	ALA	2.3
45	2n	37	PHE	2.3
6	1G	139	LEU	2.3
7	2H	64	LEU	2.3
11	1P	99	LEU	2.3
44	2m	90	LEU	2.3
26	24	5	ILE	2.3
36	2e	118	ILE	2.3
47	2p	19	ILE	2.3
1	1A	1091	A	2.3
1	1A	2803	A	2.3
1	2A	528	A	2.3
33	2b	54	THR	2.3
57	2a	969	A	2.3
57	2a	975	A	2.3
35	1d	154	ASN	2.3
26	14	57	GLU	2.3
33	2b	86	GLU	2.3
34	2c	199	LYS	2.3
51	1t	74	LYS	2.3
1	1A	2166	U	2.3
32	1a	1446	U	2.3
54	1w	66	U	2.3
1	2A	652(U)	G	2.3
7	2H	10	PRO	2.3
33	1b	232	PRO	2.3
54	1w	10	G	2.3
54	2w	69	G	2.3
57	2a	1220	G	2.3
1	1A	1126	C	2.3
1	2A	865	C	2.3

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Mol	Chain	Res	Type	RSRZ
1	2A	893	C	2.3
1	2A	2174	C	2.3
21	2Z	143	GLY	2.3
26	14	64	GLY	2.3
26	24	47	GLN	2.3
32	1a	1008	C	2.3
33	1b	72	GLY	2.3
39	2h	90	GLY	2.3
40	2i	128	ARG	2.3
47	1p	82	GLN	2.3
56	2y	56	C	2.3
57	2a	1037	C	2.3
21	2Z	165	VAL	2.3
44	2m	98	VAL	2.3
50	2s	58	VAL	2.3
21	2Z	155	LEU	2.3
34	2c	61	ALA	2.3
34	2c	87	LEU	2.3
40	2i	82	ALA	2.3
41	2j	26	ALA	2.3
8	1I	109	ILE	2.3
33	2b	127	ILE	2.3
34	2c	14	ILE	2.3
36	2e	133	TYR	2.3
41	2j	48	THR	2.3
20	2Y	34	LYS	2.3
33	2b	48	MET	2.3
35	1d	150	GLU	2.3
40	2i	118	LYS	2.3
1	1A	1119	A	2.3
54	2w	14	A	2.3
10	2O	81	ASP	2.3
35	1d	83	SER	2.3
6	1G	83	ARG	2.3
7	2H	3	ARG	2.3
51	1t	98	PRO	2.3
20	2Y	57	GLN	2.3
47	2p	48	TRP	2.3
34	2c	205	GLY	2.3
46	2o	89	GLY	2.3
51	2t	96	GLY	2.3
1	2A	2109	U	2.3

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Mol	Chain	Res	Type	RSRZ
1	2A	2150	U	2.3
7	2H	24	VAL	2.3
33	1b	15	VAL	2.3
36	2e	41	VAL	2.3
41	2j	49	VAL	2.3
4	2E	52	LEU	2.3
22	10	7	LEU	2.3
22	20	45	PHE	2.3
21	2Z	57	ILE	2.3
33	2b	201	ILE	2.3
34	2c	24	ALA	2.3
1	1A	940	C	2.3
1	1A	1104	G	2.3
1	1A	2176	G	2.3
1	1A	2182	G	2.3
1	1A	2188	G	2.3
41	1j	6	ILE	2.3
50	1s	40	ILE	2.3
1	1A	2815	C	2.3
50	2s	14	HIS	2.3
54	1w	67	C	2.3
54	2w	61	C	2.3
55	1x	68	C	2.3
55	2x	70	G	2.3
56	2y	44	G	2.3
57	2a	1039	C	2.3
33	1b	133	LYS	2.3
35	2d	86	LYS	2.3
42	2k	51	LYS	2.3
52	2u	17	THR	2.3
35	2d	20	TYR	2.3
3	2D	122	ASP	2.3
14	2S	17	ARG	2.3
34	1c	62	ASP	2.3
40	2i	123	PRO	2.3
41	1j	29	ARG	2.3
41	2j	53	PRO	2.3
1	1A	1132	A	2.3
26	24	45	GLY	2.3
32	1a	344	A	2.3
40	2i	67	GLY	2.3
54	1w	7	A	2.3

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Mol	Chain	Res	Type	RSRZ
57	2a	1287	A	2.3
50	2s	34	TRP	2.3
7	2H	44	VAL	2.3
14	2S	48	LEU	2.3
21	2Z	86	VAL	2.3
33	2b	213	LEU	2.3
41	1j	72	VAL	2.3
44	2m	96	LEU	2.3
6	2G	141	PHE	2.3
21	1Z	136	PHE	2.3
1	1A	12	U	2.2
1	1A	1985	U	2.2
7	2H	156	ALA	2.2
44	2m	4	ILE	2.2
45	2n	10	ALA	2.2
57	2a	1315	U	2.2
34	2c	135	LYS	2.2
34	2c	23	TYR	2.2
42	1k	75	TYR	2.2
55	1x	69	C	2.2
57	2a	1129	C	2.2
57	2a	1189	C	2.2
1	2A	2110	G	2.2
32	1a	630	G	2.2
56	2y	53	G	2.2
57	2a	485	G	2.2
57	2a	1370	G	2.2
7	2H	42	ARG	2.2
8	2I	50	ARG	2.2
39	2h	122	ARG	2.2
24	22	70	GLN	2.2
34	2c	171	GLY	2.2
33	1b	10	LEU	2.2
33	1b	93	VAL	2.2
33	2b	93	VAL	2.2
40	2i	41	VAL	2.2
1	1A	1554	A	2.2
33	2b	120	ALA	2.2
33	2b	132	LYS	2.2
38	2g	2	ALA	2.2
40	2i	15	ALA	2.2
41	1j	98	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
44	2m	30	ALA	2.2
45	2n	17	LYS	2.2
57	2a	1044	A	2.2
1	1A	941	U	2.2
32	1a	202	U	2.2
26	24	32	TYR	2.2
33	2b	37	ASN	2.2
33	2b	130	ARG	2.2
21	2Z	95	PRO	2.2
41	1j	77	PRO	2.2
57	2a	962	C	2.2
57	2a	1321	C	2.2
57	2a	1452	C	2.2
6	2G	49	ASP	2.2
1	1A	698	G	2.2
1	1A	1109	G	2.2
1	2A	2124	G	2.2
12	2Q	15	GLY	2.2
49	1r	78	LEU	2.2
56	1y	69	G	2.2
6	2G	38	VAL	2.2
6	2G	74	LYS	2.2
34	2c	151	VAL	2.2
45	2n	61	TRP	2.2
21	2Z	88	PHE	2.2
33	2b	58	ILE	2.2
40	2i	101	PHE	2.2
40	2i	117	HIS	2.2
41	2j	98	ILE	2.2
42	2k	48	ILE	2.2
36	2e	17	ALA	2.2
36	2e	94	ALA	2.2
40	1i	15	ALA	2.2
45	2n	59	ALA	2.2
44	2m	105	THR	2.2
57	2a	1005	A	2.2
57	2a	1092	A	2.2
1	1A	2131	U	2.2
44	1m	102	ARG	2.2
45	2n	41	ARG	2.2
26	24	67	TYR	2.2
56	2y	51	U	2.2

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Mol	Chain	Res	Type	RSRZ
33	1b	234	PRO	2.2
35	2d	37	PRO	2.2
34	2c	178	LEU	2.2
35	2d	21	LEU	2.2
40	1i	56	LEU	2.2
51	1t	102	GLY	2.2
17	2V	52	VAL	2.2
40	2i	44	VAL	2.2
41	1j	24	VAL	2.2
1	1A	2150	C	2.2
1	2A	2140	C	2.2
33	1b	200	ILE	2.2
44	2m	22	ILE	2.2
45	2n	42	ILE	2.2
6	2G	163	ALA	2.2
13	2R	101	ALA	2.2
34	2c	146	ALA	2.2
39	2h	124	ALA	2.2
44	2m	42	ALA	2.2
1	1A	569	G	2.2
1	1A	2138	G	2.2
1	2A	2894	G	2.2
2	2B	119	G	2.2
34	2c	161	GLU	2.2
54	2w	65	G	2.2
56	1y	18	G	2.2
57	2a	1190	G	2.2
50	2s	33	THR	2.2
3	2D	262	ARG	2.2
47	2p	81	ARG	2.2
1	1A	2139	A	2.2
7	2H	118	PRO	2.2
20	2Y	53	PRO	2.2
33	1b	131	PRO	2.2
34	2c	48	TYR	2.2
57	2a	1248	A	2.2
1	1A	1220	U	2.2
1	2A	271(K)	U	2.2
1	2A	1113	U	2.2
14	2S	57	LYS	2.2
26	14	69	LYS	2.2
32	1a	841	U	2.2

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Mol	Chain	Res	Type	RSRZ
42	2k	13	GLN	2.2
40	2i	97	LYS	2.2
52	2u	20	LYS	2.2
57	2a	1211	U	2.2
33	1b	227	GLY	2.2
33	2b	154	LEU	2.2
33	2b	227	GLY	2.2
41	2j	36	GLY	2.2
52	1u	16	GLY	2.2
6	2G	156	ASP	2.2
12	2Q	7	MET	2.2
7	2H	50	VAL	2.2
41	1j	38	ILE	2.2
8	2I	65	ALA	2.1
19	2X	91	ALA	2.1
49	1r	24	ALA	2.1
44	2m	58	GLU	2.1
1	2A	2163	C	2.1
1	2A	2164	C	2.1
34	2c	191	THR	2.1
44	2m	3	ARG	2.1
57	2a	1043	C	2.1
57	2a	1203	C	2.1
7	2H	128	PRO	2.1
25	13	2	PRO	2.1
32	1a	159	G	2.1
41	2j	41	PRO	2.1
56	1y	15	G	2.1
56	2y	6	G	2.1
57	2a	971	G	2.1
57	2a	1047	G	2.1
57	2a	1215	G	2.1
7	2H	83	TYR	2.1
19	2X	69	TYR	2.1
33	2b	156	LYS	2.1
42	1k	13	GLN	2.1
52	2u	3	LYS	2.1
6	2G	172	LEU	2.1
7	2H	33	LEU	2.1
20	2Y	1	MET	2.1
1	1A	554	A	2.1
1	1A	2195	A	2.1

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Mol	Chain	Res	Type	RSRZ
21	1Z	147	GLY	2.1
35	2d	16	GLY	2.1
57	2a	977	A	2.1
57	2a	978	A	2.1
1	1A	2189	U	2.1
1	2A	271(L)	U	2.1
1	2A	2130	U	2.1
36	2e	80	ILE	2.1
39	1h	4	ASP	2.1
43	2l	55	VAL	2.1
54	1w	20	U	2.1
54	1w	45	U	2.1
57	2a	1136	U	2.1
57	2a	1159	U	2.1
57	2a	1196	U	2.1
21	2Z	153	SER	2.1
51	1t	70	SER	2.1
36	2e	45	PHE	2.1
35	1d	164	ALA	2.1
41	2j	83	GLU	2.1
48	2q	96	GLU	2.1
7	2H	60	ARG	2.1
38	2g	76	ARG	2.1
47	2p	8	ARG	2.1
50	2s	78	ARG	2.1
34	2c	67	THR	2.1
40	2i	27	THR	2.1
33	2b	169	LYS	2.1
44	2m	121	LYS	2.1
1	1A	2196	C	2.1
56	2y	13	C	2.1
57	2a	1060	C	2.1
57	2a	1066	C	2.1
57	2a	1320	C	2.1
6	2G	148	MET	2.1
7	2H	71	LEU	2.1
21	2Z	1	MET	2.1
33	2b	94	ASN	2.1
35	2d	165	MET	2.1
45	2n	47	LEU	2.1
48	2q	43	LEU	2.1
22	20	13	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
50	2s	26	GLY	2.1
50	2s	82	GLY	2.1
51	1t	69	GLY	2.1
12	2Q	66	ILE	2.1
21	2Z	85	HIS	2.1
1	1A	694	G	2.1
1	1A	2153	G	2.1
1	2A	2318	G	2.1
6	2G	126	ASP	2.1
12	2Q	102	VAL	2.1
34	1c	86	VAL	2.1
34	2c	134	ILE	2.1
34	2c	202	ILE	2.1
36	2e	67	VAL	2.1
36	2e	90	VAL	2.1
36	2e	101	ILE	2.1
40	2i	63	ILE	2.1
52	2u	13	ILE	2.1
57	2a	953	G	2.1
57	2a	973	G	2.1
57	2a	1258	G	2.1
57	2a	1276	G	2.1
33	2b	70	PHE	2.1
1	2A	900	A	2.1
6	2G	46	ALA	2.1
6	2G	169	ALA	2.1
33	2b	188	ALA	2.1
34	2c	160	ALA	2.1
56	2y	14	A	2.1
56	2y	35	A	2.1
5	2F	161	GLU	2.1
20	1Y	91	GLU	2.1
21	2Z	2	GLU	2.1
57	2a	1000	U	2.1
57	2a	1040	U	2.1
57	2a	1065	U	2.1
34	2c	167	TRP	2.1
41	2j	87	THR	2.1
42	2k	57	THR	2.1
6	2G	2	PRO	2.1
21	2Z	158	PRO	2.1
33	2b	202	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
36	2e	96	PRO	2.1
7	2H	171	LEU	2.1
8	1I	44	LEU	2.1
34	1c	178	LEU	2.1
36	2e	139	LEU	2.1
44	2m	81	LEU	2.1
4	2E	10	GLY	2.1
17	2V	41	GLY	2.1
1	1A	2814	C	2.1
7	2H	26	VAL	2.1
25	23	6	VAL	2.1
33	2b	197	VAL	2.1
44	2m	60	VAL	2.1
57	2a	848	C	2.1
6	2G	4	ASP	2.1
26	24	42	PHE	2.1
50	2s	74	PHE	2.1
6	2G	151	ALA	2.1
12	1Q	6	ARG	2.1
34	2c	88	ARG	2.1
36	2e	86	ALA	2.1
40	1i	66	ARG	2.1
44	2m	75	ALA	2.1
45	2n	5	ALA	2.1
1	2A	1170	G	2.1
1	2A	2751	G	2.1
36	2e	9	LYS	2.1
56	2y	19	G	2.1
56	2y	52	G	2.1
57	2a	1057	G	2.1
1	1A	1219	A	2.1
1	2A	12	U	2.1
1	2A	2135	A	2.1
2	2B	120	A	2.1
6	2G	19	LEU	2.1
47	1p	49	LEU	2.1
34	2c	185	GLY	2.1
45	2n	49	HIS	2.1
7	2H	72	ILE	2.1
34	1c	14	ILE	2.1
35	1d	5	ILE	2.1
42	2k	75	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
44	2m	9	ILE	2.1
9	2N	140	VAL	2.1
21	1Z	139	VAL	2.1
7	2H	51	ARG	2.0
7	2H	159	GLU	2.0
12	2Q	139	GLU	2.0
21	2Z	131	ARG	2.0
33	1b	21	ARG	2.0
34	2c	126	ARG	2.0
5	1F	13	SER	2.0
33	2b	88	ALA	2.0
33	2b	233	SER	2.0
34	2c	60	ALA	2.0
45	2n	30	ALA	2.0
50	2s	4	SER	2.0
1	2A	2794	C	2.0
55	1x	67	C	2.0
41	2j	67	THR	2.0
41	2j	92	THR	2.0
33	1b	202	PRO	2.0
1	1A	1106	U	2.0
8	2I	38	LEU	2.0
11	2P	68	GLN	2.0
32	1a	203	U	2.0
39	2h	39	LEU	2.0
39	2h	63	LEU	2.0
45	2n	53	LEU	2.0
50	2s	20	LEU	2.0
1	2A	2141	G	2.0
1	2A	2152	G	2.0
53	1v	13	A	2.0
54	2w	7	A	2.0
57	2a	532	A	2.0
57	2a	983	A	2.0
57	2a	1009	G	2.0
57	2a	1180	A	2.0
57	2a	1184	G	2.0
57	2a	1310	G	2.0
41	2j	68	HIS	2.0
5	1F	208	GLY	2.0
4	2E	151	TYR	2.0
6	2G	11	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
33	2b	92	TYR	2.0
38	2g	151	TYR	2.0
6	2G	91	ARG	2.0
19	2X	68	ARG	2.0
33	2b	56	ARG	2.0
38	2g	6	ARG	2.0
39	2h	91	ARG	2.0
40	2i	42	ARG	2.0
51	1t	86	ARG	2.0
52	2u	10	ARG	2.0
8	1I	135	GLU	2.0
11	2P	149	GLU	2.0
13	2R	69	ASP	2.0
33	1b	9	GLU	2.0
34	2c	90	GLU	2.0
8	2I	131	LYS	2.0
35	2d	169	LYS	2.0
36	2e	95	ALA	2.0
50	2s	18	LYS	2.0
51	2t	30	LYS	2.0
14	2S	31	SER	2.0
14	2S	5	THR	2.0
34	1c	15	THR	2.0
1	2A	2129	C	2.0
32	1a	1006	C	2.0
33	2b	196	LEU	2.0
34	1c	94	LEU	2.0
34	2c	162	GLN	2.0
50	2s	16	LEU	2.0
50	2s	22	LEU	2.0
57	2a	1007	C	2.0
57	2a	1214	C	2.0
1	2A	958	U	2.0
50	2s	53	ASN	2.0
51	1t	75	ASN	2.0
57	2a	1313	U	2.0
4	2E	115	GLY	2.0
15	2T	69	GLY	2.0
17	2V	101	GLY	2.0
35	1d	23	GLY	2.0
36	2e	29	GLY	2.0
41	2j	38	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
41	2j	75	ILE	2.0
1	2A	866	A	2.0
1	2A	2298	A	2.0
6	2G	118	ARG	2.0
6	2G	159	VAL	2.0
11	2P	77	ARG	2.0
35	1d	3	ARG	2.0
35	2d	131	ARG	2.0
35	2d	170	VAL	2.0
36	2e	18	ARG	2.0
39	2h	84	ARG	2.0
40	2i	53	VAL	2.0
57	2a	1110	A	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	55	20/21	0.46	0.18	89,99,107,116	0
54	G7M	2w	46	24/25	0.52	0.17	80,88,101,118	0
56	5MU	2y	54	21/22	0.54	0.16	86,91,105,122	0
56	G7M	2y	46	24/25	0.54	0.18	82,90,99,118	0
56	G7M	1y	46	24/25	0.55	0.18	80,88,98,108	0
54	G7M	1w	46	24/25	0.58	0.18	70,80,100,123	0
56	PSU	1y	55	20/21	0.62	0.14	84,90,100,105	0
56	5MU	1y	54	21/22	0.66	0.15	76,85,92,104	0
56	4SU	2y	8	20/21	0.67	0.14	85,90,98,107	0
56	PSU	2y	32	20/21	0.74	0.14	74,82,94,96	0
54	4SU	2w	8	20/21	0.75	0.12	82,88,103,107	0
58	BB9	B	17	6/7	0.75	0.31	68,79,86,100	0
56	4SU	1y	8	20/21	0.77	0.14	83,88,102,104	0
54	PSU	2w	55	20/21	0.78	0.12	73,83,90,98	0
56	PSU	2y	39	20/21	0.79	0.14	72,80,86,98	0
54	4SU	1w	8	20/21	0.79	0.14	72,81,89,91	0
55	5MU	2x	54	21/22	0.82	0.14	70,77,80,92	0
55	PSU	2x	55	20/21	0.83	0.13	69,73,79,80	0
57	2MG	2a	1207	24/25	0.84	0.14	72,80,87,88	0
56	PSU	1y	32	20/21	0.84	0.13	70,78,86,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	PSU	2w	32	20/21	0.85	0.12	70,77,85,91	0
54	5MU	2w	54	21/22	0.86	0.11	67,75,81,86	0
43	0TD	1l	92	10/11	0.86	0.16	41,42,49,76	0
58	BB9	A	17	6/7	0.86	0.19	54,69,80,92	0
55	4SU	2x	8	20/21	0.86	0.12	70,75,79,81	0
56	PSU	1y	39	20/21	0.87	0.11	69,73,78,82	0
43	0TD	2l	92	10/11	0.87	0.16	58,62,66,84	0
57	M2G	2a	966	25/26	0.87	0.15	56,62,75,78	0
54	PSU	1w	55	20/21	0.89	0.10	53,69,78,80	0
57	5MC	2a	967	21/22	0.91	0.12	60,65,76,77	0
55	5MC	2x	32	21/22	0.91	0.13	62,66,70,75	0
57	PSU	2a	516	20/21	0.91	0.11	58,66,72,72	0
1	5MU	2A	1915	21/22	0.91	0.10	58,65,68,73	0
55	5MU	1x	54	21/22	0.92	0.10	54,61,65,73	0
57	5MC	2a	1400	21/22	0.92	0.14	58,64,70,74	0
57	4OC	2a	1402	22/23	0.92	0.12	48,57,64,65	0
1	PSU	2A	1911	20/21	0.92	0.10	50,55,60,77	0
54	PSU	1w	32	20/21	0.92	0.10	53,59,72,72	0
1	PSU	2A	1917	20/21	0.93	0.09	51,60,68,71	0
54	MIA	2w	37	25/30	0.93	0.10	63,70,76,77	0
57	G7M	2a	527	24/25	0.93	0.11	46,55,64,74	0
57	5MC	2a	1404	21/22	0.93	0.10	46,51,59,64	0
57	5MC	2a	1407	21/22	0.93	0.11	38,49,54,63	0
54	PSU	2w	39	20/21	0.93	0.10	65,72,79,80	0
55	PSU	1x	55	20/21	0.93	0.09	52,56,67,69	0
1	4OC	2A	1920	21/23	0.94	0.09	50,55,58,59	0
1	5MU	1A	1937	21/22	0.94	0.10	39,44,52,54	0
32	2MG	1a	1207	24/25	0.94	0.10	50,60,65,66	0
55	4SU	1x	8	20/21	0.95	0.09	48,55,66,78	0
57	UR3	2a	1498	21/22	0.95	0.11	44,50,56,60	0
57	MA6	2a	1518	24/25	0.95	0.10	42,58,62,63	0
57	MA6	2a	1519	24/25	0.95	0.12	47,54,62,63	0
54	5MU	1w	54	21/22	0.95	0.08	45,59,64,65	0
1	5MC	2A	1962	21/22	0.95	0.08	31,43,52,61	0
55	5MC	1x	32	21/22	0.96	0.09	39,46,52,57	0
1	PSU	1A	1939	20/21	0.96	0.09	36,41,45,46	0
32	MA6	1a	1519	24/25	0.96	0.09	30,35,38,42	0
1	5MC	2A	1942	21/22	0.96	0.09	39,50,56,63	0
54	MIA	1w	37	29/30	0.96	0.09	36,44,57,62	0
32	PSU	1a	516	20/21	0.96	0.07	45,49,50,51	0
32	G7M	1a	527	24/25	0.96	0.08	31,38,45,46	0
32	M2G	1a	966	25/26	0.96	0.10	39,44,51,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	OMG	2A	2251	24/25	0.97	0.07	33,37,41,47	0
1	2MA	2A	2503	23/24	0.97	0.09	26,30,33,36	0
1	PSU	2A	2605	20/21	0.97	0.08	24,33,36,37	0
1	4OC	1A	1942	21/23	0.97	0.07	29,34,37,40	0
1	5MC	1A	1964	21/22	0.97	0.07	24,31,36,43	0
32	5MC	1a	967	21/22	0.97	0.08	42,45,51,54	0
1	PSU	1A	1933	20/21	0.97	0.08	31,38,41,42	0
32	5MC	1a	1400	21/22	0.97	0.07	30,41,43,48	0
32	4OC	1a	1402	22/23	0.97	0.07	33,38,43,44	0
1	5MU	2A	1939	21/22	0.97	0.08	30,33,39,42	0
54	PSU	1w	39	20/21	0.97	0.08	44,50,59,59	0
32	5MC	1a	1404	21/22	0.97	0.07	29,33,37,40	0
32	5MC	1a	1407	21/22	0.97	0.07	27,33,37,40	0
1	5MC	1A	1984	21/22	0.98	0.05	18,26,30,37	0
1	2MU	1A	2564	21/23	0.98	0.07	16,22,26,31	0
1	PSU	1A	2617	20/21	0.98	0.06	15,18,23,24	0
1	5MU	1A	1961	21/22	0.98	0.07	15,20,24,26	0
32	UR3	1a	1498	21/22	0.98	0.06	27,33,37,39	0
58	BB9	A	6	6/7	0.98	0.05	20,21,22,23	0
58	BB9	B	9	6/7	0.98	0.07	32,35,36,37	0
1	2MU	2A	2552	21/23	0.98	0.07	32,37,41,46	0
32	MA6	1a	1518	24/25	0.98	0.07	25,33,36,39	0
58	BB9	A	9	6/7	0.99	0.05	14,16,16,19	0
1	OMG	1A	2263	24/25	0.99	0.04	15,19,22,25	0
1	2MA	1A	2515	23/24	0.99	0.05	10,14,17,22	0
58	BB9	B	6	6/7	0.99	0.05	23,30,33,35	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3445	1/1	0.33	0.29	55,55,55,55	0
59	MG	2j	8002	1/1	0.37	0.17	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3781	1/1	0.46	0.23	63,63,63,63	0
59	MG	2A	3528	1/1	0.51	0.30	81,81,81,81	0
59	MG	2A	3259	1/1	0.53	0.19	82,82,82,82	0
59	MG	1A	4115	1/1	0.53	0.23	60,60,60,60	0
59	MG	1y	104	1/1	0.54	0.41	80,80,80,80	0
59	MG	1a	3548	1/1	0.57	0.33	74,74,74,74	0
59	MG	2y	3005	1/1	0.57	0.19	98,98,98,98	0
59	MG	2A	3447	1/1	0.58	0.17	57,57,57,57	0
59	MG	2U	202	1/1	0.58	0.24	69,69,69,69	0
59	MG	2a	3113	1/1	0.59	0.28	69,69,69,69	0
59	MG	2a	3206	1/1	0.59	0.19	74,74,74,74	0
59	MG	2A	3075	1/1	0.59	0.21	73,73,73,73	0
59	MG	2v	103	1/1	0.59	0.32	70,70,70,70	0
59	MG	1a	3482	1/1	0.59	0.28	52,52,52,52	0
59	MG	2a	3221	1/1	0.60	0.30	76,76,76,76	0
59	MG	1w	111	1/1	0.60	0.30	80,80,80,80	0
59	MG	2A	3619	1/1	0.60	0.23	60,60,60,60	0
59	MG	2A	3520	1/1	0.60	0.17	79,79,79,79	0
59	MG	1y	102	1/1	0.61	0.17	77,77,77,77	0
59	MG	1y	105	1/1	0.61	0.17	80,80,80,80	0
59	MG	2a	3180	1/1	0.63	0.23	74,74,74,74	0
59	MG	2a	3212	1/1	0.64	0.26	73,73,73,73	0
59	MG	1A	4118	1/1	0.65	0.18	69,69,69,69	0
59	MG	1a	3358	1/1	0.65	0.24	73,73,73,73	0
59	MG	2A	3555	1/1	0.66	0.20	61,61,61,61	0
59	MG	1A	3420	1/1	0.66	0.18	60,60,60,60	0
59	MG	1A	3926	1/1	0.67	0.20	22,22,22,22	0
59	MG	2A	3733	1/1	0.67	0.20	71,71,71,71	0
59	MG	2A	3535	1/1	0.67	0.13	63,63,63,63	0
59	MG	2A	3347	1/1	0.67	0.19	57,57,57,57	0
59	MG	2y	3007	1/1	0.67	0.14	78,78,78,78	0
59	MG	2a	3235	1/1	0.68	0.22	80,80,80,80	0
59	MG	1Z	303	1/1	0.68	0.10	69,69,69,69	0
59	MG	1B	229	1/1	0.68	0.14	69,69,69,69	0
59	MG	2A	3018	1/1	0.68	0.22	71,71,71,71	0
59	MG	2A	3622	1/1	0.68	0.22	58,58,58,58	0
59	MG	2A	3769	1/1	0.69	0.21	56,56,56,56	0
59	MG	2j	8001	1/1	0.69	0.15	63,63,63,63	0
59	MG	1B	225	1/1	0.69	0.16	59,59,59,59	0
59	MG	1x	116	1/1	0.70	0.12	70,70,70,70	0
59	MG	2A	3588	1/1	0.71	0.19	60,60,60,60	0
59	MG	1A	3265	1/1	0.71	0.16	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3395	1/1	0.71	0.18	54,54,54,54	0
59	MG	1Y	503	1/1	0.71	0.13	69,69,69,69	0
59	MG	1A	3722	1/1	0.71	0.27	72,72,72,72	0
59	MG	2A	3774	1/1	0.71	0.22	64,64,64,64	0
59	MG	2A	3531	1/1	0.71	0.17	57,57,57,57	0
59	MG	2A	3191	1/1	0.71	0.18	59,59,59,59	0
59	MG	2a	3002	1/1	0.71	0.20	73,73,73,73	0
59	MG	1B	220	1/1	0.71	0.24	66,66,66,66	0
59	MG	1A	4011	1/1	0.72	0.19	59,59,59,59	0
59	MG	1A	4174	1/1	0.72	0.23	52,52,52,52	0
59	MG	2a	3182	1/1	0.72	0.20	67,67,67,67	0
59	MG	2A	3253	1/1	0.72	0.20	61,61,61,61	0
59	MG	1A	4072	1/1	0.72	0.17	55,55,55,55	0
59	MG	1A	3405	1/1	0.72	0.11	55,55,55,55	0
59	MG	1A	3819	1/1	0.73	0.12	23,23,23,23	0
59	MG	2A	3494	1/1	0.73	0.16	58,58,58,58	0
59	MG	2A	3789	1/1	0.73	0.22	66,66,66,66	0
59	MG	2A	3265	1/1	0.73	0.36	73,73,73,73	0
59	MG	2a	3211	1/1	0.73	0.23	65,65,65,65	0
59	MG	2w	3007	1/1	0.73	0.23	72,72,72,72	0
59	MG	1y	103	1/1	0.73	0.20	88,88,88,88	0
59	MG	2a	3220	1/1	0.73	0.29	65,65,65,65	0
59	MG	2a	3199	1/1	0.74	0.16	58,58,58,58	0
59	MG	2A	3085	1/1	0.74	0.15	62,62,62,62	0
59	MG	1A	3902	1/1	0.74	0.14	45,45,45,45	0
59	MG	2A	3243	1/1	0.74	0.20	66,66,66,66	0
59	MG	2A	3611	1/1	0.74	0.13	66,66,66,66	0
59	MG	2B	3015	1/1	0.74	0.22	64,64,64,64	0
59	MG	2S	8001	1/1	0.74	0.17	73,73,73,73	0
59	MG	2g	8001	1/1	0.74	0.11	74,74,74,74	0
59	MG	1A	3702	1/1	0.74	0.14	20,20,20,20	0
59	MG	1a	3536	1/1	0.74	0.21	58,58,58,58	0
59	MG	2a	3037	1/1	0.74	0.29	74,74,74,74	0
59	MG	2w	3003	1/1	0.74	0.15	74,74,74,74	0
59	MG	2A	3726	1/1	0.74	0.18	56,56,56,56	0
59	MG	2x	103	1/1	0.74	0.30	74,74,74,74	0
59	MG	1A	4145	1/1	0.74	0.13	45,45,45,45	0
59	MG	2A	3768	1/1	0.74	0.18	58,58,58,58	0
59	MG	1s	3001	1/1	0.75	0.25	62,62,62,62	0
59	MG	2a	3215	1/1	0.75	0.33	75,75,75,75	0
59	MG	2R	203	1/1	0.75	0.18	52,52,52,52	0
59	MG	1a	3421	1/1	0.75	0.18	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1a	3420	1/1	0.75	0.20	65,65,65,65	0
59	MG	2A	3758	1/1	0.75	0.29	63,63,63,63	0
59	MG	2A	3760	1/1	0.75	0.26	61,61,61,61	0
59	MG	2A	3765	1/1	0.75	0.18	70,70,70,70	0
59	MG	2a	3133	1/1	0.75	0.15	67,67,67,67	0
59	MG	2A	3290	1/1	0.75	0.11	67,67,67,67	0
59	MG	2A	3209	1/1	0.75	0.19	60,60,60,60	0
59	MG	2A	3376	1/1	0.75	0.15	54,54,54,54	0
59	MG	2y	3003	1/1	0.75	0.10	83,83,83,83	0
59	MG	1a	3557	1/1	0.75	0.25	63,63,63,63	0
59	MG	2A	3246	1/1	0.75	0.19	67,67,67,67	0
59	MG	1A	3578	1/1	0.76	0.17	73,73,73,73	0
59	MG	2A	3289	1/1	0.76	0.17	70,70,70,70	0
59	MG	1A	3892	1/1	0.76	0.13	62,62,62,62	0
59	MG	1a	3572	1/1	0.76	0.15	63,63,63,63	0
59	MG	2a	3005	1/1	0.76	0.33	74,74,74,74	0
59	MG	2A	3587	1/1	0.76	0.14	62,62,62,62	0
59	MG	1A	3292	1/1	0.76	0.19	71,71,71,71	0
59	MG	2q	205	1/1	0.76	0.25	69,69,69,69	0
59	MG	2A	3771	1/1	0.76	0.15	67,67,67,67	0
59	MG	1a	3492	1/1	0.76	0.11	75,75,75,75	0
59	MG	2A	3775	1/1	0.76	0.14	63,63,63,63	0
59	MG	2A	3051	1/1	0.76	0.21	67,67,67,67	0
59	MG	2A	3517	1/1	0.76	0.22	58,58,58,58	0
59	MG	2A	3795	1/1	0.76	0.22	66,66,66,66	0
59	MG	1A	3344	1/1	0.76	0.21	57,57,57,57	0
59	MG	1A	3166	1/1	0.77	0.23	54,54,54,54	0
59	MG	2A	3260	1/1	0.77	0.22	76,76,76,76	0
59	MG	2a	3108	1/1	0.77	0.24	62,62,62,62	0
59	MG	1a	3426	1/1	0.77	0.34	55,55,55,55	0
59	MG	2a	3118	1/1	0.77	0.48	71,71,71,71	0
59	MG	2A	3725	1/1	0.77	0.16	64,64,64,64	0
59	MG	2a	3176	1/1	0.77	0.34	75,75,75,75	0
59	MG	1a	3435	1/1	0.77	0.40	76,76,76,76	0
59	MG	2A	3731	1/1	0.77	0.17	72,72,72,72	0
59	MG	1A	3410	1/1	0.77	0.19	58,58,58,58	0
59	MG	2a	3205	1/1	0.77	0.19	60,60,60,60	0
59	MG	1A	3382	1/1	0.77	0.21	57,57,57,57	0
59	MG	2a	3210	1/1	0.77	0.20	65,65,65,65	0
59	MG	1A	3798	1/1	0.77	0.29	44,44,44,44	0
59	MG	2A	3402	1/1	0.77	0.26	57,57,57,57	0
59	MG	1A	4106	1/1	0.77	0.18	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1a	3550	1/1	0.77	0.21	78,78,78,78	0
59	MG	1a	3553	1/1	0.77	0.28	60,60,60,60	0
59	MG	2A	3143	1/1	0.77	0.20	77,77,77,77	0
59	MG	2A	3146	1/1	0.77	0.19	78,78,78,78	0
59	MG	1A	3801	1/1	0.77	0.09	34,34,34,34	0
59	MG	1a	3330	1/1	0.77	0.17	58,58,58,58	0
59	MG	2l	202	1/1	0.77	0.16	71,71,71,71	0
59	MG	2A	3793	1/1	0.77	0.17	62,62,62,62	0
59	MG	2v	102	1/1	0.77	0.28	69,69,69,69	0
59	MG	2A	3539	1/1	0.77	0.14	57,57,57,57	0
59	MG	2A	3836	1/1	0.77	0.27	65,65,65,65	0
59	MG	1a	3578	1/1	0.77	0.13	59,59,59,59	0
59	MG	2A	3573	1/1	0.77	0.15	64,64,64,64	0
59	MG	1A	3178	1/1	0.77	0.20	61,61,61,61	0
59	MG	1A	3577	1/1	0.77	0.19	57,57,57,57	0
59	MG	2A	3597	1/1	0.77	0.19	65,65,65,65	0
59	MG	2A	3073	1/1	0.78	0.22	63,63,63,63	0
59	MG	1x	114	1/1	0.78	0.26	58,58,58,58	0
59	MG	2A	3080	1/1	0.78	0.22	74,74,74,74	0
59	MG	1A	3740	1/1	0.78	0.19	49,49,49,49	0
59	MG	2A	3273	1/1	0.78	0.23	66,66,66,66	0
59	MG	2A	3558	1/1	0.78	0.14	56,56,56,56	0
59	MG	2A	3105	1/1	0.78	0.12	54,54,54,54	0
59	MG	1A	3806	1/1	0.78	0.23	47,47,47,47	0
59	MG	2A	3307	1/1	0.78	0.28	60,60,60,60	0
59	MG	2a	3216	1/1	0.78	0.35	63,63,63,63	0
59	MG	2A	3325	1/1	0.78	0.29	68,68,68,68	0
59	MG	1A	3911	1/1	0.78	0.13	62,62,62,62	0
59	MG	2A	3170	1/1	0.78	0.20	60,60,60,60	0
59	MG	2B	3022	1/1	0.78	0.25	72,72,72,72	0
59	MG	1A	4111	1/1	0.78	0.17	63,63,63,63	0
59	MG	2A	3663	1/1	0.78	0.14	60,60,60,60	0
59	MG	2A	3689	1/1	0.78	0.12	65,65,65,65	0
59	MG	1A	3645	1/1	0.78	0.29	63,63,63,63	0
59	MG	2A	3462	1/1	0.78	0.14	62,62,62,62	0
59	MG	2A	3218	1/1	0.78	0.19	63,63,63,63	0
59	MG	2a	3093	1/1	0.78	0.29	71,71,71,71	0
59	MG	2w	3005	1/1	0.78	0.11	73,73,73,73	0
59	MG	2w	3006	1/1	0.78	0.10	72,72,72,72	0
59	MG	2A	3516	1/1	0.78	0.30	64,64,64,64	0
59	MG	2A	3742	1/1	0.78	0.13	69,69,69,69	0
59	MG	2A	3748	1/1	0.78	0.18	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3997	1/1	0.78	0.17	41,41,41,41	0
59	MG	1w	112	1/1	0.78	0.10	65,65,65,65	0
59	MG	1a	3425	1/1	0.79	0.23	58,58,58,58	0
59	MG	2A	3792	1/1	0.79	0.17	63,63,63,63	0
59	MG	2A	3636	1/1	0.79	0.18	64,64,64,64	0
59	MG	2A	3247	1/1	0.79	0.27	52,52,52,52	0
59	MG	2A	3249	1/1	0.79	0.13	62,62,62,62	0
59	MG	2B	3003	1/1	0.79	0.27	71,71,71,71	0
59	MG	1A	3193	1/1	0.79	0.15	56,56,56,56	0
59	MG	1A	3454	1/1	0.79	0.11	55,55,55,55	0
59	MG	2A	3524	1/1	0.79	0.19	51,51,51,51	0
59	MG	2A	3084	1/1	0.79	0.32	76,76,76,76	0
59	MG	1F	310	1/1	0.79	0.21	47,47,47,47	0
59	MG	1A	3479	1/1	0.79	0.32	69,69,69,69	0
59	MG	2A	3126	1/1	0.79	0.23	59,59,59,59	0
59	MG	2a	3017	1/1	0.79	0.24	76,76,76,76	0
59	MG	2a	3019	1/1	0.79	0.30	63,63,63,63	0
59	MG	1A	3249	1/1	0.79	0.11	43,43,43,43	0
59	MG	2a	3046	1/1	0.79	0.14	70,70,70,70	0
59	MG	1A	4063	1/1	0.79	0.12	45,45,45,45	0
59	MG	2a	3106	1/1	0.79	0.34	67,67,67,67	0
59	MG	1a	3549	1/1	0.79	0.30	67,67,67,67	0
59	MG	2a	3110	1/1	0.79	0.13	71,71,71,71	0
59	MG	1A	3429	1/1	0.79	0.17	50,50,50,50	0
59	MG	1a	3416	1/1	0.79	0.34	62,62,62,62	0
59	MG	1A	4095	1/1	0.79	0.25	61,61,61,61	0
59	MG	1B	222	1/1	0.79	0.19	50,50,50,50	0
59	MG	2A	3448	1/1	0.79	0.23	70,70,70,70	0
59	MG	2a	3181	1/1	0.79	0.18	55,55,55,55	0
59	MG	2A	3564	1/1	0.80	0.20	54,54,54,54	0
59	MG	18	101	1/1	0.80	0.24	62,62,62,62	0
59	MG	2a	3209	1/1	0.80	0.17	57,57,57,57	0
59	MG	1A	4117	1/1	0.80	0.16	63,63,63,63	0
59	MG	28	102	1/1	0.80	0.29	58,58,58,58	0
59	MG	1a	3462	1/1	0.80	0.24	72,72,72,72	0
59	MG	2A	3480	1/1	0.80	0.13	24,24,24,24	0
59	MG	2A	3264	1/1	0.80	0.17	60,60,60,60	0
59	MG	1A	3869	1/1	0.80	0.12	54,54,54,54	0
59	MG	2a	3036	1/1	0.80	0.17	71,71,71,71	0
59	MG	2A	3029	1/1	0.80	0.27	66,66,66,66	0
59	MG	2a	3044	1/1	0.80	0.20	66,66,66,66	0
59	MG	2A	3626	1/1	0.80	0.14	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1a	3393	1/1	0.80	0.15	70,70,70,70	0
59	MG	2a	3101	1/1	0.80	0.26	59,59,59,59	0
59	MG	2A	3658	1/1	0.80	0.15	68,68,68,68	0
59	MG	1A	4141	1/1	0.80	0.13	36,36,36,36	0
59	MG	1a	3543	1/1	0.80	0.17	68,68,68,68	0
59	MG	1A	3673	1/1	0.80	0.15	33,33,33,33	0
59	MG	2w	3004	1/1	0.80	0.15	75,75,75,75	0
59	MG	1A	3449	1/1	0.80	0.12	54,54,54,54	0
59	MG	1A	4077	1/1	0.80	0.20	59,59,59,59	0
59	MG	2A	3399	1/1	0.80	0.17	55,55,55,55	0
59	MG	2B	3016	1/1	0.80	0.22	77,77,77,77	0
59	MG	2B	3020	1/1	0.80	0.10	80,80,80,80	0
59	MG	2A	3097	1/1	0.80	0.38	74,74,74,74	0
59	MG	2F	301	1/1	0.80	0.31	70,70,70,70	0
59	MG	2A	3687	1/1	0.81	0.12	39,39,39,39	0
59	MG	2a	3183	1/1	0.81	0.17	65,65,65,65	0
59	MG	2B	3018	1/1	0.81	0.19	62,62,62,62	0
59	MG	2A	3275	1/1	0.81	0.23	66,66,66,66	0
59	MG	1a	3567	1/1	0.81	0.10	83,83,83,83	0
59	MG	2A	3022	1/1	0.81	0.14	46,46,46,46	0
59	MG	2A	3193	1/1	0.81	0.21	40,40,40,40	0
59	MG	1E	312	1/1	0.81	0.12	56,56,56,56	0
59	MG	1A	3948	1/1	0.81	0.11	69,69,69,69	0
59	MG	2A	3747	1/1	0.81	0.29	61,61,61,61	0
59	MG	1O	3006	1/1	0.81	0.11	64,64,64,64	0
59	MG	2A	3377	1/1	0.81	0.16	36,36,36,36	0
59	MG	1a	3508	1/1	0.81	0.13	51,51,51,51	0
59	MG	2A	3583	1/1	0.81	0.15	48,48,48,48	0
59	MG	1a	3418	1/1	0.81	0.29	64,64,64,64	0
59	MG	1x	112	1/1	0.81	0.13	47,47,47,47	0
59	MG	2A	3596	1/1	0.81	0.16	60,60,60,60	0
59	MG	1V	202	1/1	0.81	0.11	54,54,54,54	0
59	MG	2a	3066	1/1	0.81	0.21	54,54,54,54	0
59	MG	2A	3605	1/1	0.81	0.20	55,55,55,55	0
59	MG	2A	3457	1/1	0.81	0.13	65,65,65,65	0
59	MG	2A	3255	1/1	0.81	0.32	65,65,65,65	0
59	MG	2A	3791	1/1	0.81	0.13	62,62,62,62	0
59	MG	1A	3907	1/1	0.81	0.16	74,74,74,74	0
59	MG	1a	3424	1/1	0.81	0.19	66,66,66,66	0
59	MG	1A	3745	1/1	0.81	0.19	48,48,48,48	0
59	MG	2A	3813	1/1	0.81	0.18	62,62,62,62	0
59	MG	2y	3002	1/1	0.81	0.14	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	4019	1/1	0.81	0.34	33,33,33,33	0
59	MG	1A	3521	1/1	0.81	0.12	54,54,54,54	0
59	MG	2A	3675	1/1	0.81	0.13	51,51,51,51	0
59	MG	2A	3776	1/1	0.82	0.16	56,56,56,56	0
59	MG	1b	3001	1/1	0.82	0.11	74,74,74,74	0
59	MG	2A	3240	1/1	0.82	0.17	62,62,62,62	0
59	MG	2A	3390	1/1	0.82	0.21	60,60,60,60	0
59	MG	1l	203	1/1	0.82	0.23	64,64,64,64	0
59	MG	2a	3146	1/1	0.82	0.19	79,79,79,79	0
59	MG	1a	3350	1/1	0.82	0.21	61,61,61,61	0
59	MG	2A	3413	1/1	0.82	0.12	43,43,43,43	0
59	MG	2A	3427	1/1	0.82	0.17	49,49,49,49	0
59	MG	2A	3438	1/1	0.82	0.25	77,77,77,77	0
59	MG	1A	3515	1/1	0.82	0.47	71,71,71,71	0
59	MG	2B	3008	1/1	0.82	0.21	66,66,66,66	0
59	MG	2B	3010	1/1	0.82	0.23	60,60,60,60	0
59	MG	1D	313	1/1	0.82	0.29	34,34,34,34	0
59	MG	1a	3402	1/1	0.82	0.22	60,60,60,60	0
59	MG	1A	3647	1/1	0.82	0.22	56,56,56,56	0
59	MG	2A	3474	1/1	0.82	0.21	55,55,55,55	0
59	MG	1A	4138	1/1	0.82	0.14	76,76,76,76	0
59	MG	1A	4074	1/1	0.82	0.16	63,63,63,63	0
59	MG	1A	3828	1/1	0.82	0.12	46,46,46,46	0
59	MG	1A	3844	1/1	0.82	0.17	35,35,35,35	0
59	MG	2A	3272	1/1	0.82	0.23	44,44,44,44	0
59	MG	25	104	1/1	0.82	0.11	61,61,61,61	0
59	MG	2A	3154	1/1	0.82	0.29	58,58,58,58	0
59	MG	2A	3526	1/1	0.82	0.14	54,54,54,54	0
59	MG	2a	3003	1/1	0.82	0.23	54,54,54,54	0
59	MG	2A	3161	1/1	0.82	0.18	67,67,67,67	0
59	MG	2A	3286	1/1	0.82	0.33	58,58,58,58	0
59	MG	2A	3749	1/1	0.82	0.19	55,55,55,55	0
59	MG	2A	3287	1/1	0.82	0.32	65,65,65,65	0
59	MG	2A	3169	1/1	0.82	0.19	53,53,53,53	0
59	MG	2A	3547	1/1	0.82	0.27	67,67,67,67	0
59	MG	1A	3656	1/1	0.82	0.18	57,57,57,57	0
59	MG	2a	3053	1/1	0.82	0.19	58,58,58,58	0
59	MG	1A	3113	1/1	0.82	0.18	37,37,37,37	0
59	MG	2a	3092	1/1	0.82	0.28	61,61,61,61	0
59	MG	1A	3641	1/1	0.82	0.15	40,40,40,40	0
59	MG	2a	3098	1/1	0.82	0.26	69,69,69,69	0
59	MG	2A	3346	1/1	0.82	0.20	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1a	3345	1/1	0.82	0.34	62,62,62,62	0
59	MG	1a	3472	1/1	0.83	0.27	64,64,64,64	0
59	MG	2a	3105	1/1	0.83	0.19	64,64,64,64	0
59	MG	1A	3904	1/1	0.83	0.13	58,58,58,58	0
59	MG	1a	3305	1/1	0.83	0.14	54,54,54,54	0
59	MG	2A	3599	1/1	0.83	0.17	65,65,65,65	0
59	MG	1A	3087	1/1	0.83	0.22	56,56,56,56	0
59	MG	2A	3606	1/1	0.83	0.12	73,73,73,73	0
59	MG	1A	4178	1/1	0.83	0.16	60,60,60,60	0
59	MG	2a	3134	1/1	0.83	0.12	80,80,80,80	0
59	MG	2A	3798	1/1	0.83	0.17	57,57,57,57	0
59	MG	2a	3163	1/1	0.83	0.12	91,91,91,91	0
59	MG	2a	3166	1/1	0.83	0.17	65,65,65,65	0
59	MG	1A	4179	1/1	0.83	0.18	60,60,60,60	0
59	MG	2A	3044	1/1	0.83	0.14	62,62,62,62	0
59	MG	1A	3910	1/1	0.83	0.15	64,64,64,64	0
59	MG	2A	3629	1/1	0.83	0.17	67,67,67,67	0
59	MG	2A	3634	1/1	0.83	0.16	41,41,41,41	0
59	MG	2a	3198	1/1	0.83	0.20	56,56,56,56	0
59	MG	1a	3363	1/1	0.83	0.27	50,50,50,50	0
59	MG	2A	3651	1/1	0.83	0.13	72,72,72,72	0
59	MG	1A	3775	1/1	0.83	0.17	46,46,46,46	0
59	MG	1a	3396	1/1	0.83	0.17	62,62,62,62	0
59	MG	1A	3503	1/1	0.83	0.17	53,53,53,53	0
59	MG	1a	3405	1/1	0.83	0.17	47,47,47,47	0
59	MG	2O	8001	1/1	0.83	0.14	53,53,53,53	0
59	MG	2A	3087	1/1	0.83	0.19	53,53,53,53	0
59	MG	2A	3712	1/1	0.83	0.11	40,40,40,40	0
59	MG	1a	3409	1/1	0.83	0.15	74,74,74,74	0
59	MG	1a	3415	1/1	0.83	0.33	56,56,56,56	0
59	MG	2a	3229	1/1	0.83	0.26	60,60,60,60	0
59	MG	2A	3110	1/1	0.83	0.17	60,60,60,60	0
59	MG	2f	3002	1/1	0.83	0.20	69,69,69,69	0
59	MG	1A	3850	1/1	0.83	0.15	46,46,46,46	0
59	MG	1B	230	1/1	0.83	0.17	59,59,59,59	0
59	MG	2A	3745	1/1	0.83	0.13	48,48,48,48	0
59	MG	1A	3955	1/1	0.83	0.10	68,68,68,68	0
59	MG	2a	3018	1/1	0.83	0.20	67,67,67,67	0
59	MG	1A	3958	1/1	0.83	0.14	45,45,45,45	0
59	MG	2a	3035	1/1	0.83	0.15	57,57,57,57	0
59	MG	1A	3971	1/1	0.83	0.10	45,45,45,45	0
59	MG	2A	3542	1/1	0.83	0.10	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3344	1/1	0.83	0.17	56,56,56,56	0
59	MG	1A	3617	1/1	0.83	0.11	47,47,47,47	0
59	MG	1A	4137	1/1	0.83	0.21	64,64,64,64	0
59	MG	2A	3348	1/1	0.83	0.25	66,66,66,66	0
59	MG	2a	3073	1/1	0.83	0.25	71,71,71,71	0
59	MG	2A	3366	1/1	0.83	0.36	70,70,70,70	0
59	MG	1A	3638	1/1	0.83	0.11	28,28,28,28	0
59	MG	1A	3809	1/1	0.83	0.10	48,48,48,48	0
59	MG	2A	3471	1/1	0.84	0.29	58,58,58,58	0
59	MG	1P	203	1/1	0.84	0.12	49,49,49,49	0
59	MG	1A	3284	1/1	0.84	0.12	37,37,37,37	0
59	MG	2A	3739	1/1	0.84	0.17	49,49,49,49	0
59	MG	2a	3055	1/1	0.84	0.30	58,58,58,58	0
59	MG	2a	3064	1/1	0.84	0.27	70,70,70,70	0
59	MG	2A	3491	1/1	0.84	0.12	53,53,53,53	0
59	MG	1B	204	1/1	0.84	0.26	48,48,48,48	0
59	MG	2a	3081	1/1	0.84	0.18	67,67,67,67	0
59	MG	1a	3414	1/1	0.84	0.30	57,57,57,57	0
59	MG	1A	3732	1/1	0.84	0.17	60,60,60,60	0
59	MG	2A	3262	1/1	0.84	0.14	56,56,56,56	0
59	MG	2A	3755	1/1	0.84	0.24	64,64,64,64	0
59	MG	2a	3102	1/1	0.84	0.15	66,66,66,66	0
59	MG	1A	4012	1/1	0.84	0.21	53,53,53,53	0
59	MG	1A	3138	1/1	0.84	0.23	59,59,59,59	0
59	MG	2a	3107	1/1	0.84	0.28	68,68,68,68	0
59	MG	2A	3764	1/1	0.84	0.16	38,38,38,38	0
59	MG	1a	3326	1/1	0.84	0.32	56,56,56,56	0
59	MG	2a	3112	1/1	0.84	0.21	51,51,51,51	0
59	MG	2A	3088	1/1	0.84	0.17	65,65,65,65	0
59	MG	2a	3116	1/1	0.84	0.26	65,65,65,65	0
59	MG	1A	3741	1/1	0.84	0.15	46,46,46,46	0
59	MG	2A	3099	1/1	0.84	0.15	51,51,51,51	0
59	MG	1A	3338	1/1	0.84	0.17	42,42,42,42	0
59	MG	2a	3138	1/1	0.84	0.11	88,88,88,88	0
59	MG	2A	3288	1/1	0.84	0.09	67,67,67,67	0
59	MG	1B	231	1/1	0.84	0.22	63,63,63,63	0
59	MG	2A	3778	1/1	0.84	0.22	63,63,63,63	0
59	MG	2A	3557	1/1	0.84	0.13	53,53,53,53	0
59	MG	2A	3783	1/1	0.84	0.11	73,73,73,73	0
59	MG	2A	3119	1/1	0.84	0.21	61,61,61,61	0
59	MG	2A	3292	1/1	0.84	0.19	66,66,66,66	0
59	MG	2A	3295	1/1	0.84	0.16	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2a	3187	1/1	0.84	0.14	71,71,71,71	0
59	MG	2A	3582	1/1	0.84	0.14	29,29,29,29	0
59	MG	1v	3001	1/1	0.84	0.14	60,60,60,60	0
59	MG	2A	3584	1/1	0.84	0.17	52,52,52,52	0
59	MG	2A	3585	1/1	0.84	0.17	59,59,59,59	0
59	MG	2A	3309	1/1	0.84	0.13	57,57,57,57	0
59	MG	2A	3845	1/1	0.84	0.52	49,49,49,49	0
59	MG	1w	109	1/1	0.84	0.17	68,68,68,68	0
59	MG	2B	3007	1/1	0.84	0.17	69,69,69,69	0
59	MG	2A	3594	1/1	0.84	0.11	64,64,64,64	0
59	MG	2A	3338	1/1	0.84	0.44	66,66,66,66	0
59	MG	1A	3254	1/1	0.84	0.23	64,64,64,64	0
59	MG	1a	3362	1/1	0.84	0.13	51,51,51,51	0
59	MG	1x	103	1/1	0.84	0.15	60,60,60,60	0
59	MG	1a	3436	1/1	0.84	0.31	56,56,56,56	0
59	MG	2A	3354	1/1	0.84	0.20	61,61,61,61	0
59	MG	2D	304	1/1	0.84	0.60	44,44,44,44	0
59	MG	2E	303	1/1	0.84	0.24	53,53,53,53	0
59	MG	1A	3778	1/1	0.84	0.12	38,38,38,38	0
59	MG	2A	3178	1/1	0.84	0.19	50,50,50,50	0
59	MG	2p	3001	1/1	0.84	0.20	63,63,63,63	0
59	MG	1a	3364	1/1	0.84	0.27	53,53,53,53	0
59	MG	1a	3369	1/1	0.84	0.17	64,64,64,64	0
59	MG	1a	3372	1/1	0.84	0.22	64,64,64,64	0
59	MG	2A	3211	1/1	0.84	0.23	61,61,61,61	0
59	MG	2A	3216	1/1	0.84	0.14	47,47,47,47	0
59	MG	1A	3102	1/1	0.84	0.13	46,46,46,46	0
59	MG	2A	3662	1/1	0.84	0.20	69,69,69,69	0
59	MG	2A	3233	1/1	0.84	0.30	66,66,66,66	0
59	MG	1a	3511	1/1	0.84	0.14	46,46,46,46	0
59	MG	2x	104	1/1	0.84	0.21	71,71,71,71	0
59	MG	2y	3001	1/1	0.84	0.14	65,65,65,65	0
59	MG	1a	3394	1/1	0.84	0.24	61,61,61,61	0
59	MG	2A	3455	1/1	0.84	0.17	65,65,65,65	0
59	MG	1A	3508	1/1	0.84	0.13	53,53,53,53	0
59	MG	1a	3544	1/1	0.84	0.23	66,66,66,66	0
59	MG	1A	4073	1/1	0.85	0.14	40,40,40,40	0
59	MG	1a	3365	1/1	0.85	0.13	62,62,62,62	0
59	MG	1A	3545	1/1	0.85	0.12	21,21,21,21	0
59	MG	2a	3080	1/1	0.85	0.18	58,58,58,58	0
59	MG	1A	3909	1/1	0.85	0.18	58,58,58,58	0
59	MG	2a	3082	1/1	0.85	0.24	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2a	3085	1/1	0.85	0.24	69,69,69,69	0
59	MG	2a	3088	1/1	0.85	0.21	61,61,61,61	0
59	MG	2a	3089	1/1	0.85	0.24	67,67,67,67	0
59	MG	1a	3381	1/1	0.85	0.22	62,62,62,62	0
59	MG	2A	3761	1/1	0.85	0.17	61,61,61,61	0
59	MG	2A	3538	1/1	0.85	0.13	47,47,47,47	0
59	MG	2A	3089	1/1	0.85	0.20	78,78,78,78	0
59	MG	2A	3095	1/1	0.85	0.21	60,60,60,60	0
59	MG	2A	3543	1/1	0.85	0.12	46,46,46,46	0
59	MG	2A	3770	1/1	0.85	0.19	53,53,53,53	0
59	MG	1a	3388	1/1	0.85	0.35	61,61,61,61	0
59	MG	2A	3551	1/1	0.85	0.14	60,60,60,60	0
59	MG	1A	3487	1/1	0.85	0.12	55,55,55,55	0
59	MG	1B	236	1/1	0.85	0.12	57,57,57,57	0
59	MG	1A	3678	1/1	0.85	0.22	57,57,57,57	0
59	MG	2A	3559	1/1	0.85	0.15	38,38,38,38	0
59	MG	2A	3782	1/1	0.85	0.10	60,60,60,60	0
59	MG	2a	3122	1/1	0.85	0.24	67,67,67,67	0
59	MG	1a	3401	1/1	0.85	0.11	48,48,48,48	0
59	MG	2A	3566	1/1	0.85	0.12	71,71,71,71	0
59	MG	2A	3306	1/1	0.85	0.28	60,60,60,60	0
59	MG	1A	3489	1/1	0.85	0.11	33,33,33,33	0
59	MG	2a	3160	1/1	0.85	0.13	73,73,73,73	0
59	MG	1a	3404	1/1	0.85	0.41	65,65,65,65	0
59	MG	2A	3315	1/1	0.85	0.34	63,63,63,63	0
59	MG	1A	3271	1/1	0.85	0.36	35,35,35,35	0
59	MG	2A	3799	1/1	0.85	0.16	60,60,60,60	0
59	MG	2A	3809	1/1	0.85	0.11	55,55,55,55	0
59	MG	1a	3406	1/1	0.85	0.22	50,50,50,50	0
59	MG	2A	3831	1/1	0.85	0.30	39,39,39,39	0
59	MG	1A	3629	1/1	0.85	0.10	17,17,17,17	0
59	MG	2a	3193	1/1	0.85	0.16	70,70,70,70	0
59	MG	1a	3410	1/1	0.85	0.20	59,59,59,59	0
59	MG	1A	3303	1/1	0.85	0.18	50,50,50,50	0
59	MG	2a	3204	1/1	0.85	0.28	62,62,62,62	0
59	MG	2A	3173	1/1	0.85	0.18	62,62,62,62	0
59	MG	1A	4125	1/1	0.85	0.18	40,40,40,40	0
59	MG	2A	3180	1/1	0.85	0.14	53,53,53,53	0
59	MG	2B	3011	1/1	0.85	0.21	62,62,62,62	0
59	MG	2A	3188	1/1	0.85	0.17	53,53,53,53	0
59	MG	1A	3394	1/1	0.85	0.12	60,60,60,60	0
59	MG	1A	3988	1/1	0.85	0.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3198	1/1	0.85	0.13	71,71,71,71	0
59	MG	2a	3219	1/1	0.85	0.13	73,73,73,73	0
59	MG	1x	111	1/1	0.85	0.19	65,65,65,65	0
59	MG	2A	3628	1/1	0.85	0.11	43,43,43,43	0
59	MG	2a	3226	1/1	0.85	0.22	59,59,59,59	0
59	MG	1A	3995	1/1	0.85	0.18	49,49,49,49	0
59	MG	2A	3422	1/1	0.85	0.14	67,67,67,67	0
59	MG	2a	3236	1/1	0.85	0.09	75,75,75,75	0
59	MG	2a	3238	1/1	0.85	0.16	62,62,62,62	0
59	MG	2F	303	1/1	0.85	0.47	54,54,54,54	0
59	MG	1A	3518	1/1	0.85	0.39	63,63,63,63	0
59	MG	2A	3637	1/1	0.85	0.11	61,61,61,61	0
59	MG	2A	3428	1/1	0.85	0.16	63,63,63,63	0
59	MG	1a	3315	1/1	0.85	0.13	48,48,48,48	0
59	MG	2A	3224	1/1	0.85	0.10	49,49,49,49	0
59	MG	2q	201	1/1	0.85	0.16	50,50,50,50	0
59	MG	1A	3857	1/1	0.85	0.11	22,22,22,22	0
59	MG	1A	3746	1/1	0.85	0.17	48,48,48,48	0
59	MG	1a	3429	1/1	0.85	0.21	61,61,61,61	0
59	MG	2w	3002	1/1	0.85	0.18	73,73,73,73	0
59	MG	1a	3336	1/1	0.85	0.26	60,60,60,60	0
59	MG	2a	3013	1/1	0.85	0.22	68,68,68,68	0
59	MG	2A	3708	1/1	0.85	0.16	29,29,29,29	0
59	MG	1A	3758	1/1	0.85	0.11	37,37,37,37	0
59	MG	1A	4036	1/1	0.85	0.09	46,46,46,46	0
59	MG	2A	3250	1/1	0.85	0.13	56,56,56,56	0
59	MG	2A	3486	1/1	0.85	0.22	61,61,61,61	0
59	MG	1a	3354	1/1	0.85	0.13	66,66,66,66	0
59	MG	1a	3478	1/1	0.85	0.11	68,68,68,68	0
59	MG	1B	217	1/1	0.85	0.11	41,41,41,41	0
59	MG	1A	3773	1/1	0.85	0.10	57,57,57,57	0
59	MG	1A	3223	1/1	0.85	0.17	40,40,40,40	0
59	MG	2A	3291	1/1	0.86	0.28	74,74,74,74	0
59	MG	1A	4112	1/1	0.86	0.14	56,56,56,56	0
59	MG	2A	3601	1/1	0.86	0.14	60,60,60,60	0
59	MG	1A	3441	1/1	0.86	0.10	62,62,62,62	0
59	MG	2A	3297	1/1	0.86	0.18	52,52,52,52	0
59	MG	2a	3006	1/1	0.86	0.47	76,76,76,76	0
59	MG	2a	3009	1/1	0.86	0.31	67,67,67,67	0
59	MG	1A	3103	1/1	0.86	0.11	34,34,34,34	0
59	MG	2A	3613	1/1	0.86	0.13	36,36,36,36	0
59	MG	2A	3614	1/1	0.86	0.15	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1a	3325	1/1	0.86	0.16	50,50,50,50	0
59	MG	1a	3439	1/1	0.86	0.15	63,63,63,63	0
59	MG	2A	3625	1/1	0.86	0.20	67,67,67,67	0
59	MG	2A	3312	1/1	0.86	0.12	55,55,55,55	0
59	MG	2A	3313	1/1	0.86	0.25	54,54,54,54	0
59	MG	2a	3045	1/1	0.86	0.23	58,58,58,58	0
59	MG	1a	3453	1/1	0.86	0.13	64,64,64,64	0
59	MG	1A	3349	1/1	0.86	0.09	49,49,49,49	0
59	MG	2A	3329	1/1	0.86	0.10	59,59,59,59	0
59	MG	2A	3336	1/1	0.86	0.34	57,57,57,57	0
59	MG	2a	3065	1/1	0.86	0.20	58,58,58,58	0
59	MG	1A	3350	1/1	0.86	0.16	57,57,57,57	0
59	MG	2A	3652	1/1	0.86	0.12	60,60,60,60	0
59	MG	2A	3654	1/1	0.86	0.14	62,62,62,62	0
59	MG	1A	4127	1/1	0.86	0.25	44,44,44,44	0
59	MG	2A	3100	1/1	0.86	0.20	65,65,65,65	0
59	MG	1A	4135	1/1	0.86	0.29	40,40,40,40	0
59	MG	2A	3669	1/1	0.86	0.11	69,69,69,69	0
59	MG	1a	3489	1/1	0.86	0.10	85,85,85,85	0
59	MG	2a	3091	1/1	0.86	0.17	77,77,77,77	0
59	MG	1A	3461	1/1	0.86	0.12	58,58,58,58	0
59	MG	1a	3504	1/1	0.86	0.12	57,57,57,57	0
59	MG	2A	3690	1/1	0.86	0.15	37,37,37,37	0
59	MG	2A	3368	1/1	0.86	0.13	63,63,63,63	0
59	MG	1A	3783	1/1	0.86	0.11	64,64,64,64	0
59	MG	1A	3788	1/1	0.86	0.22	27,27,27,27	0
59	MG	2A	3380	1/1	0.86	0.12	41,41,41,41	0
59	MG	1a	3361	1/1	0.86	0.18	68,68,68,68	0
59	MG	1A	3470	1/1	0.86	0.23	47,47,47,47	0
59	MG	2A	3162	1/1	0.86	0.12	56,56,56,56	0
59	MG	2A	3165	1/1	0.86	0.15	61,61,61,61	0
59	MG	2A	3414	1/1	0.86	0.08	43,43,43,43	0
59	MG	1A	3973	1/1	0.86	0.12	28,28,28,28	0
59	MG	1A	3800	1/1	0.86	0.15	30,30,30,30	0
59	MG	1A	3990	1/1	0.86	0.20	46,46,46,46	0
59	MG	2a	3131	1/1	0.86	0.10	77,77,77,77	0
59	MG	1A	4205	1/1	0.86	0.15	45,45,45,45	0
59	MG	2A	3179	1/1	0.86	0.12	46,46,46,46	0
59	MG	1a	3370	1/1	0.86	0.27	67,67,67,67	0
59	MG	2A	3452	1/1	0.86	0.21	56,56,56,56	0
59	MG	2a	3153	1/1	0.86	0.09	80,80,80,80	0
59	MG	2a	3158	1/1	0.86	0.13	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3644	1/1	0.86	0.09	56,56,56,56	0
59	MG	2A	3189	1/1	0.86	0.13	54,54,54,54	0
59	MG	2A	3458	1/1	0.86	0.10	53,53,53,53	0
59	MG	1a	3373	1/1	0.86	0.23	59,59,59,59	0
59	MG	2a	3179	1/1	0.86	0.20	64,64,64,64	0
59	MG	1a	3380	1/1	0.86	0.15	48,48,48,48	0
59	MG	1A	3045	1/1	0.86	0.13	53,53,53,53	0
59	MG	1a	3384	1/1	0.86	0.20	46,46,46,46	0
59	MG	1a	3385	1/1	0.86	0.33	57,57,57,57	0
59	MG	2a	3185	1/1	0.86	0.09	64,64,64,64	0
59	MG	1A	4005	1/1	0.86	0.17	52,52,52,52	0
59	MG	2A	3492	1/1	0.86	0.11	44,44,44,44	0
59	MG	1a	3391	1/1	0.86	0.16	55,55,55,55	0
59	MG	2A	3507	1/1	0.86	0.13	33,33,33,33	0
59	MG	2A	3223	1/1	0.86	0.09	59,59,59,59	0
59	MG	1w	108	1/1	0.86	0.19	59,59,59,59	0
59	MG	2A	3225	1/1	0.86	0.17	53,53,53,53	0
59	MG	2A	3231	1/1	0.86	0.10	75,75,75,75	0
59	MG	1A	3129	1/1	0.86	0.14	36,36,36,36	0
59	MG	2A	3794	1/1	0.86	0.15	61,61,61,61	0
59	MG	1A	3652	1/1	0.86	0.13	35,35,35,35	0
59	MG	1A	3132	1/1	0.86	0.14	30,30,30,30	0
59	MG	1A	3226	1/1	0.86	0.28	56,56,56,56	0
59	MG	2a	3217	1/1	0.86	0.19	58,58,58,58	0
59	MG	2A	3801	1/1	0.86	0.12	55,55,55,55	0
59	MG	1A	3062	1/1	0.86	0.24	47,47,47,47	0
59	MG	1B	232	1/1	0.86	0.10	67,67,67,67	0
59	MG	1A	3314	1/1	0.86	0.13	47,47,47,47	0
59	MG	1A	3861	1/1	0.86	0.10	39,39,39,39	0
59	MG	2A	3844	1/1	0.86	0.25	48,48,48,48	0
59	MG	1A	3516	1/1	0.86	0.21	49,49,49,49	0
59	MG	2A	3258	1/1	0.86	0.24	68,68,68,68	0
59	MG	2A	3553	1/1	0.86	0.20	63,63,63,63	0
59	MG	1A	4076	1/1	0.86	0.09	43,43,43,43	0
59	MG	2A	3556	1/1	0.86	0.12	60,60,60,60	0
59	MG	1a	3412	1/1	0.86	0.22	51,51,51,51	0
59	MG	1A	3252	1/1	0.86	0.10	28,28,28,28	0
59	MG	2A	3005	1/1	0.86	0.14	62,62,62,62	0
59	MG	2B	3017	1/1	0.86	0.15	57,57,57,57	0
59	MG	1A	3433	1/1	0.86	0.15	56,56,56,56	0
59	MG	2t	3001	1/1	0.86	0.17	53,53,53,53	0
59	MG	2B	3019	1/1	0.86	0.15	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3271	1/1	0.86	0.14	71,71,71,71	0
59	MG	1P	204	1/1	0.86	0.20	41,41,41,41	0
59	MG	1R	203	1/1	0.86	0.16	33,33,33,33	0
59	MG	1S	3001	1/1	0.86	0.30	39,39,39,39	0
59	MG	2A	3285	1/1	0.86	0.12	52,52,52,52	0
59	MG	1A	3526	1/1	0.86	0.23	59,59,59,59	0
59	MG	2G	3001	1/1	0.86	0.25	64,64,64,64	0
59	MG	2x	101	1/1	0.86	0.18	72,72,72,72	0
59	MG	2A	3067	1/1	0.86	0.16	55,55,55,55	0
59	MG	2Q	3004	1/1	0.86	0.15	45,45,45,45	0
59	MG	2R	202	1/1	0.86	0.20	61,61,61,61	0
59	MG	1A	4110	1/1	0.86	0.12	62,62,62,62	0
59	MG	1A	3440	1/1	0.86	0.17	70,70,70,70	0
59	MG	2A	3079	1/1	0.86	0.23	60,60,60,60	0
59	MG	2U	204	1/1	0.86	0.25	49,49,49,49	0
59	MG	1B	212	1/1	0.87	0.12	42,42,42,42	0
59	MG	1a	3353	1/1	0.87	0.24	58,58,58,58	0
59	MG	2a	3074	1/1	0.87	0.13	64,64,64,64	0
59	MG	1A	3556	1/1	0.87	0.14	30,30,30,30	0
59	MG	1A	3671	1/1	0.87	0.13	57,57,57,57	0
59	MG	2A	3041	1/1	0.87	0.28	60,60,60,60	0
59	MG	1B	221	1/1	0.87	0.18	52,52,52,52	0
59	MG	2a	3087	1/1	0.87	0.28	65,65,65,65	0
59	MG	2A	3510	1/1	0.87	0.10	58,58,58,58	0
59	MG	1a	3459	1/1	0.87	0.10	66,66,66,66	0
59	MG	1A	4075	1/1	0.87	0.13	21,21,21,21	0
59	MG	2A	3068	1/1	0.87	0.15	52,52,52,52	0
59	MG	1a	3466	1/1	0.87	0.32	72,72,72,72	0
59	MG	1A	3569	1/1	0.87	0.11	42,42,42,42	0
59	MG	2A	3527	1/1	0.87	0.13	65,65,65,65	0
59	MG	1A	3310	1/1	0.87	0.32	40,40,40,40	0
59	MG	1A	4082	1/1	0.87	0.10	50,50,50,50	0
59	MG	2A	3083	1/1	0.87	0.25	61,61,61,61	0
59	MG	1a	3366	1/1	0.87	0.15	57,57,57,57	0
59	MG	2A	3274	1/1	0.87	0.28	59,59,59,59	0
59	MG	1a	3490	1/1	0.87	0.11	57,57,57,57	0
59	MG	1A	4085	1/1	0.87	0.14	64,64,64,64	0
59	MG	2A	3545	1/1	0.87	0.12	61,61,61,61	0
59	MG	1a	3493	1/1	0.87	0.17	51,51,51,51	0
59	MG	2A	3550	1/1	0.87	0.09	56,56,56,56	0
59	MG	1A	3699	1/1	0.87	0.11	37,37,37,37	0
59	MG	1a	3505	1/1	0.87	0.11	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1B	233	1/1	0.87	0.16	64,64,64,64	0
59	MG	1A	3232	1/1	0.87	0.14	51,51,51,51	0
59	MG	1a	3535	1/1	0.87	0.16	59,59,59,59	0
59	MG	2A	3796	1/1	0.87	0.14	70,70,70,70	0
59	MG	1D	312	1/1	0.87	0.09	49,49,49,49	0
59	MG	1A	3612	1/1	0.87	0.11	45,45,45,45	0
59	MG	1A	3810	1/1	0.87	0.11	38,38,38,38	0
59	MG	1F	309	1/1	0.87	0.08	36,36,36,36	0
59	MG	2A	3569	1/1	0.87	0.19	59,59,59,59	0
59	MG	2a	3170	1/1	0.87	0.18	49,49,49,49	0
59	MG	2A	3137	1/1	0.87	0.28	60,60,60,60	0
59	MG	2A	3574	1/1	0.87	0.20	56,56,56,56	0
59	MG	2A	3837	1/1	0.87	0.15	61,61,61,61	0
59	MG	2A	3140	1/1	0.87	0.34	72,72,72,72	0
59	MG	1A	3504	1/1	0.87	0.20	53,53,53,53	0
59	MG	2A	3145	1/1	0.87	0.19	62,62,62,62	0
59	MG	1O	3001	1/1	0.87	0.11	54,54,54,54	0
59	MG	2a	3186	1/1	0.87	0.39	69,69,69,69	0
59	MG	2A	3324	1/1	0.87	0.21	53,53,53,53	0
59	MG	2A	3150	1/1	0.87	0.14	42,42,42,42	0
59	MG	2A	3151	1/1	0.87	0.19	74,74,74,74	0
59	MG	1A	3824	1/1	0.87	0.09	35,35,35,35	0
59	MG	1A	3986	1/1	0.87	0.12	61,61,61,61	0
59	MG	1a	3559	1/1	0.87	0.18	69,69,69,69	0
59	MG	1a	3562	1/1	0.87	0.21	63,63,63,63	0
59	MG	2a	3208	1/1	0.87	0.13	63,63,63,63	0
59	MG	1a	3565	1/1	0.87	0.16	35,35,35,35	0
59	MG	1A	3628	1/1	0.87	0.08	21,21,21,21	0
59	MG	2A	3350	1/1	0.87	0.28	57,57,57,57	0
59	MG	1a	3399	1/1	0.87	0.16	42,42,42,42	0
59	MG	2a	3214	1/1	0.87	0.25	68,68,68,68	0
59	MG	2A	3362	1/1	0.87	0.09	57,57,57,57	0
59	MG	1A	4122	1/1	0.87	0.12	44,44,44,44	0
59	MG	1A	3835	1/1	0.87	0.15	51,51,51,51	0
59	MG	1f	3003	1/1	0.87	0.29	57,57,57,57	0
59	MG	1A	3237	1/1	0.87	0.15	52,52,52,52	0
59	MG	2A	3627	1/1	0.87	0.13	53,53,53,53	0
59	MG	1A	3126	1/1	0.87	0.27	29,29,29,29	0
59	MG	1A	4003	1/1	0.87	0.13	54,54,54,54	0
59	MG	1A	3057	1/1	0.87	0.07	26,26,26,26	0
59	MG	1A	3413	1/1	0.87	0.25	49,49,49,49	0
59	MG	2A	3410	1/1	0.87	0.10	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2Z	8001	1/1	0.87	0.22	68,68,68,68	0
59	MG	1a	3314	1/1	0.87	0.10	53,53,53,53	0
59	MG	1A	3033	1/1	0.87	0.26	57,57,57,57	0
59	MG	1a	3322	1/1	0.87	0.28	51,51,51,51	0
59	MG	1A	3774	1/1	0.87	0.10	52,52,52,52	0
59	MG	1A	3896	1/1	0.87	0.15	54,54,54,54	0
59	MG	1a	3327	1/1	0.87	0.22	60,60,60,60	0
59	MG	2A	3441	1/1	0.87	0.11	29,29,29,29	0
59	MG	1A	4052	1/1	0.87	0.16	60,60,60,60	0
59	MG	2A	3686	1/1	0.87	0.10	48,48,48,48	0
59	MG	1a	3331	1/1	0.87	0.39	60,60,60,60	0
59	MG	2A	3232	1/1	0.87	0.17	63,63,63,63	0
59	MG	2a	3027	1/1	0.87	0.34	63,63,63,63	0
59	MG	2a	3031	1/1	0.87	0.19	57,57,57,57	0
59	MG	1A	3360	1/1	0.87	0.11	42,42,42,42	0
59	MG	2A	3235	1/1	0.87	0.29	62,62,62,62	0
59	MG	2A	3236	1/1	0.87	0.32	57,57,57,57	0
59	MG	2A	3718	1/1	0.87	0.10	52,52,52,52	0
59	MG	2x	102	1/1	0.87	0.17	64,64,64,64	0
59	MG	2A	3239	1/1	0.87	0.19	61,61,61,61	0
59	MG	2A	3468	1/1	0.87	0.09	32,32,32,32	0
59	MG	1A	3367	1/1	0.87	0.14	59,59,59,59	0
59	MG	2A	3473	1/1	0.87	0.20	63,63,63,63	0
59	MG	2a	3059	1/1	0.87	0.11	53,53,53,53	0
59	MG	2A	3738	1/1	0.87	0.18	60,60,60,60	0
59	MG	1a	3427	1/1	0.87	0.15	64,64,64,64	0
59	MG	1a	3476	1/1	0.88	0.09	55,55,55,55	0
59	MG	1a	3477	1/1	0.88	0.16	67,67,67,67	0
59	MG	2a	3058	1/1	0.88	0.24	70,70,70,70	0
59	MG	1a	3359	1/1	0.88	0.21	66,66,66,66	0
59	MG	2A	3477	1/1	0.88	0.19	57,57,57,57	0
59	MG	1A	4060	1/1	0.88	0.15	27,27,27,27	0
59	MG	2A	3481	1/1	0.88	0.11	37,37,37,37	0
59	MG	2a	3067	1/1	0.88	0.15	56,56,56,56	0
59	MG	1a	3487	1/1	0.88	0.21	62,62,62,62	0
59	MG	1A	3378	1/1	0.88	0.26	62,62,62,62	0
59	MG	1A	3893	1/1	0.88	0.19	39,39,39,39	0
59	MG	1A	3895	1/1	0.88	0.10	39,39,39,39	0
59	MG	1A	3177	1/1	0.88	0.17	47,47,47,47	0
59	MG	2A	3751	1/1	0.88	0.19	50,50,50,50	0
59	MG	1A	3321	1/1	0.88	0.12	49,49,49,49	0
59	MG	1A	3537	1/1	0.88	0.12	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3787	1/1	0.88	0.12	49,49,49,49	0
59	MG	2A	3270	1/1	0.88	0.14	62,62,62,62	0
59	MG	1A	4078	1/1	0.88	0.08	58,58,58,58	0
59	MG	1B	235	1/1	0.88	0.11	63,63,63,63	0
59	MG	1a	3374	1/1	0.88	0.21	53,53,53,53	0
59	MG	1A	3654	1/1	0.88	0.13	54,54,54,54	0
59	MG	1D	310	1/1	0.88	0.16	43,43,43,43	0
59	MG	2A	3533	1/1	0.88	0.11	55,55,55,55	0
59	MG	2A	3773	1/1	0.88	0.10	40,40,40,40	0
59	MG	1A	3325	1/1	0.88	0.22	31,31,31,31	0
59	MG	1A	3462	1/1	0.88	0.09	50,50,50,50	0
59	MG	1A	4098	1/1	0.88	0.12	37,37,37,37	0
59	MG	2A	3128	1/1	0.88	0.14	50,50,50,50	0
59	MG	2A	3779	1/1	0.88	0.13	67,67,67,67	0
59	MG	1F	302	1/1	0.88	0.19	50,50,50,50	0
59	MG	1A	3918	1/1	0.88	0.09	27,27,27,27	0
59	MG	1A	3561	1/1	0.88	0.14	48,48,48,48	0
59	MG	1A	3143	1/1	0.88	0.25	56,56,56,56	0
59	MG	2A	3293	1/1	0.88	0.20	55,55,55,55	0
59	MG	1A	3693	1/1	0.88	0.12	13,13,13,13	0
59	MG	2a	3135	1/1	0.88	0.16	60,60,60,60	0
59	MG	2A	3147	1/1	0.88	0.21	53,53,53,53	0
59	MG	2A	3298	1/1	0.88	0.25	41,41,41,41	0
59	MG	2A	3300	1/1	0.88	0.23	46,46,46,46	0
59	MG	1A	3573	1/1	0.88	0.10	32,32,32,32	0
59	MG	1A	3812	1/1	0.88	0.15	57,57,57,57	0
59	MG	1Q	204	1/1	0.88	0.12	46,46,46,46	0
59	MG	2A	3565	1/1	0.88	0.15	49,49,49,49	0
59	MG	2A	3310	1/1	0.88	0.19	53,53,53,53	0
59	MG	2a	3174	1/1	0.88	0.15	74,74,74,74	0
59	MG	1A	3340	1/1	0.88	0.32	46,46,46,46	0
59	MG	2A	3814	1/1	0.88	0.10	44,44,44,44	0
59	MG	2A	3822	1/1	0.88	0.09	33,33,33,33	0
59	MG	1A	3982	1/1	0.88	0.12	57,57,57,57	0
59	MG	2A	3314	1/1	0.88	0.32	60,60,60,60	0
59	MG	1A	3188	1/1	0.88	0.23	37,37,37,37	0
59	MG	2A	3168	1/1	0.88	0.12	59,59,59,59	0
59	MG	1n	503	1/1	0.88	0.15	49,49,49,49	0
59	MG	2A	3327	1/1	0.88	0.23	62,62,62,62	0
59	MG	2a	3188	1/1	0.88	0.11	64,64,64,64	0
59	MG	1A	3594	1/1	0.88	0.08	15,15,15,15	0
59	MG	2a	3196	1/1	0.88	0.14	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3332	1/1	0.88	0.40	64,64,64,64	0
59	MG	2A	3171	1/1	0.88	0.09	44,44,44,44	0
59	MG	2A	3172	1/1	0.88	0.16	54,54,54,54	0
59	MG	1A	4131	1/1	0.88	0.15	40,40,40,40	0
59	MG	1w	104	1/1	0.88	0.13	66,66,66,66	0
59	MG	2A	3600	1/1	0.88	0.15	55,55,55,55	0
59	MG	1l	101	1/1	0.88	0.14	45,45,45,45	0
59	MG	16	104	1/1	0.88	0.22	43,43,43,43	0
59	MG	2A	3185	1/1	0.88	0.12	53,53,53,53	0
59	MG	1w	110	1/1	0.88	0.13	81,81,81,81	0
59	MG	2A	3361	1/1	0.88	0.10	66,66,66,66	0
59	MG	1A	3415	1/1	0.88	0.17	45,45,45,45	0
59	MG	1A	3839	1/1	0.88	0.26	25,25,25,25	0
59	MG	2A	3367	1/1	0.88	0.16	52,52,52,52	0
59	MG	1A	3843	1/1	0.88	0.14	19,19,19,19	0
59	MG	2A	3194	1/1	0.88	0.32	38,38,38,38	0
59	MG	2O	8002	1/1	0.88	0.13	48,48,48,48	0
59	MG	2Q	3002	1/1	0.88	0.24	48,48,48,48	0
59	MG	1x	109	1/1	0.88	0.11	68,68,68,68	0
59	MG	2A	3202	1/1	0.88	0.13	51,51,51,51	0
59	MG	2A	3204	1/1	0.88	0.23	58,58,58,58	0
59	MG	2A	3205	1/1	0.88	0.36	73,73,73,73	0
59	MG	2A	3207	1/1	0.88	0.08	56,56,56,56	0
59	MG	1A	3291	1/1	0.88	0.11	43,43,43,43	0
59	MG	1A	3849	1/1	0.88	0.13	54,54,54,54	0
59	MG	20	3001	1/1	0.88	0.23	66,66,66,66	0
59	MG	1A	4148	1/1	0.88	0.26	60,60,60,60	0
59	MG	1A	3155	1/1	0.88	0.14	61,61,61,61	0
59	MG	1A	3201	1/1	0.88	0.16	55,55,55,55	0
59	MG	2q	203	1/1	0.88	0.17	53,53,53,53	0
59	MG	1A	3081	1/1	0.88	0.23	51,51,51,51	0
59	MG	1A	4187	1/1	0.88	0.18	47,47,47,47	0
59	MG	2A	3667	1/1	0.88	0.16	47,47,47,47	0
59	MG	1a	3335	1/1	0.88	0.17	57,57,57,57	0
59	MG	2A	3671	1/1	0.88	0.17	66,66,66,66	0
59	MG	2a	3014	1/1	0.88	0.19	57,57,57,57	0
59	MG	2A	3674	1/1	0.88	0.28	61,61,61,61	0
59	MG	1A	4190	1/1	0.88	0.30	42,42,42,42	0
59	MG	1A	3368	1/1	0.88	0.12	39,39,39,39	0
59	MG	1A	4210	1/1	0.88	0.18	30,30,30,30	0
59	MG	2a	3030	1/1	0.88	0.21	60,60,60,60	0
59	MG	1a	3460	1/1	0.88	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	4045	1/1	0.88	0.11	53,53,53,53	0
59	MG	2A	3706	1/1	0.88	0.08	70,70,70,70	0
59	MG	1A	4048	1/1	0.88	0.07	33,33,33,33	0
59	MG	2a	3038	1/1	0.88	0.19	78,78,78,78	0
59	MG	2A	3242	1/1	0.88	0.19	56,56,56,56	0
59	MG	2y	3004	1/1	0.88	0.10	66,66,66,66	0
59	MG	1A	3876	1/1	0.88	0.14	60,60,60,60	0
59	MG	2A	3722	1/1	0.88	0.12	72,72,72,72	0
59	MG	2A	3639	1/1	0.89	0.08	47,47,47,47	0
59	MG	1a	3542	1/1	0.89	0.12	53,53,53,53	0
59	MG	1A	3485	1/1	0.89	0.24	41,41,41,41	0
59	MG	1A	3794	1/1	0.89	0.09	57,57,57,57	0
59	MG	1A	4221	1/1	0.89	0.26	31,31,31,31	0
59	MG	2a	3028	1/1	0.89	0.22	64,64,64,64	0
59	MG	1A	3631	1/1	0.89	0.16	16,16,16,16	0
59	MG	1A	3326	1/1	0.89	0.10	49,49,49,49	0
59	MG	2a	3033	1/1	0.89	0.16	56,56,56,56	0
59	MG	2a	3034	1/1	0.89	0.21	53,53,53,53	0
59	MG	1B	214	1/1	0.89	0.09	55,55,55,55	0
59	MG	1a	3556	1/1	0.89	0.09	46,46,46,46	0
59	MG	2A	3176	1/1	0.89	0.13	44,44,44,44	0
59	MG	2A	3177	1/1	0.89	0.19	63,63,63,63	0
59	MG	2a	3040	1/1	0.89	0.23	47,47,47,47	0
59	MG	2a	3042	1/1	0.89	0.08	70,70,70,70	0
59	MG	2A	3391	1/1	0.89	0.10	41,41,41,41	0
59	MG	1A	3330	1/1	0.89	0.30	36,36,36,36	0
59	MG	1A	3642	1/1	0.89	0.11	56,56,56,56	0
59	MG	1A	3399	1/1	0.89	0.29	67,67,67,67	0
59	MG	2A	3181	1/1	0.89	0.22	57,57,57,57	0
59	MG	2A	3702	1/1	0.89	0.10	64,64,64,64	0
59	MG	1A	3400	1/1	0.89	0.12	51,51,51,51	0
59	MG	2a	3063	1/1	0.89	0.18	55,55,55,55	0
59	MG	1A	3331	1/1	0.89	0.11	41,41,41,41	0
59	MG	1A	3649	1/1	0.89	0.11	55,55,55,55	0
59	MG	2A	3717	1/1	0.89	0.09	63,63,63,63	0
59	MG	1A	3409	1/1	0.89	0.15	51,51,51,51	0
59	MG	2A	3434	1/1	0.89	0.09	24,24,24,24	0
59	MG	1A	4037	1/1	0.89	0.09	40,40,40,40	0
59	MG	2a	3078	1/1	0.89	0.20	70,70,70,70	0
59	MG	2a	3079	1/1	0.89	0.28	67,67,67,67	0
59	MG	1e	3001	1/1	0.89	0.11	67,67,67,67	0
59	MG	1a	3386	1/1	0.89	0.24	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3199	1/1	0.89	0.12	54,54,54,54	0
59	MG	2A	3735	1/1	0.89	0.19	62,62,62,62	0
59	MG	2A	3737	1/1	0.89	0.12	47,47,47,47	0
59	MG	2A	3451	1/1	0.89	0.11	46,46,46,46	0
59	MG	1l	202	1/1	0.89	0.11	82,82,82,82	0
59	MG	2A	3740	1/1	0.89	0.10	48,48,48,48	0
59	MG	1A	3332	1/1	0.89	0.20	35,35,35,35	0
59	MG	1A	3833	1/1	0.89	0.08	36,36,36,36	0
59	MG	2a	3095	1/1	0.89	0.10	52,52,52,52	0
59	MG	1A	3655	1/1	0.89	0.14	42,42,42,42	0
59	MG	1A	4057	1/1	0.89	0.12	50,50,50,50	0
59	MG	1w	102	1/1	0.89	0.16	63,63,63,63	0
59	MG	2A	3470	1/1	0.89	0.16	53,53,53,53	0
59	MG	2A	3752	1/1	0.89	0.10	61,61,61,61	0
59	MG	1A	3227	1/1	0.89	0.17	50,50,50,50	0
59	MG	2A	3757	1/1	0.89	0.18	54,54,54,54	0
59	MG	2a	3109	1/1	0.89	0.23	55,55,55,55	0
59	MG	1A	3842	1/1	0.89	0.10	15,15,15,15	0
59	MG	2a	3111	1/1	0.89	0.22	54,54,54,54	0
59	MG	1A	3657	1/1	0.89	0.17	67,67,67,67	0
59	MG	1E	308	1/1	0.89	0.24	59,59,59,59	0
59	MG	1A	3044	1/1	0.89	0.11	45,45,45,45	0
59	MG	1A	3846	1/1	0.89	0.14	57,57,57,57	0
59	MG	2a	3119	1/1	0.89	0.22	68,68,68,68	0
59	MG	2A	3485	1/1	0.89	0.11	36,36,36,36	0
59	MG	1A	3341	1/1	0.89	0.10	45,45,45,45	0
59	MG	1a	3407	1/1	0.89	0.11	36,36,36,36	0
59	MG	1x	110	1/1	0.89	0.14	59,59,59,59	0
59	MG	1A	3677	1/1	0.89	0.09	10,10,10,10	0
59	MG	2A	3498	1/1	0.89	0.09	45,45,45,45	0
59	MG	1A	3533	1/1	0.89	0.10	51,51,51,51	0
59	MG	1A	3690	1/1	0.89	0.12	14,14,14,14	0
59	MG	2a	3157	1/1	0.89	0.10	77,77,77,77	0
59	MG	1a	3413	1/1	0.89	0.22	54,54,54,54	0
59	MG	1A	3077	1/1	0.89	0.14	42,42,42,42	0
59	MG	1A	3544	1/1	0.89	0.09	44,44,44,44	0
59	MG	1A	3883	1/1	0.89	0.12	52,52,52,52	0
59	MG	1A	3889	1/1	0.89	0.06	22,22,22,22	0
59	MG	2A	3788	1/1	0.89	0.12	57,57,57,57	0
59	MG	1A	4102	1/1	0.89	0.14	50,50,50,50	0
59	MG	1A	3109	1/1	0.89	0.18	46,46,46,46	0
59	MG	2A	3021	1/1	0.89	0.16	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3711	1/1	0.89	0.11	34,34,34,34	0
59	MG	1A	3022	1/1	0.89	0.13	39,39,39,39	0
59	MG	10	106	1/1	0.89	0.22	63,63,63,63	0
59	MG	1A	3730	1/1	0.89	0.09	33,33,33,33	0
59	MG	1a	3428	1/1	0.89	0.23	56,56,56,56	0
59	MG	2A	3053	1/1	0.89	0.26	61,61,61,61	0
59	MG	2A	3060	1/1	0.89	0.21	63,63,63,63	0
59	MG	2A	3806	1/1	0.89	0.11	54,54,54,54	0
59	MG	2A	3065	1/1	0.89	0.12	47,47,47,47	0
59	MG	11	103	1/1	0.89	0.16	70,70,70,70	0
59	MG	1A	3353	1/1	0.89	0.20	51,51,51,51	0
59	MG	2a	3203	1/1	0.89	0.17	57,57,57,57	0
59	MG	1A	3308	1/1	0.89	0.16	53,53,53,53	0
59	MG	2A	3829	1/1	0.89	0.16	60,60,60,60	0
59	MG	1a	3302	1/1	0.89	0.23	53,53,53,53	0
59	MG	2A	3077	1/1	0.89	0.14	46,46,46,46	0
59	MG	1a	3441	1/1	0.89	0.10	53,53,53,53	0
59	MG	1a	3443	1/1	0.89	0.26	49,49,49,49	0
59	MG	1a	3304	1/1	0.89	0.18	58,58,58,58	0
59	MG	1A	3082	1/1	0.89	0.17	48,48,48,48	0
59	MG	2B	3006	1/1	0.89	0.26	66,66,66,66	0
59	MG	1A	3263	1/1	0.89	0.11	45,45,45,45	0
59	MG	1A	3377	1/1	0.89	0.09	62,62,62,62	0
59	MG	2A	3568	1/1	0.89	0.12	74,74,74,74	0
59	MG	1A	3584	1/1	0.89	0.11	33,33,33,33	0
59	MG	1A	3767	1/1	0.89	0.12	53,53,53,53	0
59	MG	2A	3294	1/1	0.89	0.19	47,47,47,47	0
59	MG	2a	3223	1/1	0.89	0.21	69,69,69,69	0
59	MG	1A	3921	1/1	0.89	0.11	37,37,37,37	0
59	MG	1A	3924	1/1	0.89	0.14	22,22,22,22	0
59	MG	2a	3234	1/1	0.89	0.20	62,62,62,62	0
59	MG	1A	3769	1/1	0.89	0.16	48,48,48,48	0
59	MG	2A	3299	1/1	0.89	0.23	41,41,41,41	0
59	MG	1A	3021	1/1	0.89	0.23	67,67,67,67	0
59	MG	1A	3949	1/1	0.89	0.12	52,52,52,52	0
59	MG	2D	305	1/1	0.89	0.30	44,44,44,44	0
59	MG	1A	3952	1/1	0.89	0.11	48,48,48,48	0
59	MG	2A	3111	1/1	0.89	0.12	60,60,60,60	0
59	MG	1a	3344	1/1	0.89	0.20	56,56,56,56	0
59	MG	2A	3122	1/1	0.89	0.38	67,67,67,67	0
59	MG	1A	4155	1/1	0.89	0.11	54,54,54,54	0
59	MG	2A	3127	1/1	0.89	0.36	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1a	3346	1/1	0.89	0.28	57,57,57,57	0
59	MG	2A	3318	1/1	0.89	0.27	53,53,53,53	0
59	MG	2R	201	1/1	0.89	0.13	63,63,63,63	0
59	MG	2A	3607	1/1	0.89	0.10	30,30,30,30	0
59	MG	1a	3495	1/1	0.89	0.13	63,63,63,63	0
59	MG	1A	3596	1/1	0.89	0.09	54,54,54,54	0
59	MG	1A	4176	1/1	0.89	0.14	15,15,15,15	0
59	MG	1A	3603	1/1	0.89	0.09	39,39,39,39	0
59	MG	1A	3468	1/1	0.89	0.35	41,41,41,41	0
59	MG	2A	3623	1/1	0.89	0.11	51,51,51,51	0
59	MG	1a	3514	1/1	0.89	0.10	50,50,50,50	0
59	MG	1a	3525	1/1	0.89	0.11	76,76,76,76	0
59	MG	2A	3343	1/1	0.89	0.24	60,60,60,60	0
59	MG	1A	3269	1/1	0.89	0.33	27,27,27,27	0
59	MG	2A	3153	1/1	0.89	0.13	57,57,57,57	0
59	MG	1A	3392	1/1	0.89	0.09	52,52,52,52	0
59	MG	2A	3159	1/1	0.89	0.26	62,62,62,62	0
59	MG	2a	3011	1/1	0.89	0.22	53,53,53,53	0
59	MG	2a	3012	1/1	0.89	0.16	63,63,63,63	0
59	MG	1a	3539	1/1	0.89	0.14	50,50,50,50	0
59	MG	2A	3226	1/1	0.90	0.09	53,53,53,53	0
59	MG	2a	3024	1/1	0.90	0.26	59,59,59,59	0
59	MG	1A	3626	1/1	0.90	0.10	24,24,24,24	0
59	MG	1A	3426	1/1	0.90	0.14	46,46,46,46	0
59	MG	2A	3436	1/1	0.90	0.08	28,28,28,28	0
59	MG	2A	3682	1/1	0.90	0.10	56,56,56,56	0
59	MG	2A	3684	1/1	0.90	0.07	33,33,33,33	0
59	MG	2A	3685	1/1	0.90	0.11	62,62,62,62	0
59	MG	2A	3069	1/1	0.90	0.26	45,45,45,45	0
59	MG	2A	3234	1/1	0.90	0.30	64,64,64,64	0
59	MG	2A	3445	1/1	0.90	0.12	42,42,42,42	0
59	MG	2A	3446	1/1	0.90	0.12	44,44,44,44	0
59	MG	2A	3072	1/1	0.90	0.11	42,42,42,42	0
59	MG	2a	3041	1/1	0.90	0.16	63,63,63,63	0
59	MG	1A	3427	1/1	0.90	0.18	43,43,43,43	0
59	MG	2A	3237	1/1	0.90	0.11	59,59,59,59	0
59	MG	1a	3510	1/1	0.90	0.12	53,53,53,53	0
59	MG	1A	4124	1/1	0.90	0.10	56,56,56,56	0
59	MG	2a	3047	1/1	0.90	0.20	60,60,60,60	0
59	MG	2A	3241	1/1	0.90	0.20	66,66,66,66	0
59	MG	1G	3004	1/1	0.90	0.09	40,40,40,40	0
59	MG	2a	3057	1/1	0.90	0.20	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1I	3001	1/1	0.90	0.11	62,62,62,62	0
59	MG	2A	3466	1/1	0.90	0.20	55,55,55,55	0
59	MG	2A	3728	1/1	0.90	0.09	24,24,24,24	0
59	MG	2A	3082	1/1	0.90	0.12	44,44,44,44	0
59	MG	2A	3732	1/1	0.90	0.11	47,47,47,47	0
59	MG	1A	3989	1/1	0.90	0.12	49,49,49,49	0
59	MG	1O	3003	1/1	0.90	0.14	54,54,54,54	0
59	MG	1A	3510	1/1	0.90	0.16	41,41,41,41	0
59	MG	1A	3376	1/1	0.90	0.12	48,48,48,48	0
59	MG	1A	3752	1/1	0.90	0.08	27,27,27,27	0
59	MG	1A	3289	1/1	0.90	0.34	29,29,29,29	0
59	MG	2A	3741	1/1	0.90	0.13	60,60,60,60	0
59	MG	1A	3438	1/1	0.90	0.12	57,57,57,57	0
59	MG	1A	3643	1/1	0.90	0.10	42,42,42,42	0
59	MG	2a	3084	1/1	0.90	0.10	71,71,71,71	0
59	MG	2A	3261	1/1	0.90	0.05	59,59,59,59	0
59	MG	2A	3487	1/1	0.90	0.11	48,48,48,48	0
59	MG	1T	8002	1/1	0.90	0.15	51,51,51,51	0
59	MG	1A	3071	1/1	0.90	0.37	34,34,34,34	0
59	MG	2a	3090	1/1	0.90	0.12	65,65,65,65	0
59	MG	1A	3380	1/1	0.90	0.09	33,33,33,33	0
59	MG	2A	3754	1/1	0.90	0.21	64,64,64,64	0
59	MG	2A	3266	1/1	0.90	0.09	42,42,42,42	0
59	MG	1A	3255	1/1	0.90	0.15	54,54,54,54	0
59	MG	1a	3558	1/1	0.90	0.12	63,63,63,63	0
59	MG	2A	3511	1/1	0.90	0.17	50,50,50,50	0
59	MG	1A	4162	1/1	0.90	0.12	54,54,54,54	0
59	MG	1a	3408	1/1	0.90	0.47	60,60,60,60	0
59	MG	1A	3296	1/1	0.90	0.09	55,55,55,55	0
59	MG	2A	3766	1/1	0.90	0.09	53,53,53,53	0
59	MG	2A	3521	1/1	0.90	0.13	42,42,42,42	0
59	MG	1A	3187	1/1	0.90	0.09	39,39,39,39	0
59	MG	1a	3571	1/1	0.90	0.11	57,57,57,57	0
59	MG	1A	3455	1/1	0.90	0.17	51,51,51,51	0
59	MG	1a	3575	1/1	0.90	0.22	55,55,55,55	0
59	MG	2A	3141	1/1	0.90	0.12	38,38,38,38	0
59	MG	17	101	1/1	0.90	0.13	49,49,49,49	0
59	MG	2a	3117	1/1	0.90	0.25	53,53,53,53	0
59	MG	1A	3305	1/1	0.90	0.11	50,50,50,50	0
59	MG	1d	502	1/1	0.90	0.27	52,52,52,52	0
59	MG	1A	3560	1/1	0.90	0.12	45,45,45,45	0
59	MG	2a	3126	1/1	0.90	0.08	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3780	1/1	0.90	0.21	62,62,62,62	0
59	MG	1A	4188	1/1	0.90	0.26	55,55,55,55	0
59	MG	1A	3306	1/1	0.90	0.22	47,47,47,47	0
59	MG	1A	4061	1/1	0.90	0.13	40,40,40,40	0
59	MG	2A	3786	1/1	0.90	0.20	55,55,55,55	0
59	MG	2a	3141	1/1	0.90	0.16	56,56,56,56	0
59	MG	2A	3546	1/1	0.90	0.16	60,60,60,60	0
59	MG	2a	3150	1/1	0.90	0.09	57,57,57,57	0
59	MG	2a	3151	1/1	0.90	0.09	73,73,73,73	0
59	MG	1A	3666	1/1	0.90	0.11	49,49,49,49	0
59	MG	1p	101	1/1	0.90	0.15	48,48,48,48	0
59	MG	1A	3076	1/1	0.90	0.16	30,30,30,30	0
59	MG	1A	4229	1/1	0.90	0.10	24,24,24,24	0
59	MG	2A	3303	1/1	0.90	0.12	50,50,50,50	0
59	MG	2A	3164	1/1	0.90	0.23	56,56,56,56	0
59	MG	1A	3019	1/1	0.90	0.16	33,33,33,33	0
59	MG	2A	3308	1/1	0.90	0.19	50,50,50,50	0
59	MG	1B	209	1/1	0.90	0.20	58,58,58,58	0
59	MG	2a	3177	1/1	0.90	0.12	58,58,58,58	0
59	MG	1a	3329	1/1	0.90	0.36	64,64,64,64	0
59	MG	2A	3311	1/1	0.90	0.19	44,44,44,44	0
59	MG	1A	3808	1/1	0.90	0.21	33,33,33,33	0
59	MG	2A	3567	1/1	0.90	0.12	63,63,63,63	0
59	MG	1a	3430	1/1	0.90	0.15	69,69,69,69	0
59	MG	2A	3816	1/1	0.90	0.11	43,43,43,43	0
59	MG	1B	213	1/1	0.90	0.15	43,43,43,43	0
59	MG	2A	3828	1/1	0.90	0.10	60,60,60,60	0
59	MG	1A	3474	1/1	0.90	0.18	55,55,55,55	0
59	MG	1a	3438	1/1	0.90	0.21	55,55,55,55	0
59	MG	2a	3195	1/1	0.90	0.14	54,54,54,54	0
59	MG	2A	3579	1/1	0.90	0.15	32,32,32,32	0
59	MG	2A	3581	1/1	0.90	0.07	51,51,51,51	0
59	MG	2A	3843	1/1	0.90	0.08	63,63,63,63	0
59	MG	2a	3202	1/1	0.90	0.22	67,67,67,67	0
59	MG	2A	3320	1/1	0.90	0.24	59,59,59,59	0
59	MG	1A	3051	1/1	0.90	0.21	49,49,49,49	0
59	MG	2A	3846	1/1	0.90	0.13	38,38,38,38	0
59	MG	1B	218	1/1	0.90	0.14	36,36,36,36	0
59	MG	1A	3482	1/1	0.90	0.13	42,42,42,42	0
59	MG	1A	3585	1/1	0.90	0.08	33,33,33,33	0
59	MG	1a	3454	1/1	0.90	0.09	46,46,46,46	0
59	MG	2A	3590	1/1	0.90	0.10	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3591	1/1	0.90	0.20	63,63,63,63	0
59	MG	1A	3930	1/1	0.90	0.13	71,71,71,71	0
59	MG	2A	3186	1/1	0.90	0.24	64,64,64,64	0
59	MG	2A	3340	1/1	0.90	0.26	59,59,59,59	0
59	MG	2A	3598	1/1	0.90	0.11	63,63,63,63	0
59	MG	2A	3341	1/1	0.90	0.29	53,53,53,53	0
59	MG	1x	117	1/1	0.90	0.10	63,63,63,63	0
59	MG	1A	3821	1/1	0.90	0.07	21,21,21,21	0
59	MG	2A	3602	1/1	0.90	0.11	51,51,51,51	0
59	MG	1A	4086	1/1	0.90	0.09	33,33,33,33	0
59	MG	2a	3228	1/1	0.90	0.19	56,56,56,56	0
59	MG	2E	301	1/1	0.90	0.14	66,66,66,66	0
59	MG	2A	3192	1/1	0.90	0.14	46,46,46,46	0
59	MG	2E	306	1/1	0.90	0.11	29,29,29,29	0
59	MG	1A	4091	1/1	0.90	0.13	42,42,42,42	0
59	MG	1A	3276	1/1	0.90	0.11	52,52,52,52	0
59	MG	2A	3352	1/1	0.90	0.09	64,64,64,64	0
59	MG	1A	3278	1/1	0.90	0.30	62,62,62,62	0
59	MG	2A	3618	1/1	0.90	0.32	36,36,36,36	0
59	MG	1A	3106	1/1	0.90	0.21	33,33,33,33	0
59	MG	1A	3494	1/1	0.90	0.18	49,49,49,49	0
59	MG	1A	3959	1/1	0.90	0.12	55,55,55,55	0
59	MG	2A	3025	1/1	0.90	0.07	42,42,42,42	0
59	MG	1A	3837	1/1	0.90	0.16	48,48,48,48	0
59	MG	2A	3375	1/1	0.90	0.09	45,45,45,45	0
59	MG	2r	3001	1/1	0.90	0.19	77,77,77,77	0
59	MG	2T	202	1/1	0.90	0.17	61,61,61,61	0
59	MG	2A	3208	1/1	0.90	0.13	71,71,71,71	0
59	MG	2A	3032	1/1	0.90	0.26	54,54,54,54	0
59	MG	2A	3630	1/1	0.90	0.18	66,66,66,66	0
59	MG	2A	3210	1/1	0.90	0.15	62,62,62,62	0
59	MG	23	102	1/1	0.90	0.10	45,45,45,45	0
59	MG	2A	3388	1/1	0.90	0.16	60,60,60,60	0
59	MG	1A	3375	1/1	0.90	0.12	29,29,29,29	0
59	MG	2A	3214	1/1	0.90	0.12	58,58,58,58	0
59	MG	2A	3640	1/1	0.90	0.13	49,49,49,49	0
59	MG	2A	3641	1/1	0.90	0.15	75,75,75,75	0
59	MG	2A	3215	1/1	0.90	0.12	49,49,49,49	0
59	MG	1a	3367	1/1	0.90	0.23	53,53,53,53	0
59	MG	2A	3653	1/1	0.90	0.17	60,60,60,60	0
59	MG	2A	3405	1/1	0.90	0.10	65,65,65,65	0
59	MG	1A	3977	1/1	0.90	0.12	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1E	305	1/1	0.90	0.18	42,42,42,42	0
59	MG	1A	4116	1/1	0.90	0.10	50,50,50,50	0
59	MG	1a	3499	1/1	0.90	0.12	61,61,61,61	0
59	MG	1a	3360	1/1	0.91	0.10	45,45,45,45	0
59	MG	1a	3555	1/1	0.91	0.09	47,47,47,47	0
59	MG	2a	3007	1/1	0.91	0.21	66,66,66,66	0
59	MG	1A	3830	1/1	0.91	0.10	40,40,40,40	0
59	MG	1A	4193	1/1	0.91	0.08	14,14,14,14	0
59	MG	1A	3832	1/1	0.91	0.15	47,47,47,47	0
59	MG	1A	3674	1/1	0.91	0.08	14,14,14,14	0
59	MG	2A	3349	1/1	0.91	0.09	50,50,50,50	0
59	MG	2a	3015	1/1	0.91	0.10	66,66,66,66	0
59	MG	1a	3560	1/1	0.91	0.11	53,53,53,53	0
59	MG	1a	3561	1/1	0.91	0.11	62,62,62,62	0
59	MG	1A	4009	1/1	0.91	0.08	71,71,71,71	0
59	MG	2a	3022	1/1	0.91	0.16	62,62,62,62	0
59	MG	2a	3023	1/1	0.91	0.37	54,54,54,54	0
59	MG	2A	3358	1/1	0.91	0.24	56,56,56,56	0
59	MG	2A	3359	1/1	0.91	0.08	48,48,48,48	0
59	MG	1A	3209	1/1	0.91	0.15	41,41,41,41	0
59	MG	1B	201	1/1	0.91	0.14	44,44,44,44	0
59	MG	2A	3174	1/1	0.91	0.09	60,60,60,60	0
59	MG	2A	3666	1/1	0.91	0.10	62,62,62,62	0
59	MG	1a	3569	1/1	0.91	0.15	66,66,66,66	0
59	MG	1B	203	1/1	0.91	0.19	49,49,49,49	0
59	MG	1A	3214	1/1	0.91	0.15	46,46,46,46	0
59	MG	1B	208	1/1	0.91	0.23	63,63,63,63	0
59	MG	1A	4013	1/1	0.91	0.08	50,50,50,50	0
59	MG	2A	3680	1/1	0.91	0.15	55,55,55,55	0
59	MG	2A	3378	1/1	0.91	0.26	55,55,55,55	0
59	MG	1A	4014	1/1	0.91	0.08	65,65,65,65	0
59	MG	2A	3385	1/1	0.91	0.12	63,63,63,63	0
59	MG	2A	3182	1/1	0.91	0.17	61,61,61,61	0
59	MG	2A	3184	1/1	0.91	0.18	45,45,45,45	0
59	MG	1a	3377	1/1	0.91	0.26	61,61,61,61	0
59	MG	1A	4015	1/1	0.91	0.12	52,52,52,52	0
59	MG	2A	3695	1/1	0.91	0.10	53,53,53,53	0
59	MG	1f	3001	1/1	0.91	0.18	29,29,29,29	0
59	MG	1A	4018	1/1	0.91	0.09	47,47,47,47	0
59	MG	2A	3707	1/1	0.91	0.15	64,64,64,64	0
59	MG	1A	3680	1/1	0.91	0.12	53,53,53,53	0
59	MG	1A	4025	1/1	0.91	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3358	1/1	0.91	0.25	49,49,49,49	0
59	MG	2A	3415	1/1	0.91	0.10	36,36,36,36	0
59	MG	1A	3481	1/1	0.91	0.09	38,38,38,38	0
59	MG	2A	3724	1/1	0.91	0.16	34,34,34,34	0
59	MG	1a	3389	1/1	0.91	0.14	48,48,48,48	0
59	MG	2a	3076	1/1	0.91	0.30	56,56,56,56	0
59	MG	1t	3001	1/1	0.91	0.12	43,43,43,43	0
59	MG	2A	3200	1/1	0.91	0.21	37,37,37,37	0
59	MG	2A	3201	1/1	0.91	0.24	43,43,43,43	0
59	MG	1A	4039	1/1	0.91	0.08	50,50,50,50	0
59	MG	2A	3203	1/1	0.91	0.28	61,61,61,61	0
59	MG	1A	4043	1/1	0.91	0.10	39,39,39,39	0
59	MG	1B	226	1/1	0.91	0.11	56,56,56,56	0
59	MG	2a	3086	1/1	0.91	0.25	60,60,60,60	0
59	MG	1A	3359	1/1	0.91	0.16	56,56,56,56	0
59	MG	1a	3398	1/1	0.91	0.25	58,58,58,58	0
59	MG	1A	3078	1/1	0.91	0.19	48,48,48,48	0
59	MG	1A	3586	1/1	0.91	0.13	49,49,49,49	0
59	MG	1A	4053	1/1	0.91	0.24	69,69,69,69	0
59	MG	2A	3212	1/1	0.91	0.10	49,49,49,49	0
59	MG	1x	102	1/1	0.91	0.30	59,59,59,59	0
59	MG	1A	4056	1/1	0.91	0.09	43,43,43,43	0
59	MG	1x	104	1/1	0.91	0.13	61,61,61,61	0
59	MG	2a	3099	1/1	0.91	0.22	48,48,48,48	0
59	MG	1A	3591	1/1	0.91	0.09	26,26,26,26	0
59	MG	2A	3469	1/1	0.91	0.21	60,60,60,60	0
59	MG	2a	3104	1/1	0.91	0.26	54,54,54,54	0
59	MG	2A	3219	1/1	0.91	0.08	54,54,54,54	0
59	MG	2A	3221	1/1	0.91	0.16	59,59,59,59	0
59	MG	2A	3472	1/1	0.91	0.20	50,50,50,50	0
59	MG	1A	3225	1/1	0.91	0.25	64,64,64,64	0
59	MG	1A	3595	1/1	0.91	0.08	18,18,18,18	0
59	MG	1A	3424	1/1	0.91	0.18	53,53,53,53	0
59	MG	2A	3478	1/1	0.91	0.16	56,56,56,56	0
59	MG	1A	4070	1/1	0.91	0.07	33,33,33,33	0
59	MG	1A	3490	1/1	0.91	0.23	58,58,58,58	0
59	MG	2A	3483	1/1	0.91	0.15	36,36,36,36	0
59	MG	1E	307	1/1	0.91	0.13	40,40,40,40	0
59	MG	1A	3491	1/1	0.91	0.11	47,47,47,47	0
59	MG	1A	3493	1/1	0.91	0.34	55,55,55,55	0
59	MG	1E	314	1/1	0.91	0.16	47,47,47,47	0
59	MG	2a	3124	1/1	0.91	0.12	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2a	3125	1/1	0.91	0.15	79,79,79,79	0
59	MG	1A	3623	1/1	0.91	0.09	15,15,15,15	0
59	MG	2a	3127	1/1	0.91	0.09	74,74,74,74	0
59	MG	1A	3753	1/1	0.91	0.09	25,25,25,25	0
59	MG	2A	3497	1/1	0.91	0.11	30,30,30,30	0
59	MG	2A	3777	1/1	0.91	0.10	55,55,55,55	0
59	MG	1A	3754	1/1	0.91	0.19	32,32,32,32	0
59	MG	1G	3002	1/1	0.91	0.15	53,53,53,53	0
59	MG	1A	3425	1/1	0.91	0.08	49,49,49,49	0
59	MG	2A	3023	1/1	0.91	0.07	35,35,35,35	0
59	MG	2A	3024	1/1	0.91	0.11	43,43,43,43	0
59	MG	1A	3898	1/1	0.91	0.12	49,49,49,49	0
59	MG	2A	3026	1/1	0.91	0.14	32,32,32,32	0
59	MG	2a	3154	1/1	0.91	0.14	42,42,42,42	0
59	MG	2a	3156	1/1	0.91	0.10	77,77,77,77	0
59	MG	2A	3787	1/1	0.91	0.11	58,58,58,58	0
59	MG	1A	3274	1/1	0.91	0.21	51,51,51,51	0
59	MG	2a	3159	1/1	0.91	0.17	62,62,62,62	0
59	MG	1A	3175	1/1	0.91	0.14	44,44,44,44	0
59	MG	2A	3525	1/1	0.91	0.14	55,55,55,55	0
59	MG	2A	3252	1/1	0.91	0.15	58,58,58,58	0
59	MG	2A	3033	1/1	0.91	0.16	58,58,58,58	0
59	MG	2A	3038	1/1	0.91	0.20	48,48,48,48	0
59	MG	2A	3256	1/1	0.91	0.24	53,53,53,53	0
59	MG	1A	3905	1/1	0.91	0.07	71,71,71,71	0
59	MG	2A	3797	1/1	0.91	0.11	49,49,49,49	0
59	MG	2A	3042	1/1	0.91	0.11	43,43,43,43	0
59	MG	1A	3770	1/1	0.91	0.10	40,40,40,40	0
59	MG	1A	3771	1/1	0.91	0.07	33,33,33,33	0
59	MG	1A	3505	1/1	0.91	0.10	51,51,51,51	0
59	MG	2A	3058	1/1	0.91	0.09	45,45,45,45	0
59	MG	1A	4103	1/1	0.91	0.10	42,42,42,42	0
59	MG	2A	3062	1/1	0.91	0.26	43,43,43,43	0
59	MG	1A	4104	1/1	0.91	0.14	53,53,53,53	0
59	MG	2a	3192	1/1	0.91	0.15	57,57,57,57	0
59	MG	1T	8001	1/1	0.91	0.12	43,43,43,43	0
59	MG	1A	3506	1/1	0.91	0.09	41,41,41,41	0
59	MG	1A	3913	1/1	0.91	0.11	21,21,21,21	0
59	MG	1A	3020	1/1	0.91	0.08	45,45,45,45	0
59	MG	1A	3328	1/1	0.91	0.27	27,27,27,27	0
59	MG	2a	3200	1/1	0.91	0.12	65,65,65,65	0
59	MG	1A	3228	1/1	0.91	0.17	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3838	1/1	0.91	0.18	51,51,51,51	0
59	MG	10	107	1/1	0.91	0.13	38,38,38,38	0
59	MG	1A	3786	1/1	0.91	0.07	26,26,26,26	0
59	MG	2A	3560	1/1	0.91	0.07	61,61,61,61	0
59	MG	1A	3439	1/1	0.91	0.14	39,39,39,39	0
59	MG	2B	3001	1/1	0.91	0.27	53,53,53,53	0
59	MG	1a	3467	1/1	0.91	0.14	53,53,53,53	0
59	MG	2B	3004	1/1	0.91	0.07	53,53,53,53	0
59	MG	12	3001	1/1	0.91	0.08	40,40,40,40	0
59	MG	1A	3942	1/1	0.91	0.18	45,45,45,45	0
59	MG	1A	3286	1/1	0.91	0.15	64,64,64,64	0
59	MG	1A	3005	1/1	0.91	0.13	47,47,47,47	0
59	MG	19	101	1/1	0.91	0.14	46,46,46,46	0
59	MG	2B	3012	1/1	0.91	0.12	63,63,63,63	0
59	MG	2B	3014	1/1	0.91	0.18	67,67,67,67	0
59	MG	1A	3442	1/1	0.91	0.15	63,63,63,63	0
59	MG	1A	4126	1/1	0.91	0.10	53,53,53,53	0
59	MG	1A	3650	1/1	0.91	0.12	36,36,36,36	0
59	MG	1A	4129	1/1	0.91	0.10	55,55,55,55	0
59	MG	1A	3651	1/1	0.91	0.11	37,37,37,37	0
59	MG	2A	3301	1/1	0.91	0.26	41,41,41,41	0
59	MG	1A	3387	1/1	0.91	0.18	45,45,45,45	0
59	MG	2A	3305	1/1	0.91	0.18	52,52,52,52	0
59	MG	2a	3237	1/1	0.91	0.21	56,56,56,56	0
59	MG	2A	3109	1/1	0.91	0.12	43,43,43,43	0
59	MG	2d	502	1/1	0.91	0.17	59,59,59,59	0
59	MG	1A	3966	1/1	0.91	0.12	44,44,44,44	0
59	MG	2E	302	1/1	0.91	0.10	38,38,38,38	0
59	MG	1A	3968	1/1	0.91	0.08	27,27,27,27	0
59	MG	2E	304	1/1	0.91	0.18	59,59,59,59	0
59	MG	1A	3970	1/1	0.91	0.07	41,41,41,41	0
59	MG	1A	3535	1/1	0.91	0.14	37,37,37,37	0
59	MG	2A	3124	1/1	0.91	0.18	32,32,32,32	0
59	MG	2F	304	1/1	0.91	0.12	74,74,74,74	0
59	MG	1A	4147	1/1	0.91	0.13	50,50,50,50	0
59	MG	1A	3388	1/1	0.91	0.18	47,47,47,47	0
59	MG	1A	4151	1/1	0.91	0.10	45,45,45,45	0
59	MG	1A	3015	1/1	0.91	0.11	43,43,43,43	0
59	MG	2Q	3003	1/1	0.91	0.11	54,54,54,54	0
59	MG	2w	3001	1/1	0.91	0.20	56,56,56,56	0
59	MG	2A	3317	1/1	0.91	0.18	51,51,51,51	0
59	MG	1A	3153	1/1	0.91	0.27	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3984	1/1	0.91	0.09	10,10,10,10	0
59	MG	1a	3537	1/1	0.91	0.09	46,46,46,46	0
59	MG	1A	3665	1/1	0.91	0.20	51,51,51,51	0
59	MG	2A	3326	1/1	0.91	0.15	46,46,46,46	0
59	MG	1A	3154	1/1	0.91	0.16	42,42,42,42	0
59	MG	1A	3197	1/1	0.91	0.23	32,32,32,32	0
59	MG	2A	3330	1/1	0.91	0.14	53,53,53,53	0
59	MG	1A	4184	1/1	0.91	0.14	31,31,31,31	0
59	MG	2A	3335	1/1	0.91	0.10	56,56,56,56	0
59	MG	1a	3355	1/1	0.91	0.21	51,51,51,51	0
59	MG	2A	3337	1/1	0.91	0.17	44,44,44,44	0
59	MG	2a	3001	1/1	0.91	0.08	52,52,52,52	0
59	MG	1A	3825	1/1	0.91	0.18	27,27,27,27	0
59	MG	2y	3006	1/1	0.91	0.08	89,89,89,89	0
59	MG	1A	3001	1/1	0.91	0.09	35,35,35,35	0
59	MG	1A	3351	1/1	0.92	0.11	31,31,31,31	0
59	MG	2A	3677	1/1	0.92	0.10	63,63,63,63	0
59	MG	2A	3412	1/1	0.92	0.09	40,40,40,40	0
59	MG	1A	3697	1/1	0.92	0.09	18,18,18,18	0
59	MG	2a	3025	1/1	0.92	0.28	52,52,52,52	0
59	MG	1Q	203	1/1	0.92	0.14	51,51,51,51	0
59	MG	1A	3480	1/1	0.92	0.10	40,40,40,40	0
59	MG	2a	3029	1/1	0.92	0.24	58,58,58,58	0
59	MG	1A	4128	1/1	0.92	0.12	53,53,53,53	0
59	MG	2A	3423	1/1	0.92	0.08	33,33,33,33	0
59	MG	1A	3261	1/1	0.92	0.13	48,48,48,48	0
59	MG	1A	3411	1/1	0.92	0.16	48,48,48,48	0
59	MG	2A	3692	1/1	0.92	0.09	40,40,40,40	0
59	MG	1A	4134	1/1	0.92	0.12	52,52,52,52	0
59	MG	1U	202	1/1	0.92	0.18	27,27,27,27	0
59	MG	1A	3216	1/1	0.92	0.13	36,36,36,36	0
59	MG	2A	3003	1/1	0.92	0.32	61,61,61,61	0
59	MG	1A	4007	1/1	0.92	0.14	54,54,54,54	0
59	MG	1Z	302	1/1	0.92	0.14	48,48,48,48	0
59	MG	2a	3043	1/1	0.92	0.24	66,66,66,66	0
59	MG	1a	3432	1/1	0.92	0.13	44,44,44,44	0
59	MG	1a	3433	1/1	0.92	0.40	61,61,61,61	0
59	MG	1a	3434	1/1	0.92	0.17	48,48,48,48	0
59	MG	1A	3307	1/1	0.92	0.12	50,50,50,50	0
59	MG	2a	3049	1/1	0.92	0.15	55,55,55,55	0
59	MG	1A	3416	1/1	0.92	0.14	52,52,52,52	0
59	MG	1A	3734	1/1	0.92	0.12	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3028	1/1	0.92	0.14	25,25,25,25	0
59	MG	2A	3730	1/1	0.92	0.07	53,53,53,53	0
59	MG	1A	3264	1/1	0.92	0.09	56,56,56,56	0
59	MG	2a	3061	1/1	0.92	0.16	60,60,60,60	0
59	MG	2a	3062	1/1	0.92	0.10	54,54,54,54	0
59	MG	1A	3597	1/1	0.92	0.09	34,34,34,34	0
59	MG	1A	3742	1/1	0.92	0.07	29,29,29,29	0
59	MG	2A	3734	1/1	0.92	0.10	54,54,54,54	0
59	MG	2A	3037	1/1	0.92	0.21	59,59,59,59	0
59	MG	2A	3736	1/1	0.92	0.16	58,58,58,58	0
59	MG	1a	3448	1/1	0.92	0.20	60,60,60,60	0
59	MG	13	3001	1/1	0.92	0.07	39,39,39,39	0
59	MG	1A	4153	1/1	0.92	0.08	49,49,49,49	0
59	MG	2a	3077	1/1	0.92	0.22	57,57,57,57	0
59	MG	1a	3458	1/1	0.92	0.12	51,51,51,51	0
59	MG	1A	3218	1/1	0.92	0.18	38,38,38,38	0
59	MG	1A	3222	1/1	0.92	0.09	38,38,38,38	0
59	MG	2A	3744	1/1	0.92	0.09	47,47,47,47	0
59	MG	1A	4168	1/1	0.92	0.08	36,36,36,36	0
59	MG	1A	3370	1/1	0.92	0.23	51,51,51,51	0
59	MG	1A	4175	1/1	0.92	0.12	36,36,36,36	0
59	MG	1A	3097	1/1	0.92	0.06	35,35,35,35	0
59	MG	1a	3475	1/1	0.92	0.16	48,48,48,48	0
59	MG	1A	3428	1/1	0.92	0.21	56,56,56,56	0
59	MG	1A	3053	1/1	0.92	0.17	44,44,44,44	0
59	MG	2A	3490	1/1	0.92	0.08	30,30,30,30	0
59	MG	1a	3317	1/1	0.92	0.07	41,41,41,41	0
59	MG	1A	3760	1/1	0.92	0.16	32,32,32,32	0
59	MG	2A	3493	1/1	0.92	0.07	29,29,29,29	0
59	MG	1a	3483	1/1	0.92	0.13	58,58,58,58	0
59	MG	2a	3097	1/1	0.92	0.14	48,48,48,48	0
59	MG	2A	3076	1/1	0.92	0.13	37,37,37,37	0
59	MG	1a	3484	1/1	0.92	0.12	41,41,41,41	0
59	MG	2A	3501	1/1	0.92	0.16	33,33,33,33	0
59	MG	1a	3324	1/1	0.92	0.19	57,57,57,57	0
59	MG	2a	3103	1/1	0.92	0.16	62,62,62,62	0
59	MG	1A	3125	1/1	0.92	0.24	32,32,32,32	0
59	MG	2A	3081	1/1	0.92	0.08	45,45,45,45	0
59	MG	2A	3513	1/1	0.92	0.12	67,67,67,67	0
59	MG	2A	3514	1/1	0.92	0.19	35,35,35,35	0
59	MG	1A	3436	1/1	0.92	0.34	34,34,34,34	0
59	MG	1A	3899	1/1	0.92	0.11	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3518	1/1	0.92	0.18	51,51,51,51	0
59	MG	1A	4191	1/1	0.92	0.10	27,27,27,27	0
59	MG	1A	3277	1/1	0.92	0.10	48,48,48,48	0
59	MG	2A	3522	1/1	0.92	0.10	48,48,48,48	0
59	MG	2a	3114	1/1	0.92	0.34	59,59,59,59	0
59	MG	2A	3281	1/1	0.92	0.21	67,67,67,67	0
59	MG	2A	3283	1/1	0.92	0.11	60,60,60,60	0
59	MG	2A	3284	1/1	0.92	0.10	59,59,59,59	0
59	MG	1A	3511	1/1	0.92	0.22	51,51,51,51	0
59	MG	2a	3120	1/1	0.92	0.09	51,51,51,51	0
59	MG	2a	3121	1/1	0.92	0.25	61,61,61,61	0
59	MG	2A	3784	1/1	0.92	0.08	56,56,56,56	0
59	MG	2A	3785	1/1	0.92	0.11	53,53,53,53	0
59	MG	1A	3049	1/1	0.92	0.14	54,54,54,54	0
59	MG	1A	4059	1/1	0.92	0.18	57,57,57,57	0
59	MG	1a	3506	1/1	0.92	0.12	59,59,59,59	0
59	MG	1a	3337	1/1	0.92	0.30	55,55,55,55	0
59	MG	1a	3343	1/1	0.92	0.14	40,40,40,40	0
59	MG	1A	4228	1/1	0.92	0.28	34,34,34,34	0
59	MG	2A	3102	1/1	0.92	0.15	41,41,41,41	0
59	MG	2A	3104	1/1	0.92	0.15	52,52,52,52	0
59	MG	2A	3544	1/1	0.92	0.10	64,64,64,64	0
59	MG	1A	3381	1/1	0.92	0.15	41,41,41,41	0
59	MG	2a	3148	1/1	0.92	0.12	73,73,73,73	0
59	MG	1a	3519	1/1	0.92	0.18	65,65,65,65	0
59	MG	1A	3283	1/1	0.92	0.10	45,45,45,45	0
59	MG	1a	3531	1/1	0.92	0.07	49,49,49,49	0
59	MG	1A	3128	1/1	0.92	0.19	30,30,30,30	0
59	MG	1A	4066	1/1	0.92	0.10	47,47,47,47	0
59	MG	2A	3808	1/1	0.92	0.11	54,54,54,54	0
59	MG	2A	3554	1/1	0.92	0.18	62,62,62,62	0
59	MG	2A	3810	1/1	0.92	0.10	59,59,59,59	0
59	MG	2A	3812	1/1	0.92	0.09	72,72,72,72	0
59	MG	1A	4067	1/1	0.92	0.13	36,36,36,36	0
59	MG	2a	3164	1/1	0.92	0.08	75,75,75,75	0
59	MG	1A	3781	1/1	0.92	0.13	42,42,42,42	0
59	MG	2a	3169	1/1	0.92	0.15	51,51,51,51	0
59	MG	1a	3541	1/1	0.92	0.18	61,61,61,61	0
59	MG	2a	3173	1/1	0.92	0.18	61,61,61,61	0
59	MG	1A	3522	1/1	0.92	0.22	28,28,28,28	0
59	MG	1A	3915	1/1	0.92	0.08	24,24,24,24	0
59	MG	1A	3648	1/1	0.92	0.12	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1a	3546	1/1	0.92	0.16	46,46,46,46	0
59	MG	2A	3835	1/1	0.92	0.08	48,48,48,48	0
59	MG	1A	3523	1/1	0.92	0.10	37,37,37,37	0
59	MG	2A	3144	1/1	0.92	0.15	65,65,65,65	0
59	MG	1A	3443	1/1	0.92	0.23	49,49,49,49	0
59	MG	2A	3840	1/1	0.92	0.10	30,30,30,30	0
59	MG	1A	3789	1/1	0.92	0.11	56,56,56,56	0
59	MG	1a	3551	1/1	0.92	0.17	54,54,54,54	0
59	MG	2A	3570	1/1	0.92	0.09	64,64,64,64	0
59	MG	2a	3191	1/1	0.92	0.15	55,55,55,55	0
59	MG	2A	3571	1/1	0.92	0.13	68,68,68,68	0
59	MG	1A	3195	1/1	0.92	0.11	48,48,48,48	0
59	MG	1A	3936	1/1	0.92	0.08	19,19,19,19	0
59	MG	2A	3576	1/1	0.92	0.09	64,64,64,64	0
59	MG	2A	3152	1/1	0.92	0.19	48,48,48,48	0
59	MG	1B	223	1/1	0.92	0.15	45,45,45,45	0
59	MG	1A	4083	1/1	0.92	0.11	68,68,68,68	0
59	MG	2a	3201	1/1	0.92	0.20	46,46,46,46	0
59	MG	2B	3009	1/1	0.92	0.09	54,54,54,54	0
59	MG	1A	3796	1/1	0.92	0.13	45,45,45,45	0
59	MG	1A	3945	1/1	0.92	0.08	59,59,59,59	0
59	MG	1A	4089	1/1	0.92	0.15	42,42,42,42	0
59	MG	2B	3013	1/1	0.92	0.23	63,63,63,63	0
59	MG	1A	4090	1/1	0.92	0.13	34,34,34,34	0
59	MG	1A	3446	1/1	0.92	0.14	35,35,35,35	0
59	MG	2A	3166	1/1	0.92	0.25	56,56,56,56	0
59	MG	1A	4093	1/1	0.92	0.10	40,40,40,40	0
59	MG	2A	3593	1/1	0.92	0.09	37,37,37,37	0
59	MG	1B	234	1/1	0.92	0.11	54,54,54,54	0
59	MG	1A	3536	1/1	0.92	0.12	48,48,48,48	0
59	MG	2B	3021	1/1	0.92	0.23	68,68,68,68	0
59	MG	1a	3382	1/1	0.92	0.08	63,63,63,63	0
59	MG	1A	4096	1/1	0.92	0.30	26,26,26,26	0
59	MG	1B	238	1/1	0.92	0.08	30,30,30,30	0
59	MG	1A	3163	1/1	0.92	0.09	48,48,48,48	0
59	MG	1A	4099	1/1	0.92	0.10	50,50,50,50	0
59	MG	1b	3002	1/1	0.92	0.17	69,69,69,69	0
59	MG	2A	3603	1/1	0.92	0.11	49,49,49,49	0
59	MG	1A	3543	1/1	0.92	0.09	17,17,17,17	0
59	MG	2a	3232	1/1	0.92	0.19	60,60,60,60	0
59	MG	1a	3390	1/1	0.92	0.26	53,53,53,53	0
59	MG	1E	301	1/1	0.92	0.12	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3105	1/1	0.92	0.12	30,30,30,30	0
59	MG	2A	3612	1/1	0.92	0.12	44,44,44,44	0
59	MG	1A	3661	1/1	0.92	0.08	36,36,36,36	0
59	MG	2A	3353	1/1	0.92	0.18	57,57,57,57	0
59	MG	2A	3183	1/1	0.92	0.24	52,52,52,52	0
59	MG	2A	3357	1/1	0.92	0.12	55,55,55,55	0
59	MG	2A	3621	1/1	0.92	0.11	57,57,57,57	0
59	MG	1A	3343	1/1	0.92	0.09	43,43,43,43	0
59	MG	2l	201	1/1	0.92	0.10	65,65,65,65	0
59	MG	1n	502	1/1	0.92	0.28	58,58,58,58	0
59	MG	1a	3397	1/1	0.92	0.13	60,60,60,60	0
59	MG	1A	4109	1/1	0.92	0.09	42,42,42,42	0
59	MG	2T	201	1/1	0.92	0.14	54,54,54,54	0
59	MG	2A	3364	1/1	0.92	0.13	63,63,63,63	0
59	MG	2A	3365	1/1	0.92	0.15	56,56,56,56	0
59	MG	1E	313	1/1	0.92	0.23	34,34,34,34	0
59	MG	2v	101	1/1	0.92	0.24	49,49,49,49	0
59	MG	1a	3400	1/1	0.92	0.19	54,54,54,54	0
59	MG	1A	3396	1/1	0.92	0.09	46,46,46,46	0
59	MG	2v	104	1/1	0.92	0.17	52,52,52,52	0
59	MG	2A	3370	1/1	0.92	0.07	54,54,54,54	0
59	MG	1A	3173	1/1	0.92	0.08	36,36,36,36	0
59	MG	1A	3464	1/1	0.92	0.16	51,51,51,51	0
59	MG	2A	3197	1/1	0.92	0.17	50,50,50,50	0
59	MG	1A	4113	1/1	0.92	0.07	35,35,35,35	0
59	MG	1A	3823	1/1	0.92	0.14	59,59,59,59	0
59	MG	2a	3004	1/1	0.92	0.23	56,56,56,56	0
59	MG	2A	3381	1/1	0.92	0.16	17,17,17,17	0
59	MG	1G	3003	1/1	0.92	0.06	56,56,56,56	0
59	MG	2A	3386	1/1	0.92	0.12	45,45,45,45	0
59	MG	1A	3211	1/1	0.92	0.22	47,47,47,47	0
59	MG	1A	3572	1/1	0.92	0.08	38,38,38,38	0
59	MG	1N	3006	1/1	0.92	0.19	41,41,41,41	0
59	MG	1A	3091	1/1	0.92	0.07	17,17,17,17	0
59	MG	1A	3574	1/1	0.92	0.15	52,52,52,52	0
59	MG	2A	3404	1/1	0.92	0.11	48,48,48,48	0
59	MG	1A	3406	1/1	0.92	0.10	50,50,50,50	0
59	MG	2A	3407	1/1	0.92	0.09	34,34,34,34	0
59	MG	1A	3074	1/1	0.93	0.40	28,28,28,28	0
59	MG	2A	3372	1/1	0.93	0.22	50,50,50,50	0
59	MG	2A	3648	1/1	0.93	0.14	60,60,60,60	0
59	MG	2A	3373	1/1	0.93	0.07	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1D	302	1/1	0.93	0.16	17,17,17,17	0
59	MG	1a	3387	1/1	0.93	0.24	40,40,40,40	0
59	MG	1A	3724	1/1	0.93	0.13	46,46,46,46	0
59	MG	2A	3655	1/1	0.93	0.07	62,62,62,62	0
59	MG	1A	3728	1/1	0.93	0.12	16,16,16,16	0
59	MG	2a	3020	1/1	0.93	0.20	61,61,61,61	0
59	MG	1A	3313	1/1	0.93	0.07	38,38,38,38	0
59	MG	1A	3174	1/1	0.93	0.08	23,23,23,23	0
59	MG	2A	3664	1/1	0.93	0.12	68,68,68,68	0
59	MG	1E	302	1/1	0.93	0.10	47,47,47,47	0
59	MG	1A	4088	1/1	0.93	0.11	42,42,42,42	0
59	MG	2A	3387	1/1	0.93	0.09	47,47,47,47	0
59	MG	1A	3469	1/1	0.93	0.21	33,33,33,33	0
59	MG	2A	3672	1/1	0.93	0.08	58,58,58,58	0
59	MG	1A	3317	1/1	0.93	0.27	32,32,32,32	0
59	MG	1A	3391	1/1	0.93	0.13	41,41,41,41	0
59	MG	1A	4092	1/1	0.93	0.13	45,45,45,45	0
59	MG	2A	3678	1/1	0.93	0.14	64,64,64,64	0
59	MG	2A	3190	1/1	0.93	0.12	37,37,37,37	0
59	MG	1A	3589	1/1	0.93	0.09	40,40,40,40	0
59	MG	1F	301	1/1	0.93	0.14	50,50,50,50	0
59	MG	1w	107	1/1	0.93	0.10	62,62,62,62	0
59	MG	1A	3075	1/1	0.93	0.27	29,29,29,29	0
59	MG	1F	307	1/1	0.93	0.10	44,44,44,44	0
59	MG	1A	3217	1/1	0.93	0.16	47,47,47,47	0
59	MG	1A	4097	1/1	0.93	0.10	45,45,45,45	0
59	MG	1A	3748	1/1	0.93	0.28	24,24,24,24	0
59	MG	1x	101	1/1	0.93	0.10	38,38,38,38	0
59	MG	2A	3696	1/1	0.93	0.08	73,73,73,73	0
59	MG	2A	3699	1/1	0.93	0.08	38,38,38,38	0
59	MG	2a	3051	1/1	0.93	0.21	55,55,55,55	0
59	MG	1A	3266	1/1	0.93	0.17	45,45,45,45	0
59	MG	1A	3327	1/1	0.93	0.39	42,42,42,42	0
59	MG	1A	3042	1/1	0.93	0.07	17,17,17,17	0
59	MG	2A	3431	1/1	0.93	0.12	54,54,54,54	0
59	MG	1N	3004	1/1	0.93	0.10	41,41,41,41	0
59	MG	2A	3435	1/1	0.93	0.08	47,47,47,47	0
59	MG	1A	3756	1/1	0.93	0.07	26,26,26,26	0
59	MG	1N	3009	1/1	0.93	0.16	28,28,28,28	0
59	MG	2A	3440	1/1	0.93	0.16	58,58,58,58	0
59	MG	1A	3599	1/1	0.93	0.12	21,21,21,21	0
59	MG	1x	113	1/1	0.93	0.12	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3270	1/1	0.93	0.09	45,45,45,45	0
59	MG	2a	3068	1/1	0.93	0.16	52,52,52,52	0
59	MG	2a	3069	1/1	0.93	0.34	68,68,68,68	0
59	MG	2a	3072	1/1	0.93	0.31	50,50,50,50	0
59	MG	1A	3608	1/1	0.93	0.10	16,16,16,16	0
59	MG	2A	3213	1/1	0.93	0.28	52,52,52,52	0
59	MG	2A	3450	1/1	0.93	0.09	53,53,53,53	0
59	MG	1a	3419	1/1	0.93	0.20	49,49,49,49	0
59	MG	1A	3768	1/1	0.93	0.14	56,56,56,56	0
59	MG	1A	3404	1/1	0.93	0.16	34,34,34,34	0
59	MG	1a	3423	1/1	0.93	0.27	53,53,53,53	0
59	MG	1A	3220	1/1	0.93	0.21	25,25,25,25	0
59	MG	2A	3459	1/1	0.93	0.18	55,55,55,55	0
59	MG	1A	3947	1/1	0.93	0.11	58,58,58,58	0
59	MG	2A	3464	1/1	0.93	0.15	46,46,46,46	0
59	MG	1R	201	1/1	0.93	0.09	28,28,28,28	0
59	MG	2A	3467	1/1	0.93	0.16	54,54,54,54	0
59	MG	2A	3017	1/1	0.93	0.18	39,39,39,39	0
59	MG	1A	3622	1/1	0.93	0.13	17,17,17,17	0
59	MG	1A	3133	1/1	0.93	0.09	41,41,41,41	0
59	MG	2A	3229	1/1	0.93	0.12	54,54,54,54	0
59	MG	1A	3950	1/1	0.93	0.14	47,47,47,47	0
59	MG	1A	3625	1/1	0.93	0.10	63,63,63,63	0
59	MG	1A	3275	1/1	0.93	0.10	38,38,38,38	0
59	MG	1A	3777	1/1	0.93	0.12	45,45,45,45	0
59	MG	1W	201	1/1	0.93	0.20	39,39,39,39	0
59	MG	1A	3339	1/1	0.93	0.10	45,45,45,45	0
59	MG	2a	3100	1/1	0.93	0.25	51,51,51,51	0
59	MG	1Y	504	1/1	0.93	0.24	45,45,45,45	0
59	MG	1A	3962	1/1	0.93	0.17	55,55,55,55	0
59	MG	1A	3182	1/1	0.93	0.07	38,38,38,38	0
59	MG	2A	3763	1/1	0.93	0.14	66,66,66,66	0
59	MG	2A	3035	1/1	0.93	0.24	67,67,67,67	0
59	MG	2A	3036	1/1	0.93	0.09	49,49,49,49	0
59	MG	10	105	1/1	0.93	0.14	40,40,40,40	0
59	MG	1A	3967	1/1	0.93	0.10	42,42,42,42	0
59	MG	1A	3782	1/1	0.93	0.10	60,60,60,60	0
59	MG	1A	3969	1/1	0.93	0.09	36,36,36,36	0
59	MG	1A	3186	1/1	0.93	0.26	35,35,35,35	0
59	MG	2A	3045	1/1	0.93	0.09	49,49,49,49	0
59	MG	2A	3046	1/1	0.93	0.18	58,58,58,58	0
59	MG	2A	3499	1/1	0.93	0.18	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3047	1/1	0.93	0.12	47,47,47,47	0
59	MG	2A	3049	1/1	0.93	0.08	44,44,44,44	0
59	MG	1A	3784	1/1	0.93	0.09	14,14,14,14	0
59	MG	1A	3632	1/1	0.93	0.19	53,53,53,53	0
59	MG	2A	3057	1/1	0.93	0.21	51,51,51,51	0
59	MG	1A	3636	1/1	0.93	0.13	46,46,46,46	0
59	MG	2A	3515	1/1	0.93	0.08	39,39,39,39	0
59	MG	1A	3088	1/1	0.93	0.15	44,44,44,44	0
59	MG	1A	3639	1/1	0.93	0.08	51,51,51,51	0
59	MG	18	103	1/1	0.93	0.11	38,38,38,38	0
59	MG	2A	3066	1/1	0.93	0.14	54,54,54,54	0
59	MG	2A	3267	1/1	0.93	0.10	55,55,55,55	0
59	MG	1A	3792	1/1	0.93	0.10	42,42,42,42	0
59	MG	1A	3089	1/1	0.93	0.07	28,28,28,28	0
59	MG	1a	3303	1/1	0.93	0.17	55,55,55,55	0
59	MG	2a	3136	1/1	0.93	0.08	64,64,64,64	0
59	MG	1A	3345	1/1	0.93	0.20	37,37,37,37	0
59	MG	1A	3110	1/1	0.93	0.06	29,29,29,29	0
59	MG	2A	3074	1/1	0.93	0.07	49,49,49,49	0
59	MG	2A	3530	1/1	0.93	0.10	35,35,35,35	0
59	MG	2A	3277	1/1	0.93	0.29	51,51,51,51	0
59	MG	2A	3532	1/1	0.93	0.10	53,53,53,53	0
59	MG	2a	3152	1/1	0.93	0.07	65,65,65,65	0
59	MG	2A	3279	1/1	0.93	0.24	43,43,43,43	0
59	MG	1A	3799	1/1	0.93	0.14	22,22,22,22	0
59	MG	2A	3800	1/1	0.93	0.08	62,62,62,62	0
59	MG	1A	3285	1/1	0.93	0.14	42,42,42,42	0
59	MG	2A	3804	1/1	0.93	0.10	59,59,59,59	0
59	MG	1A	3513	1/1	0.93	0.12	44,44,44,44	0
59	MG	2A	3541	1/1	0.93	0.11	30,30,30,30	0
59	MG	1a	3321	1/1	0.93	0.12	50,50,50,50	0
59	MG	1A	3802	1/1	0.93	0.23	31,31,31,31	0
59	MG	1A	3111	1/1	0.93	0.12	56,56,56,56	0
59	MG	2a	3167	1/1	0.93	0.07	74,74,74,74	0
59	MG	1A	3233	1/1	0.93	0.14	51,51,51,51	0
59	MG	1A	3356	1/1	0.93	0.08	38,38,38,38	0
59	MG	2a	3171	1/1	0.93	0.08	55,55,55,55	0
59	MG	1a	3494	1/1	0.93	0.10	48,48,48,48	0
59	MG	2A	3819	1/1	0.93	0.09	47,47,47,47	0
59	MG	2A	3549	1/1	0.93	0.15	55,55,55,55	0
59	MG	2A	3827	1/1	0.93	0.10	62,62,62,62	0
59	MG	1A	3357	1/1	0.93	0.24	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3290	1/1	0.93	0.20	37,37,37,37	0
59	MG	1A	3002	1/1	0.93	0.12	53,53,53,53	0
59	MG	2A	3832	1/1	0.93	0.17	53,53,53,53	0
59	MG	1A	3239	1/1	0.93	0.25	49,49,49,49	0
59	MG	2a	3184	1/1	0.93	0.23	61,61,61,61	0
59	MG	2A	3093	1/1	0.93	0.25	56,56,56,56	0
59	MG	2A	3094	1/1	0.93	0.14	43,43,43,43	0
59	MG	1a	3333	1/1	0.93	0.23	54,54,54,54	0
59	MG	2A	3096	1/1	0.93	0.17	55,55,55,55	0
59	MG	2a	3189	1/1	0.93	0.20	57,57,57,57	0
59	MG	2A	3842	1/1	0.93	0.32	46,46,46,46	0
59	MG	1a	3334	1/1	0.93	0.20	49,49,49,49	0
59	MG	1A	3822	1/1	0.93	0.06	11,11,11,11	0
59	MG	2a	3194	1/1	0.93	0.14	68,68,68,68	0
59	MG	2A	3561	1/1	0.93	0.09	31,31,31,31	0
59	MG	2A	3562	1/1	0.93	0.09	57,57,57,57	0
59	MG	2A	3847	1/1	0.93	0.30	37,37,37,37	0
59	MG	2A	3302	1/1	0.93	0.35	57,57,57,57	0
59	MG	1A	3529	1/1	0.93	0.39	33,33,33,33	0
59	MG	2A	3304	1/1	0.93	0.33	56,56,56,56	0
59	MG	2B	3005	1/1	0.93	0.28	61,61,61,61	0
59	MG	1A	4021	1/1	0.93	0.07	27,27,27,27	0
59	MG	2A	3103	1/1	0.93	0.24	62,62,62,62	0
59	MG	1a	3341	1/1	0.93	0.16	50,50,50,50	0
59	MG	1A	3530	1/1	0.93	0.08	32,32,32,32	0
59	MG	2a	3207	1/1	0.93	0.22	55,55,55,55	0
59	MG	1a	3526	1/1	0.93	0.18	50,50,50,50	0
59	MG	2A	3572	1/1	0.93	0.08	24,24,24,24	0
59	MG	1A	4030	1/1	0.93	0.18	58,58,58,58	0
59	MG	1a	3532	1/1	0.93	0.08	57,57,57,57	0
59	MG	1A	3362	1/1	0.93	0.10	53,53,53,53	0
59	MG	2a	3213	1/1	0.93	0.12	66,66,66,66	0
59	MG	1A	3534	1/1	0.93	0.07	38,38,38,38	0
59	MG	1a	3348	1/1	0.93	0.20	41,41,41,41	0
59	MG	1A	3363	1/1	0.93	0.11	30,30,30,30	0
59	MG	2A	3316	1/1	0.93	0.25	49,49,49,49	0
59	MG	1a	3351	1/1	0.93	0.14	42,42,42,42	0
59	MG	1A	4041	1/1	0.93	0.08	42,42,42,42	0
59	MG	2A	3131	1/1	0.93	0.22	51,51,51,51	0
59	MG	2a	3222	1/1	0.93	0.17	57,57,57,57	0
59	MG	2A	3323	1/1	0.93	0.25	47,47,47,47	0
59	MG	2D	302	1/1	0.93	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3589	1/1	0.93	0.08	46,46,46,46	0
59	MG	1A	3366	1/1	0.93	0.13	58,58,58,58	0
59	MG	2A	3138	1/1	0.93	0.19	45,45,45,45	0
59	MG	1A	4044	1/1	0.93	0.10	54,54,54,54	0
59	MG	1A	3670	1/1	0.93	0.12	43,43,43,43	0
59	MG	2A	3142	1/1	0.93	0.11	58,58,58,58	0
59	MG	2E	305	1/1	0.93	0.12	43,43,43,43	0
59	MG	1a	3547	1/1	0.93	0.08	48,48,48,48	0
59	MG	2E	307	1/1	0.93	0.11	62,62,62,62	0
59	MG	2e	3001	1/1	0.93	0.12	62,62,62,62	0
59	MG	1A	3247	1/1	0.93	0.18	47,47,47,47	0
59	MG	2A	3334	1/1	0.93	0.17	61,61,61,61	0
59	MG	1A	3300	1/1	0.93	0.11	42,42,42,42	0
59	MG	1A	3302	1/1	0.93	0.14	54,54,54,54	0
59	MG	2k	3001	1/1	0.93	0.23	50,50,50,50	0
59	MG	1A	3036	1/1	0.93	0.16	23,23,23,23	0
59	MG	1A	3547	1/1	0.93	0.10	29,29,29,29	0
59	MG	1A	3551	1/1	0.93	0.09	29,29,29,29	0
59	MG	1A	3688	1/1	0.93	0.12	43,43,43,43	0
59	MG	2q	202	1/1	0.93	0.18	57,57,57,57	0
59	MG	1A	3847	1/1	0.93	0.06	25,25,25,25	0
59	MG	1A	3202	1/1	0.93	0.08	43,43,43,43	0
59	MG	2A	3155	1/1	0.93	0.13	44,44,44,44	0
59	MG	2A	3156	1/1	0.93	0.11	39,39,39,39	0
59	MG	2A	3158	1/1	0.93	0.11	50,50,50,50	0
59	MG	2A	3617	1/1	0.93	0.10	40,40,40,40	0
59	MG	1a	3368	1/1	0.93	0.33	63,63,63,63	0
59	MG	2T	203	1/1	0.93	0.22	50,50,50,50	0
59	MG	1A	4065	1/1	0.93	0.08	45,45,45,45	0
59	MG	2U	203	1/1	0.93	0.23	56,56,56,56	0
59	MG	1A	3451	1/1	0.93	0.16	38,38,38,38	0
59	MG	2V	201	1/1	0.93	0.16	60,60,60,60	0
59	MG	2X	3001	1/1	0.93	0.16	59,59,59,59	0
59	MG	1a	3371	1/1	0.93	0.12	55,55,55,55	0
59	MG	1A	3203	1/1	0.93	0.16	53,53,53,53	0
59	MG	1a	3566	1/1	0.93	0.10	57,57,57,57	0
59	MG	2A	3167	1/1	0.93	0.32	57,57,57,57	0
59	MG	1A	3698	1/1	0.93	0.09	16,16,16,16	0
59	MG	1A	3100	1/1	0.93	0.23	23,23,23,23	0
59	MG	1A	3874	1/1	0.93	0.09	13,13,13,13	0
59	MG	1A	3459	1/1	0.93	0.09	58,58,58,58	0
59	MG	1A	3258	1/1	0.93	0.15	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3713	1/1	0.93	0.11	49,49,49,49	0
59	MG	1A	3717	1/1	0.93	0.06	21,21,21,21	0
59	MG	2A	3175	1/1	0.93	0.09	63,63,63,63	0
59	MG	2a	3008	1/1	0.93	0.18	63,63,63,63	0
59	MG	A	8001	1/1	0.93	0.10	57,57,57,57	0
59	MG	1a	3437	1/1	0.94	0.33	58,58,58,58	0
59	MG	25	103	1/1	0.94	0.15	42,42,42,42	0
59	MG	2A	3071	1/1	0.94	0.11	50,50,50,50	0
59	MG	28	101	1/1	0.94	0.30	54,54,54,54	0
59	MG	1A	3167	1/1	0.94	0.09	38,38,38,38	0
59	MG	1A	3457	1/1	0.94	0.29	55,55,55,55	0
59	MG	1a	3440	1/1	0.94	0.07	50,50,50,50	0
59	MG	1A	3729	1/1	0.94	0.12	11,11,11,11	0
59	MG	2A	3608	1/1	0.94	0.14	60,60,60,60	0
59	MG	1A	3115	1/1	0.94	0.08	24,24,24,24	0
59	MG	1a	3444	1/1	0.94	0.15	33,33,33,33	0
59	MG	2A	3078	1/1	0.94	0.08	33,33,33,33	0
59	MG	1a	3447	1/1	0.94	0.12	51,51,51,51	0
59	MG	2A	3615	1/1	0.94	0.09	46,46,46,46	0
59	MG	2a	3010	1/1	0.94	0.23	62,62,62,62	0
59	MG	1A	3897	1/1	0.94	0.09	38,38,38,38	0
59	MG	2A	3319	1/1	0.94	0.21	36,36,36,36	0
59	MG	1A	3575	1/1	0.94	0.07	13,13,13,13	0
59	MG	2A	3322	1/1	0.94	0.32	42,42,42,42	0
59	MG	1A	3116	1/1	0.94	0.10	43,43,43,43	0
59	MG	2a	3016	1/1	0.94	0.07	46,46,46,46	0
59	MG	1A	3735	1/1	0.94	0.06	20,20,20,20	0
59	MG	1A	3903	1/1	0.94	0.08	29,29,29,29	0
59	MG	1S	3002	1/1	0.94	0.16	48,48,48,48	0
59	MG	1a	3461	1/1	0.94	0.10	41,41,41,41	0
59	MG	2a	3021	1/1	0.94	0.12	62,62,62,62	0
59	MG	2A	3328	1/1	0.94	0.27	51,51,51,51	0
59	MG	1A	3318	1/1	0.94	0.09	49,49,49,49	0
59	MG	1A	3319	1/1	0.94	0.06	38,38,38,38	0
59	MG	2A	3632	1/1	0.94	0.08	29,29,29,29	0
59	MG	1A	3385	1/1	0.94	0.16	39,39,39,39	0
59	MG	2A	3333	1/1	0.94	0.09	60,60,60,60	0
59	MG	1a	3470	1/1	0.94	0.08	49,49,49,49	0
59	MG	1a	3471	1/1	0.94	0.11	51,51,51,51	0
59	MG	1A	3744	1/1	0.94	0.08	44,44,44,44	0
59	MG	1a	3473	1/1	0.94	0.16	37,37,37,37	0
59	MG	1A	3124	1/1	0.94	0.09	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1Y	502	1/1	0.94	0.16	53,53,53,53	0
59	MG	1A	4107	1/1	0.94	0.11	17,17,17,17	0
59	MG	1A	3322	1/1	0.94	0.21	47,47,47,47	0
59	MG	1A	3473	1/1	0.94	0.31	54,54,54,54	0
59	MG	2A	3345	1/1	0.94	0.14	59,59,59,59	0
59	MG	1A	3389	1/1	0.94	0.27	36,36,36,36	0
59	MG	2A	3661	1/1	0.94	0.10	54,54,54,54	0
59	MG	10	101	1/1	0.94	0.16	41,41,41,41	0
59	MG	1a	3486	1/1	0.94	0.12	59,59,59,59	0
59	MG	1A	3916	1/1	0.94	0.08	12,12,12,12	0
59	MG	2A	3114	1/1	0.94	0.15	39,39,39,39	0
59	MG	2A	3117	1/1	0.94	0.12	60,60,60,60	0
59	MG	1A	3476	1/1	0.94	0.29	44,44,44,44	0
59	MG	2A	3121	1/1	0.94	0.17	49,49,49,49	0
59	MG	2a	3052	1/1	0.94	0.17	52,52,52,52	0
59	MG	1A	4114	1/1	0.94	0.13	57,57,57,57	0
59	MG	1A	3324	1/1	0.94	0.19	39,39,39,39	0
59	MG	1A	3221	1/1	0.94	0.14	40,40,40,40	0
59	MG	2A	3676	1/1	0.94	0.08	60,60,60,60	0
59	MG	1A	3065	1/1	0.94	0.28	37,37,37,37	0
59	MG	1A	3600	1/1	0.94	0.07	21,21,21,21	0
59	MG	2A	3363	1/1	0.94	0.14	47,47,47,47	0
59	MG	13	3003	1/1	0.94	0.09	42,42,42,42	0
59	MG	2A	3134	1/1	0.94	0.19	58,58,58,58	0
59	MG	1a	3501	1/1	0.94	0.07	57,57,57,57	0
59	MG	1a	3503	1/1	0.94	0.09	71,71,71,71	0
59	MG	2A	3139	1/1	0.94	0.14	33,33,33,33	0
59	MG	15	103	1/1	0.94	0.09	54,54,54,54	0
59	MG	1A	3761	1/1	0.94	0.12	49,49,49,49	0
59	MG	1A	3763	1/1	0.94	0.11	46,46,46,46	0
59	MG	1a	3507	1/1	0.94	0.08	64,64,64,64	0
59	MG	1A	3943	1/1	0.94	0.08	33,33,33,33	0
59	MG	1A	3765	1/1	0.94	0.14	33,33,33,33	0
59	MG	1A	3068	1/1	0.94	0.17	53,53,53,53	0
59	MG	1a	3301	1/1	0.94	0.22	49,49,49,49	0
59	MG	1A	3483	1/1	0.94	0.11	56,56,56,56	0
59	MG	1A	3092	1/1	0.94	0.21	32,32,32,32	0
59	MG	1A	3184	1/1	0.94	0.10	42,42,42,42	0
59	MG	1a	3527	1/1	0.94	0.07	62,62,62,62	0
59	MG	2a	3083	1/1	0.94	0.12	59,59,59,59	0
59	MG	1a	3528	1/1	0.94	0.07	59,59,59,59	0
59	MG	1a	3530	1/1	0.94	0.08	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3951	1/1	0.94	0.08	52,52,52,52	0
59	MG	2A	3397	1/1	0.94	0.07	23,23,23,23	0
59	MG	2A	3157	1/1	0.94	0.19	47,47,47,47	0
59	MG	2A	3401	1/1	0.94	0.10	59,59,59,59	0
59	MG	2A	3729	1/1	0.94	0.08	57,57,57,57	0
59	MG	1a	3309	1/1	0.94	0.23	61,61,61,61	0
59	MG	1a	3313	1/1	0.94	0.22	42,42,42,42	0
59	MG	1A	3488	1/1	0.94	0.07	45,45,45,45	0
59	MG	1A	3772	1/1	0.94	0.19	46,46,46,46	0
59	MG	2a	3096	1/1	0.94	0.46	56,56,56,56	0
59	MG	1A	3034	1/1	0.94	0.06	27,27,27,27	0
59	MG	1a	3540	1/1	0.94	0.07	36,36,36,36	0
59	MG	1A	3048	1/1	0.94	0.07	39,39,39,39	0
59	MG	1A	4142	1/1	0.94	0.06	47,47,47,47	0
59	MG	1A	3333	1/1	0.94	0.14	35,35,35,35	0
59	MG	1A	3965	1/1	0.94	0.10	46,46,46,46	0
59	MG	1a	3545	1/1	0.94	0.06	46,46,46,46	0
59	MG	1A	3492	1/1	0.94	0.16	55,55,55,55	0
59	MG	1A	3281	1/1	0.94	0.22	43,43,43,43	0
59	MG	2A	3430	1/1	0.94	0.07	29,29,29,29	0
59	MG	1A	3229	1/1	0.94	0.06	45,45,45,45	0
59	MG	1A	4154	1/1	0.94	0.07	38,38,38,38	0
59	MG	1A	3496	1/1	0.94	0.18	50,50,50,50	0
59	MG	1A	4156	1/1	0.94	0.16	37,37,37,37	0
59	MG	1A	4161	1/1	0.94	0.07	35,35,35,35	0
59	MG	1a	3554	1/1	0.94	0.12	58,58,58,58	0
59	MG	1A	3498	1/1	0.94	0.17	51,51,51,51	0
59	MG	1A	4167	1/1	0.94	0.05	19,19,19,19	0
59	MG	1A	3500	1/1	0.94	0.10	54,54,54,54	0
59	MG	1a	3340	1/1	0.94	0.10	53,53,53,53	0
59	MG	1A	4172	1/1	0.94	0.30	44,44,44,44	0
59	MG	1A	3502	1/1	0.94	0.15	35,35,35,35	0
59	MG	1A	3023	1/1	0.94	0.37	24,24,24,24	0
59	MG	1A	3050	1/1	0.94	0.14	31,31,31,31	0
59	MG	1A	3342	1/1	0.94	0.08	42,42,42,42	0
59	MG	1A	3985	1/1	0.94	0.10	53,53,53,53	0
59	MG	1a	3349	1/1	0.94	0.11	45,45,45,45	0
59	MG	1A	3234	1/1	0.94	0.10	33,33,33,33	0
59	MG	1a	3570	1/1	0.94	0.20	47,47,47,47	0
59	MG	2a	3128	1/1	0.94	0.06	59,59,59,59	0
59	MG	1A	3987	1/1	0.94	0.07	47,47,47,47	0
59	MG	2A	3465	1/1	0.94	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3507	1/1	0.94	0.12	45,45,45,45	0
59	MG	2A	3196	1/1	0.94	0.10	51,51,51,51	0
59	MG	1A	4189	1/1	0.94	0.10	44,44,44,44	0
59	MG	1a	3576	1/1	0.94	0.18	53,53,53,53	0
59	MG	1A	3795	1/1	0.94	0.10	23,23,23,23	0
59	MG	1a	3356	1/1	0.94	0.09	41,41,41,41	0
59	MG	1a	3357	1/1	0.94	0.11	58,58,58,58	0
59	MG	2a	3149	1/1	0.94	0.07	58,58,58,58	0
59	MG	1A	3287	1/1	0.94	0.21	38,38,38,38	0
59	MG	1A	4192	1/1	0.94	0.30	29,29,29,29	0
59	MG	1A	3991	1/1	0.94	0.12	40,40,40,40	0
59	MG	1A	4194	1/1	0.94	0.25	33,33,33,33	0
59	MG	2A	3479	1/1	0.94	0.08	26,26,26,26	0
59	MG	2A	3206	1/1	0.94	0.23	50,50,50,50	0
59	MG	1A	4197	1/1	0.94	0.25	25,25,25,25	0
59	MG	2A	3482	1/1	0.94	0.08	40,40,40,40	0
59	MG	1A	4203	1/1	0.94	0.18	33,33,33,33	0
59	MG	2A	3484	1/1	0.94	0.10	33,33,33,33	0
59	MG	2a	3162	1/1	0.94	0.09	55,55,55,55	0
59	MG	1A	3418	1/1	0.94	0.16	22,22,22,22	0
59	MG	1A	3037	1/1	0.94	0.18	37,37,37,37	0
59	MG	1A	3423	1/1	0.94	0.09	41,41,41,41	0
59	MG	1A	3052	1/1	0.94	0.25	45,45,45,45	0
59	MG	1A	4006	1/1	0.94	0.06	31,31,31,31	0
59	MG	1A	3039	1/1	0.94	0.05	22,22,22,22	0
59	MG	1B	202	1/1	0.94	0.22	37,37,37,37	0
59	MG	2a	3172	1/1	0.94	0.14	42,42,42,42	0
59	MG	1A	3803	1/1	0.94	0.18	33,33,33,33	0
59	MG	2A	3217	1/1	0.94	0.14	48,48,48,48	0
59	MG	2a	3175	1/1	0.94	0.09	58,58,58,58	0
59	MG	1w	105	1/1	0.94	0.11	39,39,39,39	0
59	MG	2A	3803	1/1	0.94	0.08	50,50,50,50	0
59	MG	2a	3178	1/1	0.94	0.20	52,52,52,52	0
59	MG	1w	106	1/1	0.94	0.15	61,61,61,61	0
59	MG	1A	4010	1/1	0.94	0.11	50,50,50,50	0
59	MG	2A	3505	1/1	0.94	0.12	35,35,35,35	0
59	MG	1A	3804	1/1	0.94	0.22	27,27,27,27	0
59	MG	2A	3508	1/1	0.94	0.10	43,43,43,43	0
59	MG	2A	3509	1/1	0.94	0.10	40,40,40,40	0
59	MG	1A	3517	1/1	0.94	0.15	41,41,41,41	0
59	MG	1a	3375	1/1	0.94	0.10	37,37,37,37	0
59	MG	1B	210	1/1	0.94	0.10	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3227	1/1	0.94	0.20	47,47,47,47	0
59	MG	2A	3820	1/1	0.94	0.17	35,35,35,35	0
59	MG	1a	3378	1/1	0.94	0.19	63,63,63,63	0
59	MG	2A	3823	1/1	0.94	0.18	47,47,47,47	0
59	MG	2A	3824	1/1	0.94	0.10	43,43,43,43	0
59	MG	1a	3379	1/1	0.94	0.08	49,49,49,49	0
59	MG	1A	3028	1/1	0.94	0.05	34,34,34,34	0
59	MG	1A	3352	1/1	0.94	0.08	43,43,43,43	0
59	MG	1A	3295	1/1	0.94	0.07	47,47,47,47	0
59	MG	1x	107	1/1	0.94	0.12	50,50,50,50	0
59	MG	2A	3834	1/1	0.94	0.09	42,42,42,42	0
59	MG	1x	108	1/1	0.94	0.23	53,53,53,53	0
59	MG	1A	3354	1/1	0.94	0.21	37,37,37,37	0
59	MG	1A	3813	1/1	0.94	0.06	15,15,15,15	0
59	MG	1A	3815	1/1	0.94	0.10	25,25,25,25	0
59	MG	1A	4024	1/1	0.94	0.09	46,46,46,46	0
59	MG	2A	3841	1/1	0.94	0.08	59,59,59,59	0
59	MG	1A	3430	1/1	0.94	0.23	32,32,32,32	0
59	MG	1A	4026	1/1	0.94	0.07	45,45,45,45	0
59	MG	2A	3245	1/1	0.94	0.12	48,48,48,48	0
59	MG	1A	4027	1/1	0.94	0.05	45,45,45,45	0
59	MG	1A	3431	1/1	0.94	0.08	45,45,45,45	0
59	MG	1A	3250	1/1	0.94	0.11	49,49,49,49	0
59	MG	1A	3299	1/1	0.94	0.07	49,49,49,49	0
59	MG	2A	3251	1/1	0.94	0.07	40,40,40,40	0
59	MG	1A	3157	1/1	0.94	0.10	37,37,37,37	0
59	MG	1A	3301	1/1	0.94	0.26	37,37,37,37	0
59	MG	2A	3254	1/1	0.94	0.06	47,47,47,47	0
59	MG	1A	4042	1/1	0.94	0.07	42,42,42,42	0
59	MG	1A	3675	1/1	0.94	0.16	21,21,21,21	0
59	MG	2A	3257	1/1	0.94	0.08	49,49,49,49	0
59	MG	2A	3008	1/1	0.94	0.13	44,44,44,44	0
59	MG	2A	3548	1/1	0.94	0.08	36,36,36,36	0
59	MG	2a	3225	1/1	0.94	0.13	59,59,59,59	0
59	MG	2A	3015	1/1	0.94	0.09	57,57,57,57	0
59	MG	1A	3253	1/1	0.94	0.15	37,37,37,37	0
59	MG	1A	3161	1/1	0.94	0.16	25,25,25,25	0
59	MG	2a	3231	1/1	0.94	0.16	57,57,57,57	0
59	MG	2A	3019	1/1	0.94	0.11	54,54,54,54	0
59	MG	2a	3233	1/1	0.94	0.07	50,50,50,50	0
59	MG	1A	3540	1/1	0.94	0.09	47,47,47,47	0
59	MG	1A	3686	1/1	0.94	0.08	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1D	305	1/1	0.94	0.10	29,29,29,29	0
59	MG	1D	308	1/1	0.94	0.18	27,27,27,27	0
59	MG	2A	3268	1/1	0.94	0.21	61,61,61,61	0
59	MG	2A	3269	1/1	0.94	0.12	50,50,50,50	0
59	MG	1A	3304	1/1	0.94	0.15	36,36,36,36	0
59	MG	2D	301	1/1	0.94	0.20	47,47,47,47	0
59	MG	1A	3058	1/1	0.94	0.10	50,50,50,50	0
59	MG	1A	3212	1/1	0.94	0.12	49,49,49,49	0
59	MG	1A	4058	1/1	0.94	0.13	47,47,47,47	0
59	MG	1A	3695	1/1	0.94	0.07	20,20,20,20	0
59	MG	1A	3004	1/1	0.94	0.09	47,47,47,47	0
59	MG	1E	306	1/1	0.94	0.10	31,31,31,31	0
59	MG	1A	3447	1/1	0.94	0.27	38,38,38,38	0
59	MG	1A	3552	1/1	0.94	0.09	7,7,7,7	0
59	MG	1A	3848	1/1	0.94	0.07	72,72,72,72	0
59	MG	1A	3262	1/1	0.94	0.21	41,41,41,41	0
59	MG	2q	204	1/1	0.94	0.09	70,70,70,70	0
59	MG	1A	3705	1/1	0.94	0.07	17,17,17,17	0
59	MG	1A	3215	1/1	0.94	0.27	33,33,33,33	0
59	MG	1A	3859	1/1	0.94	0.08	37,37,37,37	0
59	MG	2A	3575	1/1	0.94	0.13	60,60,60,60	0
59	MG	1A	3860	1/1	0.94	0.07	37,37,37,37	0
59	MG	1A	3452	1/1	0.94	0.16	32,32,32,32	0
59	MG	2P	201	1/1	0.94	0.24	51,51,51,51	0
59	MG	2Q	3001	1/1	0.94	0.07	52,52,52,52	0
59	MG	2A	3048	1/1	0.94	0.20	53,53,53,53	0
59	MG	1A	3714	1/1	0.94	0.07	10,10,10,10	0
59	MG	2A	3050	1/1	0.94	0.13	48,48,48,48	0
59	MG	1A	3564	1/1	0.94	0.05	26,26,26,26	0
59	MG	2A	3052	1/1	0.94	0.14	56,56,56,56	0
59	MG	1A	3720	1/1	0.94	0.07	34,34,34,34	0
59	MG	2A	3054	1/1	0.94	0.08	43,43,43,43	0
59	MG	2A	3055	1/1	0.94	0.06	24,24,24,24	0
59	MG	2A	3056	1/1	0.94	0.13	56,56,56,56	0
59	MG	1A	3880	1/1	0.94	0.09	64,64,64,64	0
59	MG	1A	3881	1/1	0.94	0.13	47,47,47,47	0
59	MG	1a	3431	1/1	0.94	0.12	38,38,38,38	0
59	MG	1A	3311	1/1	0.94	0.12	39,39,39,39	0
59	MG	1A	3884	1/1	0.94	0.11	41,41,41,41	0
59	MG	1N	3007	1/1	0.94	0.27	49,49,49,49	0
59	MG	1A	3888	1/1	0.94	0.06	31,31,31,31	0
59	MG	1A	3723	1/1	0.94	0.11	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	23	101	1/1	0.94	0.11	51,51,51,51	0
59	MG	13	3002	1/1	0.95	0.07	37,37,37,37	0
59	MG	1a	3497	1/1	0.95	0.10	65,65,65,65	0
59	MG	2A	3101	1/1	0.95	0.10	27,27,27,27	0
59	MG	27	3001	1/1	0.95	0.25	56,56,56,56	0
59	MG	1A	3981	1/1	0.95	0.07	13,13,13,13	0
59	MG	2A	3610	1/1	0.95	0.18	40,40,40,40	0
59	MG	1A	3691	1/1	0.95	0.12	39,39,39,39	0
59	MG	1A	4139	1/1	0.95	0.06	28,28,28,28	0
59	MG	1A	4140	1/1	0.95	0.05	31,31,31,31	0
59	MG	2A	3106	1/1	0.95	0.09	57,57,57,57	0
59	MG	1A	3983	1/1	0.95	0.11	63,63,63,63	0
59	MG	1A	3140	1/1	0.95	0.24	28,28,28,28	0
59	MG	1A	4144	1/1	0.95	0.10	42,42,42,42	0
59	MG	1A	3141	1/1	0.95	0.09	26,26,26,26	0
59	MG	2A	3620	1/1	0.95	0.14	50,50,50,50	0
59	MG	1A	3817	1/1	0.95	0.06	31,31,31,31	0
59	MG	1A	3818	1/1	0.95	0.07	14,14,14,14	0
59	MG	2A	3339	1/1	0.95	0.31	50,50,50,50	0
59	MG	1A	4149	1/1	0.95	0.09	47,47,47,47	0
59	MG	1a	3517	1/1	0.95	0.06	60,60,60,60	0
59	MG	2A	3342	1/1	0.95	0.05	41,41,41,41	0
59	MG	2A	3123	1/1	0.95	0.20	46,46,46,46	0
59	MG	1A	4150	1/1	0.95	0.07	35,35,35,35	0
59	MG	2A	3125	1/1	0.95	0.07	30,30,30,30	0
59	MG	2A	3631	1/1	0.95	0.17	54,54,54,54	0
59	MG	1A	3579	1/1	0.95	0.07	30,30,30,30	0
59	MG	2A	3633	1/1	0.95	0.07	37,37,37,37	0
59	MG	1A	4152	1/1	0.95	0.08	21,21,21,21	0
59	MG	1A	3230	1/1	0.95	0.21	40,40,40,40	0
59	MG	1A	3231	1/1	0.95	0.16	39,39,39,39	0
59	MG	2A	3133	1/1	0.95	0.16	48,48,48,48	0
59	MG	2a	3026	1/1	0.95	0.26	47,47,47,47	0
59	MG	1A	3422	1/1	0.95	0.18	56,56,56,56	0
59	MG	1a	3320	1/1	0.95	0.17	51,51,51,51	0
59	MG	2A	3643	1/1	0.95	0.06	48,48,48,48	0
59	MG	1A	3992	1/1	0.95	0.05	30,30,30,30	0
59	MG	2A	3355	1/1	0.95	0.12	44,44,44,44	0
59	MG	2a	3032	1/1	0.95	0.07	54,54,54,54	0
59	MG	1A	4160	1/1	0.95	0.08	53,53,53,53	0
59	MG	1a	3323	1/1	0.95	0.13	43,43,43,43	0
59	MG	1A	3272	1/1	0.95	0.12	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3996	1/1	0.95	0.08	35,35,35,35	0
59	MG	2A	3656	1/1	0.95	0.06	40,40,40,40	0
59	MG	2A	3657	1/1	0.95	0.07	60,60,60,60	0
59	MG	2a	3039	1/1	0.95	0.08	55,55,55,55	0
59	MG	1A	3708	1/1	0.95	0.08	37,37,37,37	0
59	MG	1A	4000	1/1	0.95	0.10	47,47,47,47	0
59	MG	1A	4171	1/1	0.95	0.23	26,26,26,26	0
59	MG	1A	4002	1/1	0.95	0.06	44,44,44,44	0
59	MG	1A	4173	1/1	0.95	0.32	36,36,36,36	0
59	MG	2A	3665	1/1	0.95	0.09	38,38,38,38	0
59	MG	2A	3148	1/1	0.95	0.10	65,65,65,65	0
59	MG	2A	3149	1/1	0.95	0.13	29,29,29,29	0
59	MG	1A	3709	1/1	0.95	0.06	20,20,20,20	0
59	MG	1A	3273	1/1	0.95	0.19	49,49,49,49	0
59	MG	1A	3831	1/1	0.95	0.24	17,17,17,17	0
59	MG	2A	3673	1/1	0.95	0.07	55,55,55,55	0
59	MG	1A	4177	1/1	0.95	0.19	29,29,29,29	0
59	MG	1A	3205	1/1	0.95	0.19	24,24,24,24	0
59	MG	1a	3338	1/1	0.95	0.18	51,51,51,51	0
59	MG	1a	3339	1/1	0.95	0.14	54,54,54,54	0
59	MG	2a	3060	1/1	0.95	0.20	49,49,49,49	0
59	MG	1A	3206	1/1	0.95	0.10	35,35,35,35	0
59	MG	1A	3107	1/1	0.95	0.28	32,32,32,32	0
59	MG	1A	4185	1/1	0.95	0.18	46,46,46,46	0
59	MG	1A	3719	1/1	0.95	0.05	44,44,44,44	0
59	MG	1A	3235	1/1	0.95	0.17	34,34,34,34	0
59	MG	1A	3721	1/1	0.95	0.08	14,14,14,14	0
59	MG	1A	3364	1/1	0.95	0.27	34,34,34,34	0
59	MG	1A	3365	1/1	0.95	0.21	40,40,40,40	0
59	MG	2A	3392	1/1	0.95	0.08	58,58,58,58	0
59	MG	2a	3071	1/1	0.95	0.15	51,51,51,51	0
59	MG	2A	3395	1/1	0.95	0.07	28,28,28,28	0
59	MG	1A	4016	1/1	0.95	0.11	24,24,24,24	0
59	MG	1A	4017	1/1	0.95	0.07	44,44,44,44	0
59	MG	2A	3697	1/1	0.95	0.07	25,25,25,25	0
59	MG	2A	3400	1/1	0.95	0.08	21,21,21,21	0
59	MG	1a	3564	1/1	0.95	0.08	54,54,54,54	0
59	MG	1A	3210	1/1	0.95	0.07	35,35,35,35	0
59	MG	2A	3403	1/1	0.95	0.11	38,38,38,38	0
59	MG	1A	4195	1/1	0.95	0.17	27,27,27,27	0
59	MG	2A	3709	1/1	0.95	0.07	46,46,46,46	0
59	MG	1A	3607	1/1	0.95	0.04	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1a	3568	1/1	0.95	0.06	53,53,53,53	0
59	MG	1A	3432	1/1	0.95	0.21	47,47,47,47	0
59	MG	1A	3320	1/1	0.95	0.07	41,41,41,41	0
59	MG	1A	4207	1/1	0.95	0.15	26,26,26,26	0
59	MG	1A	3614	1/1	0.95	0.06	24,24,24,24	0
59	MG	1a	3573	1/1	0.95	0.18	37,37,37,37	0
59	MG	2A	3416	1/1	0.95	0.07	34,34,34,34	0
59	MG	2A	3417	1/1	0.95	0.10	31,31,31,31	0
59	MG	2A	3418	1/1	0.95	0.07	46,46,46,46	0
59	MG	1A	4212	1/1	0.95	0.11	32,32,32,32	0
59	MG	1A	3615	1/1	0.95	0.15	55,55,55,55	0
59	MG	1A	4225	1/1	0.95	0.19	34,34,34,34	0
59	MG	1A	3280	1/1	0.95	0.07	39,39,39,39	0
59	MG	1A	3145	1/1	0.95	0.09	44,44,44,44	0
59	MG	1A	4031	1/1	0.95	0.09	47,47,47,47	0
59	MG	1A	4033	1/1	0.95	0.06	45,45,45,45	0
59	MG	1A	3371	1/1	0.95	0.21	39,39,39,39	0
59	MG	2A	3187	1/1	0.95	0.41	37,37,37,37	0
59	MG	1A	3372	1/1	0.95	0.19	37,37,37,37	0
59	MG	1B	205	1/1	0.95	0.10	40,40,40,40	0
59	MG	1A	4038	1/1	0.95	0.10	25,25,25,25	0
59	MG	2A	3443	1/1	0.95	0.07	30,30,30,30	0
59	MG	1A	3242	1/1	0.95	0.22	24,24,24,24	0
59	MG	1A	3875	1/1	0.95	0.14	54,54,54,54	0
59	MG	1B	211	1/1	0.95	0.31	52,52,52,52	0
59	MG	1A	3246	1/1	0.95	0.11	47,47,47,47	0
59	MG	2A	3195	1/1	0.95	0.21	36,36,36,36	0
59	MG	1A	3877	1/1	0.95	0.06	44,44,44,44	0
59	MG	2A	3753	1/1	0.95	0.12	52,52,52,52	0
59	MG	1A	3879	1/1	0.95	0.08	51,51,51,51	0
59	MG	2a	3115	1/1	0.95	0.27	59,59,59,59	0
59	MG	2A	3453	1/1	0.95	0.10	60,60,60,60	0
59	MG	1w	101	1/1	0.95	0.10	56,56,56,56	0
59	MG	1B	215	1/1	0.95	0.06	44,44,44,44	0
59	MG	1w	103	1/1	0.95	0.14	56,56,56,56	0
59	MG	1A	3149	1/1	0.95	0.06	20,20,20,20	0
59	MG	1A	4046	1/1	0.95	0.09	36,36,36,36	0
59	MG	1B	219	1/1	0.95	0.05	28,28,28,28	0
59	MG	2a	3123	1/1	0.95	0.15	55,55,55,55	0
59	MG	1A	3630	1/1	0.95	0.09	16,16,16,16	0
59	MG	1A	3751	1/1	0.95	0.07	21,21,21,21	0
59	MG	2A	3767	1/1	0.95	0.13	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3444	1/1	0.95	0.09	45,45,45,45	0
59	MG	1A	4054	1/1	0.95	0.19	57,57,57,57	0
59	MG	1A	3180	1/1	0.95	0.08	39,39,39,39	0
59	MG	2a	3132	1/1	0.95	0.07	68,68,68,68	0
59	MG	1A	3084	1/1	0.95	0.09	31,31,31,31	0
59	MG	2A	3772	1/1	0.95	0.11	35,35,35,35	0
59	MG	1A	3891	1/1	0.95	0.06	15,15,15,15	0
59	MG	1A	3329	1/1	0.95	0.08	51,51,51,51	0
59	MG	1A	3288	1/1	0.95	0.22	50,50,50,50	0
59	MG	2a	3139	1/1	0.95	0.08	65,65,65,65	0
59	MG	2a	3140	1/1	0.95	0.09	68,68,68,68	0
59	MG	1a	3392	1/1	0.95	0.22	45,45,45,45	0
59	MG	2a	3143	1/1	0.95	0.07	43,43,43,43	0
59	MG	2a	3144	1/1	0.95	0.17	50,50,50,50	0
59	MG	1x	105	1/1	0.95	0.16	47,47,47,47	0
59	MG	1A	3759	1/1	0.95	0.12	41,41,41,41	0
59	MG	1A	3640	1/1	0.95	0.10	25,25,25,25	0
59	MG	1a	3395	1/1	0.95	0.06	40,40,40,40	0
59	MG	1A	4064	1/1	0.95	0.11	30,30,30,30	0
59	MG	1A	3525	1/1	0.95	0.21	48,48,48,48	0
59	MG	2A	3220	1/1	0.95	0.17	68,68,68,68	0
59	MG	1A	3762	1/1	0.95	0.12	48,48,48,48	0
59	MG	1A	3086	1/1	0.95	0.07	31,31,31,31	0
59	MG	1A	4068	1/1	0.95	0.05	38,38,38,38	0
59	MG	1x	115	1/1	0.95	0.11	56,56,56,56	0
59	MG	2A	3488	1/1	0.95	0.22	54,54,54,54	0
59	MG	1A	3900	1/1	0.95	0.09	53,53,53,53	0
59	MG	2a	3161	1/1	0.95	0.09	72,72,72,72	0
59	MG	1A	3013	1/1	0.95	0.22	44,44,44,44	0
59	MG	1A	3766	1/1	0.95	0.06	21,21,21,21	0
59	MG	2A	3230	1/1	0.95	0.12	42,42,42,42	0
59	MG	2a	3165	1/1	0.95	0.07	68,68,68,68	0
59	MG	1A	3104	1/1	0.95	0.26	32,32,32,32	0
59	MG	2A	3495	1/1	0.95	0.13	37,37,37,37	0
59	MG	2A	3496	1/1	0.95	0.12	49,49,49,49	0
59	MG	1A	3335	1/1	0.95	0.10	46,46,46,46	0
59	MG	1A	3456	1/1	0.95	0.09	50,50,50,50	0
59	MG	2A	3002	1/1	0.95	0.27	46,46,46,46	0
59	MG	2A	3500	1/1	0.95	0.11	27,27,27,27	0
59	MG	1A	3336	1/1	0.95	0.07	36,36,36,36	0
59	MG	2A	3503	1/1	0.95	0.06	32,32,32,32	0
59	MG	2A	3504	1/1	0.95	0.11	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3805	1/1	0.95	0.10	53,53,53,53	0
59	MG	2A	3004	1/1	0.95	0.16	46,46,46,46	0
59	MG	1A	3159	1/1	0.95	0.17	32,32,32,32	0
59	MG	2A	3238	1/1	0.95	0.26	53,53,53,53	0
59	MG	1A	4079	1/1	0.95	0.15	68,68,68,68	0
59	MG	2A	3010	1/1	0.95	0.06	36,36,36,36	0
59	MG	1a	3411	1/1	0.95	0.28	47,47,47,47	0
59	MG	1A	3393	1/1	0.95	0.14	47,47,47,47	0
59	MG	1A	3539	1/1	0.95	0.08	26,26,26,26	0
59	MG	2A	3817	1/1	0.95	0.12	32,32,32,32	0
59	MG	1E	309	1/1	0.95	0.09	47,47,47,47	0
59	MG	1A	4084	1/1	0.95	0.10	45,45,45,45	0
59	MG	1A	3914	1/1	0.95	0.06	21,21,21,21	0
59	MG	2a	3190	1/1	0.95	0.17	56,56,56,56	0
59	MG	1A	3294	1/1	0.95	0.12	30,30,30,30	0
59	MG	1A	4087	1/1	0.95	0.10	34,34,34,34	0
59	MG	1A	3541	1/1	0.95	0.09	20,20,20,20	0
59	MG	1F	306	1/1	0.95	0.08	40,40,40,40	0
59	MG	2A	3523	1/1	0.95	0.11	63,63,63,63	0
59	MG	1A	3257	1/1	0.95	0.12	24,24,24,24	0
59	MG	1A	3919	1/1	0.95	0.05	67,67,67,67	0
59	MG	2A	3030	1/1	0.95	0.12	50,50,50,50	0
59	MG	2A	3031	1/1	0.95	0.22	44,44,44,44	0
59	MG	1A	3191	1/1	0.95	0.15	45,45,45,45	0
59	MG	2A	3529	1/1	0.95	0.10	47,47,47,47	0
59	MG	1A	3779	1/1	0.95	0.17	36,36,36,36	0
59	MG	2A	3839	1/1	0.95	0.21	39,39,39,39	0
59	MG	1A	3925	1/1	0.95	0.07	10,10,10,10	0
59	MG	1A	3780	1/1	0.95	0.07	10,10,10,10	0
59	MG	1A	3397	1/1	0.95	0.15	38,38,38,38	0
59	MG	2A	3534	1/1	0.95	0.13	58,58,58,58	0
59	MG	1N	3001	1/1	0.95	0.27	52,52,52,52	0
59	MG	2A	3536	1/1	0.95	0.09	41,41,41,41	0
59	MG	2A	3537	1/1	0.95	0.16	59,59,59,59	0
59	MG	2A	3263	1/1	0.95	0.20	47,47,47,47	0
59	MG	2A	3848	1/1	0.95	0.11	47,47,47,47	0
59	MG	2A	3040	1/1	0.95	0.12	40,40,40,40	0
59	MG	2B	3002	1/1	0.95	0.30	56,56,56,56	0
59	MG	1A	3934	1/1	0.95	0.07	16,16,16,16	0
59	MG	1N	3005	1/1	0.95	0.10	51,51,51,51	0
59	MG	2A	3043	1/1	0.95	0.12	57,57,57,57	0
59	MG	1A	3659	1/1	0.95	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3940	1/1	0.95	0.06	27,27,27,27	0
59	MG	1A	3298	1/1	0.95	0.15	57,57,57,57	0
59	MG	1A	3664	1/1	0.95	0.07	46,46,46,46	0
59	MG	2a	3224	1/1	0.95	0.19	58,58,58,58	0
59	MG	1O	3002	1/1	0.95	0.29	41,41,41,41	0
59	MG	1A	3259	1/1	0.95	0.19	41,41,41,41	0
59	MG	1A	3402	1/1	0.95	0.11	42,42,42,42	0
59	MG	1A	3554	1/1	0.95	0.11	26,26,26,26	0
59	MG	1A	4108	1/1	0.95	0.06	32,32,32,32	0
59	MG	1a	3442	1/1	0.95	0.12	59,59,59,59	0
59	MG	2A	3280	1/1	0.95	0.07	49,49,49,49	0
59	MG	1A	3095	1/1	0.95	0.08	23,23,23,23	0
59	MG	1A	3478	1/1	0.95	0.26	42,42,42,42	0
59	MG	1a	3446	1/1	0.95	0.08	48,48,48,48	0
59	MG	1A	3014	1/1	0.95	0.14	38,38,38,38	0
59	MG	1A	3347	1/1	0.95	0.17	40,40,40,40	0
59	MG	2A	3059	1/1	0.95	0.06	37,37,37,37	0
59	MG	1a	3449	1/1	0.95	0.12	53,53,53,53	0
59	MG	1A	3676	1/1	0.95	0.06	29,29,29,29	0
59	MG	1A	3567	1/1	0.95	0.06	27,27,27,27	0
59	MG	1S	3003	1/1	0.95	0.06	61,61,61,61	0
59	MG	1A	3348	1/1	0.95	0.07	56,56,56,56	0
59	MG	1A	3679	1/1	0.95	0.07	50,50,50,50	0
59	MG	1A	3964	1/1	0.95	0.10	36,36,36,36	0
59	MG	2A	3070	1/1	0.95	0.07	42,42,42,42	0
59	MG	1U	204	1/1	0.95	0.06	36,36,36,36	0
59	MG	1A	3137	1/1	0.95	0.20	43,43,43,43	0
59	MG	1A	4119	1/1	0.95	0.08	22,22,22,22	0
59	MG	1a	3468	1/1	0.95	0.13	51,51,51,51	0
59	MG	2F	302	1/1	0.95	0.13	41,41,41,41	0
59	MG	1W	202	1/1	0.95	0.08	39,39,39,39	0
59	MG	1X	3004	1/1	0.95	0.08	49,49,49,49	0
59	MG	1A	4121	1/1	0.95	0.10	30,30,30,30	0
59	MG	2A	3580	1/1	0.95	0.08	29,29,29,29	0
59	MG	1A	3681	1/1	0.95	0.05	23,23,23,23	0
59	MG	1A	3682	1/1	0.95	0.09	48,48,48,48	0
59	MG	1A	3199	1/1	0.95	0.06	32,32,32,32	0
59	MG	1A	3687	1/1	0.95	0.16	54,54,54,54	0
59	MG	1Z	304	1/1	0.95	0.19	50,50,50,50	0
59	MG	1A	3807	1/1	0.95	0.14	21,21,21,21	0
59	MG	1O	104	1/1	0.95	0.05	39,39,39,39	0
59	MG	1A	3484	1/1	0.95	0.17	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3086	1/1	0.95	0.18	30,30,30,30	0
59	MG	1A	3972	1/1	0.95	0.11	24,24,24,24	0
59	MG	1A	4130	1/1	0.95	0.09	65,65,65,65	0
59	MG	10	108	1/1	0.95	0.04	39,39,39,39	0
59	MG	2A	3090	1/1	0.95	0.17	53,53,53,53	0
59	MG	2U	201	1/1	0.95	0.13	47,47,47,47	0
59	MG	2A	3091	1/1	0.95	0.10	44,44,44,44	0
59	MG	1A	3689	1/1	0.95	0.07	41,41,41,41	0
59	MG	1a	3491	1/1	0.95	0.08	75,75,75,75	0
59	MG	1A	3121	1/1	0.95	0.09	37,37,37,37	0
59	MG	2A	3321	1/1	0.95	0.07	58,58,58,58	0
59	MG	1A	3980	1/1	0.95	0.09	39,39,39,39	0
59	MG	1A	4136	1/1	0.95	0.08	50,50,50,50	0
59	MG	2A	3604	1/1	0.95	0.10	46,46,46,46	0
59	MG	1A	3633	1/1	0.96	0.08	22,22,22,22	0
59	MG	2A	3660	1/1	0.96	0.07	76,76,76,76	0
59	MG	1A	3634	1/1	0.96	0.06	12,12,12,12	0
59	MG	1D	301	1/1	0.96	0.22	24,24,24,24	0
59	MG	1A	3635	1/1	0.96	0.07	8,8,8,8	0
59	MG	1A	3083	1/1	0.96	0.16	36,36,36,36	0
59	MG	1D	306	1/1	0.96	0.15	40,40,40,40	0
59	MG	2A	3408	1/1	0.96	0.11	56,56,56,56	0
59	MG	2A	3409	1/1	0.96	0.10	50,50,50,50	0
59	MG	1A	3922	1/1	0.96	0.08	41,41,41,41	0
59	MG	2A	3670	1/1	0.96	0.09	64,64,64,64	0
59	MG	1A	3923	1/1	0.96	0.06	46,46,46,46	0
59	MG	1A	3041	1/1	0.96	0.07	20,20,20,20	0
59	MG	1A	3369	1/1	0.96	0.27	31,31,31,31	0
59	MG	1A	3055	1/1	0.96	0.13	50,50,50,50	0
59	MG	1A	3520	1/1	0.96	0.13	16,16,16,16	0
59	MG	1A	3931	1/1	0.96	0.06	64,64,64,64	0
59	MG	1A	3932	1/1	0.96	0.05	49,49,49,49	0
59	MG	2A	3420	1/1	0.96	0.09	28,28,28,28	0
59	MG	2A	3679	1/1	0.96	0.10	79,79,79,79	0
59	MG	2A	3421	1/1	0.96	0.14	42,42,42,42	0
59	MG	1A	3933	1/1	0.96	0.08	25,25,25,25	0
59	MG	1A	3224	1/1	0.96	0.13	49,49,49,49	0
59	MG	2A	3424	1/1	0.96	0.08	31,31,31,31	0
59	MG	1x	106	1/1	0.96	0.20	57,57,57,57	0
59	MG	1A	3072	1/1	0.96	0.10	34,34,34,34	0
59	MG	2A	3429	1/1	0.96	0.06	56,56,56,56	0
59	MG	1E	310	1/1	0.96	0.11	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1E	311	1/1	0.96	0.10	15,15,15,15	0
59	MG	2A	3433	1/1	0.96	0.08	38,38,38,38	0
59	MG	1A	3776	1/1	0.96	0.07	55,55,55,55	0
59	MG	1A	4100	1/1	0.96	0.08	50,50,50,50	0
59	MG	1A	3941	1/1	0.96	0.08	30,30,30,30	0
59	MG	2A	3700	1/1	0.96	0.07	35,35,35,35	0
59	MG	2A	3437	1/1	0.96	0.13	48,48,48,48	0
59	MG	2A	3704	1/1	0.96	0.06	53,53,53,53	0
59	MG	1A	3135	1/1	0.96	0.19	22,22,22,22	0
59	MG	2A	3439	1/1	0.96	0.06	32,32,32,32	0
59	MG	2a	3056	1/1	0.96	0.08	47,47,47,47	0
59	MG	1A	3524	1/1	0.96	0.13	31,31,31,31	0
59	MG	1F	304	1/1	0.96	0.11	21,21,21,21	0
59	MG	1F	305	1/1	0.96	0.16	27,27,27,27	0
59	MG	2A	3715	1/1	0.96	0.08	61,61,61,61	0
59	MG	2A	3444	1/1	0.96	0.10	31,31,31,31	0
59	MG	1A	3944	1/1	0.96	0.07	39,39,39,39	0
59	MG	2A	3719	1/1	0.96	0.06	64,64,64,64	0
59	MG	2A	3720	1/1	0.96	0.06	42,42,42,42	0
59	MG	1y	101	1/1	0.96	0.12	32,32,32,32	0
59	MG	1A	3056	1/1	0.96	0.11	24,24,24,24	0
59	MG	1A	3183	1/1	0.96	0.08	39,39,39,39	0
59	MG	2A	3449	1/1	0.96	0.11	17,17,17,17	0
59	MG	1A	3527	1/1	0.96	0.16	22,22,22,22	0
59	MG	1A	3279	1/1	0.96	0.13	45,45,45,45	0
59	MG	2A	3001	1/1	0.96	0.31	49,49,49,49	0
59	MG	1A	3038	1/1	0.96	0.10	30,30,30,30	0
59	MG	1A	3448	1/1	0.96	0.28	36,36,36,36	0
59	MG	1A	3139	1/1	0.96	0.09	29,29,29,29	0
59	MG	1A	3282	1/1	0.96	0.19	36,36,36,36	0
59	MG	1a	3417	1/1	0.96	0.32	50,50,50,50	0
59	MG	2A	3009	1/1	0.96	0.05	31,31,31,31	0
59	MG	2A	3463	1/1	0.96	0.08	43,43,43,43	0
59	MG	1N	3002	1/1	0.96	0.08	44,44,44,44	0
59	MG	2A	3013	1/1	0.96	0.09	47,47,47,47	0
59	MG	1N	3003	1/1	0.96	0.23	37,37,37,37	0
59	MG	1A	3384	1/1	0.96	0.07	40,40,40,40	0
59	MG	2A	3228	1/1	0.96	0.05	36,36,36,36	0
59	MG	1A	3453	1/1	0.96	0.09	18,18,18,18	0
59	MG	1A	3538	1/1	0.96	0.09	20,20,20,20	0
59	MG	2A	3746	1/1	0.96	0.09	48,48,48,48	0
59	MG	1A	3090	1/1	0.96	0.10	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3386	1/1	0.96	0.07	47,47,47,47	0
59	MG	1A	4120	1/1	0.96	0.06	33,33,33,33	0
59	MG	1A	3043	1/1	0.96	0.10	21,21,21,21	0
59	MG	1A	3542	1/1	0.96	0.09	41,41,41,41	0
59	MG	1O	3005	1/1	0.96	0.13	40,40,40,40	0
59	MG	2A	3027	1/1	0.96	0.10	39,39,39,39	0
59	MG	1A	4123	1/1	0.96	0.06	46,46,46,46	0
59	MG	1A	3190	1/1	0.96	0.09	39,39,39,39	0
59	MG	1A	3458	1/1	0.96	0.07	38,38,38,38	0
59	MG	2A	3759	1/1	0.96	0.08	52,52,52,52	0
59	MG	1Q	201	1/1	0.96	0.07	25,25,25,25	0
59	MG	1A	3112	1/1	0.96	0.13	33,33,33,33	0
59	MG	2A	3762	1/1	0.96	0.08	47,47,47,47	0
59	MG	1A	3460	1/1	0.96	0.12	50,50,50,50	0
59	MG	2A	3244	1/1	0.96	0.16	47,47,47,47	0
59	MG	1Q	206	1/1	0.96	0.07	39,39,39,39	0
59	MG	1A	3390	1/1	0.96	0.07	43,43,43,43	0
59	MG	1A	3334	1/1	0.96	0.11	39,39,39,39	0
59	MG	2A	3248	1/1	0.96	0.13	52,52,52,52	0
59	MG	1A	3974	1/1	0.96	0.07	17,17,17,17	0
59	MG	1A	3975	1/1	0.96	0.15	23,23,23,23	0
59	MG	1A	3805	1/1	0.96	0.25	30,30,30,30	0
59	MG	1A	3979	1/1	0.96	0.06	35,35,35,35	0
59	MG	1A	3144	1/1	0.96	0.39	35,35,35,35	0
59	MG	1A	3555	1/1	0.96	0.09	48,48,48,48	0
59	MG	1A	3194	1/1	0.96	0.20	45,45,45,45	0
59	MG	1A	3558	1/1	0.96	0.07	15,15,15,15	0
59	MG	1A	3337	1/1	0.96	0.17	48,48,48,48	0
59	MG	1A	3060	1/1	0.96	0.31	26,26,26,26	0
59	MG	2A	3502	1/1	0.96	0.15	42,42,42,42	0
59	MG	1a	3450	1/1	0.96	0.13	51,51,51,51	0
59	MG	1a	3452	1/1	0.96	0.06	40,40,40,40	0
59	MG	1W	203	1/1	0.96	0.18	29,29,29,29	0
59	MG	1X	3001	1/1	0.96	0.13	30,30,30,30	0
59	MG	1a	3455	1/1	0.96	0.05	27,27,27,27	0
59	MG	1a	3456	1/1	0.96	0.14	32,32,32,32	0
59	MG	1A	3471	1/1	0.96	0.11	30,30,30,30	0
59	MG	1A	3565	1/1	0.96	0.06	28,28,28,28	0
59	MG	2a	3129	1/1	0.96	0.09	75,75,75,75	0
59	MG	1A	3472	1/1	0.96	0.10	26,26,26,26	0
59	MG	1A	3568	1/1	0.96	0.07	15,15,15,15	0
59	MG	1Z	301	1/1	0.96	0.11	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3146	1/1	0.96	0.12	34,34,34,34	0
59	MG	1A	3820	1/1	0.96	0.08	13,13,13,13	0
59	MG	2A	3063	1/1	0.96	0.05	40,40,40,40	0
59	MG	2A	3519	1/1	0.96	0.11	62,62,62,62	0
59	MG	1A	3570	1/1	0.96	0.10	24,24,24,24	0
59	MG	1A	3198	1/1	0.96	0.21	27,27,27,27	0
59	MG	10	103	1/1	0.96	0.11	35,35,35,35	0
59	MG	2a	3142	1/1	0.96	0.06	67,67,67,67	0
59	MG	2A	3276	1/1	0.96	0.12	32,32,32,32	0
59	MG	1A	3694	1/1	0.96	0.08	29,29,29,29	0
59	MG	1A	3475	1/1	0.96	0.11	53,53,53,53	0
59	MG	2A	3802	1/1	0.96	0.07	35,35,35,35	0
59	MG	1A	3696	1/1	0.96	0.09	30,30,30,30	0
59	MG	1A	3398	1/1	0.96	0.10	49,49,49,49	0
59	MG	2A	3282	1/1	0.96	0.28	54,54,54,54	0
59	MG	1A	3114	1/1	0.96	0.11	36,36,36,36	0
59	MG	2A	3807	1/1	0.96	0.09	38,38,38,38	0
59	MG	1A	4159	1/1	0.96	0.08	34,34,34,34	0
59	MG	11	102	1/1	0.96	0.07	25,25,25,25	0
59	MG	1A	3293	1/1	0.96	0.09	49,49,49,49	0
59	MG	1A	3700	1/1	0.96	0.06	20,20,20,20	0
59	MG	1a	3485	1/1	0.96	0.06	49,49,49,49	0
59	MG	1A	3094	1/1	0.96	0.25	28,28,28,28	0
59	MG	1A	4163	1/1	0.96	0.15	53,53,53,53	0
59	MG	1A	4164	1/1	0.96	0.07	39,39,39,39	0
59	MG	1A	3704	1/1	0.96	0.08	13,13,13,13	0
59	MG	16	101	1/1	0.96	0.10	32,32,32,32	0
59	MG	2A	3540	1/1	0.96	0.11	48,48,48,48	0
59	MG	1A	3836	1/1	0.96	0.07	36,36,36,36	0
59	MG	1A	3403	1/1	0.96	0.22	33,33,33,33	0
59	MG	2A	3825	1/1	0.96	0.07	42,42,42,42	0
59	MG	2A	3826	1/1	0.96	0.07	54,54,54,54	0
59	MG	2A	3296	1/1	0.96	0.15	33,33,33,33	0
59	MG	1A	3838	1/1	0.96	0.13	26,26,26,26	0
59	MG	18	102	1/1	0.96	0.21	37,37,37,37	0
59	MG	2A	3830	1/1	0.96	0.21	32,32,32,32	0
59	MG	1A	3707	1/1	0.96	0.07	57,57,57,57	0
59	MG	1A	3581	1/1	0.96	0.07	22,22,22,22	0
59	MG	1a	3500	1/1	0.96	0.07	64,64,64,64	0
59	MG	1A	3583	1/1	0.96	0.06	50,50,50,50	0
59	MG	1A	3018	1/1	0.96	0.05	8,8,8,8	0
59	MG	1A	3119	1/1	0.96	0.06	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3552	1/1	0.96	0.06	54,54,54,54	0
59	MG	1A	3346	1/1	0.96	0.19	52,52,52,52	0
59	MG	1A	3715	1/1	0.96	0.06	62,62,62,62	0
59	MG	1a	3306	1/1	0.96	0.14	48,48,48,48	0
59	MG	1a	3307	1/1	0.96	0.24	51,51,51,51	0
59	MG	2A	3098	1/1	0.96	0.19	47,47,47,47	0
59	MG	1a	3308	1/1	0.96	0.07	44,44,44,44	0
59	MG	1A	4182	1/1	0.96	0.20	23,23,23,23	0
59	MG	1a	3512	1/1	0.96	0.07	45,45,45,45	0
59	MG	1A	3587	1/1	0.96	0.07	51,51,51,51	0
59	MG	1A	4022	1/1	0.96	0.08	39,39,39,39	0
59	MG	1A	3588	1/1	0.96	0.07	30,30,30,30	0
59	MG	1A	3407	1/1	0.96	0.11	46,46,46,46	0
59	MG	1a	3319	1/1	0.96	0.05	34,34,34,34	0
59	MG	2A	3107	1/1	0.96	0.21	44,44,44,44	0
59	MG	1A	3590	1/1	0.96	0.09	40,40,40,40	0
59	MG	2a	3197	1/1	0.96	0.10	54,54,54,54	0
59	MG	1A	3156	1/1	0.96	0.10	58,58,58,58	0
59	MG	1A	3593	1/1	0.96	0.07	18,18,18,18	0
59	MG	1A	3864	1/1	0.96	0.09	43,43,43,43	0
59	MG	1A	4032	1/1	0.96	0.07	48,48,48,48	0
59	MG	1A	3868	1/1	0.96	0.06	30,30,30,30	0
59	MG	1A	4034	1/1	0.96	0.07	61,61,61,61	0
59	MG	1A	3096	1/1	0.96	0.14	32,32,32,32	0
59	MG	1A	4198	1/1	0.96	0.12	22,22,22,22	0
59	MG	1A	3871	1/1	0.96	0.05	54,54,54,54	0
59	MG	1A	3726	1/1	0.96	0.06	14,14,14,14	0
59	MG	1a	3332	1/1	0.96	0.12	38,38,38,38	0
59	MG	2A	3331	1/1	0.96	0.06	58,58,58,58	0
59	MG	1A	3208	1/1	0.96	0.19	33,33,33,33	0
59	MG	1A	4208	1/1	0.96	0.29	29,29,29,29	0
59	MG	2A	3129	1/1	0.96	0.17	48,48,48,48	0
59	MG	2A	3130	1/1	0.96	0.24	46,46,46,46	0
59	MG	1A	3158	1/1	0.96	0.10	44,44,44,44	0
59	MG	1A	3122	1/1	0.96	0.22	28,28,28,28	0
59	MG	1A	4213	1/1	0.96	0.12	24,24,24,24	0
59	MG	2A	3135	1/1	0.96	0.16	58,58,58,58	0
59	MG	2a	3218	1/1	0.96	0.07	63,63,63,63	0
59	MG	1A	4220	1/1	0.96	0.12	24,24,24,24	0
59	MG	1A	3123	1/1	0.96	0.23	28,28,28,28	0
59	MG	1A	4223	1/1	0.96	0.13	39,39,39,39	0
59	MG	1A	3417	1/1	0.96	0.17	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1a	3342	1/1	0.96	0.06	42,42,42,42	0
59	MG	1A	4227	1/1	0.96	0.17	32,32,32,32	0
59	MG	1A	3602	1/1	0.96	0.06	19,19,19,19	0
59	MG	1A	3736	1/1	0.96	0.11	15,15,15,15	0
59	MG	2a	3227	1/1	0.96	0.17	45,45,45,45	0
59	MG	1A	4047	1/1	0.96	0.12	31,31,31,31	0
59	MG	1a	3347	1/1	0.96	0.12	40,40,40,40	0
59	MG	2a	3230	1/1	0.96	0.07	68,68,68,68	0
59	MG	1A	3739	1/1	0.96	0.30	26,26,26,26	0
59	MG	2A	3351	1/1	0.96	0.07	56,56,56,56	0
59	MG	1A	4049	1/1	0.96	0.06	36,36,36,36	0
59	MG	1A	3886	1/1	0.96	0.06	38,38,38,38	0
59	MG	1A	3079	1/1	0.96	0.11	46,46,46,46	0
59	MG	1a	3352	1/1	0.96	0.16	42,42,42,42	0
59	MG	1B	206	1/1	0.96	0.25	50,50,50,50	0
59	MG	1A	3165	1/1	0.96	0.23	22,22,22,22	0
59	MG	1A	3355	1/1	0.96	0.12	30,30,30,30	0
59	MG	2A	3360	1/1	0.96	0.12	50,50,50,50	0
59	MG	2f	3001	1/1	0.96	0.08	38,38,38,38	0
59	MG	1A	3743	1/1	0.96	0.09	38,38,38,38	0
59	MG	2A	3616	1/1	0.96	0.08	37,37,37,37	0
59	MG	1A	3499	1/1	0.96	0.07	46,46,46,46	0
59	MG	1A	3894	1/1	0.96	0.06	43,43,43,43	0
59	MG	1A	3064	1/1	0.96	0.12	19,19,19,19	0
59	MG	1A	3040	1/1	0.96	0.12	30,30,30,30	0
59	MG	2A	3160	1/1	0.96	0.06	48,48,48,48	0
59	MG	1A	3747	1/1	0.96	0.15	26,26,26,26	0
59	MG	1A	3168	1/1	0.96	0.35	38,38,38,38	0
59	MG	2A	3163	1/1	0.96	0.07	57,57,57,57	0
59	MG	1A	3619	1/1	0.96	0.07	19,19,19,19	0
59	MG	1a	3577	1/1	0.96	0.08	50,50,50,50	0
59	MG	1A	3621	1/1	0.96	0.11	25,25,25,25	0
59	MG	1A	3901	1/1	0.96	0.06	59,59,59,59	0
59	MG	1A	3309	1/1	0.96	0.10	56,56,56,56	0
59	MG	20	3003	1/1	0.96	0.10	50,50,50,50	0
59	MG	1A	4069	1/1	0.96	0.08	48,48,48,48	0
59	MG	2A	3379	1/1	0.96	0.07	24,24,24,24	0
59	MG	25	102	1/1	0.96	0.18	53,53,53,53	0
59	MG	1A	3169	1/1	0.96	0.06	34,34,34,34	0
59	MG	1B	224	1/1	0.96	0.16	52,52,52,52	0
59	MG	2A	3383	1/1	0.96	0.14	31,31,31,31	0
59	MG	1A	3755	1/1	0.96	0.06	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3638	1/1	0.96	0.11	55,55,55,55	0
59	MG	1k	201	1/1	0.96	0.10	39,39,39,39	0
59	MG	1A	3624	1/1	0.96	0.05	14,14,14,14	0
59	MG	1A	3361	1/1	0.96	0.09	35,35,35,35	0
59	MG	1A	3267	1/1	0.96	0.12	42,42,42,42	0
59	MG	2A	3645	1/1	0.96	0.06	51,51,51,51	0
59	MG	1A	3219	1/1	0.96	0.07	51,51,51,51	0
59	MG	2A	3649	1/1	0.96	0.08	47,47,47,47	0
59	MG	1A	3509	1/1	0.96	0.16	40,40,40,40	0
59	MG	1a	3376	1/1	0.96	0.15	62,62,62,62	0
59	MG	2A	3396	1/1	0.96	0.07	41,41,41,41	0
59	MG	1A	3127	1/1	0.96	0.17	37,37,37,37	0
59	MG	2A	3398	1/1	0.96	0.15	50,50,50,50	0
59	MG	1A	3315	1/1	0.96	0.19	34,34,34,34	0
59	MG	1A	3316	1/1	0.96	0.10	15,15,15,15	0
59	MG	B	3001	1/1	0.96	0.14	46,46,46,46	0
60	ZN	24	501	1/1	0.96	0.10	111,111,111,111	0
59	MG	1G	3005	1/1	0.97	0.08	51,51,51,51	0
59	MG	1A	4023	1/1	0.97	0.04	49,49,49,49	0
59	MG	1a	3383	1/1	0.97	0.21	43,43,43,43	0
59	MG	1A	3610	1/1	0.97	0.06	19,19,19,19	0
59	MG	1A	3027	1/1	0.97	0.20	30,30,30,30	0
59	MG	1A	3613	1/1	0.97	0.09	36,36,36,36	0
59	MG	1A	3243	1/1	0.97	0.32	28,28,28,28	0
59	MG	2a	3070	1/1	0.97	0.15	60,60,60,60	0
59	MG	1A	4029	1/1	0.97	0.06	46,46,46,46	0
59	MG	1A	3421	1/1	0.97	0.13	33,33,33,33	0
59	MG	1A	3477	1/1	0.97	0.10	31,31,31,31	0
59	MG	1A	3703	1/1	0.97	0.06	55,55,55,55	0
59	MG	1A	3908	1/1	0.97	0.06	55,55,55,55	0
59	MG	1A	3244	1/1	0.97	0.16	24,24,24,24	0
59	MG	1l	201	1/1	0.97	0.12	30,30,30,30	0
59	MG	1A	4035	1/1	0.97	0.10	35,35,35,35	0
59	MG	1O	3004	1/1	0.97	0.05	48,48,48,48	0
59	MG	1A	3204	1/1	0.97	0.18	23,23,23,23	0
59	MG	1A	3797	1/1	0.97	0.14	35,35,35,35	0
59	MG	1P	201	1/1	0.97	0.21	23,23,23,23	0
59	MG	1P	202	1/1	0.97	0.30	25,25,25,25	0
59	MG	1A	3706	1/1	0.97	0.04	28,28,28,28	0
59	MG	1A	3136	1/1	0.97	0.25	26,26,26,26	0
59	MG	1A	4040	1/1	0.97	0.06	36,36,36,36	0
59	MG	1a	3403	1/1	0.97	0.10	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1Q	202	1/1	0.97	0.10	37,37,37,37	0
59	MG	1A	4169	1/1	0.97	0.08	22,22,22,22	0
59	MG	1A	4170	1/1	0.97	0.10	23,23,23,23	0
59	MG	1Q	205	1/1	0.97	0.06	37,37,37,37	0
59	MG	1A	3248	1/1	0.97	0.11	36,36,36,36	0
59	MG	2a	3094	1/1	0.97	0.15	48,48,48,48	0
59	MG	1A	3069	1/1	0.97	0.12	28,28,28,28	0
59	MG	2A	3356	1/1	0.97	0.10	18,18,18,18	0
59	MG	1R	202	1/1	0.97	0.41	33,33,33,33	0
59	MG	1A	3917	1/1	0.97	0.09	15,15,15,15	0
59	MG	1A	3710	1/1	0.97	0.06	18,18,18,18	0
59	MG	1A	3070	1/1	0.97	0.13	25,25,25,25	0
59	MG	1A	3379	1/1	0.97	0.09	37,37,37,37	0
59	MG	1A	3098	1/1	0.97	0.19	30,30,30,30	0
59	MG	1A	3099	1/1	0.97	0.19	31,31,31,31	0
59	MG	1U	201	1/1	0.97	0.19	27,27,27,27	0
59	MG	1A	3548	1/1	0.97	0.07	38,38,38,38	0
59	MG	1A	4181	1/1	0.97	0.27	33,33,33,33	0
59	MG	1U	205	1/1	0.97	0.23	29,29,29,29	0
59	MG	1V	201	1/1	0.97	0.13	33,33,33,33	0
59	MG	1a	3422	1/1	0.97	0.17	50,50,50,50	0
59	MG	1A	3718	1/1	0.97	0.05	39,39,39,39	0
59	MG	1A	4183	1/1	0.97	0.06	34,34,34,34	0
59	MG	1A	3549	1/1	0.97	0.07	40,40,40,40	0
59	MG	1A	3929	1/1	0.97	0.09	52,52,52,52	0
59	MG	2A	3818	1/1	0.97	0.07	63,63,63,63	0
59	MG	1W	204	1/1	0.97	0.13	32,32,32,32	0
59	MG	1W	205	1/1	0.97	0.16	23,23,23,23	0
59	MG	1A	3117	1/1	0.97	0.20	25,25,25,25	0
59	MG	1A	3383	1/1	0.97	0.11	38,38,38,38	0
59	MG	1A	3142	1/1	0.97	0.14	36,36,36,36	0
59	MG	1A	3256	1/1	0.97	0.05	27,27,27,27	0
59	MG	1A	3176	1/1	0.97	0.06	35,35,35,35	0
59	MG	1A	3725	1/1	0.97	0.06	41,41,41,41	0
59	MG	1A	4062	1/1	0.97	0.05	34,34,34,34	0
59	MG	1A	3939	1/1	0.97	0.06	36,36,36,36	0
59	MG	2A	3389	1/1	0.97	0.06	33,33,33,33	0
59	MG	1A	3557	1/1	0.97	0.04	23,23,23,23	0
59	MG	1A	3118	1/1	0.97	0.22	33,33,33,33	0
59	MG	2A	3833	1/1	0.97	0.07	47,47,47,47	0
59	MG	10	102	1/1	0.97	0.08	43,43,43,43	0
59	MG	2A	3393	1/1	0.97	0.06	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3559	1/1	0.97	0.08	28,28,28,28	0
59	MG	2A	3007	1/1	0.97	0.12	40,40,40,40	0
59	MG	1A	4201	1/1	0.97	0.07	32,32,32,32	0
59	MG	1A	3009	1/1	0.97	0.09	25,25,25,25	0
59	MG	1A	4204	1/1	0.97	0.09	29,29,29,29	0
59	MG	1A	3731	1/1	0.97	0.07	33,33,33,33	0
59	MG	2A	3014	1/1	0.97	0.06	29,29,29,29	0
59	MG	1A	3495	1/1	0.97	0.06	46,46,46,46	0
59	MG	1A	3733	1/1	0.97	0.04	47,47,47,47	0
59	MG	1A	4209	1/1	0.97	0.12	21,21,21,21	0
59	MG	1A	4071	1/1	0.97	0.07	50,50,50,50	0
59	MG	1A	4211	1/1	0.97	0.14	23,23,23,23	0
59	MG	1a	3451	1/1	0.97	0.10	43,43,43,43	0
59	MG	1A	3260	1/1	0.97	0.06	32,32,32,32	0
59	MG	1A	3829	1/1	0.97	0.08	38,38,38,38	0
59	MG	1A	4214	1/1	0.97	0.29	36,36,36,36	0
59	MG	15	102	1/1	0.97	0.13	25,25,25,25	0
59	MG	1A	4215	1/1	0.97	0.35	31,31,31,31	0
59	MG	1A	4218	1/1	0.97	0.18	24,24,24,24	0
59	MG	16	103	1/1	0.97	0.05	49,49,49,49	0
59	MG	1A	3101	1/1	0.97	0.18	30,30,30,30	0
59	MG	1A	3566	1/1	0.97	0.06	13,13,13,13	0
59	MG	17	102	1/1	0.97	0.06	46,46,46,46	0
59	MG	1a	3463	1/1	0.97	0.16	44,44,44,44	0
59	MG	2A	3034	1/1	0.97	0.08	50,50,50,50	0
59	MG	1A	4222	1/1	0.97	0.22	31,31,31,31	0
59	MG	1A	3646	1/1	0.97	0.06	8,8,8,8	0
59	MG	2A	3426	1/1	0.97	0.06	23,23,23,23	0
59	MG	2A	3635	1/1	0.97	0.07	62,62,62,62	0
59	MG	1A	3953	1/1	0.97	0.05	64,64,64,64	0
59	MG	1A	3954	1/1	0.97	0.06	49,49,49,49	0
59	MG	2A	3039	1/1	0.97	0.14	23,23,23,23	0
59	MG	2a	3168	1/1	0.97	0.18	54,54,54,54	0
59	MG	1A	3032	1/1	0.97	0.19	26,26,26,26	0
59	MG	1A	4080	1/1	0.97	0.09	28,28,28,28	0
59	MG	1A	3148	1/1	0.97	0.18	26,26,26,26	0
59	MG	1a	3474	1/1	0.97	0.07	42,42,42,42	0
59	MG	1A	3501	1/1	0.97	0.16	41,41,41,41	0
59	MG	2D	303	1/1	0.97	0.03	20,20,20,20	0
59	MG	2A	3647	1/1	0.97	0.06	39,39,39,39	0
59	MG	1A	3008	1/1	0.97	0.04	16,16,16,16	0
59	MG	1A	3963	1/1	0.97	0.07	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3185	1/1	0.97	0.22	36,36,36,36	0
59	MG	1A	3150	1/1	0.97	0.13	30,30,30,30	0
59	MG	1A	3151	1/1	0.97	0.05	15,15,15,15	0
59	MG	1a	3312	1/1	0.97	0.11	62,62,62,62	0
59	MG	2A	3442	1/1	0.97	0.11	24,24,24,24	0
59	MG	1A	3017	1/1	0.97	0.04	28,28,28,28	0
59	MG	1A	3189	1/1	0.97	0.29	43,43,43,43	0
59	MG	1A	3845	1/1	0.97	0.19	33,33,33,33	0
59	MG	2A	3659	1/1	0.97	0.05	66,66,66,66	0
59	MG	1a	3316	1/1	0.97	0.10	40,40,40,40	0
59	MG	1A	3750	1/1	0.97	0.09	42,42,42,42	0
59	MG	2N	8001	1/1	0.97	0.07	45,45,45,45	0
59	MG	1a	3318	1/1	0.97	0.04	43,43,43,43	0
59	MG	1A	3024	1/1	0.97	0.24	19,19,19,19	0
59	MG	1A	4094	1/1	0.97	0.10	35,35,35,35	0
59	MG	1A	3658	1/1	0.97	0.04	39,39,39,39	0
59	MG	1A	3026	1/1	0.97	0.36	28,28,28,28	0
59	MG	2A	3061	1/1	0.97	0.10	42,42,42,42	0
59	MG	2A	3454	1/1	0.97	0.07	36,36,36,36	0
59	MG	1a	3496	1/1	0.97	0.11	66,66,66,66	0
59	MG	1A	3660	1/1	0.97	0.06	40,40,40,40	0
59	MG	1a	3498	1/1	0.97	0.07	63,63,63,63	0
59	MG	1A	3851	1/1	0.97	0.09	43,43,43,43	0
59	MG	1A	3852	1/1	0.97	0.12	36,36,36,36	0
59	MG	1A	3978	1/1	0.97	0.06	38,38,38,38	0
59	MG	1A	3853	1/1	0.97	0.05	33,33,33,33	0
59	MG	1A	3856	1/1	0.97	0.06	39,39,39,39	0
59	MG	1A	3580	1/1	0.97	0.04	23,23,23,23	0
59	MG	1A	3858	1/1	0.97	0.07	22,22,22,22	0
59	MG	1A	3054	1/1	0.97	0.11	24,24,24,24	0
59	MG	1B	228	1/1	0.97	0.06	30,30,30,30	0
59	MG	2A	3683	1/1	0.97	0.08	53,53,53,53	0
59	MG	1A	3757	1/1	0.97	0.04	39,39,39,39	0
59	MG	1A	3108	1/1	0.97	0.23	26,26,26,26	0
59	MG	1A	3863	1/1	0.97	0.04	9,9,9,9	0
59	MG	1A	3512	1/1	0.97	0.09	40,40,40,40	0
59	MG	1A	3867	1/1	0.97	0.05	36,36,36,36	0
59	MG	2A	3476	1/1	0.97	0.07	43,43,43,43	0
59	MG	1a	3518	1/1	0.97	0.06	32,32,32,32	0
59	MG	2A	3693	1/1	0.97	0.10	32,32,32,32	0
59	MG	2A	3694	1/1	0.97	0.05	28,28,28,28	0
59	MG	1A	3667	1/1	0.97	0.06	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1a	3520	1/1	0.97	0.06	60,60,60,60	0
59	MG	1a	3524	1/1	0.97	0.05	71,71,71,71	0
59	MG	1A	3669	1/1	0.97	0.06	38,38,38,38	0
59	MG	1A	3066	1/1	0.97	0.15	27,27,27,27	0
59	MG	1B	237	1/1	0.97	0.06	39,39,39,39	0
59	MG	1A	3873	1/1	0.97	0.04	30,30,30,30	0
59	MG	2A	3705	1/1	0.97	0.05	49,49,49,49	0
59	MG	1A	3993	1/1	0.97	0.05	20,20,20,20	0
59	MG	1A	3994	1/1	0.97	0.05	31,31,31,31	0
59	MG	1D	303	1/1	0.97	0.19	35,35,35,35	0
59	MG	1a	3533	1/1	0.97	0.06	59,59,59,59	0
59	MG	2A	3710	1/1	0.97	0.08	34,34,34,34	0
59	MG	2A	3489	1/1	0.97	0.07	32,32,32,32	0
59	MG	2A	3092	1/1	0.97	0.13	32,32,32,32	0
59	MG	1a	3534	1/1	0.97	0.06	45,45,45,45	0
59	MG	1D	304	1/1	0.97	0.14	38,38,38,38	0
59	MG	1A	3514	1/1	0.97	0.29	53,53,53,53	0
59	MG	1A	3764	1/1	0.97	0.06	54,54,54,54	0
59	MG	1A	3196	1/1	0.97	0.17	26,26,26,26	0
59	MG	2a	3239	1/1	0.97	0.13	42,42,42,42	0
59	MG	1A	3998	1/1	0.97	0.06	13,13,13,13	0
59	MG	1A	3093	1/1	0.97	0.06	35,35,35,35	0
59	MG	1A	3080	1/1	0.97	0.12	16,16,16,16	0
59	MG	1A	3408	1/1	0.97	0.18	32,32,32,32	0
59	MG	1A	4004	1/1	0.97	0.06	43,43,43,43	0
59	MG	1E	303	1/1	0.97	0.21	33,33,33,33	0
59	MG	1E	304	1/1	0.97	0.13	27,27,27,27	0
59	MG	1A	3519	1/1	0.97	0.10	46,46,46,46	0
59	MG	1A	3592	1/1	0.97	0.04	17,17,17,17	0
59	MG	1A	3162	1/1	0.97	0.29	30,30,30,30	0
59	MG	2A	3506	1/1	0.97	0.13	42,42,42,42	0
59	MG	1A	4008	1/1	0.97	0.10	54,54,54,54	0
59	MG	1A	3885	1/1	0.97	0.10	47,47,47,47	0
59	MG	1a	3552	1/1	0.97	0.13	55,55,55,55	0
59	MG	2A	3112	1/1	0.97	0.04	33,33,33,33	0
59	MG	2A	3113	1/1	0.97	0.10	38,38,38,38	0
59	MG	1A	4132	1/1	0.97	0.12	37,37,37,37	0
59	MG	2A	3115	1/1	0.97	0.28	36,36,36,36	0
59	MG	2A	3743	1/1	0.97	0.04	40,40,40,40	0
59	MG	2A	3116	1/1	0.97	0.24	35,35,35,35	0
59	MG	1A	4133	1/1	0.97	0.04	35,35,35,35	0
59	MG	1A	3200	1/1	0.97	0.15	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3120	1/1	0.97	0.12	34,34,34,34	0
59	MG	1A	3323	1/1	0.97	0.45	28,28,28,28	0
59	MG	1A	3466	1/1	0.97	0.22	24,24,24,24	0
59	MG	1A	3467	1/1	0.97	0.09	28,28,28,28	0
59	MG	1A	3598	1/1	0.97	0.06	24,24,24,24	0
59	MG	1A	3412	1/1	0.97	0.08	37,37,37,37	0
59	MG	1A	3236	1/1	0.97	0.15	34,34,34,34	0
59	MG	2a	3048	1/1	0.97	0.16	42,42,42,42	0
59	MG	1A	3601	1/1	0.97	0.05	12,12,12,12	0
59	MG	2A	3756	1/1	0.97	0.10	51,51,51,51	0
59	MG	1a	3563	1/1	0.97	0.10	50,50,50,50	0
59	MG	1A	3414	1/1	0.97	0.05	42,42,42,42	0
59	MG	2a	3054	1/1	0.97	0.17	41,41,41,41	0
59	MG	1F	308	1/1	0.97	0.08	45,45,45,45	0
59	MG	1A	4143	1/1	0.97	0.12	16,16,16,16	0
59	MG	1A	3134	1/1	0.97	0.15	24,24,24,24	0
59	MG	1G	3001	1/1	0.97	0.14	32,32,32,32	0
59	MG	1A	3164	1/1	0.97	0.26	27,27,27,27	0
59	MG	2A	3136	1/1	0.97	0.19	33,33,33,33	0
59	MG	1A	4146	1/1	0.97	0.06	26,26,26,26	0
60	ZN	14	501	1/1	0.97	0.06	87,87,87,87	0
59	MG	1A	3240	1/1	0.97	0.17	31,31,31,31	0
60	ZN	2n	501	1/1	0.97	0.05	90,90,90,90	0
62	K	2A	3849	1/1	0.97	0.05	47,47,47,47	0
59	MG	1A	3073	1/1	0.98	0.17	26,26,26,26	0
59	MG	1A	3238	1/1	0.98	0.23	41,41,41,41	0
59	MG	1a	3488	1/1	0.98	0.05	39,39,39,39	0
59	MG	1A	3712	1/1	0.98	0.05	43,43,43,43	0
59	MG	1U	203	1/1	0.98	0.21	22,22,22,22	0
59	MG	1A	3061	1/1	0.98	0.09	8,8,8,8	0
59	MG	1B	207	1/1	0.98	0.03	32,32,32,32	0
59	MG	2A	3711	1/1	0.98	0.05	50,50,50,50	0
59	MG	1A	3855	1/1	0.98	0.07	51,51,51,51	0
59	MG	2A	3714	1/1	0.98	0.06	66,66,66,66	0
59	MG	1A	3463	1/1	0.98	0.18	24,24,24,24	0
59	MG	2A	3716	1/1	0.98	0.07	56,56,56,56	0
59	MG	2A	3132	1/1	0.98	0.07	21,21,21,21	0
59	MG	2A	3406	1/1	0.98	0.07	39,39,39,39	0
59	MG	1A	3003	1/1	0.98	0.06	16,16,16,16	0
59	MG	2a	3130	1/1	0.98	0.06	79,79,79,79	0
59	MG	1A	3465	1/1	0.98	0.18	27,27,27,27	0
59	MG	2A	3721	1/1	0.98	0.03	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3241	1/1	0.98	0.15	24,24,24,24	0
59	MG	1A	3546	1/1	0.98	0.05	37,37,37,37	0
59	MG	1A	3401	1/1	0.98	0.06	28,28,28,28	0
59	MG	1A	3862	1/1	0.98	0.04	38,38,38,38	0
59	MG	2a	3137	1/1	0.98	0.07	68,68,68,68	0
59	MG	1X	3002	1/1	0.98	0.06	28,28,28,28	0
59	MG	1a	3502	1/1	0.98	0.06	67,67,67,67	0
59	MG	1X	3003	1/1	0.98	0.14	32,32,32,32	0
59	MG	1A	3785	1/1	0.98	0.10	18,18,18,18	0
59	MG	2A	3563	1/1	0.98	0.04	52,52,52,52	0
59	MG	1A	3029	1/1	0.98	0.07	29,29,29,29	0
59	MG	2A	3419	1/1	0.98	0.06	28,28,28,28	0
59	MG	1A	3865	1/1	0.98	0.04	42,42,42,42	0
59	MG	2a	3147	1/1	0.98	0.04	59,59,59,59	0
59	MG	2A	3011	1/1	0.98	0.06	38,38,38,38	0
59	MG	2A	3012	1/1	0.98	0.05	35,35,35,35	0
59	MG	1A	3373	1/1	0.98	0.12	29,29,29,29	0
59	MG	1A	3550	1/1	0.98	0.06	14,14,14,14	0
59	MG	2A	3425	1/1	0.98	0.09	47,47,47,47	0
59	MG	1a	3509	1/1	0.98	0.04	61,61,61,61	0
59	MG	1A	3434	1/1	0.98	0.14	21,21,21,21	0
59	MG	2a	3155	1/1	0.98	0.05	72,72,72,72	0
59	MG	1A	3960	1/1	0.98	0.07	16,16,16,16	0
59	MG	1A	4050	1/1	0.98	0.08	45,45,45,45	0
59	MG	2A	3020	1/1	0.98	0.05	24,24,24,24	0
59	MG	2X	3002	1/1	0.98	0.08	47,47,47,47	0
59	MG	2A	3577	1/1	0.98	0.05	36,36,36,36	0
59	MG	1A	3961	1/1	0.98	0.04	37,37,37,37	0
59	MG	20	3002	1/1	0.98	0.09	51,51,51,51	0
59	MG	2A	3432	1/1	0.98	0.07	26,26,26,26	0
59	MG	1a	3516	1/1	0.98	0.10	64,64,64,64	0
59	MG	2A	3750	1/1	0.98	0.05	51,51,51,51	0
59	MG	1A	3870	1/1	0.98	0.04	29,29,29,29	0
59	MG	1A	3790	1/1	0.98	0.12	35,35,35,35	0
59	MG	1A	3872	1/1	0.98	0.09	48,48,48,48	0
59	MG	1A	3791	1/1	0.98	0.04	34,34,34,34	0
59	MG	2A	3586	1/1	0.98	0.04	46,46,46,46	0
59	MG	1a	3522	1/1	0.98	0.06	66,66,66,66	0
59	MG	1A	3435	1/1	0.98	0.22	28,28,28,28	0
59	MG	1A	3793	1/1	0.98	0.09	46,46,46,46	0
59	MG	1A	3553	1/1	0.98	0.05	20,20,20,20	0
59	MG	1A	3727	1/1	0.98	0.08	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3592	1/1	0.98	0.04	23,23,23,23	0
59	MG	1A	3160	1/1	0.98	0.32	36,36,36,36	0
59	MG	1a	3529	1/1	0.98	0.04	53,53,53,53	0
59	MG	1A	3437	1/1	0.98	0.12	48,48,48,48	0
59	MG	1A	3604	1/1	0.98	0.05	27,27,27,27	0
59	MG	12	3002	1/1	0.98	0.13	36,36,36,36	0
59	MG	1A	3882	1/1	0.98	0.06	45,45,45,45	0
59	MG	1A	3605	1/1	0.98	0.05	14,14,14,14	0
59	MG	1A	3606	1/1	0.98	0.07	17,17,17,17	0
59	MG	1A	3268	1/1	0.98	0.12	32,32,32,32	0
59	MG	1A	3030	1/1	0.98	0.16	14,14,14,14	0
59	MG	1a	3538	1/1	0.98	0.09	44,44,44,44	0
59	MG	1A	3887	1/1	0.98	0.08	50,50,50,50	0
59	MG	1A	4165	1/1	0.98	0.09	9,9,9,9	0
59	MG	2A	3456	1/1	0.98	0.04	50,50,50,50	0
59	MG	1D	307	1/1	0.98	0.18	24,24,24,24	0
59	MG	2A	3609	1/1	0.98	0.03	44,44,44,44	0
59	MG	1A	4166	1/1	0.98	0.07	11,11,11,11	0
59	MG	1D	309	1/1	0.98	0.10	37,37,37,37	0
59	MG	1A	3609	1/1	0.98	0.04	17,17,17,17	0
59	MG	1A	3672	1/1	0.98	0.04	42,42,42,42	0
59	MG	1A	3890	1/1	0.98	0.05	50,50,50,50	0
59	MG	1A	3738	1/1	0.98	0.03	27,27,27,27	0
59	MG	1A	3245	1/1	0.98	0.24	21,21,21,21	0
59	MG	1A	3611	1/1	0.98	0.06	17,17,17,17	0
59	MG	1A	3047	1/1	0.98	0.05	19,19,19,19	0
59	MG	1A	3297	1/1	0.98	0.05	43,43,43,43	0
59	MG	1A	3147	1/1	0.98	0.36	26,26,26,26	0
59	MG	1A	3562	1/1	0.98	0.08	18,18,18,18	0
59	MG	2A	3790	1/1	0.98	0.11	37,37,37,37	0
59	MG	1A	4081	1/1	0.98	0.04	14,14,14,14	0
59	MG	1A	3563	1/1	0.98	0.05	37,37,37,37	0
59	MG	2A	3624	1/1	0.98	0.05	44,44,44,44	0
59	MG	1A	3814	1/1	0.98	0.03	22,22,22,22	0
59	MG	2A	3475	1/1	0.98	0.04	48,48,48,48	0
59	MG	1a	3310	1/1	0.98	0.08	19,19,19,19	0
59	MG	1a	3311	1/1	0.98	0.04	45,45,45,45	0
59	MG	1A	4180	1/1	0.98	0.19	28,28,28,28	0
59	MG	1A	3067	1/1	0.98	0.11	19,19,19,19	0
59	MG	1A	3620	1/1	0.98	0.06	15,15,15,15	0
59	MG	1A	3031	1/1	0.98	0.27	24,24,24,24	0
59	MG	1A	3749	1/1	0.98	0.03	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3683	1/1	0.98	0.03	29,29,29,29	0
59	MG	1A	3684	1/1	0.98	0.04	28,28,28,28	0
59	MG	1A	3025	1/1	0.98	0.11	21,21,21,21	0
59	MG	2a	3050	1/1	0.98	0.04	54,54,54,54	0
59	MG	1A	3999	1/1	0.98	0.03	20,20,20,20	0
59	MG	1A	3251	1/1	0.98	0.15	47,47,47,47	0
59	MG	1A	4001	1/1	0.98	0.09	37,37,37,37	0
59	MG	1A	3207	1/1	0.98	0.20	24,24,24,24	0
59	MG	1A	3016	1/1	0.98	0.03	20,20,20,20	0
59	MG	2A	3811	1/1	0.98	0.09	62,62,62,62	0
59	MG	2A	3642	1/1	0.98	0.12	63,63,63,63	0
59	MG	1A	3826	1/1	0.98	0.06	42,42,42,42	0
59	MG	1A	3912	1/1	0.98	0.09	47,47,47,47	0
59	MG	1A	4196	1/1	0.98	0.21	29,29,29,29	0
59	MG	1a	3328	1/1	0.98	0.12	17,17,17,17	0
59	MG	1A	3486	1/1	0.98	0.21	31,31,31,31	0
59	MG	2A	3650	1/1	0.98	0.14	60,60,60,60	0
59	MG	1A	3571	1/1	0.98	0.10	13,13,13,13	0
59	MG	2A	3821	1/1	0.98	0.06	35,35,35,35	0
59	MG	1a	3445	1/1	0.98	0.09	32,32,32,32	0
59	MG	1A	4199	1/1	0.98	0.19	32,32,32,32	0
59	MG	1A	4200	1/1	0.98	0.25	27,27,27,27	0
59	MG	1A	3450	1/1	0.98	0.21	31,31,31,31	0
59	MG	1A	4202	1/1	0.98	0.18	27,27,27,27	0
59	MG	1A	4101	1/1	0.98	0.07	41,41,41,41	0
59	MG	1A	3152	1/1	0.98	0.07	25,25,25,25	0
59	MG	2A	3222	1/1	0.98	0.06	45,45,45,45	0
59	MG	1A	3059	1/1	0.98	0.15	10,10,10,10	0
59	MG	2a	3075	1/1	0.98	0.16	33,33,33,33	0
59	MG	1A	3528	1/1	0.98	0.13	35,35,35,35	0
59	MG	1N	3008	1/1	0.98	0.08	36,36,36,36	0
59	MG	1A	3576	1/1	0.98	0.11	9,9,9,9	0
59	MG	1A	3419	1/1	0.98	0.24	30,30,30,30	0
59	MG	1A	3171	1/1	0.98	0.06	25,25,25,25	0
59	MG	1A	3531	1/1	0.98	0.25	28,28,28,28	0
59	MG	2A	3512	1/1	0.98	0.05	45,45,45,45	0
59	MG	2A	3668	1/1	0.98	0.09	43,43,43,43	0
59	MG	1A	3701	1/1	0.98	0.05	17,17,17,17	0
59	MG	1A	3841	1/1	0.98	0.03	24,24,24,24	0
59	MG	1A	3637	1/1	0.98	0.05	18,18,18,18	0
59	MG	1A	3927	1/1	0.98	0.09	12,12,12,12	0
59	MG	1a	3464	1/1	0.98	0.03	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	2A	3369	1/1	0.98	0.04	67,67,67,67	0
59	MG	1A	4216	1/1	0.98	0.08	24,24,24,24	0
59	MG	2A	3371	1/1	0.98	0.06	48,48,48,48	0
59	MG	1A	4217	1/1	0.98	0.13	35,35,35,35	0
59	MG	1A	4020	1/1	0.98	0.14	34,34,34,34	0
59	MG	2A	3374	1/1	0.98	0.07	49,49,49,49	0
59	MG	1A	4219	1/1	0.98	0.19	32,32,32,32	0
59	MG	2A	3681	1/1	0.98	0.06	62,62,62,62	0
59	MG	1A	3192	1/1	0.98	0.18	27,27,27,27	0
59	MG	1A	3172	1/1	0.98	0.04	25,25,25,25	0
59	MG	2A	3108	1/1	0.98	0.08	43,43,43,43	0
59	MG	1A	3582	1/1	0.98	0.03	24,24,24,24	0
59	MG	1A	3012	1/1	0.98	0.09	18,18,18,18	0
59	MG	1A	4224	1/1	0.98	0.04	23,23,23,23	0
59	MG	1A	3085	1/1	0.98	0.17	15,15,15,15	0
59	MG	1A	4226	1/1	0.98	0.06	24,24,24,24	0
59	MG	1A	3312	1/1	0.98	0.21	33,33,33,33	0
59	MG	1a	3479	1/1	0.98	0.08	48,48,48,48	0
59	MG	1a	3480	1/1	0.98	0.04	37,37,37,37	0
59	MG	1a	3481	1/1	0.98	0.10	44,44,44,44	0
59	MG	2A	3118	1/1	0.98	0.17	37,37,37,37	0
59	MG	1A	3935	1/1	0.98	0.03	24,24,24,24	0
59	MG	1A	4028	1/1	0.98	0.10	50,50,50,50	0
60	ZN	2Y	501	1/1	0.98	0.04	86,86,86,86	0
59	MG	1A	3497	1/1	0.98	0.19	38,38,38,38	0
60	ZN	29	501	1/1	0.98	0.04	69,69,69,69	0
59	MG	1A	3937	1/1	0.98	0.06	22,22,22,22	0
61	SF4	2d	501	8/8	0.98	0.05	56,66,80,82	0
59	MG	2A	3703	1/1	0.98	0.03	30,30,30,30	0
59	MG	1A	3663	1/1	0.99	0.05	14,14,14,14	0
59	MG	1a	3515	1/1	0.99	0.04	39,39,39,39	0
59	MG	2A	3064	1/1	0.99	0.11	16,16,16,16	0
59	MG	1B	227	1/1	0.99	0.05	31,31,31,31	0
59	MG	1a	3574	1/1	0.99	0.05	43,43,43,43	0
59	MG	1A	3685	1/1	0.99	0.04	14,14,14,14	0
59	MG	2A	3815	1/1	0.99	0.03	56,56,56,56	0
59	MG	2A	3006	1/1	0.99	0.05	30,30,30,30	0
59	MG	1A	3011	1/1	0.99	0.20	16,16,16,16	0
59	MG	2A	3382	1/1	0.99	0.04	58,58,58,58	0
59	MG	1A	3834	1/1	0.99	0.06	34,34,34,34	0
59	MG	2A	3384	1/1	0.99	0.06	28,28,28,28	0
59	MG	1a	3465	1/1	0.99	0.03	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1a	3521	1/1	0.99	0.04	46,46,46,46	0
59	MG	1A	3120	1/1	0.99	0.10	10,10,10,10	0
59	MG	1a	3523	1/1	0.99	0.02	54,54,54,54	0
59	MG	1A	3627	1/1	0.99	0.05	28,28,28,28	0
59	MG	2A	3595	1/1	0.99	0.04	34,34,34,34	0
59	MG	1X	3005	1/1	0.99	0.06	26,26,26,26	0
59	MG	1f	3002	1/1	0.99	0.08	33,33,33,33	0
59	MG	2A	3016	1/1	0.99	0.07	21,21,21,21	0
59	MG	2A	3461	1/1	0.99	0.03	27,27,27,27	0
59	MG	1a	3469	1/1	0.99	0.06	48,48,48,48	0
59	MG	2A	3394	1/1	0.99	0.03	40,40,40,40	0
59	MG	1A	3006	1/1	0.99	0.04	23,23,23,23	0
59	MG	1A	3668	1/1	0.99	0.04	38,38,38,38	0
59	MG	1A	3811	1/1	0.99	0.03	30,30,30,30	0
59	MG	1A	3840	1/1	0.99	0.05	16,16,16,16	0
59	MG	1A	3046	1/1	0.99	0.08	28,28,28,28	0
59	MG	1A	4051	1/1	0.99	0.04	38,38,38,38	0
59	MG	1A	3938	1/1	0.99	0.02	22,22,22,22	0
59	MG	1A	3976	1/1	0.99	0.10	56,56,56,56	0
59	MG	1A	3692	1/1	0.99	0.07	37,37,37,37	0
59	MG	1A	4055	1/1	0.99	0.06	32,32,32,32	0
59	MG	1A	3716	1/1	0.99	0.04	34,34,34,34	0
59	MG	1A	3906	1/1	0.99	0.06	36,36,36,36	0
59	MG	2A	3278	1/1	0.99	0.16	40,40,40,40	0
59	MG	1A	3130	1/1	0.99	0.16	32,32,32,32	0
59	MG	2A	3688	1/1	0.99	0.07	38,38,38,38	0
59	MG	1A	3816	1/1	0.99	0.06	35,35,35,35	0
59	MG	1A	3213	1/1	0.99	0.20	27,27,27,27	0
59	MG	2A	3691	1/1	0.99	0.04	29,29,29,29	0
59	MG	2A	3411	1/1	0.99	0.05	40,40,40,40	0
59	MG	1A	3878	1/1	0.99	0.02	38,38,38,38	0
59	MG	1D	311	1/1	0.99	0.21	19,19,19,19	0
59	MG	1A	4186	1/1	0.99	0.09	27,27,27,27	0
59	MG	1A	3946	1/1	0.99	0.03	46,46,46,46	0
59	MG	1A	3131	1/1	0.99	0.29	33,33,33,33	0
59	MG	2A	3698	1/1	0.99	0.05	49,49,49,49	0
59	MG	1A	3007	1/1	0.99	0.11	17,17,17,17	0
59	MG	1A	4105	1/1	0.99	0.09	53,53,53,53	0
59	MG	2A	3701	1/1	0.99	0.03	26,26,26,26	0
59	MG	1A	3616	1/1	0.99	0.09	16,16,16,16	0
59	MG	1A	3179	1/1	0.99	0.04	25,25,25,25	0
59	MG	1A	3618	1/1	0.99	0.04	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	1A	3063	1/1	0.99	0.06	15,15,15,15	0
59	MG	1A	3374	1/1	0.99	0.16	27,27,27,27	0
59	MG	1A	3854	1/1	0.99	0.04	52,52,52,52	0
59	MG	1A	3181	1/1	0.99	0.22	25,25,25,25	0
59	MG	1A	3956	1/1	0.99	0.06	26,26,26,26	0
59	MG	1A	3957	1/1	0.99	0.02	33,33,33,33	0
59	MG	1B	216	1/1	0.99	0.09	38,38,38,38	0
59	MG	1A	3920	1/1	0.99	0.06	45,45,45,45	0
59	MG	2A	3713	1/1	0.99	0.04	29,29,29,29	0
59	MG	1A	4157	1/1	0.99	0.04	24,24,24,24	0
59	MG	1A	4158	1/1	0.99	0.07	20,20,20,20	0
59	MG	1F	303	1/1	0.99	0.03	24,24,24,24	0
59	MG	1A	3170	1/1	0.99	0.15	10,10,10,10	0
59	MG	1A	3827	1/1	0.99	0.04	23,23,23,23	0
59	MG	1A	3035	1/1	0.99	0.27	24,24,24,24	0
59	MG	1A	4206	1/1	0.99	0.16	21,21,21,21	0
59	MG	2A	3644	1/1	0.99	0.04	69,69,69,69	0
59	MG	1a	3457	1/1	0.99	0.07	28,28,28,28	0
60	ZN	1Y	501	1/1	0.99	0.02	58,58,58,58	0
59	MG	2A	3723	1/1	0.99	0.03	47,47,47,47	0
60	ZN	16	102	1/1	0.99	0.05	36,36,36,36	0
60	ZN	1n	501	1/1	0.99	0.02	54,54,54,54	0
59	MG	2A	3646	1/1	0.99	0.04	53,53,53,53	0
59	MG	1A	3532	1/1	0.99	0.21	25,25,25,25	0
60	ZN	25	101	1/1	0.99	0.03	49,49,49,49	0
60	ZN	26	501	1/1	0.99	0.03	57,57,57,57	0
59	MG	1A	3662	1/1	0.99	0.05	15,15,15,15	0
59	MG	2A	3727	1/1	0.99	0.03	31,31,31,31	0
61	SF4	1d	501	8/8	0.99	0.06	52,55,64,66	0
59	MG	1a	3513	1/1	0.99	0.03	61,61,61,61	0
59	MG	2A	3578	1/1	0.99	0.04	25,25,25,25	0
59	MG	2A	3460	1/1	1.00	0.04	25,25,25,25	0
59	MG	1A	3928	1/1	1.00	0.02	16,16,16,16	0
59	MG	1A	3653	1/1	1.00	0.03	12,12,12,12	0
59	MG	1A	3010	1/1	1.00	0.04	16,16,16,16	0
59	MG	1A	3866	1/1	1.00	0.04	15,15,15,15	0
60	ZN	15	101	1/1	1.00	0.04	34,34,34,34	0
59	MG	1A	3737	1/1	1.00	0.03	34,34,34,34	0
60	ZN	19	102	1/1	1.00	0.07	40,40,40,40	0
59	MG	2a	3145	1/1	1.00	0.04	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.