



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 05:54 AM EDT

PDB ID : 7U2J / pdb_00007u2j
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with mRNA, aminoacylated A-site Gly-NH-tRNA^{Gly}, peptidyl P-site fMAC-NH-tRNA^{Met}, deacylated E-site tRNA^{Gly}, and chloramphenicol at 2.55Å resolution
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Deposited on : 2022-02-24
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) were used in the production of this report:

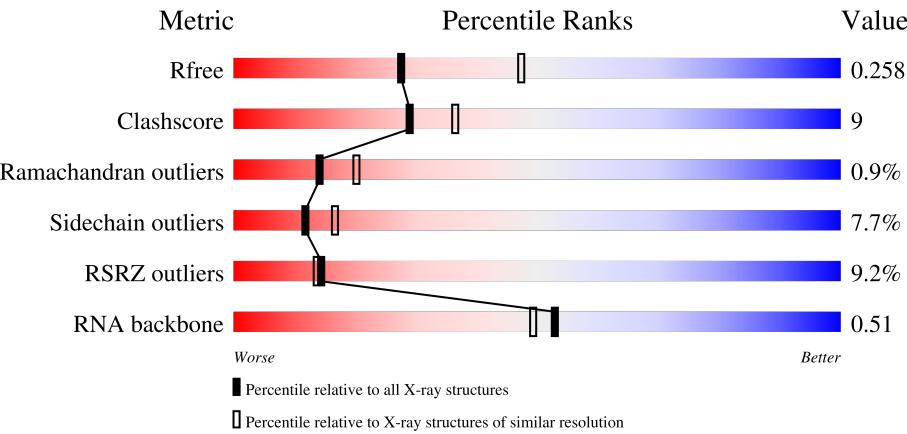
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)
RNA backbone	3983	1112 (2.80-2.28)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	4% 68% 25% 6% .
1	2A	2915	4% 60% 30% 7% .
2	1B	121	75% 21% ..
2	2B	121	3% 60% 28% 12% .

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Mol	Chain	Length	Quality of chain
3	1D	276	 % 82% 16% .
3	2D	276	 3% 83% 15% .
4	1E	206	 84% 13% ..
4	2E	206	 6% 78% 19% ..
5	1F	210	 % 78% 16% . .
5	2F	210	 2% 65% 31% .
6	1G	182	 7% 69% 29% ..
6	2G	182	 14% 57% 35% 8% .
7	1H	180	 2% 75% 18% . .
7	2H	180	 29% 62% 31% . .
8	1I	148	 4% 70% 24% 5% .
8	2I	148	 9% 69% 24% 5% .
9	1N	140	 % 85% 14% .
9	2N	140	 10% 73% 26% .
10	1O	122	 2% 82% 18%
10	2O	122	 75% 25%
11	1P	150	 % 78% 19% ...
11	2P	150	 5% 80% 17% ...
12	1Q	141	 % 82% 18%
12	2Q	141	 18% 64% 33% .
13	1R	118	 82% 15% .
13	2R	118	 84% 14% .
14	1S	112	 2% 86% 12% ..
14	2S	112	 17% 60% 37% ..
15	1T	146	 3% 71% 18% . 10%

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

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

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

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Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1w	74	
54	2w	74	
55	1x	77	
55	2x	77	
56	1z	3	
56	2z	3	
57	1y	74	
57	2y	74	

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
58	MG	1A	3247	-	-	-	X
58	MG	1a	1697	-	-	-	X
58	MG	1a	1727	-	-	-	X
58	MG	1a	1771	-	-	-	X
58	MG	1a	1777	-	-	-	X
58	MG	2A	3330	-	-	-	X
58	MG	2A	3390	-	-	-	X
58	MG	2A	3413	-	-	-	X
58	MG	2A	3416	-	-	-	X
58	MG	2a	1608	-	-	-	X
58	MG	2a	1633	-	-	-	X
58	MG	2a	1711	-	-	-	X
58	MG	2a	1822	-	-	-	X
58	MG	2v	101	-	-	-	X

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 299751 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	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
5	2F	202	Total	C	N	O	S	0	0	0
			1579	1007	296	274	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called MG-mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			286	128	59	86	13			
53	2v	13	Total	C	N	O	P	0	0	0
			286	128	59	86	13			

- Molecule 54 is a RNA chain called A-site Aminoacyl-tRNA Gly-NH-tRNAgly.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	73	Total	C	N	O	P	S	0	0	0
			1556	695	275	512	73	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1536	686	273	504	72	1			

- Molecule 55 is a RNA chain called P-site Peptidyl-tRNA fMAC-NH-tRNAmet RNA-part.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			

- Molecule 56 is a protein called P-site Peptidyl-tRNA fMAC-NH-tRNAmet Peptide-part.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1z	3	Total	C	N	O	S	0	0	0
			21	12	3	4	2			
56	2z	3	Total	C	N	O	S	0	0	0
			21	12	3	4	2			

- Molecule 57 is a RNA chain called E-site Deacylated tRNAgly.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
57	1y	73	Total	C	N	O	P	S	0	0	0
			1552	693	273	512	73	1			
57	2y	73	Total	C	N	O	P	S	0	0	0
			1552	693	273	512	73	1			

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1085	Total	Mg	0	0
			1085	1085		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1B	37	Total 37	Mg 37	0	0
58	1D	11	Total 11	Mg 11	0	0
58	1E	15	Total 15	Mg 15	0	0
58	1F	11	Total 11	Mg 11	0	0
58	1G	4	Total 4	Mg 4	0	0
58	1H	1	Total 1	Mg 1	0	0
58	1I	1	Total 1	Mg 1	0	0
58	1N	5	Total 5	Mg 5	0	0
58	1O	6	Total 6	Mg 6	0	0
58	1P	5	Total 5	Mg 5	0	0
58	1Q	8	Total 8	Mg 8	0	0
58	1R	7	Total 7	Mg 7	0	0
58	1S	3	Total 3	Mg 3	0	0
58	1T	2	Total 2	Mg 2	0	0
58	1U	10	Total 10	Mg 10	0	0
58	1V	6	Total 6	Mg 6	0	0
58	1W	7	Total 7	Mg 7	0	0
58	1X	6	Total 6	Mg 6	0	0
58	1Y	3	Total 3	Mg 3	0	0
58	1Z	3	Total 3	Mg 3	0	0
58	10	8	Total 8	Mg 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	11	4	Total 4	Mg 4	0	0
58	12	2	Total 2	Mg 2	0	0
58	13	4	Total 4	Mg 4	0	0
58	15	8	Total 8	Mg 8	0	0
58	16	3	Total 3	Mg 3	0	0
58	17	5	Total 5	Mg 5	0	0
58	18	6	Total 6	Mg 6	0	0
58	19	1	Total 1	Mg 1	0	0
58	1a	214	Total 214	Mg 214	0	0
58	1b	2	Total 2	Mg 2	0	0
58	1d	1	Total 1	Mg 1	0	0
58	1e	3	Total 3	Mg 3	0	0
58	1f	2	Total 2	Mg 2	0	0
58	1k	1	Total 1	Mg 1	0	0
58	1l	2	Total 2	Mg 2	0	0
58	1m	1	Total 1	Mg 1	0	0
58	1n	2	Total 2	Mg 2	0	0
58	1p	1	Total 1	Mg 1	0	0
58	1s	1	Total 1	Mg 1	0	0
58	1t	1	Total 1	Mg 1	0	0
58	1w	9	Total 9	Mg 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1x	12	Total 12	Mg 12	0	0
58	1y	1	Total 1	Mg 1	0	0
58	2A	800	Total 800	Mg 800	0	0
58	2B	18	Total 18	Mg 18	0	0
58	2D	5	Total 5	Mg 5	0	0
58	2E	8	Total 8	Mg 8	0	0
58	2F	8	Total 8	Mg 8	0	0
58	2G	1	Total 1	Mg 1	0	0
58	2N	1	Total 1	Mg 1	0	0
58	2O	1	Total 1	Mg 1	0	0
58	2Q	3	Total 3	Mg 3	0	0
58	2R	2	Total 2	Mg 2	0	0
58	2T	4	Total 4	Mg 4	0	0
58	2U	1	Total 1	Mg 1	0	0
58	2V	1	Total 1	Mg 1	0	0
58	2W	2	Total 2	Mg 2	0	0
58	2X	1	Total 1	Mg 1	0	0
58	2Y	1	Total 1	Mg 1	0	0
58	2Z	1	Total 1	Mg 1	0	0
58	20	3	Total 3	Mg 3	0	0
58	21	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	23	2	Total Mg 2 2	0	0
58	25	4	Total Mg 4 4	0	0
58	26	1	Total Mg 1 1	0	0
58	27	2	Total Mg 2 2	0	0
58	28	3	Total Mg 3 3	0	0
58	2a	223	Total Mg 223 223	0	0
58	2d	2	Total Mg 2 2	0	0
58	2e	1	Total Mg 1 1	0	0
58	2f	2	Total Mg 2 2	0	0
58	2g	1	Total Mg 1 1	0	0
58	2j	1	Total Mg 1 1	0	0
58	2l	2	Total Mg 2 2	0	0
58	2q	2	Total Mg 2 2	0	0
58	2r	1	Total Mg 1 1	0	0
58	2t	1	Total Mg 1 1	0	0
58	2v	1	Total Mg 1 1	0	0
58	2w	2	Total Mg 2 2	0	0
58	2x	8	Total Mg 8 8	0	0

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

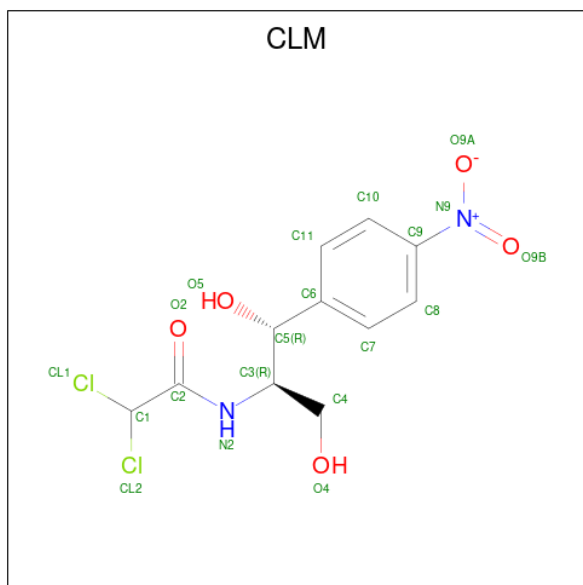
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1A	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	2A	1	Total K 1 1	0	0

- Molecule 60 is CHLORAMPHENICOL (CCD ID: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	1A	1	Total C Cl N O 20 11 2 2 5	0	0
60	2w	1	Total C Cl N O 20 11 2 2 5	0	0

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

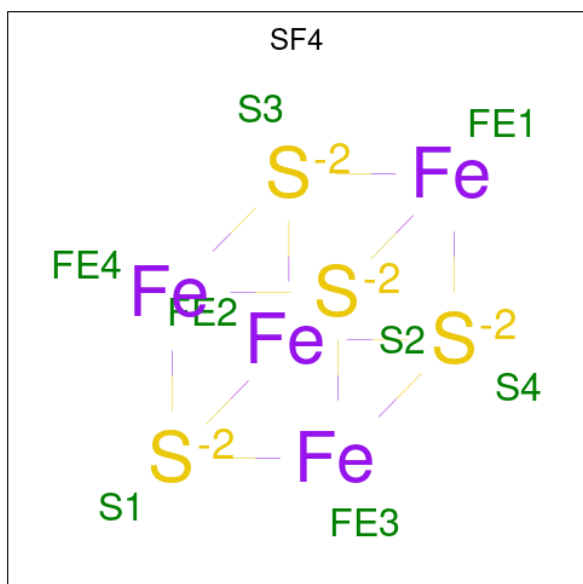
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1Y	1	Total Zn 1 1	0	0
61	14	1	Total Zn 1 1	0	0
61	15	1	Total Zn 1 1	0	0
61	16	1	Total Zn 1 1	0	0
61	19	1	Total Zn 1 1	0	0
61	1n	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2Y	1	Total	Zn	0	0
			1	1		
61	24	1	Total	Zn	0	0
			1	1		
61	25	1	Total	Zn	0	0
			1	1		
61	26	1	Total	Zn	0	0
			1	1		
61	29	1	Total	Zn	0	0
			1	1		
61	2n	1	Total	Zn	0	0
			1	1		

- Molecule 62 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
62	1d	1	Total	Fe	S	0	0
			8	4	4		
62	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 63 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1A	1977	Total	O	0	0
			1977	1977		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1B	66	Total 66	O 66	0	0
63	1D	30	Total 30	O 30	0	0
63	1E	23	Total 23	O 23	0	0
63	1F	17	Total 17	O 17	0	0
63	1G	6	Total 6	O 6	0	0
63	1H	1	Total 1	O 1	0	0
63	1N	4	Total 4	O 4	0	0
63	1O	7	Total 7	O 7	0	0
63	1P	20	Total 20	O 20	0	0
63	1Q	7	Total 7	O 7	0	0
63	1R	9	Total 9	O 9	0	0
63	1S	5	Total 5	O 5	0	0
63	1T	8	Total 8	O 8	0	0
63	1U	11	Total 11	O 11	0	0
63	1V	9	Total 9	O 9	0	0
63	1W	7	Total 7	O 7	0	0
63	1X	7	Total 7	O 7	0	0
63	1Y	2	Total 2	O 2	0	0
63	10	11	Total 11	O 11	0	0
63	11	8	Total 8	O 8	0	0
63	12	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	13	5	Total 5	O 5	0	0
63	14	1	Total 1	O 1	0	0
63	15	6	Total 6	O 6	0	0
63	16	2	Total 2	O 2	0	0
63	17	8	Total 8	O 8	0	0
63	18	12	Total 12	O 12	0	0
63	1a	263	Total 263	O 263	0	0
63	1b	1	Total 1	O 1	0	0
63	1d	1	Total 1	O 1	0	0
63	1e	1	Total 1	O 1	0	0
63	1f	1	Total 1	O 1	0	0
63	1g	1	Total 1	O 1	0	0
63	1l	6	Total 6	O 6	0	0
63	1m	2	Total 2	O 2	0	0
63	1n	1	Total 1	O 1	0	0
63	1o	1	Total 1	O 1	0	0
63	1q	3	Total 3	O 3	0	0
63	1u	1	Total 1	O 1	0	0
63	1v	3	Total 3	O 3	0	0
63	1w	5	Total 5	O 5	0	0
63	1x	11	Total 11	O 11	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	1y	1	Total 1	O 1	0	0
63	2A	1074	Total 1074	O 1074	0	0
63	2B	18	Total 18	O 18	0	0
63	2D	22	Total 22	O 22	0	0
63	2E	13	Total 13	O 13	0	0
63	2F	12	Total 12	O 12	0	0
63	2I	2	Total 2	O 2	0	0
63	2N	1	Total 1	O 1	0	0
63	2O	3	Total 3	O 3	0	0
63	2P	11	Total 11	O 11	0	0
63	2Q	2	Total 2	O 2	0	0
63	2R	3	Total 3	O 3	0	0
63	2T	2	Total 2	O 2	0	0
63	2U	3	Total 3	O 3	0	0
63	2W	2	Total 2	O 2	0	0
63	2X	5	Total 5	O 5	0	0
63	2Y	1	Total 1	O 1	0	0
63	2Z	1	Total 1	O 1	0	0
63	20	3	Total 3	O 3	0	0
63	21	5	Total 5	O 5	0	0
63	23	1	Total 1	O 1	0	0

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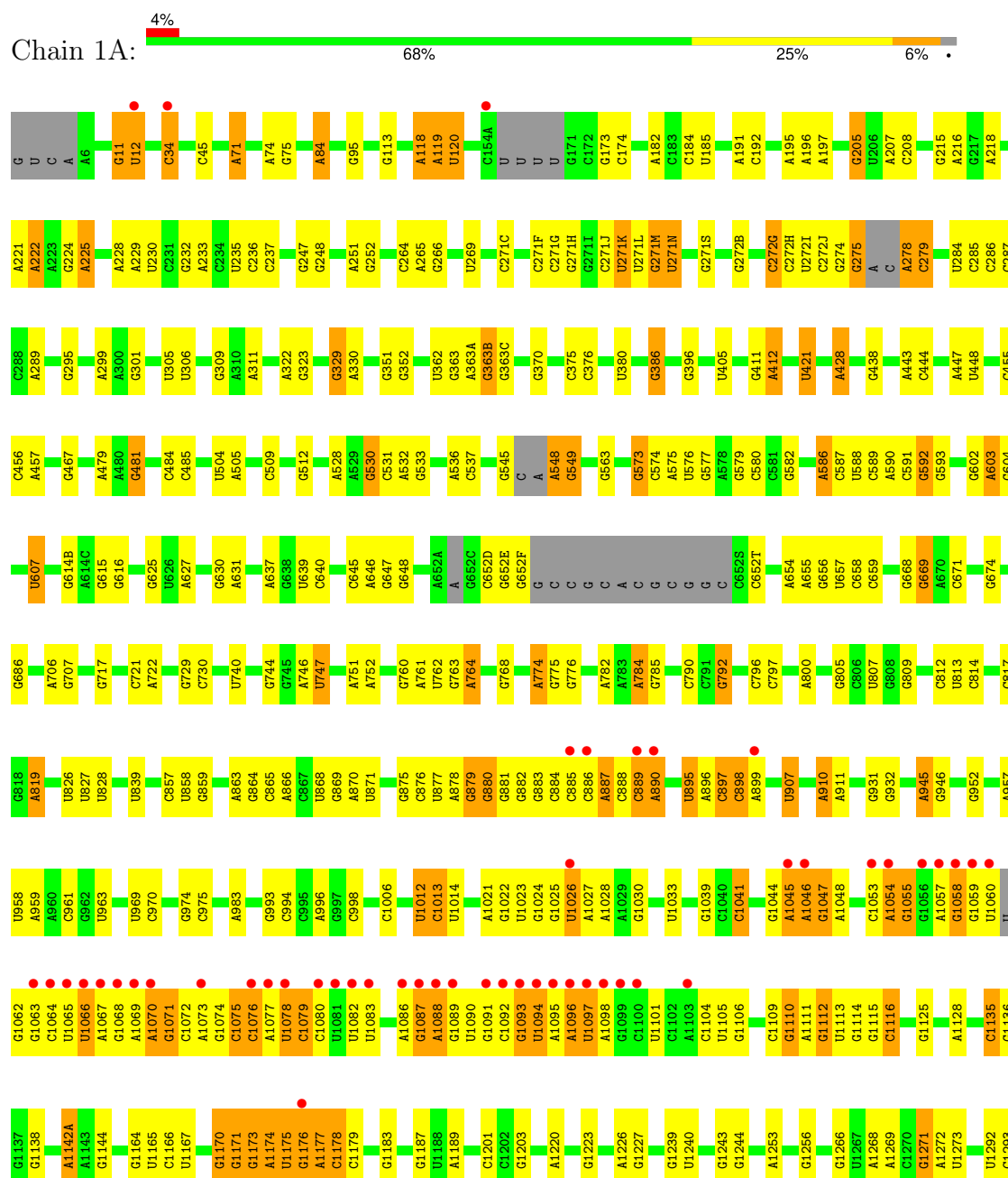
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
63	27	2	Total 2	O 2	0	0
63	28	6	Total 6	O 6	0	0
63	29	1	Total 1	O 1	0	0
63	2a	245	Total 245	O 245	0	0
63	2d	2	Total 2	O 2	0	0
63	2j	1	Total 1	O 1	0	0
63	2l	3	Total 3	O 3	0	0
63	2o	1	Total 1	O 1	0	0
63	2p	2	Total 2	O 2	0	0
63	2q	1	Total 1	O 1	0	0
63	2r	1	Total 1	O 1	0	0
63	2t	2	Total 2	O 2	0	0
63	2v	1	Total 1	O 1	0	0
63	2w	2	Total 2	O 2	0	0
63	2x	6	Total 6	O 6	0	0
63	2z	1	Total 1	O 1	0	0

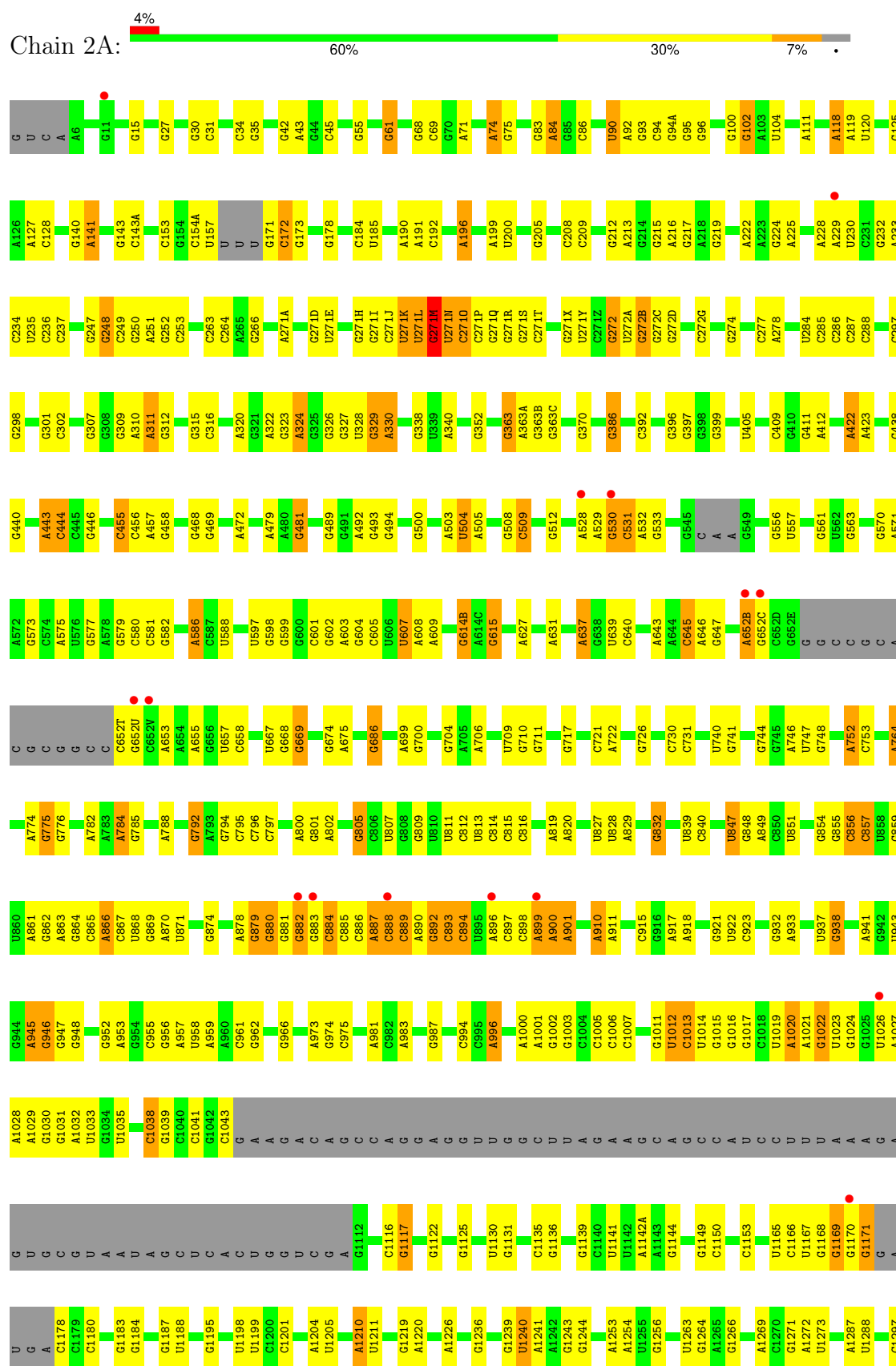
3 Residue-property plots

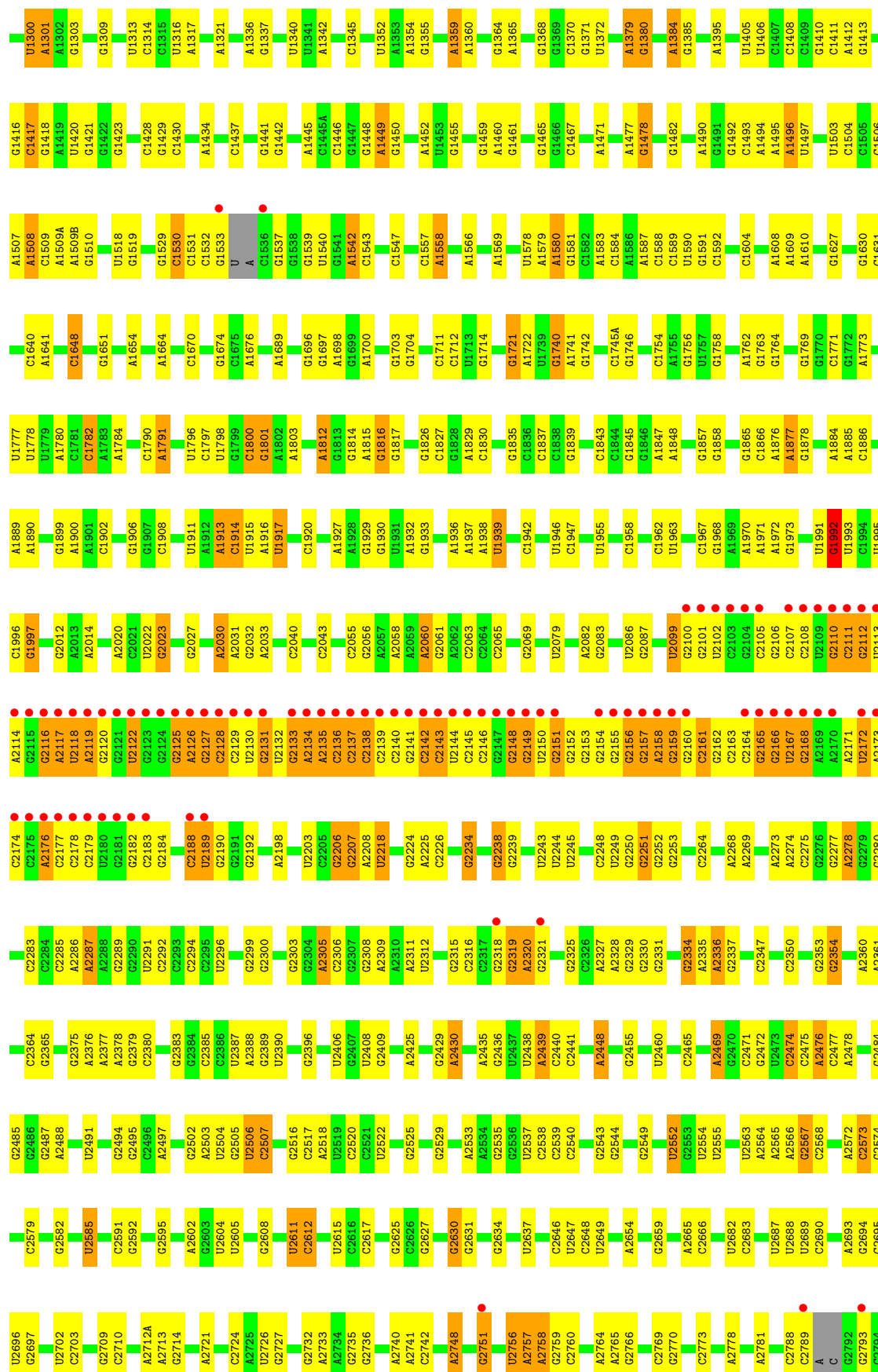
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

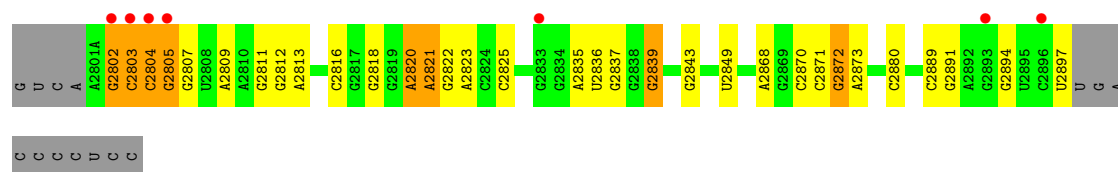
• Molecule 1: 23S Ribosomal RNA





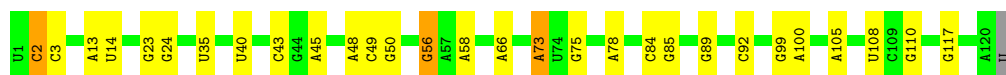






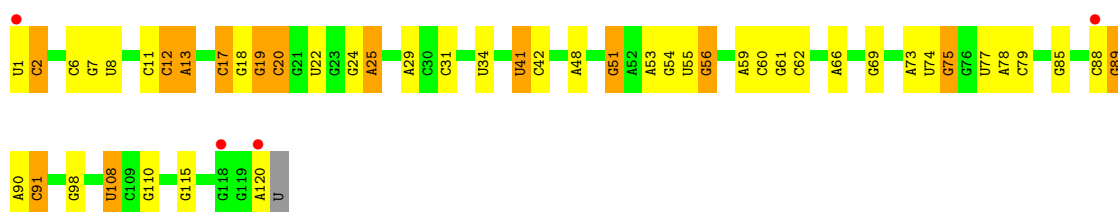
- Molecule 2: 5S Ribosomal RNA

Chain 1B: 75% 21% ..



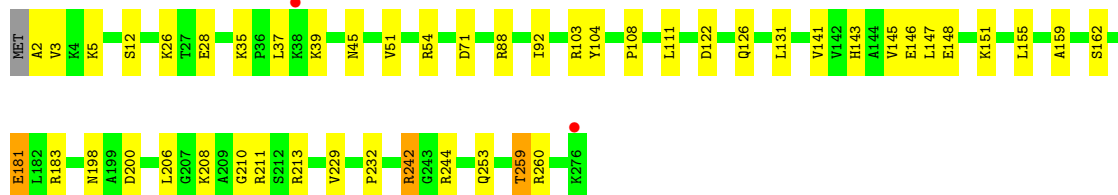
- Molecule 2: 5S Ribosomal RNA

Chain 2B: 3% 60% 28% 12% .



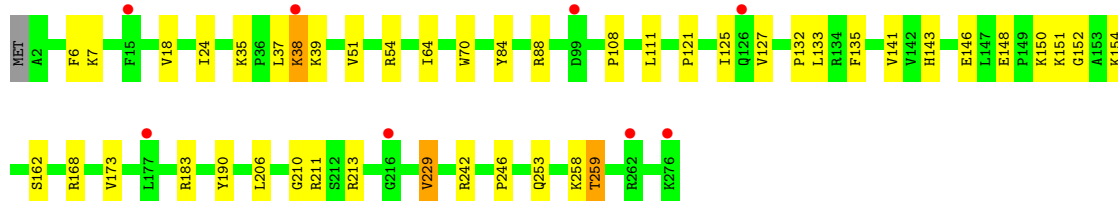
- Molecule 3: 50S ribosomal protein L2

Chain 1D: % 82% 16% .



- Molecule 3: 50S ribosomal protein L2

Chain 2D: 3% 83% 15% .

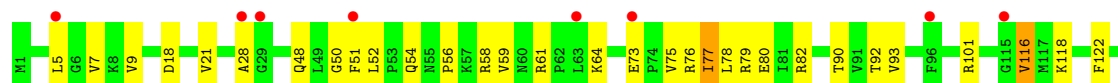
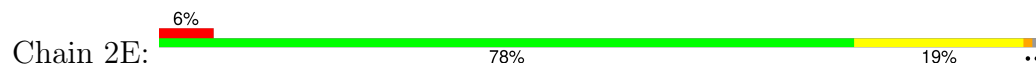


- Molecule 4: 50S ribosomal protein L3

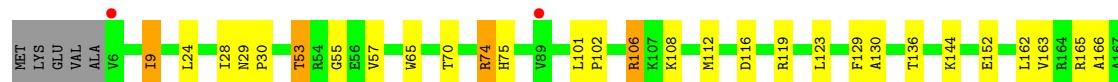
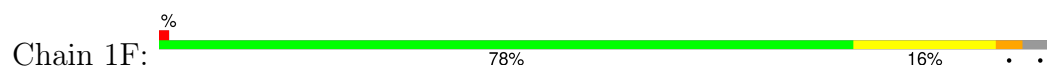
Chain 1E: 84% 13% ..



- Molecule 4: 50S ribosomal protein L3



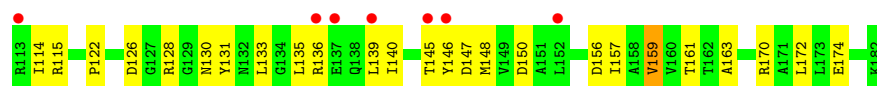
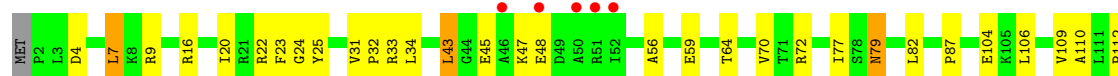
- Molecule 5: 50S ribosomal protein L4



- Molecule 5: 50S ribosomal protein L4

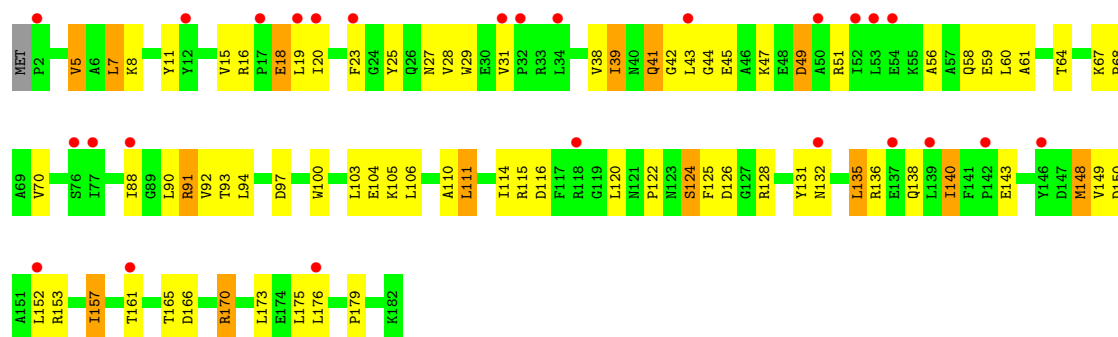


- Molecule 6: 50S ribosomal protein L5

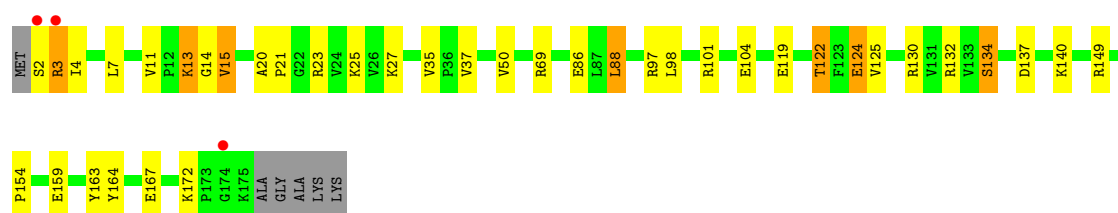
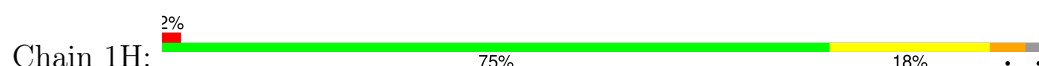


- Molecule 6: 50S ribosomal protein L5

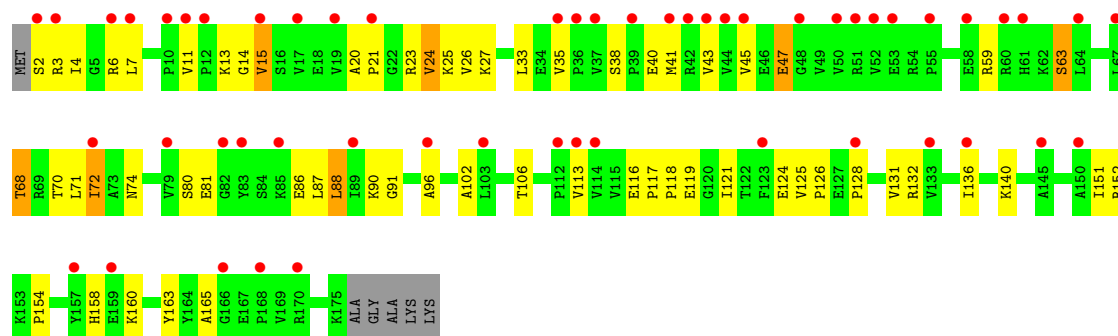




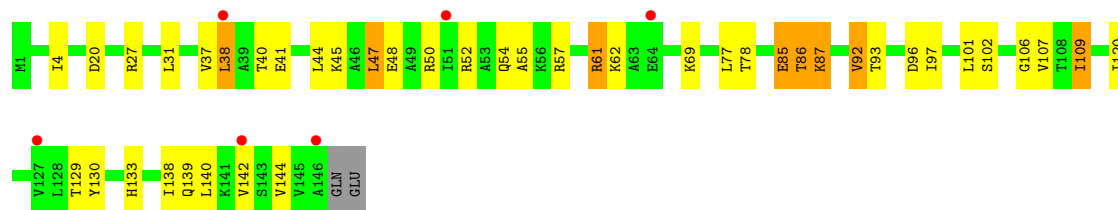
• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6

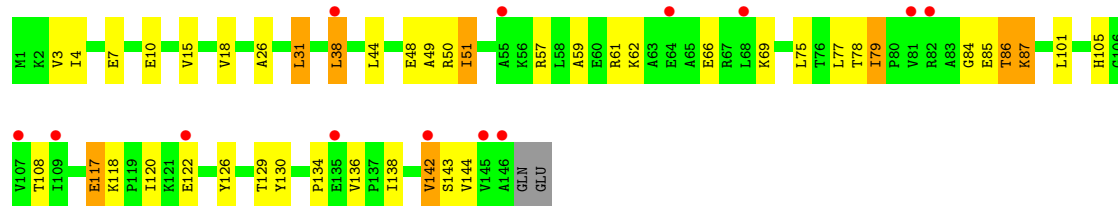


• Molecule 8: 50S ribosomal protein L9

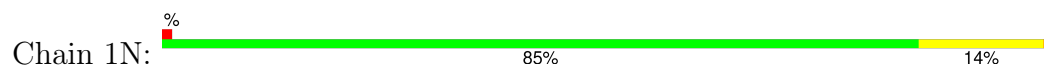


• Molecule 8: 50S ribosomal protein L9

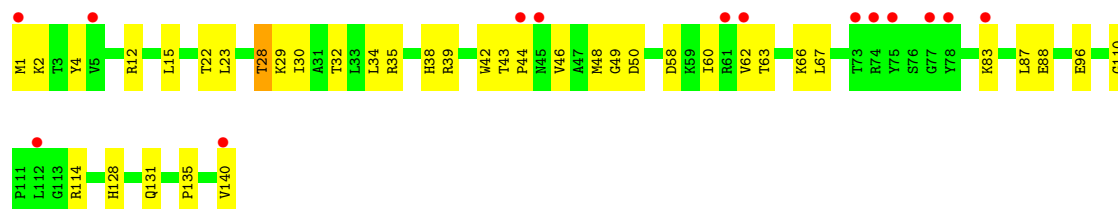
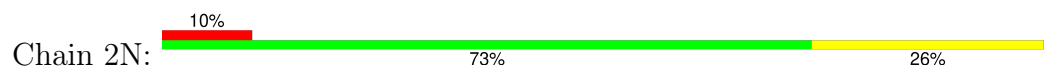




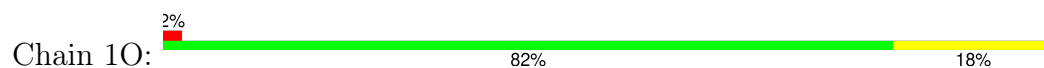
- Molecule 9: 50S ribosomal protein L13



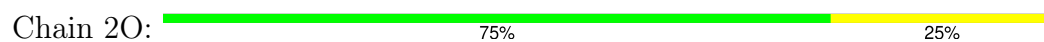
- Molecule 9: 50S ribosomal protein L13



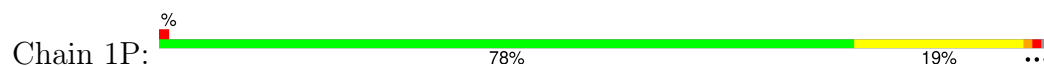
- Molecule 10: 50S ribosomal protein L14



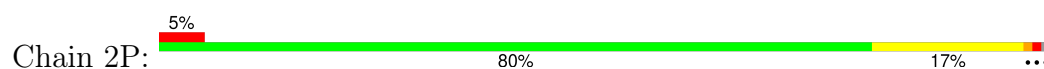
- Molecule 10: 50S ribosomal protein L14

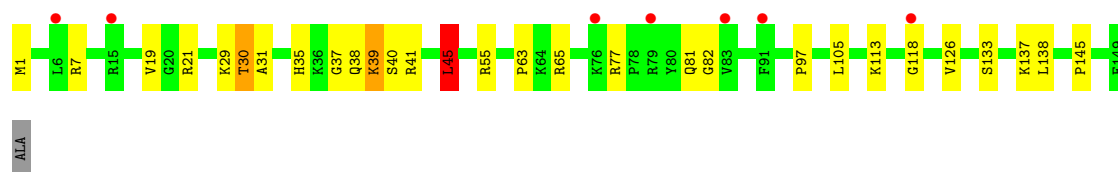


- Molecule 11: 50S ribosomal protein L15

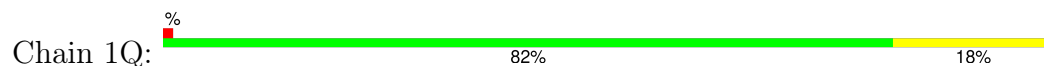


- Molecule 11: 50S ribosomal protein L15

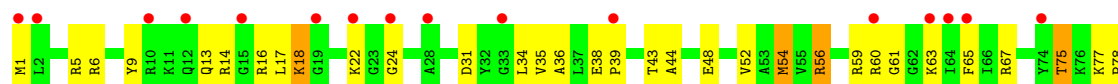




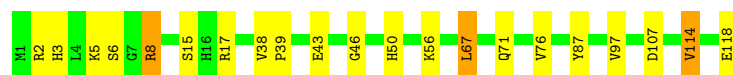
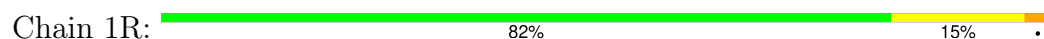
- Molecule 12: 50S ribosomal protein L16



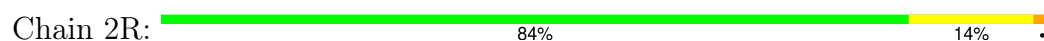
- Molecule 12: 50S ribosomal protein L16



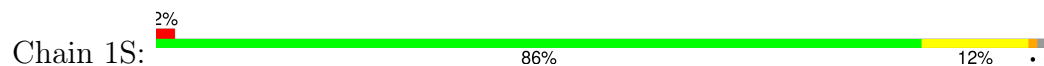
- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17

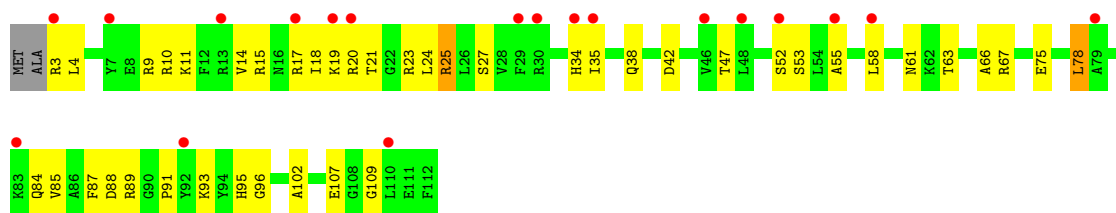


- Molecule 14: 50S ribosomal protein L18

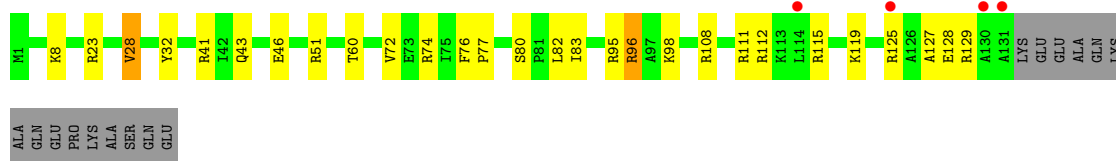
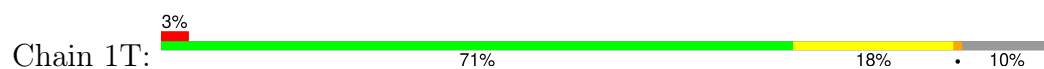


- Molecule 14: 50S ribosomal protein L18

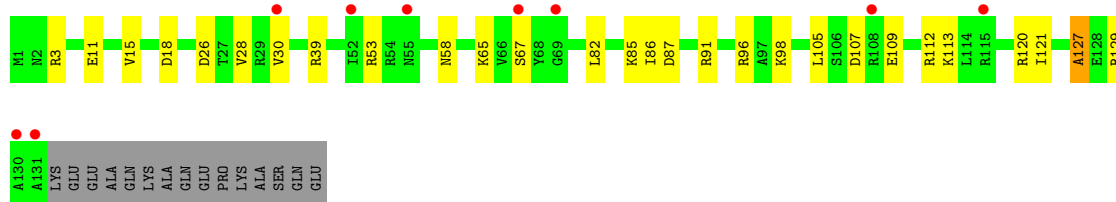




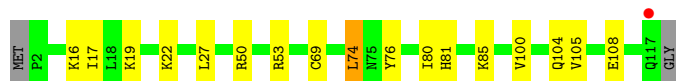
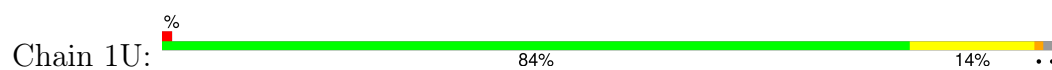
• Molecule 15: 50S ribosomal protein L19



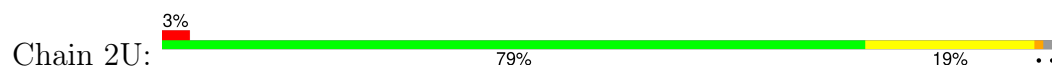
• Molecule 15: 50S ribosomal protein L19



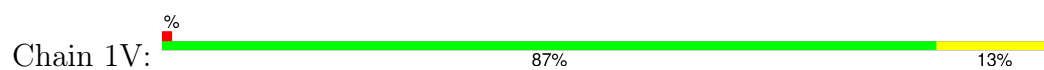
• Molecule 16: 50S ribosomal protein L20



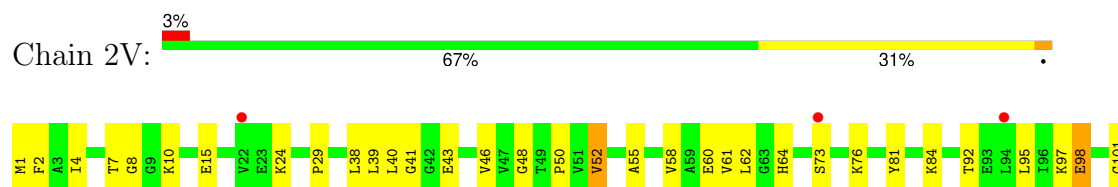
• Molecule 16: 50S ribosomal protein L20



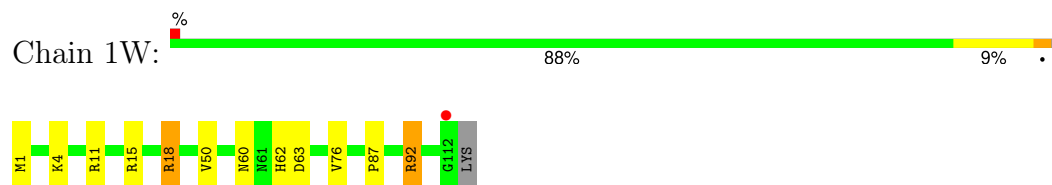
• Molecule 17: 50S ribosomal protein L21



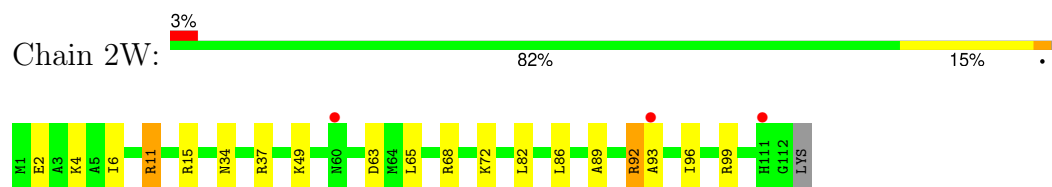
• Molecule 17: 50S ribosomal protein L21



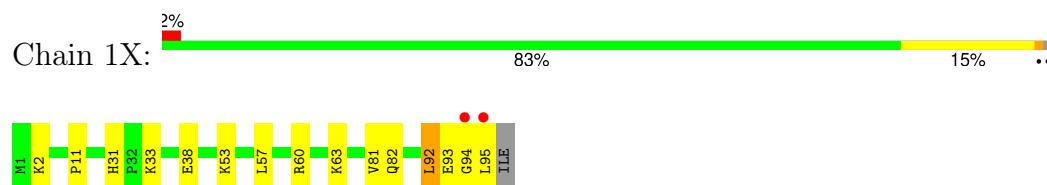
• Molecule 18: 50S ribosomal protein L22



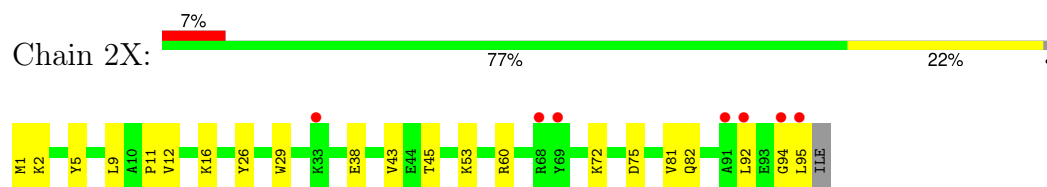
• Molecule 18: 50S ribosomal protein L22



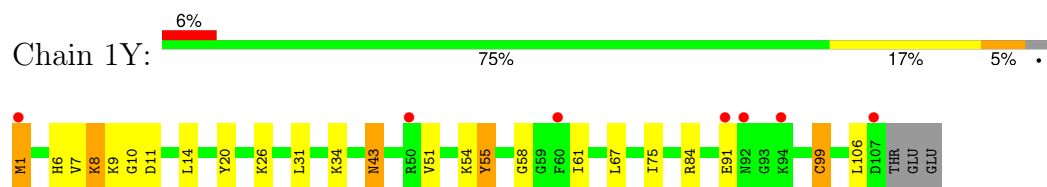
• Molecule 19: 50S ribosomal protein L23



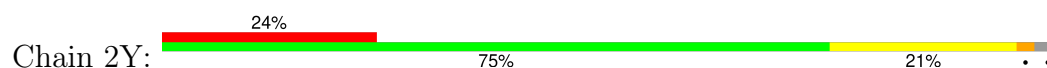
• Molecule 19: 50S ribosomal protein L23

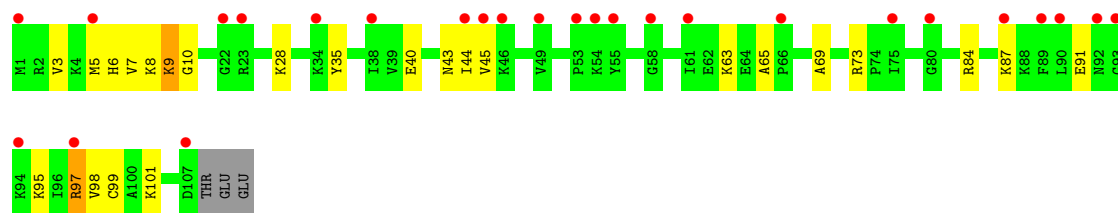


• Molecule 20: 50S ribosomal protein L24

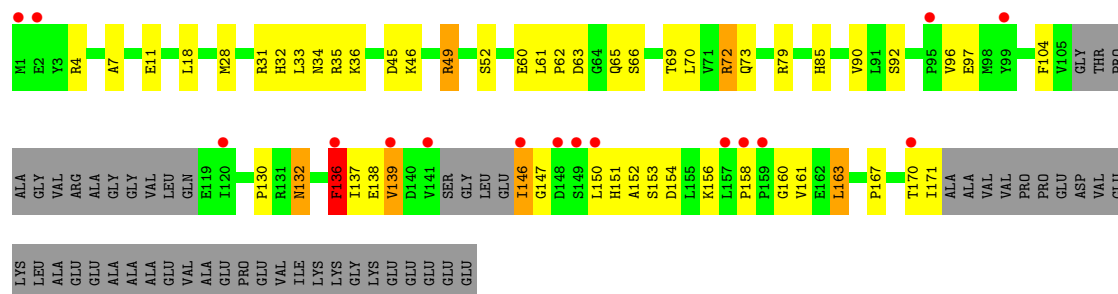


• Molecule 20: 50S ribosomal protein L24

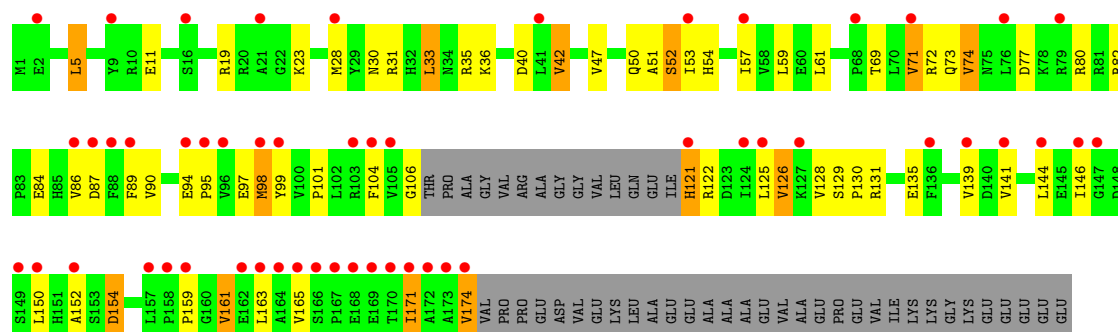




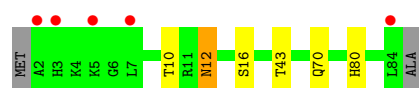
• Molecule 21: 50S ribosomal protein L25



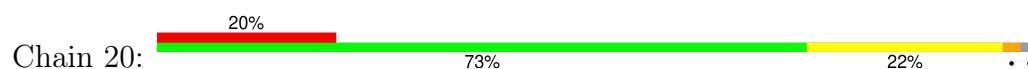
• Molecule 21: 50S ribosomal protein L25



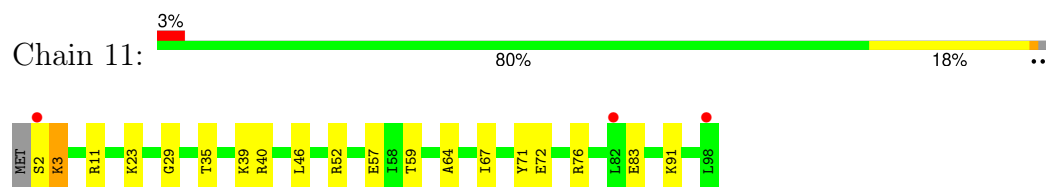
• Molecule 22: 50S ribosomal protein L27



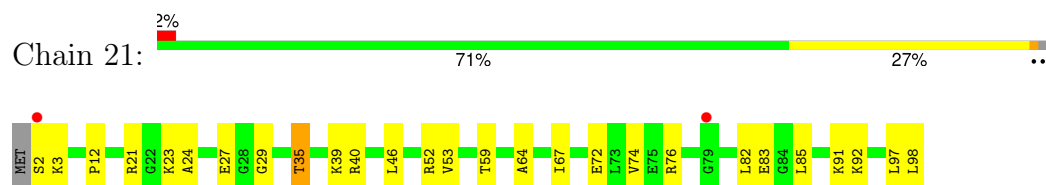
• Molecule 22: 50S ribosomal protein L27



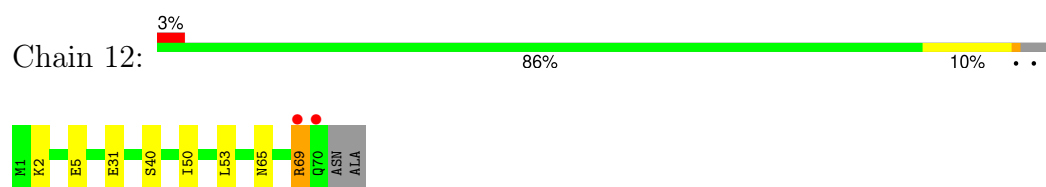
- Molecule 23: 50S ribosomal protein L28



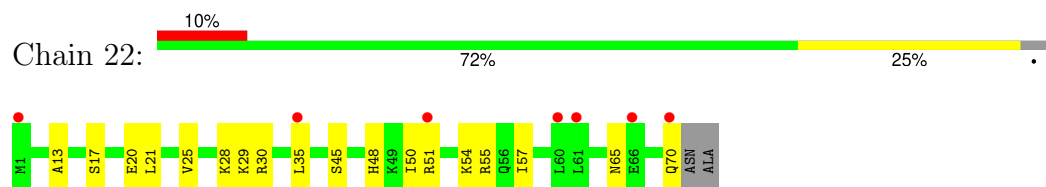
- Molecule 23: 50S ribosomal protein L28



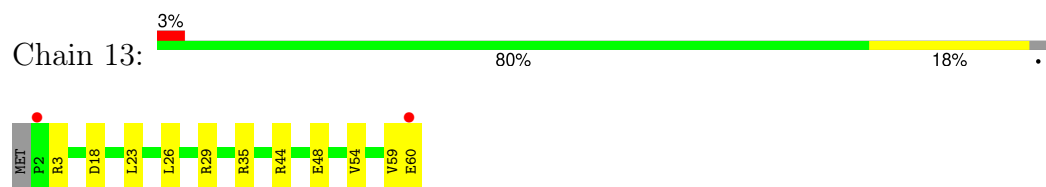
- Molecule 24: 50S ribosomal protein L29



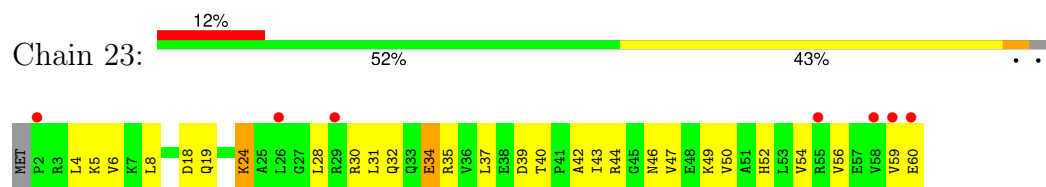
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30

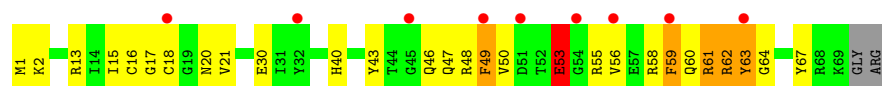


- Molecule 25: 50S ribosomal protein L30

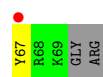
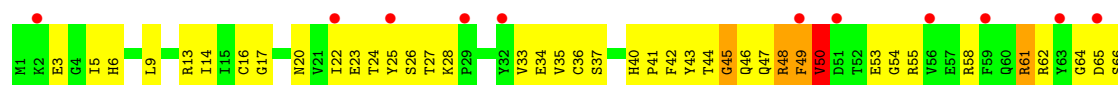


- Molecule 26: 50S ribosomal protein L31

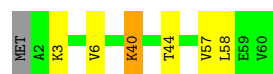
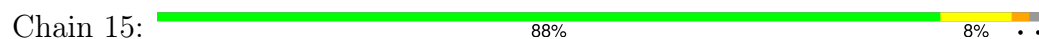




- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



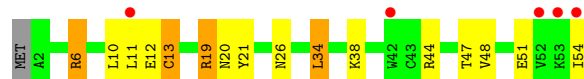
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



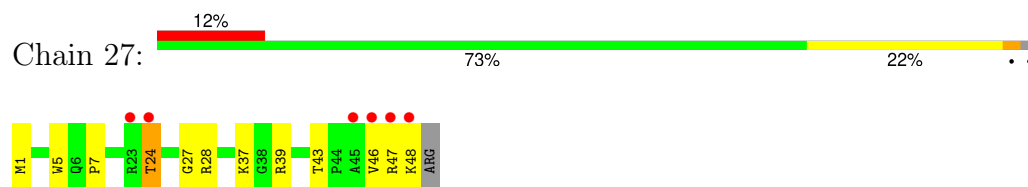
- Molecule 28: 50S ribosomal protein L33



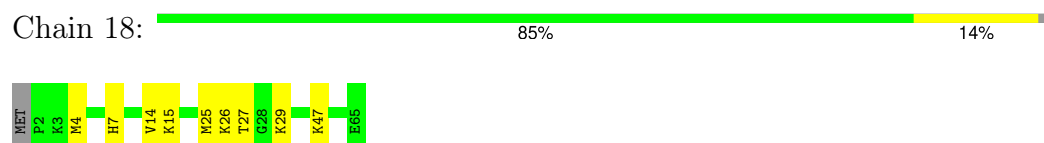
- Molecule 29: 50S ribosomal protein L34



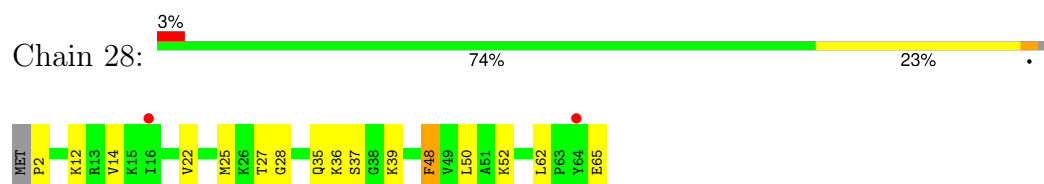
- Molecule 29: 50S ribosomal protein L34



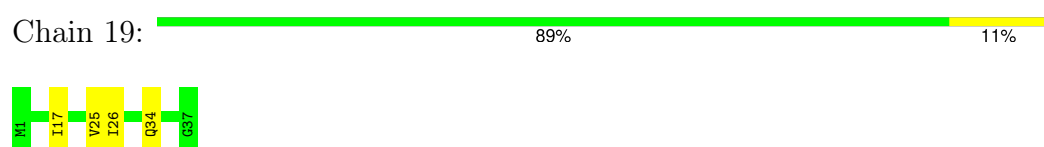
- Molecule 30: 50S ribosomal protein L35



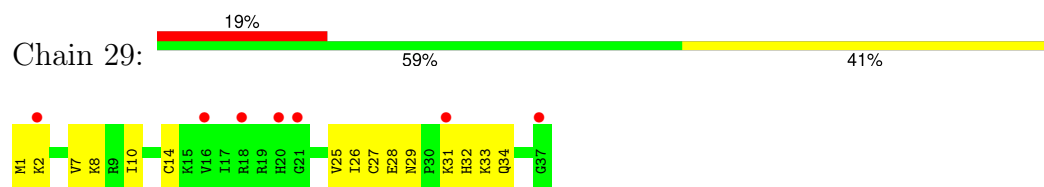
- Molecule 30: 50S ribosomal protein L35



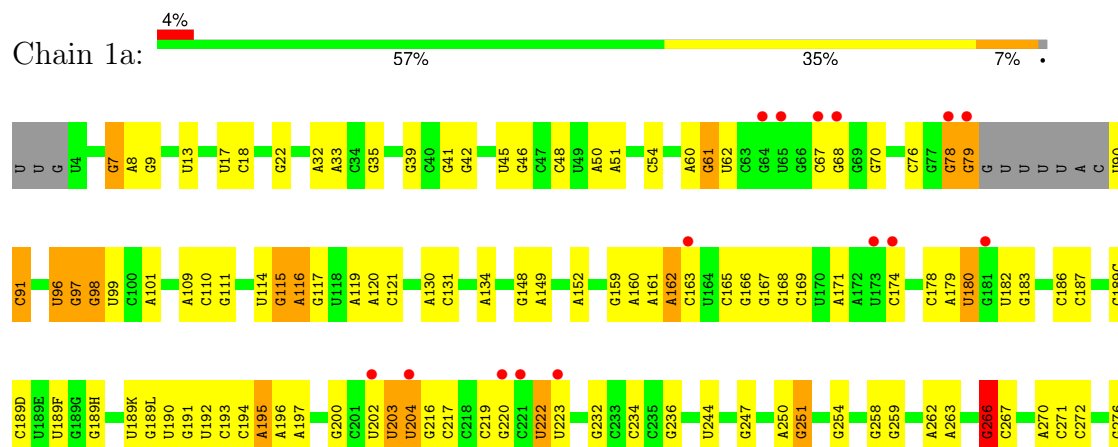
- Molecule 31: 50S ribosomal protein L36

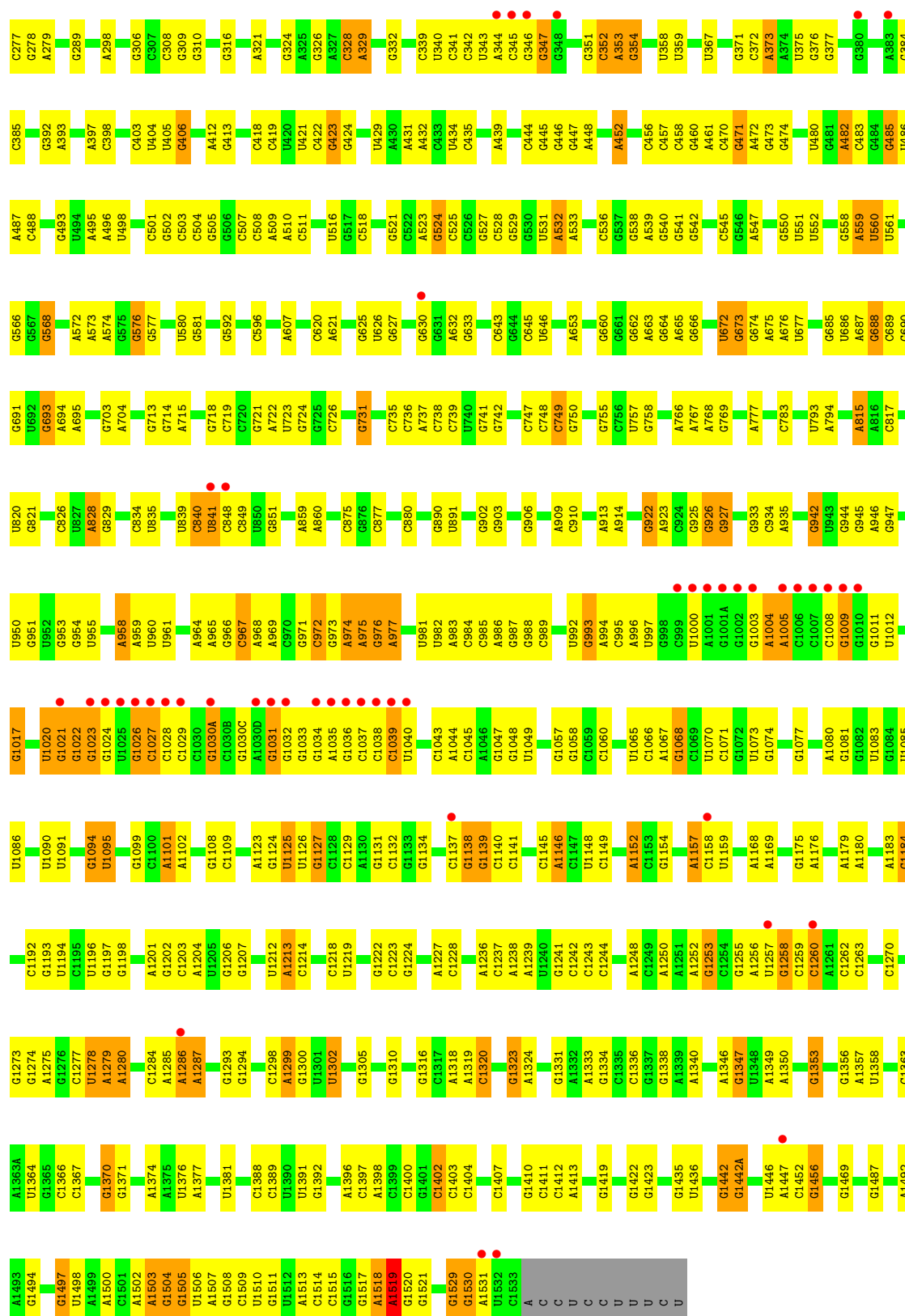


- Molecule 31: 50S ribosomal protein L36

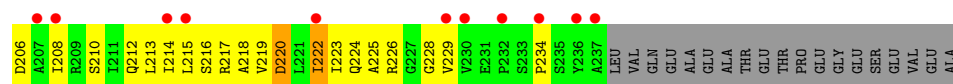


- Molecule 32: 16S Ribosomal RNA

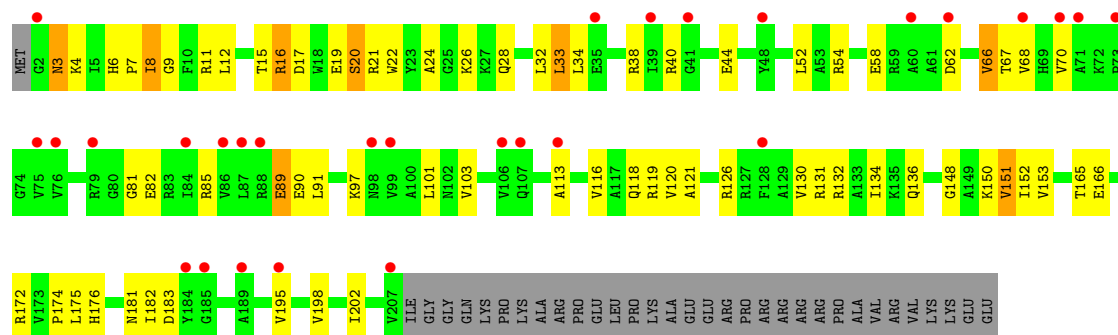




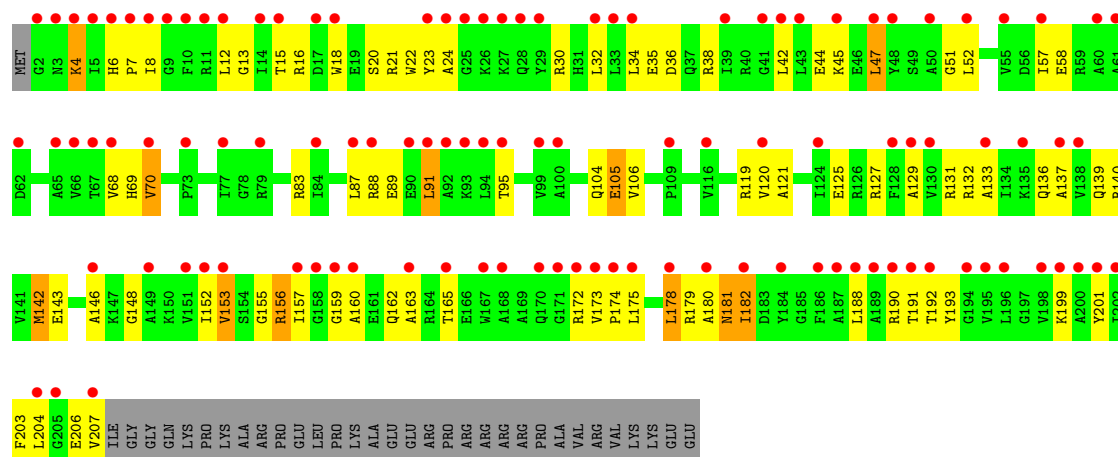




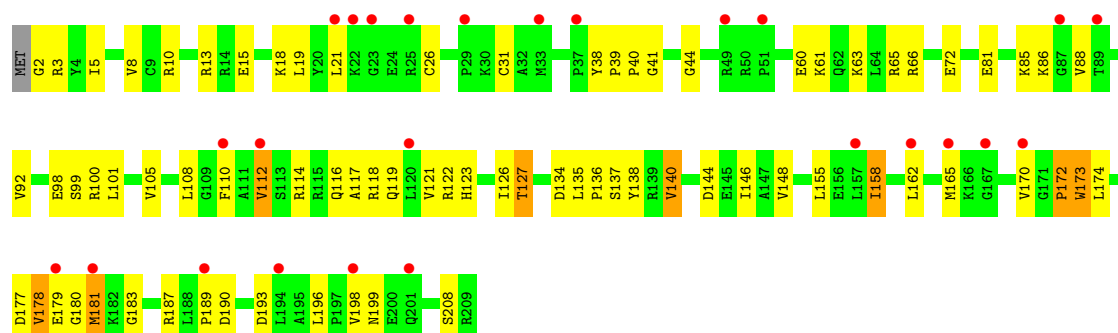
• Molecule 34: 30S ribosomal protein S3



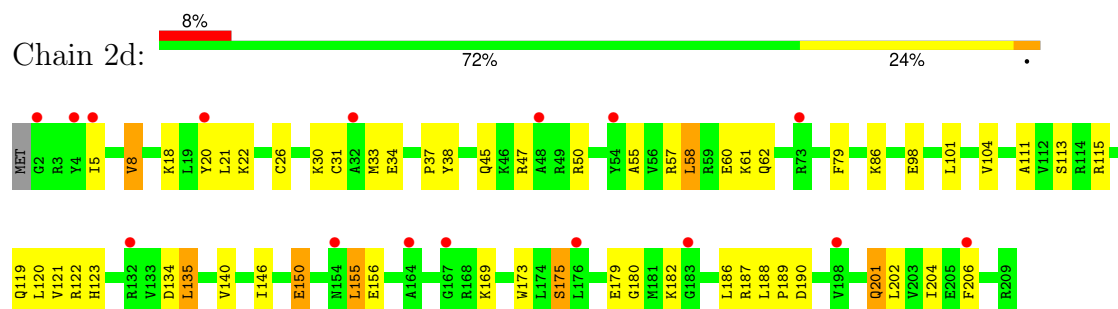
• Molecule 34: 30S ribosomal protein S3



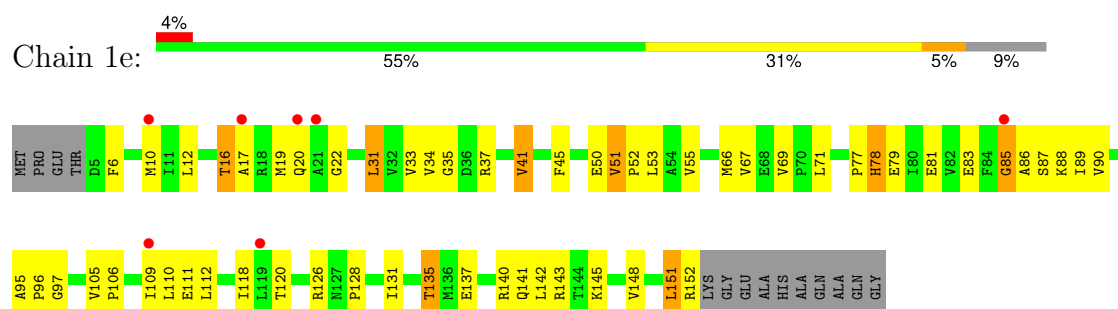
• Molecule 35: 30S ribosomal protein S4



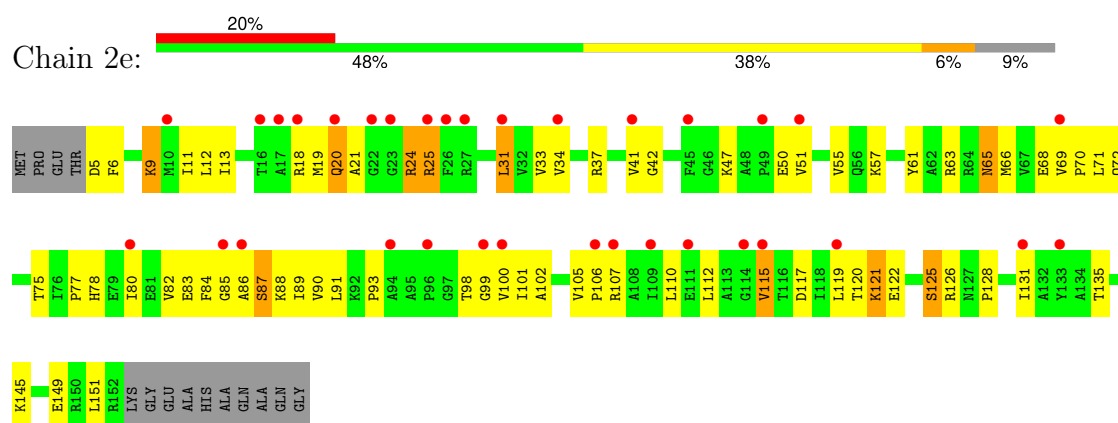
- Molecule 35: 30S ribosomal protein S4



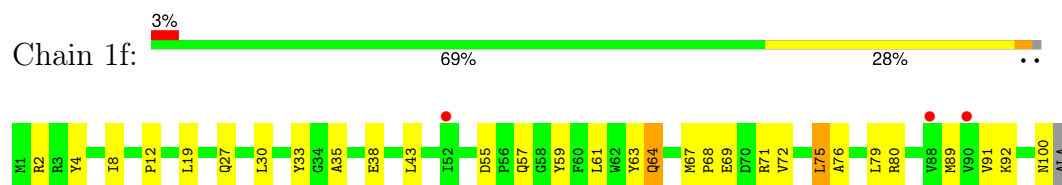
- Molecule 36: 30S ribosomal protein S5



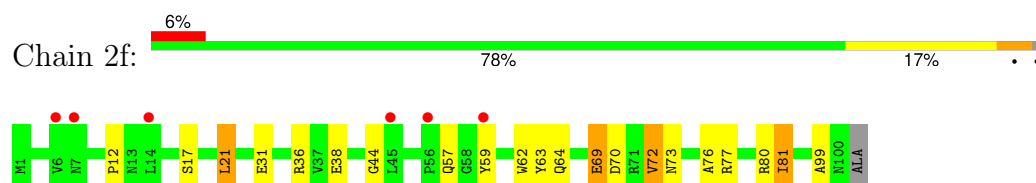
- Molecule 36: 30S ribosomal protein S5



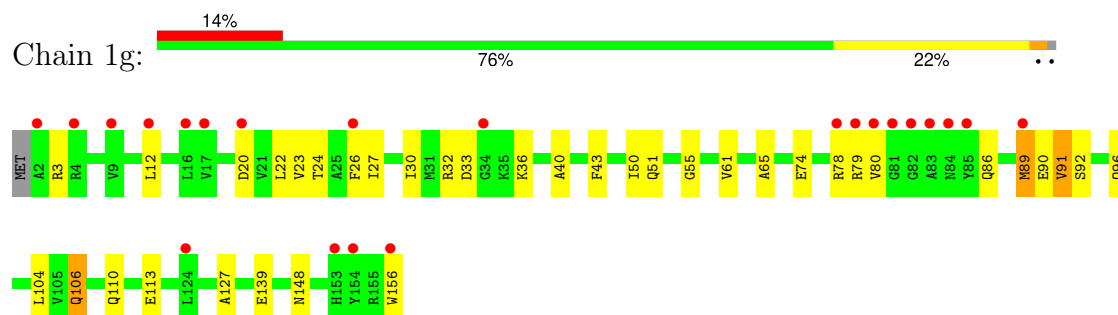
- Molecule 37: 30S ribosomal protein S6



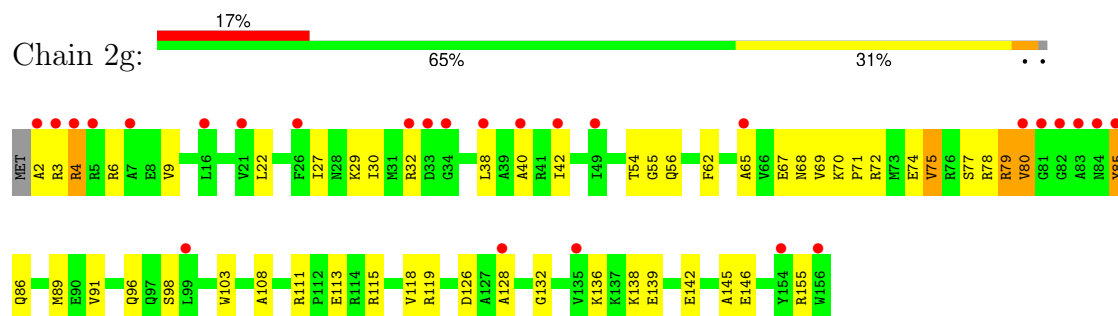
- Molecule 37: 30S ribosomal protein S6



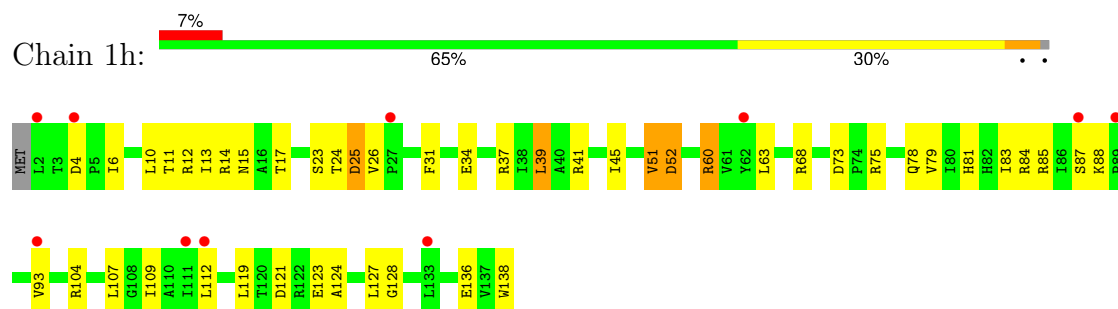
- Molecule 38: 30S ribosomal protein S7



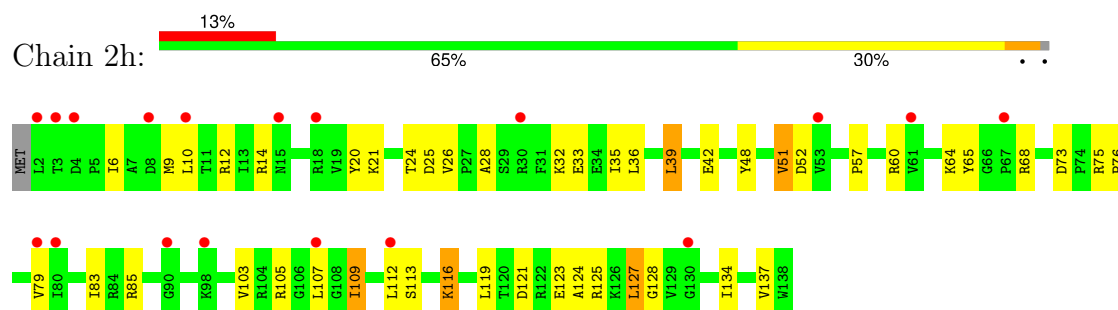
- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8

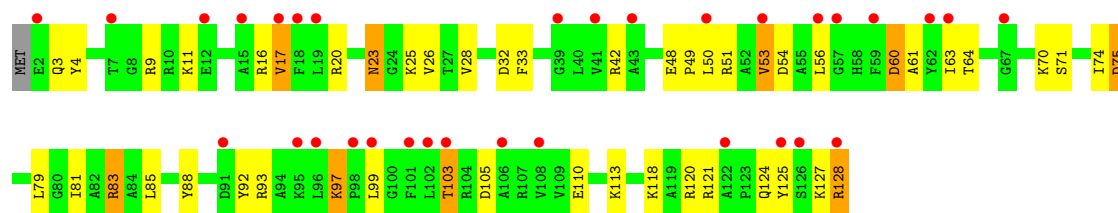


- Molecule 39: 30S ribosomal protein S8

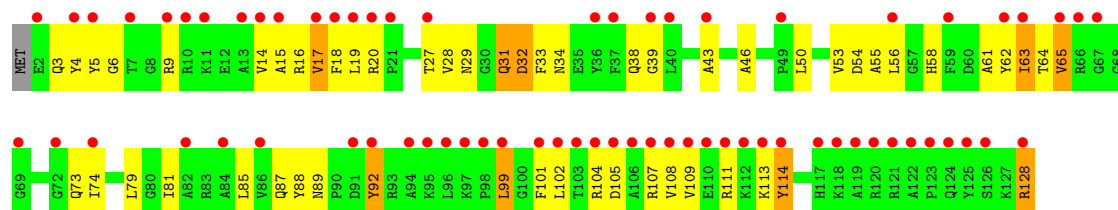


- Molecule 40: 30S ribosomal protein S9

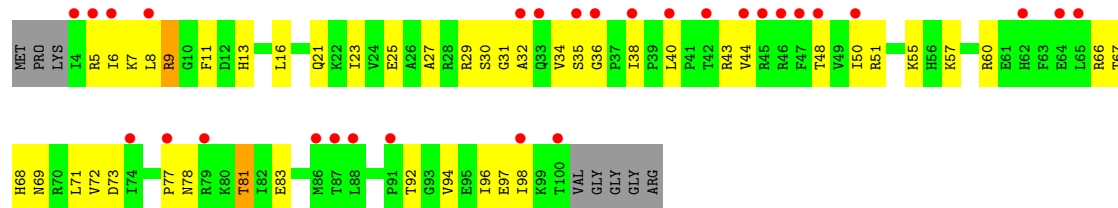




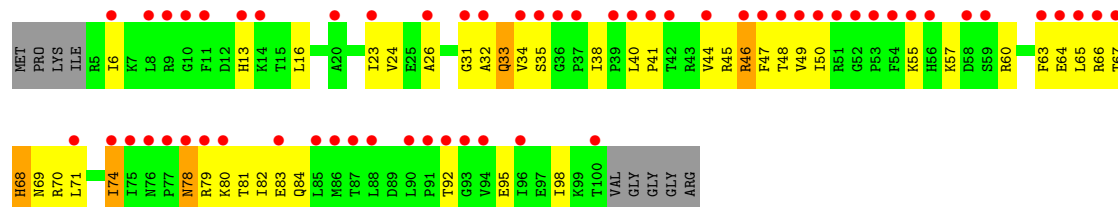
• Molecule 40: 30S ribosomal protein S9



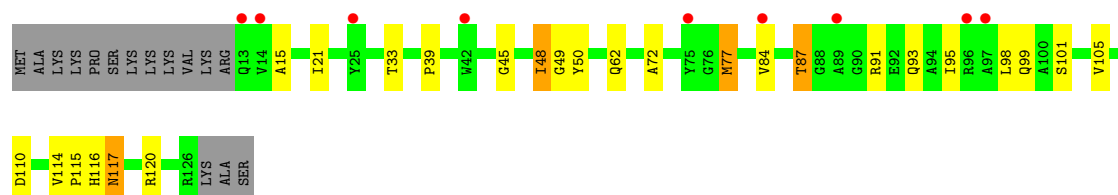
• Molecule 41: 30S ribosomal protein S10



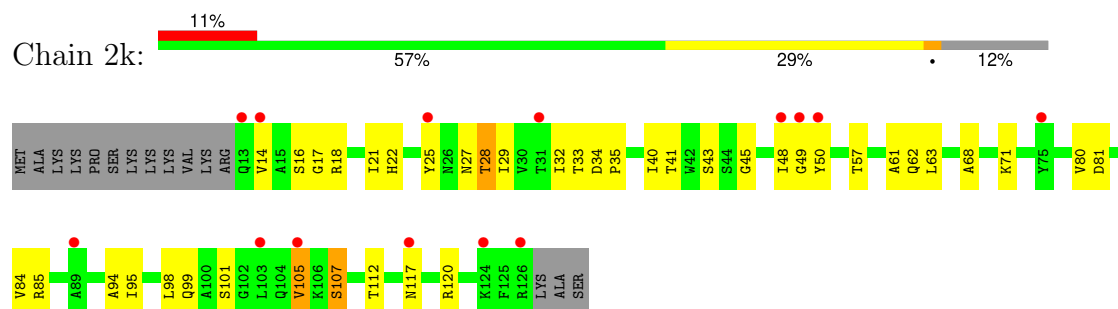
• Molecule 41: 30S ribosomal protein S10



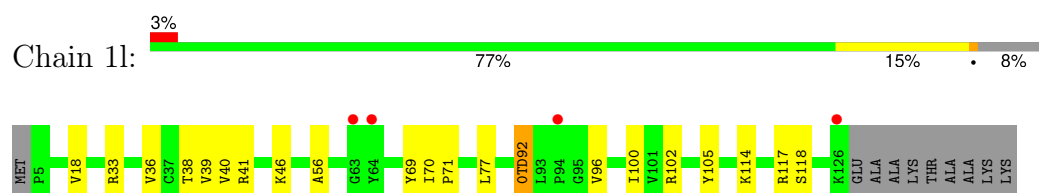
• Molecule 42: 30S ribosomal protein S11



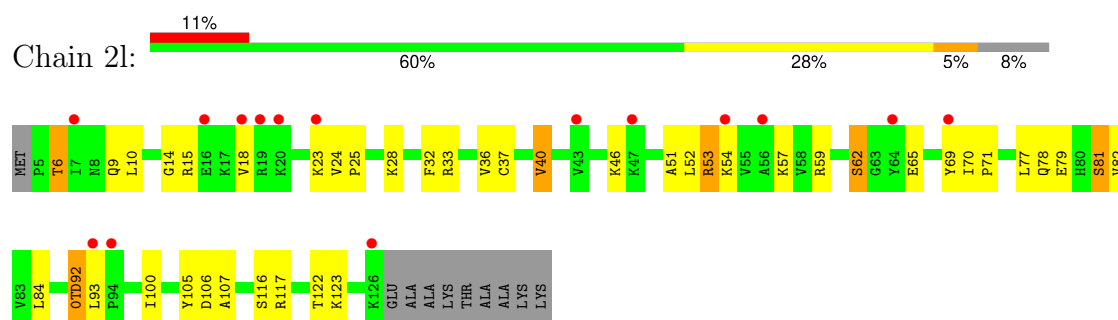
- Molecule 42: 30S ribosomal protein S11



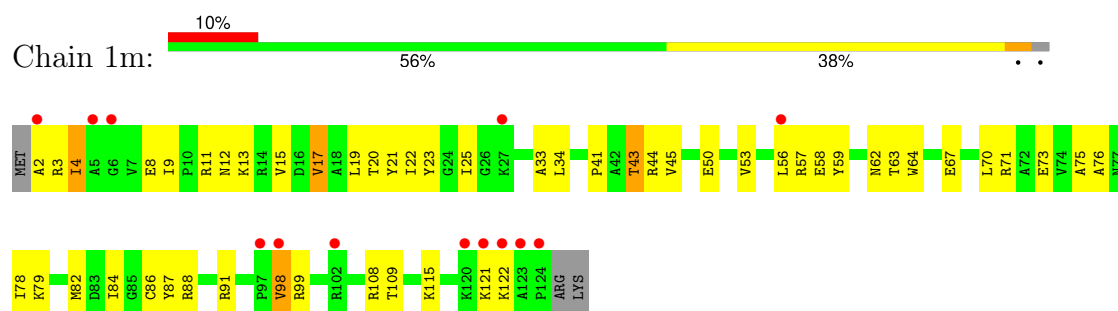
- Molecule 43: 30S ribosomal protein S12



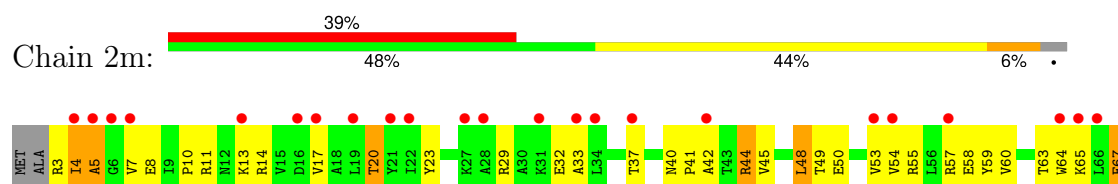
- Molecule 43: 30S ribosomal protein S12

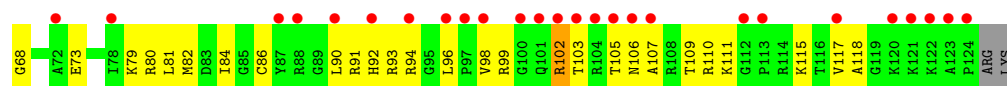


- Molecule 44: 30S ribosomal protein S13

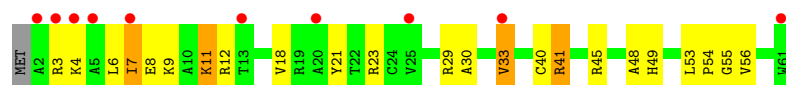


- Molecule 44: 30S ribosomal protein S13

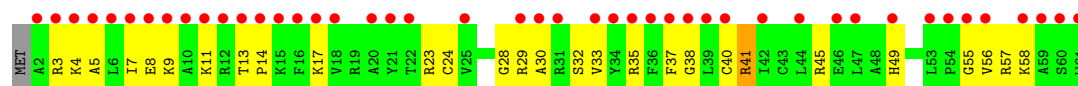
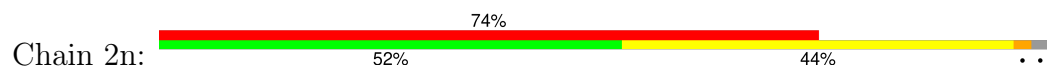




- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



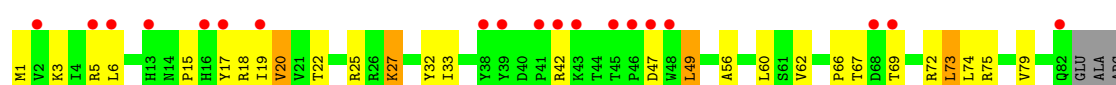
- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15



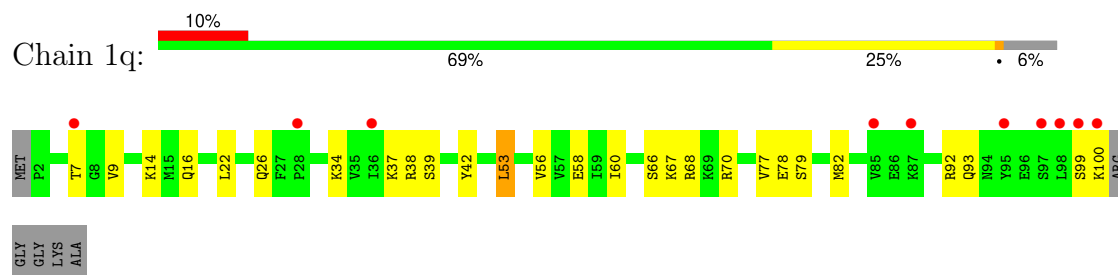
- Molecule 47: 30S ribosomal protein S16



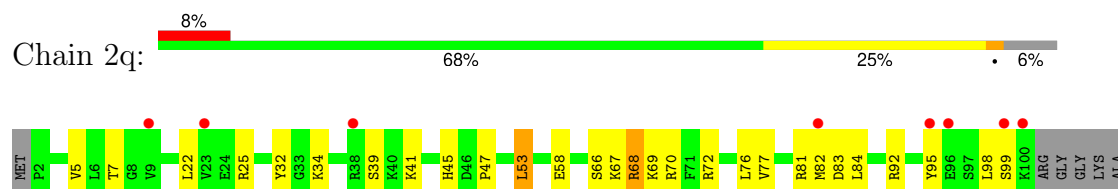
- Molecule 47: 30S ribosomal protein S16



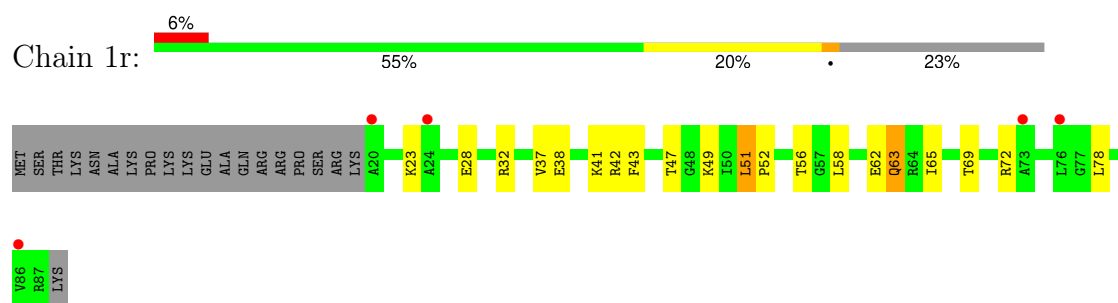
- Molecule 48: 30S ribosomal protein S17



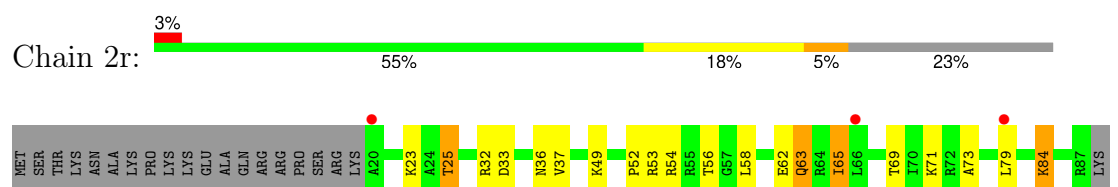
- Molecule 48: 30S ribosomal protein S17



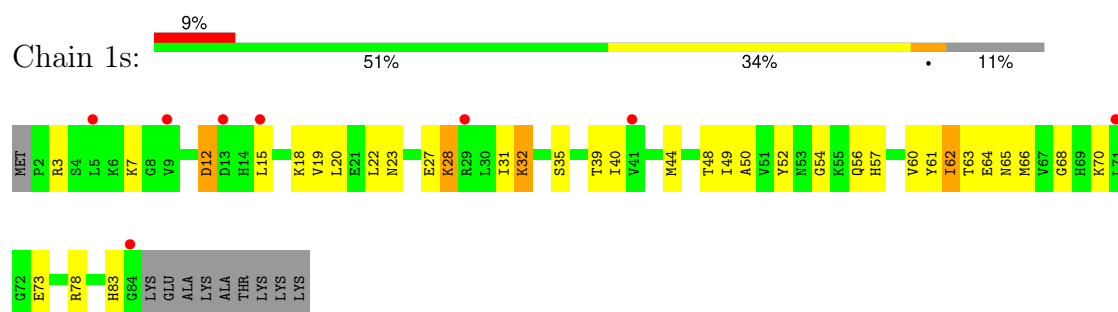
- Molecule 49: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S18

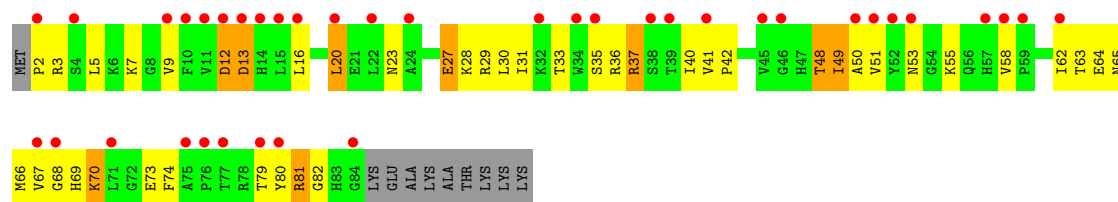


- Molecule 50: 30S ribosomal protein S19

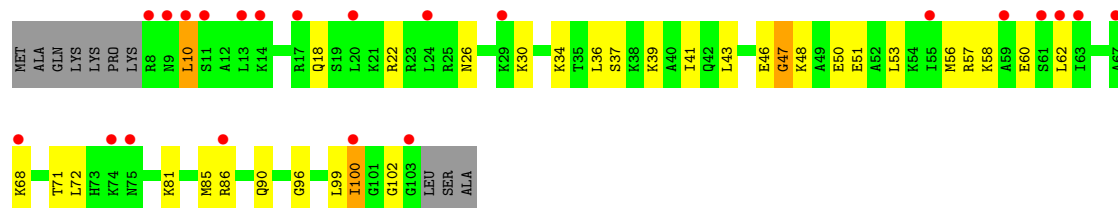


- Molecule 50: 30S ribosomal protein S19

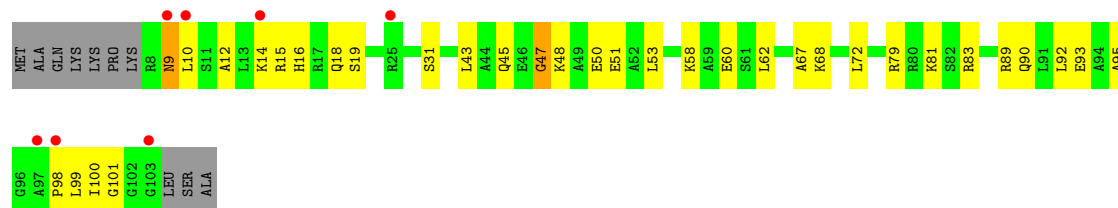




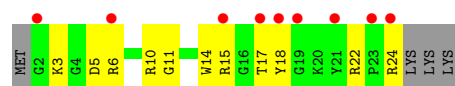
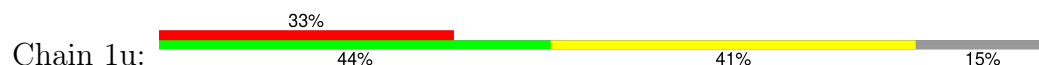
• Molecule 51: 30S ribosomal protein S20



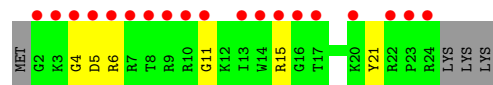
• Molecule 51: 30S ribosomal protein S20



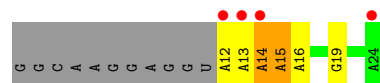
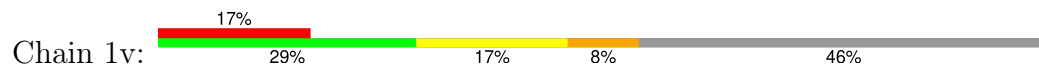
• Molecule 52: 30S ribosomal protein Thx



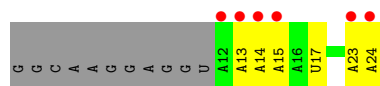
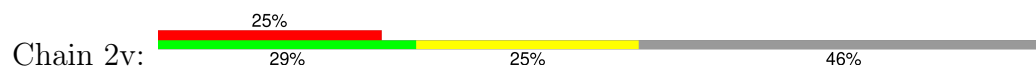
• Molecule 52: 30S ribosomal protein Thx



• Molecule 53: MG-mRNA



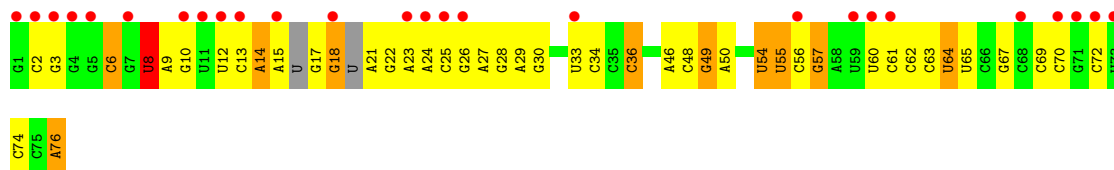
- Molecule 53: MG-mRNA



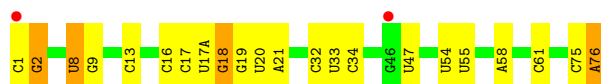
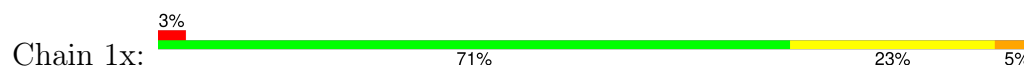
- Molecule 54: A-site Aminoacyl-tRNA Gly-NH-tRNAgly



- Molecule 54: A-site Aminoacyl-tRNA Gly-NH-tRNAgly



- Molecule 55: P-site Peptidyl-tRNA fMAC-NH-tRNAmet RNA-part



- Molecule 55: P-site Peptidyl-tRNA fMAC-NH-tRNAmet RNA-part



- Molecule 56: P-site Peptidyl-tRNA fMAC-NH-tRNAmet Peptide-part



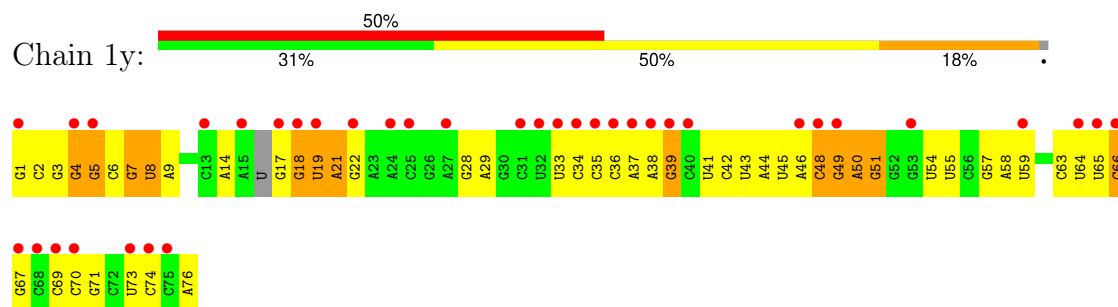
There are no outlier residues recorded for this chain.

- Molecule 56: P-site Peptidyl-tRNA fMAC-NH-tRNAmet Peptide-part



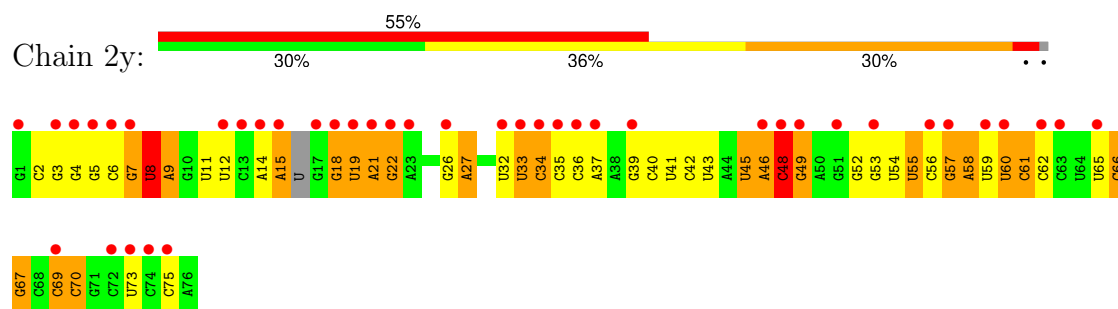
● Molecule 57: E-site Deacylated tRNAgly

Chain 1y:



● Molecule 57: E-site Deacylated tRNAgly

Chain 2y:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.93Å 451.24Å 622.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	125.00 – 2.55 125.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (125.00-2.55) 99.5 (125.00-2.55)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.213 , 0.256 0.216 , 0.258	Depositor DCC
R_{free} test set	94560 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	299751	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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: CLM, MG, 5MC, G7M, FME, 2MG, MA6, ZN, OMU, 4OC, 5MU, K, OMC, 0TD, PSU, 2MA, M2G, SF4, UR3, L3X, 8AN, 4SU, OMG

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	0.29	0/69011	0.47	1/107720 (0.0%)
1	2A	0.21	0/67295	0.40	3/105042 (0.0%)
2	1B	0.22	0/2882	0.40	0/4494
2	2B	0.18	0/2879	0.36	0/4487
3	1D	0.27	0/2186	0.51	0/2944
3	2D	0.21	0/2186	0.43	0/2944
4	1E	0.27	0/1592	0.49	0/2149
4	2E	0.20	0/1592	0.43	0/2149
5	1F	0.26	0/1618	0.49	0/2191
5	2F	0.19	0/1614	0.45	0/2186
6	1G	0.20	0/1448	0.44	0/1957
6	2G	0.20	0/1453	0.44	0/1963
7	1H	0.21	0/1356	0.40	0/1834
7	2H	0.20	0/1356	0.37	0/1834
8	1I	0.20	0/1112	0.46	0/1514
8	2I	0.17	0/1079	0.41	0/1475
9	1N	0.25	0/1144	0.45	0/1543
9	2N	0.19	0/1144	0.38	0/1543
10	1O	0.25	0/943	0.45	0/1269
10	2O	0.18	0/943	0.42	0/1269
11	1P	0.26	0/1152	0.53	0/1533
11	2P	0.21	0/1152	0.45	0/1533
12	1Q	0.27	0/1143	0.48	0/1527
12	2Q	0.19	0/1143	0.41	0/1527
13	1R	0.27	0/982	0.49	0/1312
13	2R	0.20	0/982	0.43	0/1312
14	1S	0.23	0/883	0.47	0/1176
14	2S	0.24	0/880	0.48	0/1172
15	1T	0.23	0/1105	0.46	0/1477
15	2T	0.20	0/1097	0.41	0/1468
16	1U	0.26	0/977	0.45	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.18	0/977	0.41	0/1301
17	1V	0.25	0/782	0.48	0/1049
17	2V	0.17	0/782	0.38	0/1049
18	1W	0.28	0/897	0.44	0/1205
18	2W	0.20	0/897	0.40	0/1205
19	1X	0.27	0/764	0.52	0/1025
19	2X	0.20	0/764	0.45	0/1025
20	1Y	0.23	0/819	0.47	0/1095
20	2Y	0.19	0/819	0.43	0/1095
21	1Z	0.22	0/1267	0.46	0/1717
21	2Z	0.24	0/1299	0.44	1/1763 (0.1%)
22	10	0.27	0/662	0.54	2/881 (0.2%)
22	20	0.21	0/662	0.45	0/881
23	11	0.26	0/762	0.45	0/1014
23	21	0.22	0/762	0.39	0/1014
24	12	0.24	0/590	0.42	0/781
24	22	0.18	0/590	0.39	0/781
25	13	0.26	0/474	0.47	0/635
25	23	0.18	0/469	0.39	0/630
26	14	0.24	0/565	0.61	0/761
26	24	0.24	0/545	0.55	0/737
27	15	0.26	0/469	0.49	0/635
27	25	0.22	0/469	0.42	0/635
28	16	0.26	0/460	0.48	0/613
28	26	0.18	0/456	0.40	0/608
29	17	0.30	0/426	0.51	0/561
29	27	0.24	0/426	0.51	0/561
30	18	0.26	0/525	0.47	0/691
30	28	0.21	0/525	0.39	0/691
31	19	0.28	0/310	0.50	0/407
31	29	0.19	0/310	0.42	0/407
32	1a	0.20	1/35795 (0.0%)	0.39	1/55864 (0.0%)
32	2a	0.19	0/35886	0.37	0/56005
33	1b	0.21	0/1881	0.48	0/2542
33	2b	0.22	0/1860	0.49	1/2518 (0.0%)
34	1c	0.18	0/1572	0.39	0/2126
34	2c	0.22	0/1566	0.43	0/2119
35	1d	0.19	0/1685	0.43	0/2262
35	2d	0.19	0/1704	0.42	0/2284
36	1e	0.21	0/1145	0.48	0/1543
36	2e	0.21	0/1149	0.46	0/1548
37	1f	0.18	0/823	0.39	0/1115
37	2f	0.18	0/829	0.38	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.18	0/1250	0.39	0/1679
38	2g	0.18	0/1254	0.40	0/1683
39	1h	0.19	0/1108	0.42	0/1494
39	2h	0.18	0/1108	0.41	0/1494
40	1i	0.19	0/1002	0.49	0/1346
40	2i	0.21	0/997	0.48	0/1343
41	1j	0.20	0/722	0.42	0/982
41	2j	0.22	0/727	0.51	1/988 (0.1%)
42	1k	0.18	0/844	0.42	0/1145
42	2k	0.18	0/848	0.40	0/1149
43	1l	0.19	0/937	0.42	0/1260
43	2l	0.18	0/937	0.42	0/1260
44	1m	0.19	0/969	0.46	0/1302
44	2m	0.19	0/961	0.44	0/1291
45	1n	0.19	0/501	0.42	0/664
45	2n	0.20	0/501	0.47	0/664
46	1o	0.20	0/739	0.39	0/985
46	2o	0.17	0/739	0.37	0/985
47	1p	0.21	0/697	0.46	0/939
47	2p	0.19	0/693	0.44	0/935
48	1q	0.17	0/836	0.40	0/1117
48	2q	0.18	0/836	0.41	0/1117
49	1r	0.19	0/560	0.42	0/746
49	2r	0.17	0/560	0.39	0/746
50	1s	0.18	0/667	0.48	0/900
50	2s	0.28	0/661	0.60	0/893
51	1t	0.23	0/730	0.56	1/965 (0.1%)
51	2t	0.18	0/729	0.43	0/965
52	1u	0.19	0/203	0.42	0/266
52	2u	0.23	0/203	0.43	0/266
53	1v	0.23	0/322	0.34	0/501
53	2v	0.19	0/322	0.26	0/501
54	1w	0.26	0/1639	0.39	0/2548
54	2w	0.27	1/1616 (0.1%)	0.37	0/2510
55	1x	0.26	0/1723	0.40	0/2684
55	2x	0.24	1/1723 (0.1%)	0.38	0/2684
56	1z	0.28	0/10	0.56	0/12
56	2z	0.15	0/10	0.27	0/12
57	1y	0.29	1/1664 (0.1%)	0.39	0/2587
57	2y	0.29	1/1664 (0.1%)	0.43	1/2587 (0.0%)
All	All	0.23	5/316960 (0.0%)	0.43	12/474542 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	2F	0	1
11	1P	0	1
11	2P	0	1
21	1Z	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2y	8	4SU	O3'-P	5.39	1.61	1.56
57	1y	8	4SU	O3'-P	5.29	1.61	1.56
32	1a	1498	UR3	O3'-P	5.25	1.61	1.56
54	2w	8	4SU	O3'-P	5.17	1.61	1.56
55	2x	8	4SU	O3'-P	5.07	1.61	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	1t	96	GLY	N-CA-C	7.32	116.87	110.21
1	1A	1992	G	C2'-C3'-O3'	7.16	120.24	109.50
1	2A	1992	G	C2'-C3'-O3'	6.29	118.93	109.50
33	2b	222	ILE	N-CA-C	-5.62	106.20	111.48
57	2y	48	C	P-O3'-C3'	5.55	128.52	120.20
21	2Z	135	GLU	N-CA-C	-5.35	108.52	114.62
1	2A	271(M)	G	P-O3'-C3'	5.33	126.09	119.70
1	2A	271(M)	G	OP1-P-O3'	5.17	116.58	105.20
41	2j	82	ILE	N-CA-C	-5.17	106.19	112.76
32	1a	266	G	C2'-C3'-O3'	5.17	117.25	109.50
22	10	12	ASN	CA-C-N	-5.05	108.82	122.46
22	10	12	ASN	C-N-CA	-5.05	108.82	122.46

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
21	1Z	136	PHE	Peptide
5	2F	20	LEU	Peptide
11	2P	35	HIS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31195	561	0
1	2A	60322	0	30429	675	0
2	1B	2577	0	1305	20	0
2	2B	2575	0	1303	35	0
3	1D	2136	0	2218	37	0
3	2D	2136	0	2218	36	0
4	1E	1559	0	1618	18	0
4	2E	1559	0	1618	30	0
5	1F	1583	0	1625	24	0
5	2F	1579	0	1619	46	0
6	1G	1423	0	1436	29	0
6	2G	1428	0	1438	58	0
7	1H	1330	0	1407	22	0
7	2H	1330	0	1407	34	0
8	1I	1097	0	1140	30	0
8	2I	1064	0	1082	26	0
9	1N	1117	0	1184	12	0
9	2N	1117	0	1184	22	0
10	1O	933	0	996	14	0
10	2O	933	0	996	21	0
11	1P	1135	0	1212	26	0
11	2P	1135	0	1212	20	0
12	1Q	1122	0	1179	17	0
12	2Q	1122	0	1179	33	0
13	1R	968	0	1033	14	0
13	2R	968	0	1033	13	0
14	1S	873	0	927	11	0
14	2S	870	0	923	32	0
15	1T	1091	0	1151	18	0
15	2T	1083	0	1136	17	0
16	1U	959	0	1019	9	0
16	2U	959	0	1019	14	0
17	1V	771	0	830	9	0
17	2V	771	0	830	18	0
18	1W	886	0	940	7	0
18	2W	886	0	940	14	0
19	1X	750	0	814	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2X	750	0	814	15	0
20	1Y	806	0	881	14	0
20	2Y	806	0	881	12	0
21	1Z	1240	0	1240	29	0
21	2Z	1271	0	1273	48	0
22	10	653	0	674	8	0
22	20	653	0	674	20	0
23	11	755	0	826	13	0
23	21	755	0	826	19	0
24	12	588	0	643	5	0
24	22	588	0	643	12	0
25	13	469	0	518	5	0
25	23	464	0	514	19	0
26	14	552	0	533	22	0
26	24	532	0	503	32	0
27	15	455	0	465	2	0
27	25	455	0	465	5	0
28	16	453	0	473	12	0
28	26	449	0	469	9	0
29	17	418	0	467	9	0
29	27	418	0	467	10	0
30	18	517	0	582	6	0
30	28	517	0	582	11	0
31	19	307	0	335	2	0
31	29	307	0	335	7	0
32	1a	32246	0	16295	408	0
32	2a	32327	0	16338	558	0
33	1b	1846	0	1867	66	0
33	2b	1825	0	1828	93	0
34	1c	1548	0	1535	36	0
34	2c	1542	0	1517	62	0
35	1d	1655	0	1672	56	0
35	2d	1674	0	1714	40	0
36	1e	1129	0	1185	43	0
36	2e	1133	0	1191	51	0
37	1f	810	0	804	17	0
37	2f	816	0	808	12	0
38	1g	1231	0	1238	22	0
38	2g	1235	0	1249	33	0
39	1h	1088	0	1126	34	0
39	2h	1088	0	1126	33	0
40	1i	983	0	986	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	2i	978	0	966	50	0
41	1j	709	0	650	35	0
41	2j	714	0	672	32	0
42	1k	829	0	825	19	0
42	2k	833	0	836	22	0
43	1l	932	0	980	13	0
43	2l	932	0	979	21	0
44	1m	958	0	1002	32	0
44	2m	950	0	988	51	0
45	1n	492	0	529	17	0
45	2n	492	0	529	28	0
46	1o	728	0	760	14	0
46	2o	728	0	760	19	0
47	1p	681	0	697	23	0
47	2p	677	0	686	20	0
48	1q	823	0	891	15	0
48	2q	823	0	891	21	0
49	1r	555	0	618	13	0
49	2r	555	0	618	13	0
50	1s	652	0	662	28	0
50	2s	646	0	644	39	0
51	1t	728	0	798	23	0
51	2t	727	0	796	24	0
52	1u	199	0	208	7	0
52	2u	199	0	208	4	0
53	1v	286	0	142	6	0
53	2v	286	0	142	5	0
54	1w	1556	0	778	26	0
54	2w	1536	0	770	27	0
55	1x	1646	0	839	12	0
55	2x	1646	0	838	19	0
56	1z	21	0	20	0	0
56	2z	21	0	20	2	0
57	1y	1552	0	791	25	0
57	2y	1552	0	790	44	0
58	10	8	0	0	0	0
58	11	4	0	0	0	0
58	12	2	0	0	0	0
58	13	4	0	0	0	0
58	15	8	0	0	0	0
58	16	3	0	0	0	0
58	17	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	18	6	0	0	0	0
58	19	1	0	0	0	0
58	1A	1085	0	0	0	0
58	1B	37	0	0	0	0
58	1D	11	0	0	0	0
58	1E	15	0	0	0	0
58	1F	11	0	0	0	0
58	1G	4	0	0	0	0
58	1H	1	0	0	0	0
58	1I	1	0	0	0	0
58	1N	5	0	0	0	0
58	1O	6	0	0	0	0
58	1P	5	0	0	0	0
58	1Q	8	0	0	0	0
58	1R	7	0	0	0	0
58	1S	3	0	0	0	0
58	1T	2	0	0	0	0
58	1U	10	0	0	0	0
58	1V	6	0	0	0	0
58	1W	7	0	0	0	0
58	1X	6	0	0	0	0
58	1Y	3	0	0	0	0
58	1Z	3	0	0	0	0
58	1a	214	0	0	0	0
58	1b	2	0	0	0	0
58	1d	1	0	0	0	0
58	1e	3	0	0	0	0
58	1f	2	0	0	0	0
58	1k	1	0	0	0	0
58	1l	2	0	0	0	0
58	1m	1	0	0	0	0
58	1n	2	0	0	0	0
58	1p	1	0	0	0	0
58	1s	1	0	0	0	0
58	1t	1	0	0	0	0
58	1w	9	0	0	0	0
58	1x	12	0	0	0	0
58	1y	1	0	0	0	0
58	20	3	0	0	0	0
58	21	1	0	0	0	0
58	23	2	0	0	0	0
58	25	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	26	1	0	0	0	0
58	27	2	0	0	0	0
58	28	3	0	0	0	0
58	2A	800	0	0	0	0
58	2B	18	0	0	0	0
58	2D	5	0	0	0	0
58	2E	8	0	0	0	0
58	2F	8	0	0	0	0
58	2G	1	0	0	0	0
58	2N	1	0	0	0	0
58	2O	1	0	0	0	0
58	2Q	3	0	0	0	0
58	2R	2	0	0	0	0
58	2T	4	0	0	0	0
58	2U	1	0	0	0	0
58	2V	1	0	0	0	0
58	2W	2	0	0	0	0
58	2X	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2Z	1	0	0	0	0
58	2a	223	0	0	0	0
58	2d	2	0	0	0	0
58	2e	1	0	0	0	0
58	2f	2	0	0	0	0
58	2g	1	0	0	0	0
58	2j	1	0	0	0	0
58	2l	2	0	0	0	0
58	2q	2	0	0	0	0
58	2r	1	0	0	0	0
58	2t	1	0	0	0	0
58	2v	1	0	0	0	0
58	2w	2	0	0	0	0
58	2x	8	0	0	0	0
59	1A	1	0	0	0	0
59	2A	1	0	0	0	0
60	1A	20	0	11	1	0
60	2w	20	0	11	1	0
61	14	1	0	0	0	0
61	15	1	0	0	0	0
61	16	1	0	0	0	0
61	19	1	0	0	0	0
61	1Y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1n	1	0	0	0	0
61	24	1	0	0	0	0
61	25	1	0	0	0	0
61	26	1	0	0	0	0
61	29	1	0	0	0	0
61	2Y	1	0	0	0	0
61	2n	1	0	0	0	0
62	1d	8	0	0	1	0
62	2d	8	0	0	0	0
63	10	11	0	0	1	0
63	11	8	0	0	0	0
63	12	3	0	0	0	0
63	13	5	0	0	0	0
63	14	1	0	0	0	0
63	15	6	0	0	0	0
63	16	2	0	0	0	0
63	17	8	0	0	1	0
63	18	12	0	0	0	0
63	1A	1977	0	0	75	0
63	1B	66	0	0	5	0
63	1D	30	0	0	0	0
63	1E	23	0	0	0	0
63	1F	17	0	0	0	0
63	1G	6	0	0	2	0
63	1H	1	0	0	0	0
63	1N	4	0	0	0	0
63	1O	7	0	0	0	0
63	1P	20	0	0	1	0
63	1Q	7	0	0	0	0
63	1R	9	0	0	3	0
63	1S	5	0	0	0	0
63	1T	8	0	0	1	0
63	1U	11	0	0	0	0
63	1V	9	0	0	0	0
63	1W	7	0	0	1	0
63	1X	7	0	0	1	0
63	1Y	2	0	0	1	0
63	1a	263	0	0	22	0
63	1b	1	0	0	0	0
63	1d	1	0	0	0	0
63	1e	1	0	0	0	0
63	1f	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	1g	1	0	0	0	0
63	1l	6	0	0	0	0
63	1m	2	0	0	0	0
63	1n	1	0	0	0	0
63	1o	1	0	0	0	0
63	1q	3	0	0	0	0
63	1u	1	0	0	1	0
63	1v	3	0	0	0	0
63	1w	5	0	0	0	0
63	1x	11	0	0	1	0
63	1y	1	0	0	0	0
63	20	3	0	0	1	0
63	21	5	0	0	0	0
63	23	1	0	0	0	0
63	27	2	0	0	0	0
63	28	6	0	0	0	0
63	29	1	0	0	0	0
63	2A	1074	0	0	72	0
63	2B	18	0	0	0	0
63	2D	22	0	0	0	0
63	2E	13	0	0	3	0
63	2F	12	0	0	0	0
63	2I	2	0	0	0	0
63	2N	1	0	0	0	0
63	2O	3	0	0	0	0
63	2P	11	0	0	1	0
63	2Q	2	0	0	0	0
63	2R	3	0	0	0	0
63	2T	2	0	0	0	0
63	2U	3	0	0	0	0
63	2W	2	0	0	0	0
63	2X	5	0	0	0	0
63	2Y	1	0	0	0	0
63	2Z	1	0	0	0	0
63	2a	245	0	0	30	0
63	2d	2	0	0	0	0
63	2j	1	0	0	1	0
63	2l	3	0	0	0	0
63	2o	1	0	0	0	0
63	2p	2	0	0	0	0
63	2q	1	0	0	0	0
63	2r	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	2t	2	0	0	0	0
63	2v	1	0	0	0	0
63	2w	2	0	0	0	0
63	2x	6	0	0	0	0
63	2z	1	0	0	0	0
All	All	299751	0	196702	4115	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (4115) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.28	1.31
1:1A:1054:A:N6	1:1A:1105:U:H3	1.49	1.10
1:1A:1059:G:H1	1:1A:1079:C:N4	1.57	1.03
1:1A:1082:U:O4	1:1A:1086:A:N1	1.91	1.02
1:1A:1062:G:H1	1:1A:1077:A:H61	1.09	0.98
29:17:24:THR:HG22	29:17:27:GLY:H	1.29	0.96
1:2A:1604:C:OP2	63:2A:3902:HOH:O	1.86	0.93
54:2w:6:C:H42	54:2w:67:G:H1	1.18	0.92
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.49	0.91
22:10:10:THR:HG22	22:10:12:ASN:H	1.35	0.91
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.53	0.91
1:1A:2427:C:OP1	63:1A:4102:HOH:O	1.89	0.90
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.18	0.89
54:1w:49:G:H1	54:1w:65:U:H3	1.18	0.89
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.53	0.89
32:2a:1286:A:H8	32:2a:1287:A:H4'	1.37	0.88
1:1A:1059:G:H1	1:1A:1079:C:H42	0.90	0.87
1:1A:1054:A:H61	1:1A:1105:U:H3	0.92	0.87
1:2A:2138:C:H42	1:2A:2153:G:H1	1.23	0.87
54:2w:49:G:H1	54:2w:65:U:H3	0.88	0.87
1:1A:2099:U:H3	1:1A:2190:G:H1	1.19	0.87
32:1a:116:A:OP1	63:1a:1901:HOH:O	1.92	0.86
32:2a:1086:U:H3	32:2a:1099:G:H22	1.24	0.86
1:2A:1204:A:H2	1:2A:1241:A:H62	1.25	0.84
1:1A:1055:G:H1	1:1A:1104:C:H42	1.25	0.84
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.13	0.84
32:2a:1029:C:C4	32:2a:1032:G:N1	2.47	0.83
1:2A:880:G:N2	1:2A:898:C:O2	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1395:A:OP1	63:1A:4104:HOH:O	1.97	0.83
32:2a:975:A:H4'	32:2a:976:G:H5''	1.58	0.83
1:2A:1689:A:H62	1:2A:1698:A:H2	1.27	0.83
1:1A:1332:G:OP1	63:1A:4103:HOH:O	1.96	0.82
34:2c:47:LEU:HB3	34:2c:52:LEU:HB2	1.61	0.82
32:1a:70:G:H1	32:1a:99:U:H3	1.28	0.82
1:1A:2136:C:N3	1:1A:2155:G:C2	2.48	0.81
26:14:16:CYS:SG	26:14:17:GLY:N	2.51	0.81
41:1j:30:SER:HB3	41:1j:81:THR:HG23	1.63	0.81
29:27:24:THR:HG22	29:27:27:GLY:H	1.42	0.81
32:2a:951:G:N7	44:2m:102:ARG:NH2	2.29	0.81
1:2A:2100:G:H1	1:2A:2189:U:H3	0.83	0.81
1:1A:878:A:N6	1:1A:899:A:O2'	2.11	0.81
1:1A:1058:G:H1	1:1A:1080:C:N4	1.79	0.81
32:1a:574:A:OP2	63:1a:1902:HOH:O	1.98	0.81
57:2y:18:G:C2	57:2y:56:C:C2	2.69	0.81
1:2A:805:G:OP1	63:2A:3903:HOH:O	1.99	0.80
1:1A:2550:G:OP1	63:1A:4105:HOH:O	1.99	0.80
48:2q:7:THR:HG22	48:2q:58:GLU:HG2	1.64	0.80
1:2A:1995:U:OP1	63:2A:3904:HOH:O	2.00	0.79
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.16	0.79
1:1A:826:U:OP1	63:1A:4102:HOH:O	1.99	0.79
1:2A:1371:G:N7	63:2A:3936:HOH:O	2.15	0.79
54:1w:15:A:H2	54:1w:21:A:H1'	1.48	0.79
1:1A:2821:A:OP2	63:1A:4106:HOH:O	2.00	0.79
1:2A:2709:G:O6	63:2A:3905:HOH:O	2.01	0.78
32:1a:405:U:O4	35:1d:2:GLY:N	2.17	0.78
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.65	0.78
32:1a:165:C:H2'	32:1a:166:G:H8	1.47	0.78
50:2s:49:ILE:HG22	50:2s:62:ILE:HD11	1.66	0.78
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.17	0.77
32:1a:975:A:H4'	32:1a:976:G:H5''	1.67	0.77
1:1A:1059:G:N2	1:1A:1079:C:N3	2.31	0.77
49:1r:38:GLU:HA	49:1r:41:LYS:HD3	1.66	0.77
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.67	0.77
32:2a:266:G:H5''	32:2a:268:C:H41	1.48	0.77
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.18	0.77
1:2A:570:G:O6	63:2A:3906:HOH:O	2.02	0.77
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.67	0.76
26:24:40:HIS:HB3	26:24:43:TYR:HB2	1.66	0.76
54:2w:6:C:N4	54:2w:67:G:H1	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.19	0.76
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.66	0.76
38:2g:70:LYS:HG2	38:2g:96:GLN:HB3	1.67	0.76
1:1A:1069:A:H5'	1:1A:1070:A:H8	1.49	0.76
1:1A:1670:C:OP2	63:1A:4105:HOH:O	2.03	0.76
1:2A:2430:A:OP2	63:2A:3907:HOH:O	2.02	0.76
1:2A:2316:C:O2'	6:2G:128:ARG:NH2	2.19	0.76
1:2A:2448:A:OP1	63:2A:3906:HOH:O	2.02	0.76
1:1A:2128:C:N3	1:1A:2160:G:N2	2.33	0.76
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.21	0.76
1:2A:2319:G:H22	14:2S:3:ARG:HH11	1.33	0.76
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.67	0.76
1:2A:2063:C:OP1	63:2A:3908:HOH:O	2.04	0.75
32:2a:344:A:H5''	32:2a:345:C:H5	1.51	0.75
1:1A:1058:G:H1	1:1A:1080:C:H42	1.30	0.75
32:1a:558:G:OP1	63:1a:1903:HOH:O	2.04	0.75
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.20	0.75
1:1A:582:G:N7	63:1A:4133:HOH:O	2.18	0.75
33:1b:21:ARG:O	33:1b:23:ARG:N	2.20	0.75
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.66	0.75
48:1q:53:LEU:HD23	48:1q:82:MET:HE1	1.67	0.75
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.22	0.75
44:2m:37:THR:O	44:2m:55:ARG:NH1	2.20	0.75
1:1A:2128:C:N4	1:1A:2160:G:N1	2.34	0.75
1:2A:2218:U:O2	23:21:52:ARG:NH1	2.20	0.75
36:2e:20:GLN:OE1	36:2e:25:ARG:NH1	2.20	0.74
44:2m:80:ARG:HH22	50:2s:69:HIS:HE1	1.32	0.74
8:1I:77:LEU:HB3	8:1I:142:VAL:HG12	1.69	0.74
1:2A:854:G:O6	63:2A:3909:HOH:O	2.04	0.74
1:2A:1648:C:OP1	63:2A:3913:HOH:O	2.06	0.74
32:2a:1056:U:H5'	34:2c:163:ALA:HB2	1.69	0.74
1:1A:1060:U:H3	1:1A:1088:A:H8	1.34	0.74
1:1A:2807:G:N1	1:1A:2893:G:O6	2.19	0.74
32:2a:731:G:OP1	63:2a:1902:HOH:O	2.05	0.74
38:2g:113:GLU:HB2	38:2g:119:ARG:HG2	1.70	0.74
39:1h:34:GLU:OE1	39:1h:37:ARG:NH1	2.19	0.74
1:2A:1812:A:OP2	63:2A:3910:HOH:O	2.05	0.74
1:1A:2185:C:H2'	1:1A:2186:G:H8	1.53	0.74
1:1A:1058:G:N2	1:1A:1080:C:N3	2.34	0.74
35:1d:112:VAL:HG23	35:1d:116:GLN:HE22	1.51	0.74
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.70	0.74
1:2A:962:G:OP1	63:2A:3911:HOH:O	2.05	0.74
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.52	0.74
38:2g:115:ARG:HG2	38:2g:118:VAL:HG22	1.70	0.73
1:1A:1669:A:OP2	63:1A:4105:HOH:O	2.05	0.73
32:1a:1505:G:OP2	63:1a:1904:HOH:O	2.06	0.73
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.20	0.73
1:1A:1023:U:OP2	63:1A:4108:HOH:O	2.06	0.73
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.70	0.73
1:1A:1603:A:OP1	63:1A:4104:HOH:O	2.04	0.73
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.52	0.73
32:2a:1040:U:H2'	32:2a:1041:A:H8	1.54	0.73
1:1A:998:C:OP1	63:1A:4107:HOH:O	2.06	0.73
32:1a:664:G:H22	32:1a:741:G:H1	1.36	0.73
1:1A:2822:G:OP2	63:1A:4106:HOH:O	2.06	0.73
1:2A:792:G:O6	63:2A:3912:HOH:O	2.06	0.73
33:1b:15:VAL:HG13	33:1b:209:ARG:HG3	1.71	0.73
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.71	0.73
42:2k:81:ASP:OD1	42:2k:107:SER:OG	2.06	0.73
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.70	0.72
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.06	0.72
42:2k:48:ILE:O	42:2k:50:TYR:N	2.21	0.72
57:2y:18:G:N2	57:2y:56:C:C2	2.57	0.72
1:1A:592:G:O6	63:1A:4109:HOH:O	2.07	0.72
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.22	0.72
57:2y:18:G:C2	57:2y:56:C:N3	2.56	0.72
1:2A:323:G:HO2'	1:2A:1205:U:H3	1.35	0.72
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.23	0.72
32:2a:673:G:H2'	32:2a:674:G:C8	2.23	0.72
32:2a:814:A:H2'	32:2a:816:A:H5'	1.71	0.72
32:1a:1027:C:C2	32:1a:1034:G:N2	2.57	0.72
33:1b:87:ARG:NH1	33:1b:233:SER:OG	2.22	0.72
1:2A:921:G:O6	63:2A:3917:HOH:O	2.07	0.72
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.22	0.72
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.70	0.72
32:1a:375:U:OP1	47:1p:69:THR:OG1	2.07	0.72
40:1i:42:ARG:NH2	40:1i:75:ASP:OD1	2.22	0.72
1:2A:1024:G:HO2'	1:2A:1144:G:HO2'	1.36	0.72
1:2A:1670:C:OP1	63:2A:3915:HOH:O	2.06	0.72
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.70	0.72
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1O:48:PRO:HB3	32:1a:1422:G:H5''	1.71	0.72
1:2A:297:C:OP2	63:2A:3916:HOH:O	2.07	0.72
1:1A:1452:A:OP2	63:1A:4110:HOH:O	2.07	0.72
2:1B:58:A:OP2	63:1B:301:HOH:O	2.07	0.72
32:1a:1469:G:N7	63:1a:1916:HOH:O	2.22	0.72
1:2A:775:G:O3'	63:2A:3918:HOH:O	2.08	0.72
32:2a:596:C:OP2	63:2a:1903:HOH:O	2.07	0.72
35:2d:18:LYS:NZ	35:2d:31:CYS:SG	2.63	0.72
1:2A:948:G:OP1	63:2A:3911:HOH:O	2.08	0.71
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.22	0.71
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.24	0.71
1:1A:744:G:OP1	63:1A:4111:HOH:O	2.08	0.71
41:1j:5:ARG:HG3	41:1j:71:LEU:HD11	1.72	0.71
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.22	0.71
40:2i:16:ARG:HB2	40:2i:64:THR:HG22	1.72	0.71
33:1b:100:GLY:O	33:1b:104:ASN:N	2.18	0.71
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.73	0.71
1:1A:582:G:OP2	63:1A:4114:HOH:O	2.09	0.71
1:1A:2629:A:O2'	1:1A:2630:G:OP2	2.08	0.71
1:1A:1469:A:OP2	63:1A:4112:HOH:O	2.08	0.71
32:1a:117:G:OP2	63:1a:1901:HOH:O	2.09	0.71
1:2A:1676:A:OP2	63:2A:3920:HOH:O	2.09	0.71
32:2a:953:G:H5'	32:2a:965:A:H61	1.54	0.71
1:1A:11:G:H2'	1:1A:12:U:H5'	1.72	0.71
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	1.73	0.71
39:2h:64:LYS:HG2	39:2h:79:VAL:HG21	1.71	0.71
1:1A:2100:G:H1	1:1A:2189:U:H3	1.36	0.70
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.23	0.70
1:1A:2142:C:N3	1:1A:2149:G:O6	2.24	0.70
21:2Z:141:VAL:HG13	21:2Z:144:LEU:HB3	1.71	0.70
15:1T:77:PRO:HG2	15:1T:80:SER:HB2	1.73	0.70
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.08	0.70
9:2N:15:LEU:HB2	9:2N:135:PRO:HB2	1.73	0.70
1:1A:762:U:OP1	63:1A:4115:HOH:O	2.09	0.70
63:1A:4106:HOH:O	13:1R:3:HIS:NE2	2.23	0.70
28:16:53:LYS:NZ	57:1y:1:G:OP1	2.22	0.70
52:1u:5:ASP:OD2	63:1u:101:HOH:O	2.09	0.70
1:1A:84:A:H5''	20:1Y:8:LYS:HE3	1.72	0.70
32:1a:324:G:N7	63:1a:1919:HOH:O	2.24	0.70
34:1c:62:ASP:HA	34:1c:97:LYS:HD3	1.74	0.70
32:2a:148:G:H2'	32:2a:149:A:H8	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:88:ALA:HA	33:2b:223:ILE:HD11	1.72	0.70
1:1A:654:A:OP2	63:1A:4113:HOH:O	2.09	0.70
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.54	0.70
1:1A:1865:G:N2	1:1A:1877:A:OP2	2.23	0.70
43:1l:39:VAL:HG11	43:1l:41:ARG:HH11	1.57	0.70
55:1x:75:C:OP1	63:1x:201:HOH:O	2.09	0.70
42:2k:99:GLN:HG2	42:2k:105:VAL:HG21	1.74	0.70
1:2A:1890:A:OP2	63:2A:3921:HOH:O	2.09	0.70
32:2a:860:A:OP2	63:2a:1904:HOH:O	2.09	0.70
1:1A:2222:G:OP2	63:1A:4117:HOH:O	2.10	0.70
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.40	0.70
32:1a:1381:U:H1'	38:1g:79:ARG:HG2	1.74	0.70
50:2s:51:VAL:O	50:2s:58:VAL:N	2.23	0.70
1:2A:2522:U:OP2	63:2A:3923:HOH:O	2.10	0.69
1:1A:1082:U:N3	1:1A:1086:A:N6	2.06	0.69
1:1A:2141:G:O6	1:1A:2150:U:O2	2.11	0.69
1:2A:2143:C:H42	1:2A:2148:G:H1	1.40	0.69
6:2G:114:ILE:HA	6:2G:140:ILE:HD11	1.73	0.69
47:2p:15:PRO:HD2	47:2p:42:ARG:HD2	1.74	0.69
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.24	0.69
1:2A:2595:G:N7	63:2A:3969:HOH:O	2.25	0.69
1:1A:2101:G:H1	1:1A:2188:C:H42	1.40	0.69
44:1m:3:ARG:HG2	44:1m:8:GLU:HA	1.74	0.69
1:1A:1013:C:OP2	63:1A:4121:HOH:O	2.11	0.69
6:2G:18:GLU:HG2	6:2G:175:LEU:HD21	1.73	0.69
1:2A:955:C:OP1	12:2Q:87:LYS:NZ	2.26	0.69
1:2A:2134:A:H62	1:2A:2157:G:H4'	1.58	0.69
15:2T:39:ARG:NH2	32:2a:345:C:OP2	2.24	0.69
40:1i:16:ARG:HB2	40:1i:64:THR:HG22	1.73	0.69
1:2A:2582:G:OP2	63:2A:3919:HOH:O	2.08	0.69
1:1A:2751:G:C2	7:1H:2:SER:HB3	2.27	0.69
27:15:40:LYS:NZ	27:15:44:THR:O	2.24	0.69
1:2A:83:G:H1	1:2A:102:G:HO2'	1.38	0.69
1:2A:2592:G:OP1	63:2A:3924:HOH:O	2.11	0.69
26:24:58:ARG:HD2	50:2s:68:GLY:H	1.57	0.69
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.09	0.69
32:2a:1029:C:N3	32:2a:1032:G:N2	2.41	0.69
32:2a:1029:C:N4	32:2a:1032:G:N1	2.41	0.69
1:1A:1762:A:H2'	63:1A:5731:HOH:O	1.92	0.69
1:1A:2552:OMU:OP2	63:1A:4120:HOH:O	2.11	0.69
57:1y:37:A:H2'	57:1y:38:A:H8	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1024:G:OP2	63:2A:3914:HOH:O	2.10	0.69
32:2a:73:G:H1	32:2a:96:U:H3	1.37	0.69
1:1A:1648:C:OP1	63:1A:4116:HOH:O	2.10	0.69
32:1a:171:A:OP1	63:1a:1905:HOH:O	2.09	0.69
1:2A:794:G:OP1	63:2A:3922:HOH:O	2.10	0.69
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.26	0.69
1:1A:1359:A:H2	1:1A:1372:U:O4	1.75	0.68
6:1G:45:GLU:OE2	63:1G:301:HOH:O	2.10	0.68
32:1a:258:G:H2'	32:1a:259:G:H8	1.58	0.68
32:1a:532:A:N6	32:1a:1206:G:O2'	2.26	0.68
32:1a:953:G:H5'	32:1a:965:A:H61	1.57	0.68
46:1o:16:ALA:HB1	46:1o:21:ASP:HB3	1.73	0.68
1:2A:1968:G:OP1	63:2A:3924:HOH:O	2.10	0.68
25:23:6:VAL:HA	25:23:56:VAL:HG12	1.75	0.68
32:2a:504:C:OP1	63:2a:1905:HOH:O	2.10	0.68
35:2d:140:VAL:HG11	35:2d:146:ILE:HD11	1.75	0.68
52:2u:6:ARG:HG2	52:2u:15:ARG:HD2	1.76	0.68
1:1A:2128:C:N4	1:1A:2160:G:H1	1.90	0.68
1:2A:2721:A:OP1	63:2A:3925:HOH:O	2.11	0.68
34:2c:125:GLU:HB3	34:2c:190:ARG:HE	1.57	0.68
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.28	0.68
1:2A:2014:A:H4'	18:2W:92:ARG:HH11	1.58	0.68
21:2Z:47:VAL:O	21:2Z:50:GLN:NE2	2.26	0.68
32:2a:255:G:OP2	63:2a:1906:HOH:O	2.10	0.68
1:1A:2702:U:OP2	63:1A:4118:HOH:O	2.11	0.68
32:1a:545:C:OP1	35:1d:61:LYS:NZ	2.27	0.68
1:2A:1395:A:OP1	63:2A:3902:HOH:O	2.12	0.68
1:1A:1026:U:OP1	63:1A:4108:HOH:O	2.11	0.68
1:2A:1762:A:N1	63:2A:3976:HOH:O	2.26	0.68
1:2A:2079:U:OP1	23:21:21:ARG:NH2	2.24	0.68
1:2A:2138:C:N4	1:2A:2153:G:H1	1.89	0.68
50:2s:64:GLU:OE2	50:2s:65:ASN:ND2	2.26	0.68
1:1A:1647:G:OP1	63:1A:4116:HOH:O	2.10	0.68
8:1I:129:THR:HG22	8:1I:139:GLN:HE22	1.56	0.68
54:1w:66:C:H2'	54:1w:67:G:H8	1.58	0.68
1:2A:883:G:N2	1:2A:894:C:O2	2.26	0.68
14:2S:67:ARG:NH1	14:2S:107:GLU:OE2	2.26	0.68
32:2a:1004:A:N6	32:2a:1037:C:O2	2.26	0.68
34:2c:181:ASN:HD21	34:2c:204:LEU:HD12	1.57	0.68
1:1A:1614:A:OP1	63:1A:4122:HOH:O	2.12	0.68
41:2j:38:ILE:HD11	41:2j:71:LEU:HD23	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:49:G:N2	54:2w:65:U:O2	2.21	0.68
1:1A:2136:C:N4	1:1A:2155:G:N1	2.42	0.67
1:2A:946:G:OP1	63:2A:3928:HOH:O	2.12	0.67
1:2A:2110:G:OP1	1:2A:2118:U:N3	2.25	0.67
54:2w:8:4SU:S4	54:2w:14:A:N7	2.67	0.67
32:1a:944:G:OP1	63:1a:1907:HOH:O	2.12	0.67
36:1e:137:GLU:OE2	36:1e:141:GLN:NE2	2.27	0.67
38:1g:78:ARG:HH11	38:1g:156:TRP:HE3	1.42	0.67
32:1a:1083:U:OP1	63:1a:1906:HOH:O	2.11	0.67
1:2A:298:G:OP2	63:2A:3926:HOH:O	2.12	0.67
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.75	0.67
1:1A:751:A:OP1	63:1A:4122:HOH:O	2.11	0.67
33:1b:195:ASP:O	39:1h:68:ARG:NH2	2.27	0.67
1:1A:1170:G:N7	63:1A:4165:HOH:O	2.27	0.67
1:1A:2790:A:H3'	1:1A:2790:A:N3	2.10	0.67
8:1I:40:THR:O	8:1I:44:LEU:HB2	1.94	0.67
39:2h:113:SER:HB2	39:2h:134:ILE:HD11	1.77	0.67
32:2a:533:A:OP1	63:2a:1907:HOH:O	2.12	0.67
32:2a:664:G:H22	32:2a:741:G:H1	1.42	0.67
32:2a:999:C:H42	32:2a:1042:G:H1	1.42	0.67
47:1p:15:PRO:HD2	47:1p:42:ARG:HD3	1.76	0.67
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.76	0.67
1:2A:2058:A:N7	63:2A:3981:HOH:O	2.27	0.67
1:2A:2816:C:O3'	13:2R:99:LYS:NZ	2.27	0.67
18:1W:1:MET:HE2	18:1W:62:HIS:HB3	1.77	0.67
36:1e:50:GLU:HB2	36:1e:53:LEU:HD13	1.77	0.67
44:1m:11:ARG:HA	44:1m:45:VAL:HB	1.76	0.67
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.77	0.67
32:2a:1272:G:N2	32:2a:1273:G:N7	2.43	0.67
5:1F:165:ARG:HA	5:1F:168:ARG:HD2	1.77	0.67
1:1A:2096:U:H3	1:1A:2193:G:H1	1.43	0.66
1:2A:307:G:H21	1:2A:330:A:H62	1.42	0.66
32:2a:671:G:H5'	37:2f:77:ARG:HH22	1.58	0.66
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.30	0.66
32:1a:166:G:N7	63:1a:1929:HOH:O	2.27	0.66
1:2A:879:G:H3'	1:2A:880:G:H8	1.60	0.66
32:2a:406:G:H5'	35:2d:5:ILE:HD13	1.78	0.66
34:2c:58:GLU:HB3	41:2j:92:THR:HG21	1.76	0.66
1:1A:309:G:N3	1:1A:329:G:O2'	2.27	0.66
32:1a:1129:C:H5''	40:1i:16:ARG:HH12	1.60	0.66
1:1A:1014:U:OP2	63:1A:4121:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1198:G:OP1	63:1a:1908:HOH:O	2.13	0.66
32:2a:532:A:N6	32:2a:1206:G:O2'	2.29	0.66
2:1B:48:A:H4'	14:1S:95:HIS:HD2	1.60	0.66
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.14	0.66
33:2b:48:MET:HA	33:2b:51:LEU:HB2	1.78	0.66
40:1i:110:GLU:OE2	40:1i:113:LYS:NZ	2.29	0.66
47:1p:22:THR:HA	47:1p:33:ILE:HG13	1.76	0.66
1:2A:2504:U:OP2	63:2A:3932:HOH:O	2.14	0.66
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.77	0.66
39:1h:51:VAL:HG21	39:1h:60:ARG:HD2	1.78	0.66
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.78	0.66
1:2A:219:G:OP2	63:2A:3927:HOH:O	2.12	0.66
1:2A:2136:C:HO2'	1:2A:2137:C:H6	1.44	0.66
32:2a:976:G:H5'	32:2a:1358:U:O2'	1.95	0.66
32:2a:1257:U:O4	45:2n:17:LYS:NZ	2.28	0.66
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.12	0.66
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.77	0.66
34:1c:89:GLU:OE1	34:1c:90:GLU:N	2.27	0.66
1:2A:1452:A:OP2	63:2A:3929:HOH:O	2.13	0.66
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.78	0.66
33:2b:121:LEU:HD21	33:2b:130:ARG:HH21	1.60	0.66
2:1B:89:G:OP1	63:1B:302:HOH:O	2.14	0.65
32:1a:977:A:O2'	32:1a:981:U:N3	2.29	0.65
33:1b:87:ARG:NH2	33:1b:220:ASP:OD1	2.26	0.65
32:2a:56:U:H2'	32:2a:57:G:C8	2.31	0.65
40:2i:128:ARG:NH2	55:2x:33:U:OP2	2.28	0.65
1:1A:2755:C:OP2	63:1A:4123:HOH:O	2.15	0.65
8:1I:38:LEU:HD23	8:1I:38:LEU:H	1.60	0.65
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.29	0.65
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.77	0.65
32:1a:1456:G:N2	51:1t:51:GLU:OE2	2.28	0.65
41:1j:38:ILE:HD11	41:1j:71:LEU:HD23	1.77	0.65
1:2A:1664:A:OP1	63:2A:3933:HOH:O	2.14	0.65
5:2F:124:LEU:HB3	5:2F:193:VAL:HG12	1.78	0.65
32:2a:1305:G:H22	32:2a:1331:G:H1'	1.60	0.65
34:2c:179:ARG:HG2	34:2c:206:GLU:HB2	1.79	0.65
39:2h:119:LEU:HB3	39:2h:123:GLU:HB2	1.77	0.65
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.31	0.65
32:1a:1500:A:OP1	63:1a:1909:HOH:O	2.14	0.65
1:2A:2167:U:H3'	1:2A:2168:G:H21	1.60	0.65
21:2Z:11:GLU:O	21:2Z:36:LYS:NZ	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1118:C:OP1	40:2i:104:ARG:NH1	2.29	0.65
32:2a:1174:G:N7	63:2a:1934:HOH:O	2.28	0.65
35:2d:119:GLN:HG2	35:2d:123:HIS:CD2	2.31	0.65
1:1A:2136:C:N3	1:1A:2155:G:N2	2.45	0.65
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.61	0.65
32:1a:1320:C:OP1	50:1s:70:LYS:NZ	2.29	0.65
47:1p:60:LEU:HD11	47:1p:66:PRO:HD3	1.78	0.65
1:2A:2697:G:O6	63:2A:3905:HOH:O	2.12	0.65
34:2c:7:PRO:HG3	34:2c:201:TYR:HE1	1.61	0.65
1:1A:1948:G:O6	63:1A:4119:HOH:O	2.11	0.65
32:1a:967:5MC:HO2'	40:1i:125:TYR:HH	1.37	0.65
54:1w:2:C:H2'	54:1w:3:G:H8	1.61	0.65
1:2A:832:G:H5'	11:2P:45:LEU:HD11	1.78	0.65
1:2A:2579:C:OP1	63:2A:3930:HOH:O	2.13	0.65
10:2O:64:ARG:NH2	10:2O:99:PHE:O	2.30	0.65
26:24:44:THR:O	26:24:46:GLN:N	2.29	0.65
29:27:5:TRP:NE1	29:27:7:PRO:HG3	2.12	0.65
32:2a:1203:C:OP1	45:2n:3:ARG:NH2	2.29	0.65
41:2j:6:ILE:HG12	41:2j:98:ILE:HD13	1.77	0.65
1:1A:1053:C:H42	1:1A:1106:G:H1	1.44	0.65
32:1a:1530:G:H2'	32:1a:1531:A:C8	2.32	0.65
32:2a:662:G:H2'	32:2a:663:A:C8	2.32	0.65
1:1A:881:G:N2	1:1A:897:C:O2	2.29	0.65
1:2A:1023:U:OP2	63:2A:3914:HOH:O	2.13	0.65
17:2V:40:LEU:HB2	17:2V:46:VAL:HB	1.79	0.65
40:2i:28:VAL:HG12	40:2i:63:ILE:HB	1.78	0.65
40:1i:3:GLN:HG2	40:1i:20:ARG:HE	1.62	0.65
42:1k:62:GLN:HB2	42:1k:93:GLN:HE21	1.62	0.65
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.28	0.65
32:2a:944:G:OP1	63:2a:1909:HOH:O	2.13	0.65
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.12	0.65
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.28	0.65
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.62	0.65
51:1t:22:ARG:O	51:1t:26:ASN:ND2	2.30	0.65
57:1y:66:C:H2'	57:1y:67:G:C8	2.32	0.65
1:2A:973:A:OP2	63:2A:3931:HOH:O	2.14	0.65
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.30	0.65
6:2G:105:LYS:NZ	6:2G:143:GLU:OE2	2.28	0.65
1:1A:1176:G:H1'	1:1A:1177:A:H5''	1.78	0.64
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.14	0.64
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:2o:4:THR:N	46:2o:7:GLU:OE1	2.29	0.64
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.79	0.64
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.15	0.64
1:1A:668:G:N7	63:1A:4175:HOH:O	2.29	0.64
1:2A:330:A:H2	1:2A:1210:A:HO2'	1.44	0.64
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.61	0.64
57:2y:18:G:N1	57:2y:56:C:C4	2.65	0.64
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.78	0.64
26:24:16:CYS:HA	26:24:33:VAL:HG12	1.78	0.64
32:2a:662:G:O2'	32:2a:836:G:OP1	2.15	0.64
35:2d:175:SER:HB3	35:2d:186:LEU:HD21	1.80	0.64
32:2a:460:G:N2	32:2a:471:G:N7	2.45	0.64
33:2b:43:ASP:OD2	33:2b:46:LYS:N	2.29	0.64
1:1A:1055:G:H1	1:1A:1104:C:N4	1.95	0.64
1:1A:2499:C:OP1	63:1A:4125:HOH:O	2.15	0.64
8:1I:86:THR:OG1	8:1I:87:LYS:N	2.30	0.64
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.20	0.64
54:1w:66:C:H2'	54:1w:67:G:C8	2.32	0.64
32:2a:187:C:O2'	51:2t:89:ARG:NH2	2.30	0.64
32:2a:289:G:OP2	63:2a:1910:HOH:O	2.14	0.64
32:2a:372:C:O2	63:2a:1911:HOH:O	2.14	0.64
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	1.97	0.64
32:1a:1009:G:O6	32:1a:1020:U:O2	2.15	0.64
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.80	0.64
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	1.79	0.64
11:2P:39:LYS:HB2	11:2P:45:LEU:HD22	1.80	0.64
1:1A:192:C:OP1	63:1A:4124:HOH:O	2.15	0.64
39:1h:81:HIS:ND1	39:1h:138:TRP:OXT	2.29	0.64
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.15	0.64
10:2O:49:ARG:NH1	32:2a:1422:G:O3'	2.30	0.64
15:2T:109:GLU:HG2	15:2T:112:ARG:HH22	1.63	0.64
38:2g:68:ASN:HD22	38:2g:128:ALA:HA	1.63	0.64
3:1D:71:ASP:HB2	3:1D:103:ARG:HH12	1.62	0.64
13:1R:15:SER:OG	63:1R:301:HOH:O	2.15	0.64
26:14:55:ARG:H	26:14:56:VAL:HA	1.62	0.64
33:1b:77:ALA:HB2	33:1b:211:ILE:HD13	1.80	0.64
39:1h:39:LEU:HB3	39:1h:45:ILE:HG12	1.80	0.64
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.30	0.64
32:2a:771:G:N7	63:2a:1936:HOH:O	2.29	0.64
40:2i:18:PHE:HB3	40:2i:20:ARG:HE	1.62	0.64
57:2y:18:G:C6	57:2y:56:C:N4	2.66	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.13	0.63
40:1i:93:ARG:HH11	40:1i:97:LYS:HD2	1.63	0.63
1:2A:1354:A:OP1	3:2D:38:LYS:NZ	2.25	0.63
1:2A:1627:G:OP1	63:2A:3935:HOH:O	2.15	0.63
17:2V:60:GLU:HB2	17:2V:97:LYS:HE2	1.80	0.63
44:2m:23:TYR:HB3	44:2m:67:GLU:HA	1.81	0.63
1:1A:880:G:H1	1:1A:898:C:N4	1.96	0.63
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.46	0.63
1:2A:2100:G:O6	1:2A:2189:U:O4	2.17	0.63
1:2A:2805:G:H2'	1:2A:2807:G:H8	1.63	0.63
32:2a:651:C:N4	32:2a:753:A:OP2	2.31	0.63
1:1A:1309:G:H4'	29:17:7:PRO:HB2	1.79	0.63
32:2a:573:A:OP2	63:2a:1913:HOH:O	2.15	0.63
44:2m:3:ARG:N	44:2m:7:VAL:O	2.31	0.63
32:1a:148:G:H2'	32:1a:149:A:H8	1.63	0.63
32:1a:159:G:N2	32:1a:162:A:OP2	2.30	0.63
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.13	0.63
34:1c:44:GLU:HA	34:1c:52:LEU:HD23	1.78	0.63
40:1i:20:ARG:O	40:1i:60:ASP:N	2.24	0.63
34:2c:30:ARG:O	34:2c:34:LEU:N	2.28	0.63
1:1A:1938:A:OP2	63:1A:4126:HOH:O	2.16	0.63
34:2c:6:HIS:HD2	34:2c:8:ILE:H	1.47	0.63
24:12:65:ASN:HD22	24:12:69:ARG:HH11	1.46	0.63
2:2B:12:C:H2'	22:20:73:GLY:HA3	1.79	0.63
46:2o:7:GLU:OE2	46:2o:38:ARG:NH2	2.31	0.63
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.31	0.63
26:14:55:ARG:N	26:14:56:VAL:HA	2.14	0.63
57:1y:36:C:H2'	57:1y:37:A:O4'	1.99	0.63
1:2A:271(L):U:H4'	8:2I:50:ARG:HH11	1.63	0.63
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.80	0.63
39:2h:10:LEU:HD22	39:2h:83:ILE:HD11	1.81	0.63
40:2i:9:ARG:H	40:2i:79:LEU:HD23	1.62	0.63
50:2s:33:THR:HG22	50:2s:35:SER:H	1.64	0.63
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.33	0.63
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.32	0.63
14:2S:11:LYS:HE3	14:2S:15:ARG:HH12	1.63	0.63
32:2a:48:C:OP2	63:2a:1912:HOH:O	2.15	0.63
32:2a:624:C:H2'	32:2a:625:G:H8	1.63	0.63
36:2e:106:PRO:HB3	36:2e:135:THR:HG21	1.80	0.63
1:1A:1075:C:H2'	1:1A:1076:C:H5'	1.81	0.63
1:2A:652(T):C:H2'	1:2A:652(U):G:C8	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1011:G:OP1	16:2U:77:SER:OG	2.16	0.63
1:2A:2133:G:O2'	1:2A:2157:G:N2	2.32	0.63
1:1A:1271:G:OP2	63:1A:4116:HOH:O	2.16	0.62
33:2b:178:ARG:HH22	39:2h:68:ARG:HH12	1.45	0.62
20:1Y:34:LYS:NZ	63:1Y:301:HOH:O	2.32	0.62
32:1a:1145:C:H4'	32:1a:1146:A:H5'	1.81	0.62
1:2A:607:U:OP1	5:2F:102:PRO:HA	1.99	0.62
2:2B:75:G:N2	21:2Z:87:ASP:OD1	2.32	0.62
18:2W:2:GLU:OE2	18:2W:72:LYS:NZ	2.22	0.62
51:2t:9:ASN:OD1	51:2t:9:ASN:N	2.32	0.62
1:1A:1171:G:OP2	1:1A:1174:A:N6	2.32	0.62
32:1a:1318:A:OP1	50:1s:7:LYS:NZ	2.25	0.62
39:1h:84:ARG:NH1	39:1h:136:GLU:OE2	2.32	0.62
41:1j:8:LEU:HD22	41:1j:96:ILE:HG12	1.80	0.62
22:20:11:ARG:O	22:20:14:ARG:NH2	2.32	0.62
32:2a:6:G:H1	36:2e:98:THR:HG21	1.65	0.62
32:2a:134:A:H61	47:2p:25:ARG:NH1	1.95	0.62
35:2d:187:ARG:HH12	35:2d:190:ASP:H	1.46	0.62
36:2e:33:VAL:HG13	36:2e:112:LEU:HD22	1.81	0.62
1:1A:2140:C:H2'	1:1A:2141:G:H8	1.64	0.62
32:1a:913:A:OP1	43:1l:46:LYS:NZ	2.32	0.62
41:2j:32:ALA:HB1	41:2j:33:GLN:HG2	1.82	0.62
42:2k:21:ILE:HB	42:2k:84:VAL:HG12	1.80	0.62
43:2l:53:ARG:HG3	43:2l:93:LEU:HD21	1.80	0.62
1:1A:2123:G:H2'	1:1A:2124:G:H8	1.63	0.62
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.31	0.62
36:1e:131:ILE:O	36:1e:135:THR:OG1	2.17	0.62
1:2A:2114:A:H2	1:2A:2171:A:H61	1.47	0.62
32:2a:17:U:H2'	32:2a:18:C:C6	2.34	0.62
32:2a:742:G:OP2	46:2o:35:ARG:NH2	2.32	0.62
33:2b:74:LYS:NZ	33:2b:206:ASP:OD1	2.33	0.62
1:1A:1893:C:OP1	63:1A:4127:HOH:O	2.16	0.62
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.32	0.62
19:1X:2:LYS:NZ	19:1X:38:GLU:OE2	2.25	0.62
33:1b:8:LYS:O	33:1b:217:ARG:NH1	2.33	0.62
32:2a:1314:C:N4	50:2s:2:PRO:O	2.30	0.62
1:1A:2136:C:N4	1:1A:2155:G:C6	2.67	0.62
33:1b:165:VAL:HG13	33:1b:166:ASP:H	1.63	0.62
32:2a:737:A:H2'	32:2a:738:C:C6	2.35	0.62
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.17	0.62
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:148:G:H2'	32:2a:149:A:C8	2.35	0.62
32:2a:1417:G:O6	63:2a:1908:HOH:O	2.12	0.62
33:2b:219:VAL:HA	33:2b:222:ILE:HB	1.82	0.62
44:1m:58:GLU:O	44:1m:62:ASN:ND2	2.22	0.62
1:2A:1012:U:C5	9:2N:28:THR:HG21	2.35	0.62
18:1W:92:ARG:NH1	63:1W:301:HOH:O	2.08	0.62
5:2F:195:ASP:OD1	5:2F:196:LEU:N	2.32	0.62
6:2G:39:ILE:HG23	6:2G:157:ILE:HG23	1.82	0.62
32:2a:1144:G:H21	32:2a:1146:A:H62	1.48	0.62
1:1A:1066:U:H2'	1:1A:1068:G:OP2	2.00	0.61
63:1A:4106:HOH:O	4:1E:110:GLY:O	2.16	0.61
32:2a:64:G:H4'	32:2a:65:U:H3'	1.82	0.61
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.14	0.61
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.35	0.61
36:2e:20:GLN:NE2	36:2e:21:ALA:O	2.32	0.61
38:2g:22:LEU:HG	38:2g:62:PHE:HE2	1.64	0.61
1:1A:1096:A:N6	1:1A:1097:U:O2	2.33	0.61
1:1A:1506:C:H2'	1:1A:1507:A:H8	1.65	0.61
32:1a:1374:A:OP1	38:1g:36:LYS:NZ	2.32	0.61
1:2A:870:A:OP1	12:2Q:6:ARG:NH1	2.33	0.61
1:2A:2126:A:N6	1:2A:2163:C:O4'	2.33	0.61
1:2A:2151:G:H2'	1:2A:2152:G:H8	1.64	0.61
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.64	0.61
32:2a:437:U:H5''	35:2d:155:LEU:HD11	1.81	0.61
32:2a:523:A:H61	43:2l:92:OTD:CG	2.13	0.61
32:2a:1134:G:C2	32:2a:1135:U:H1'	2.35	0.61
29:17:23:ARG:NH1	63:17:201:HOH:O	2.32	0.61
44:2m:14:ARG:HG3	44:2m:44:ARG:HH21	1.66	0.61
32:1a:542:G:H5'	35:1d:41:GLY:HA3	1.82	0.61
1:2A:675:A:OP1	5:2F:63:LYS:NZ	2.32	0.61
32:2a:1147:C:O2	40:2i:16:ARG:NH1	2.33	0.61
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.35	0.61
32:1a:309:G:O2'	32:1a:607:A:N1	2.32	0.61
5:2F:12:LEU:HD12	5:2F:124:LEU:HD21	1.82	0.61
36:2e:100:VAL:O	36:2e:107:ARG:NH2	2.29	0.61
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.34	0.61
2:2B:41:U:H5	6:2G:70:VAL:H	1.47	0.61
5:2F:122:LYS:HB3	5:2F:191:ARG:HG2	1.82	0.61
32:2a:979:C:OP1	32:2a:1223:C:N4	2.34	0.61
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.23	0.61
32:2a:26:A:N6	32:2a:558:G:O2'	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.33	0.61
35:2d:50:ARG:HH21	36:2e:9:LYS:HE2	1.64	0.61
54:2w:14:A:N6	54:2w:21:A:C2	2.68	0.61
32:1a:17:U:H2'	32:1a:18:C:C6	2.35	0.61
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.00	0.61
32:2a:1060:C:H5'	45:2n:45:ARG:HH12	1.66	0.61
44:2m:107:ALA:HB3	44:2m:111:LYS:HE2	1.82	0.61
32:1a:1027:C:N4	32:1a:1034:G:H1	1.98	0.61
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.01	0.61
32:1a:766:A:OP2	63:1a:1910:HOH:O	2.16	0.61
1:2A:2137:C:N4	1:2A:2155:G:O6	2.34	0.61
32:2a:1055:A:N7	32:2a:1200:C:N4	2.48	0.61
42:2k:34:ASP:HB2	42:2k:35:PRO:HD2	1.81	0.61
45:2n:23:ARG:NH1	45:2n:28:GLY:O	2.34	0.61
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.36	0.60
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	1.83	0.60
21:1Z:104:PHE:HA	21:1Z:139:VAL:HB	1.82	0.60
1:1A:278:A:P	1:1A:278:A:H8	2.25	0.60
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.36	0.60
40:1i:32:ASP:OD1	40:1i:33:PHE:N	2.34	0.60
2:2B:54:G:H21	6:2G:29:TRP:HE1	1.48	0.60
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.83	0.60
32:2a:1187:G:H5'	40:2i:113:LYS:HE3	1.82	0.60
10:1O:115:VAL:HG13	10:1O:121:VAL:HG11	1.82	0.60
23:11:23:LYS:NZ	57:1y:73:U:O2'	2.31	0.60
32:1a:1086:U:H3	32:1a:1099:G:H22	1.47	0.60
47:1p:72:ARG:HA	47:1p:75:ARG:HB3	1.83	0.60
32:2a:1004:A:H5''	32:2a:1024:G:H22	1.67	0.60
32:1a:1036:G:H5''	32:1a:1037:C:C5	2.36	0.60
32:1a:1060:C:H5''	41:1j:51:ARG:HG2	1.82	0.60
1:2A:938:G:OP2	30:28:52:LYS:NZ	2.28	0.60
11:2P:29:LYS:HD3	11:2P:30:THR:HG23	1.81	0.60
1:2A:309:G:N3	1:2A:329:G:O2'	2.35	0.60
1:2A:2100:G:H2'	1:2A:2101:G:H8	1.66	0.60
1:2A:2105:C:H2'	1:2A:2106:G:H8	1.66	0.60
2:2B:22:U:H3	2:2B:61:G:H1	1.48	0.60
32:2a:984:C:H2'	32:2a:985:C:C6	2.37	0.60
41:1j:27:ALA:HA	41:1j:81:THR:HG21	1.81	0.60
7:2H:11:VAL:HG13	7:2H:15:VAL:HG22	1.81	0.60
34:2c:180:ALA:HA	34:2c:206:GLU:HB3	1.83	0.60
36:2e:78:HIS:HB3	39:2h:107:LEU:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:588:U:H2'	1:1A:589:C:C6	2.37	0.60
1:1A:2445:G:OP1	5:1F:74:ARG:NH2	2.30	0.60
1:1A:2690:C:OP2	13:1R:17:ARG:NH2	2.34	0.60
36:1e:12:LEU:HB3	36:1e:31:LEU:HB2	1.81	0.60
52:1u:17:THR:O	52:1u:22:ARG:NH1	2.34	0.60
1:2A:987:G:O2'	1:2A:1000:A:N3	2.30	0.60
3:2D:125:ILE:HB	37:2f:81:ILE:HD11	1.83	0.60
21:2Z:146:ILE:HG12	21:2Z:174:VAL:HG13	1.83	0.60
32:2a:770:C:OP1	63:2a:1915:HOH:O	2.16	0.60
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.36	0.60
26:14:56:VAL:HG22	26:14:60:GLN:HG3	1.83	0.60
33:1b:15:VAL:HG21	33:1b:213:LEU:HD22	1.84	0.60
1:2A:668:G:H5'	1:2A:669:G:OP2	2.02	0.60
32:2a:782:A:OP1	63:2a:1919:HOH:O	2.17	0.60
1:1A:530:G:N1	1:1A:2023:G:OP1	2.26	0.60
32:1a:96:U:H2'	32:1a:97:G:C8	2.36	0.60
47:1p:72:ARG:HG3	47:1p:73:LEU:HD13	1.84	0.60
51:1t:57:ARG:HH12	51:1t:100:ILE:HD12	1.65	0.60
1:2A:686:G:N2	1:2A:788:A:H61	1.99	0.60
18:2W:11:ARG:NH1	18:2W:99:ARG:O	2.34	0.60
32:2a:562:C:H1'	43:2l:15:ARG:HB3	1.83	0.60
41:2j:44:VAL:HG13	41:2j:66:ARG:HG2	1.82	0.60
1:1A:1062:G:N2	1:1A:1077:A:N1	2.41	0.60
1:1A:1069:A:H4'	1:1A:1070:A:H5''	1.84	0.60
7:1H:86:GLU:OE2	7:1H:132:ARG:NH1	2.35	0.60
1:1A:2110:G:OP1	1:1A:2118:U:N3	2.35	0.59
1:2A:1354:A:OP2	63:2A:3939:HOH:O	2.17	0.59
1:2A:1837:C:O2'	1:2A:1927:A:N3	2.29	0.59
13:2R:67:LEU:HD13	13:2R:76:VAL:HG21	1.82	0.59
14:2S:15:ARG:O	14:2S:19:LYS:HG2	2.02	0.59
32:2a:820:U:OP1	63:2a:1914:HOH:O	2.15	0.59
32:2a:839:U:H3'	32:2a:840:C:H5'	1.84	0.59
57:2y:65:U:H2'	57:2y:66:C:C6	2.36	0.59
1:1A:1466:G:HO2'	1:1A:1546:C:HO2'	1.46	0.59
33:1b:78:GLN:NE2	33:1b:94:ASN:O	2.35	0.59
51:2t:14:LYS:HG2	51:2t:18:GLN:HE21	1.67	0.59
33:1b:52:GLU:OE2	33:1b:56:ARG:NH2	2.34	0.59
34:1c:15:THR:HG21	34:1c:181:ASN:HA	1.83	0.59
44:1m:12:ASN:O	44:1m:44:ARG:NH1	2.34	0.59
1:2A:851:U:H5'	25:23:49:LYS:HD2	1.84	0.59
1:2A:2625:G:O6	63:2A:3934:HOH:O	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:254:G:OP1	48:2q:66:SER:OG	2.18	0.59
39:2h:73:ASP:OD1	39:2h:75:ARG:NE	2.35	0.59
40:2i:27:THR:HA	40:2i:32:ASP:HA	1.85	0.59
1:1A:438:G:OP2	63:1A:4128:HOH:O	2.16	0.59
32:1a:677:U:H3	32:1a:713:G:H22	1.50	0.59
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.66	0.59
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.84	0.59
54:1w:2:C:H2'	54:1w:3:G:C8	2.37	0.59
19:2X:60:ARG:HH12	29:27:47:ARG:HH12	1.50	0.59
32:2a:1273:G:H3'	32:2a:1274:G:H8	1.68	0.59
1:1A:1816:G:O6	3:1D:35:LYS:NZ	2.35	0.59
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.84	0.59
17:1V:1:MET:HE2	17:1V:43:GLU:H	1.68	0.59
1:2A:509:C:OP1	63:2A:3940:HOH:O	2.17	0.59
32:2a:1181:G:O2'	32:2a:1182:G:N7	2.35	0.59
36:2e:57:LYS:HG2	36:2e:61:TYR:CE2	2.37	0.59
3:1D:147:LEU:HD13	3:1D:155:LEU:HD11	1.83	0.59
20:1Y:51:VAL:HG12	20:1Y:58:GLY:HA3	1.85	0.59
32:1a:945:G:OP1	63:1a:1911:HOH:O	2.17	0.59
36:1e:71:LEU:HD12	36:1e:71:LEU:H	1.67	0.59
42:1k:62:GLN:OE1	42:1k:93:GLN:NE2	2.35	0.59
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.33	0.59
1:2A:615:G:OP1	5:2F:40:GLN:NE2	2.30	0.59
1:2A:794:G:OP2	63:2A:3942:HOH:O	2.17	0.59
1:2A:2291:U:OP1	1:2A:2380:C:O2'	2.20	0.59
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.36	0.59
13:1R:50:HIS:ND1	63:1R:302:HOH:O	2.32	0.59
42:1k:15:ALA:HA	42:1k:77:MET:H	1.67	0.59
1:2A:706:A:OP1	3:2D:7:LYS:NZ	2.34	0.59
23:21:76:ARG:NH1	23:21:97:LEU:O	2.35	0.59
32:2a:130:A:O2'	32:2a:131:C:O5'	2.19	0.59
32:2a:547:A:OP1	63:2a:1917:HOH:O	2.16	0.59
32:2a:865:A:N3	32:2a:918:A:O2'	2.31	0.59
32:2a:972:C:O2'	41:2j:55:LYS:O	2.17	0.59
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.21	0.59
28:26:12:GLU:OE1	28:26:19:ARG:NH1	2.36	0.59
32:2a:548:G:OP1	63:2a:1918:HOH:O	2.17	0.59
1:1A:1970:A:OP1	63:1A:4129:HOH:O	2.17	0.59
57:1y:8:4SU:O2'	57:1y:21:A:N1	2.34	0.59
5:2F:137:LYS:HA	5:2F:140:LEU:HD12	1.84	0.59
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:111:GLU:OE2	12:2Q:133:ARG:NH1	2.36	0.59
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.16	0.59
34:2c:88:ARG:HA	34:2c:91:LEU:HD13	1.84	0.59
1:1A:2140:C:N3	1:1A:2151:G:O6	2.36	0.59
1:2A:2100:G:H2'	1:2A:2101:G:C8	2.37	0.59
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.38	0.59
6:2G:38:VAL:HG12	6:2G:93:THR:HA	1.84	0.59
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.68	0.58
1:1A:1095:A:H62	1:1A:1097:U:H3	1.51	0.58
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.38	0.58
50:1s:49:ILE:HG13	50:1s:62:ILE:HD11	1.85	0.58
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.84	0.58
32:2a:646:U:H2'	32:2a:647:C:C6	2.38	0.58
32:2a:1263:C:N3	32:2a:1272:G:O6	2.36	0.58
32:2a:1518:MA6:H93	32:2a:1519:MA6:H92	1.84	0.58
47:2p:18:ARG:HD3	47:2p:35:LYS:HD2	1.84	0.58
1:1A:1243:G:O2'	11:1P:7:ARG:NH2	2.36	0.58
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.39	0.58
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.84	0.58
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.85	0.58
34:2c:172:ARG:HG3	34:2c:174:PRO:HD3	1.84	0.58
1:2A:2133:G:HO2'	1:2A:2157:G:N2	2.02	0.58
47:2p:1:MET:HE3	47:2p:3:LYS:HD3	1.85	0.58
54:2w:6:C:N3	54:2w:67:G:N2	2.50	0.58
2:1B:92:C:OP1	21:1Z:79:ARG:NH1	2.36	0.58
24:12:65:ASN:HD22	24:12:69:ARG:NH1	2.00	0.58
32:1a:460:G:N2	32:1a:471:G:OP2	2.23	0.58
1:2A:2278:A:OP2	22:20:12:ASN:ND2	2.37	0.58
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.84	0.58
21:2Z:152:ALA:HB1	21:2Z:163:LEU:HD11	1.86	0.58
36:2e:89:ILE:HG12	36:2e:135:THR:HG22	1.85	0.58
45:2n:3:ARG:HE	45:2n:3:ARG:HA	1.68	0.58
57:2y:18:G:C6	57:2y:56:C:C4	2.92	0.58
1:1A:763:G:OP1	63:1A:4130:HOH:O	2.17	0.58
1:1A:1062:G:H1	1:1A:1077:A:N6	1.91	0.58
16:1U:81:HIS:CE1	16:1U:85:LYS:HD2	2.38	0.58
32:1a:559:A:OP1	36:1e:126:ARG:NH2	2.36	0.58
10:2O:87:ILE:HD12	10:2O:91:LEU:HA	1.86	0.58
21:2Z:154:ASP:N	21:2Z:154:ASP:OD1	2.35	0.58
44:2m:94:ARG:NH2	50:2s:81:ARG:HA	2.17	0.58
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:1q:22:LEU:HD11	48:1q:39:SER:HB2	1.84	0.58
4:2E:59:VAL:HG23	4:2E:64:LYS:HE3	1.84	0.58
11:2P:38:GLN:O	11:2P:39:LYS:HB3	2.03	0.58
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.37	0.58
21:2Z:73:GLN:O	21:2Z:87:ASP:N	2.34	0.58
32:2a:56:U:H2'	32:2a:57:G:H8	1.69	0.58
32:2a:1272:G:N2	32:2a:1273:G:C5	2.71	0.58
32:2a:1316:G:N7	50:2s:7:LYS:NZ	2.50	0.58
33:2b:58:ILE:O	33:2b:62:ALA:N	2.30	0.58
1:1A:1466:G:O2'	1:1A:1546:C:O2'	2.15	0.58
11:1P:39:LYS:HB2	11:1P:45:LEU:HD22	1.85	0.58
1:2A:247:G:H4'	1:2A:386:G:C5	2.39	0.58
32:2a:259:G:OP2	51:2t:83:ARG:NH1	2.34	0.58
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.19	0.58
14:1S:84:GLN:HA	14:1S:111:GLU:HB2	1.84	0.58
33:1b:17:PHE:HB3	33:1b:44:LEU:HD11	1.85	0.58
35:1d:187:ARG:NH2	35:1d:193:ASP:OD2	2.36	0.58
22:20:32:ARG:H	22:20:35:ASN:ND2	2.02	0.58
25:23:5:LYS:NZ	25:23:34:GLU:OE2	2.35	0.58
38:2g:79:ARG:NH2	38:2g:80:VAL:HA	2.18	0.58
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.37	0.58
37:1f:38:GLU:HB2	37:1f:64:GLN:HG2	1.86	0.58
1:2A:468:G:N7	29:27:39:ARG:NH2	2.48	0.58
1:2A:801:G:O6	5:2F:53:THR:OG1	2.21	0.58
1:2A:994:C:O2'	1:2A:996:A:OP1	2.21	0.58
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.01	0.58
21:2Z:77:ASP:OD2	21:2Z:80:ARG:NH1	2.37	0.58
26:24:26:SER:OG	26:24:28:LYS:O	2.21	0.58
32:2a:1279:A:H4'	32:2a:1280:A:OP1	2.03	0.58
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.03	0.58
33:1b:166:ASP:HB3	33:1b:169:LYS:HB3	1.85	0.58
53:1v:14:A:H3'	53:1v:15:A:C8	2.39	0.58
1:2A:2659:G:OP1	7:2H:158:HIS:NE2	2.35	0.58
7:2H:90:LYS:HG3	7:2H:163:TYR:CE2	2.39	0.58
12:2Q:35:VAL:HG22	12:2Q:102:VAL:HG22	1.85	0.58
12:2Q:78:PRO:HG2	12:2Q:81:VAL:HG11	1.84	0.58
33:2b:91:PRO:HG2	33:2b:155:LEU:HD13	1.86	0.58
34:2c:12:LEU:O	45:2n:57:ARG:NH1	2.37	0.58
1:1A:278:A:O2'	1:1A:279:C:OP1	2.17	0.57
1:1A:2344:U:OP1	28:16:37:ARG:NH1	2.36	0.57
52:1u:6:ARG:HG2	52:1u:15:ARG:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:752:A:H3'	29:27:1:MET:HE1	1.85	0.57
8:2I:77:LEU:HB3	8:2I:142:VAL:HG12	1.86	0.57
17:2V:55:ALA:HA	17:2V:101:GLY:HA2	1.86	0.57
54:2w:17:G:H4'	54:2w:60:U:C4	2.38	0.57
1:1A:764:A:H5'	3:1D:210:GLY:HA2	1.86	0.57
1:1A:1057:A:N6	1:1A:1087:G:OP1	2.36	0.57
1:1A:2185:C:H2'	1:1A:2186:G:C8	2.36	0.57
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.85	0.57
26:14:18:CYS:SG	26:14:20:ASN:HB2	2.44	0.57
32:1a:204:U:H4'	32:1a:216:G:H5''	1.86	0.57
48:1q:37:LYS:O	48:1q:38:ARG:NH2	2.37	0.57
1:2A:2751:G:C8	7:2H:2:SER:HB3	2.39	0.57
15:2T:65:LYS:HE3	15:2T:67:SER:HB2	1.87	0.57
1:1A:2110:G:P	1:1A:2118:U:H3	2.26	0.57
3:1D:2:ALA:N	3:1D:200:ASP:OD2	2.37	0.57
22:10:70:GLN:OE1	22:10:80:HIS:NE2	2.37	0.57
34:1c:134:ILE:HG23	34:1c:151:VAL:HG13	1.86	0.57
35:1d:112:VAL:HG23	35:1d:116:GLN:NE2	2.18	0.57
1:2A:639:U:H2'	1:2A:640:C:C6	2.39	0.57
1:2A:796:C:H2'	1:2A:797:C:C6	2.39	0.57
12:2Q:31:ASP:OD1	12:2Q:134:ARG:NH1	2.37	0.57
43:2l:117:ARG:HB3	43:2l:122:THR:HB	1.87	0.57
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.19	0.57
45:1n:33:VAL:HA	45:1n:40:CYS:HA	1.87	0.57
1:2A:2189:U:H2'	1:2A:2190:G:C8	2.40	0.57
2:2B:31:C:H4'	6:2G:29:TRP:CZ2	2.39	0.57
6:2G:44:GLY:HA2	6:2G:88:ILE:HG23	1.85	0.57
40:2i:6:GLY:N	40:2i:17:VAL:O	2.37	0.57
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.04	0.57
36:1e:35:GLY:HA3	36:1e:112:LEU:HB3	1.86	0.57
42:1k:48:ILE:O	42:1k:50:TYR:N	2.37	0.57
54:1w:18:G:H4'	54:1w:19:U:OP2	2.04	0.57
1:2A:1313:U:OP1	63:2A:3944:HOH:O	2.18	0.57
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.39	0.57
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.84	0.57
32:2a:1402:4OC:HM22	32:2a:1403:C:H5'	1.85	0.57
44:2m:45:VAL:HA	44:2m:48:LEU:HG	1.86	0.57
1:1A:2428:G:OP1	63:1A:4102:HOH:O	2.17	0.57
33:1b:45:GLN:NE2	33:1b:49:GLU:OE2	2.38	0.57
46:2o:5:LYS:O	46:2o:9:GLN:HG2	2.05	0.57
50:2s:28:LYS:HB3	50:2s:29:ARG:CB	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1025:G:O2'	63:1A:4108:HOH:O	2.14	0.57
32:1a:933:G:O6	38:1g:3:ARG:NH2	2.38	0.57
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.37	0.57
1:2A:1171:G:H1	1:2A:1178:C:H42	1.52	0.57
1:2A:2156:G:H2'	1:2A:2157:G:C2	2.39	0.57
7:2H:86:GLU:OE2	7:2H:132:ARG:NH2	2.37	0.57
51:2t:60:GLU:HG3	51:2t:81:LYS:HD2	1.85	0.57
32:1a:1125:U:H4'	41:1j:5:ARG:HH22	1.70	0.57
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.05	0.57
1:2A:1269:A:N7	63:2A:4010:HOH:O	2.33	0.57
36:2e:87:SER:HB3	36:2e:125:SER:O	2.05	0.57
1:1A:2105:C:H2'	1:1A:2106:G:H8	1.69	0.57
1:1A:2123:G:H2'	1:1A:2124:G:C8	2.40	0.57
6:1G:133:LEU:HD11	6:1G:157:ILE:HD12	1.85	0.57
1:2A:2455:G:O6	63:2A:3938:HOH:O	2.16	0.57
6:2G:124:SER:O	6:2G:124:SER:OG	2.20	0.57
6:2G:179:PRO:HB2	26:24:42:PHE:HE2	1.70	0.57
1:1A:1187:G:H5''	17:1V:81:TYR:CE1	2.39	0.57
1:1A:2125:G:N1	1:1A:2172:U:OP1	2.23	0.57
32:1a:539:A:H2'	32:1a:540:G:C8	2.39	0.57
32:2a:576:G:OP1	63:2a:1920:HOH:O	2.18	0.57
32:2a:1144:G:N2	32:2a:1146:A:H62	2.03	0.57
48:2q:81:ARG:HB3	48:2q:84:LEU:HD12	1.87	0.57
1:1A:1054:A:N6	1:1A:1105:U:N3	2.30	0.56
1:1A:1058:G:N1	1:1A:1080:C:N4	2.40	0.56
1:2A:1011:G:OP2	16:2U:66:ASN:ND2	2.32	0.56
1:2A:1533:G:H1'	1:2A:1537:G:H22	1.69	0.56
1:2A:2135:A:C8	1:2A:2136:C:H5	2.23	0.56
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.52	0.56
1:2A:2637:U:OP1	4:2E:82:ARG:NH1	2.38	0.56
20:2Y:8:LYS:HD3	20:2Y:97:ARG:NH1	2.20	0.56
32:2a:1292:U:H2'	32:2a:1293:G:C8	2.40	0.56
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.37	0.56
1:1A:1021:A:OP2	9:1N:65:LYS:NZ	2.29	0.56
16:1U:69:CYS:HB3	16:1U:74:LEU:HD13	1.87	0.56
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.52	0.56
35:1d:173:TRP:CD2	35:1d:189:PRO:HG3	2.39	0.56
38:1g:86:GLN:HB2	38:1g:148:ASN:ND2	2.20	0.56
51:1t:60:GLU:HG3	51:1t:81:LYS:HD2	1.88	0.56
1:2A:153:C:OP2	23:21:92:LYS:NZ	2.37	0.56
1:2A:855:G:O2'	22:20:27:GLU:OE2	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:933:A:OP1	25:23:24:LYS:NZ	2.37	0.56
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.41	0.56
12:2Q:1:MET:HB3	12:2Q:44:ALA:HB1	1.86	0.56
32:2a:959:A:HO2'	32:2a:984:C:HO2'	1.52	0.56
32:2a:1105:A:H2'	32:2a:1106:G:H8	1.69	0.56
32:2a:1320:C:N3	50:2s:36:ARG:NH2	2.53	0.56
34:2c:182:ILE:HG22	34:2c:203:PHE:HA	1.87	0.56
57:2y:42:C:H2'	57:2y:43:U:H6	1.69	0.56
1:1A:11:G:C2'	1:1A:12:U:H5'	2.35	0.56
10:1O:24:VAL:HG13	10:1O:33:ALA:HB2	1.87	0.56
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.87	0.56
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.40	0.56
32:1a:67:C:H2'	32:1a:68:G:C8	2.39	0.56
32:1a:1183:A:O2'	32:1a:1184:G:OP1	2.21	0.56
34:1c:24:ALA:HB2	34:1c:32:LEU:HD12	1.87	0.56
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.87	0.56
1:2A:248:G:OP1	63:2A:3943:HOH:O	2.17	0.56
5:2F:148:LEU:HD11	5:2F:193:VAL:HG11	1.87	0.56
17:2V:1:MET:HE2	17:2V:43:GLU:HB2	1.85	0.56
39:2h:51:VAL:HG11	39:2h:60:ARG:HH11	1.70	0.56
43:2l:40:VAL:HG21	43:2l:78:GLN:HA	1.87	0.56
44:2m:14:ARG:NE	44:2m:42:ALA:HA	2.20	0.56
50:2s:63:THR:HG23	50:2s:66:MET:HE3	1.88	0.56
1:1A:1183:G:O2'	25:13:29:ARG:NH1	2.38	0.56
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.41	0.56
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.87	0.56
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.21	0.56
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.87	0.56
33:1b:178:ARG:NH1	33:1b:196:LEU:O	2.35	0.56
42:1k:72:ALA:HB1	42:1k:77:MET:HG2	1.88	0.56
54:1w:27:A:H2'	54:1w:28:G:H8	1.71	0.56
1:2A:861:A:N3	2:2B:79:C:O2'	2.38	0.56
1:2A:918:A:H5''	2:2B:98:G:O2'	2.05	0.56
2:2B:7:G:H21	14:2S:38:GLN:NE2	1.97	0.56
32:2a:1278:U:H5'	32:2a:1279:A:H5'	1.86	0.56
34:2c:47:LEU:HD11	34:2c:68:VAL:HG11	1.87	0.56
9:1N:46:VAL:HG23	9:1N:48:MET:HG2	1.87	0.56
32:1a:1035:A:N3	32:1a:1036:G:N2	2.52	0.56
32:1a:1140:C:H2'	32:1a:1141:C:H6	1.71	0.56
33:1b:125:PRO:C	33:1b:127:ILE:H	2.14	0.56
36:1e:81:GLU:HG2	36:1e:90:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.70	0.56
1:1A:1024:G:OP2	63:1A:4108:HOH:O	2.18	0.56
1:1A:2142:C:O2	1:1A:2149:G:N1	2.33	0.56
32:1a:165:C:H2'	32:1a:166:G:C8	2.36	0.56
32:1a:179:A:H2'	32:1a:180:U:C6	2.41	0.56
32:1a:1497:G:N7	63:1a:1937:HOH:O	2.32	0.56
50:1s:12:ASP:OD2	50:1s:35:SER:OG	2.22	0.56
25:23:40:THR:HG22	25:23:42:ALA:H	1.69	0.56
32:2a:1010:G:H2'	32:2a:1011:G:H8	1.71	0.56
32:2a:1255:G:OP1	41:2j:45:ARG:NH2	2.36	0.56
46:2o:87:ILE:HG22	46:2o:88:ARG:H	1.70	0.56
45:1n:4:LYS:HA	45:1n:7:ILE:HG22	1.88	0.56
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.52	0.56
21:2Z:77:ASP:N	21:2Z:82:ARG:O	2.38	0.56
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.40	0.56
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.41	0.56
1:1A:2165:G:N1	1:1A:2171:A:H8	2.04	0.56
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.87	0.56
24:12:31:GLU:HB3	24:12:53:LEU:HD21	1.87	0.56
32:1a:1284:C:H3'	32:1a:1285:A:H8	1.71	0.56
35:1d:172:PRO:O	35:1d:174:LEU:N	2.36	0.56
44:1m:4:ILE:HD12	44:1m:57:ARG:HA	1.87	0.56
1:2A:200:U:O2	1:2A:386:G:N2	2.39	0.56
1:2A:249:C:O2	30:28:12:LYS:NZ	2.36	0.56
1:2A:882:G:H1	1:2A:894:C:H42	1.54	0.56
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.41	0.56
32:2a:1479:C:H2'	32:2a:1480:G:H8	1.70	0.56
33:2b:63:MET:HG3	33:2b:225:ALA:HB1	1.88	0.56
36:2e:12:LEU:HB3	36:2e:31:LEU:HB2	1.86	0.56
1:1A:1300:U:H4'	1:1A:1301:A:H5''	1.88	0.56
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.41	0.56
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.87	0.56
32:1a:473:G:OP2	47:1p:75:ARG:NH1	2.39	0.56
32:1a:974:A:H8	32:1a:974:A:OP1	1.88	0.56
35:1d:187:ARG:NH2	35:1d:190:ASP:OD1	2.37	0.56
45:1n:23:ARG:NH1	45:1n:30:ALA:HB2	2.21	0.56
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.05	0.56
1:2A:884:C:H3'	1:2A:885:C:H6	1.71	0.56
1:2A:898:C:H2'	1:2A:899:A:H5'	1.87	0.56
1:2A:1021:A:H62	1:2A:1141:U:H3	1.52	0.56
3:2D:168:ARG:HG2	3:2D:173:VAL:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:49:ASP:N	6:2G:49:ASP:OD1	2.38	0.56
7:2H:20:ALA:HB3	7:2H:23:ARG:HB2	1.86	0.56
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.39	0.56
32:2a:390:C:O3'	47:2p:28:ARG:NH2	2.39	0.56
38:2g:27:ILE:HD13	38:2g:40:ALA:HA	1.88	0.56
1:1A:2447:G:OP2	63:1A:4131:HOH:O	2.17	0.56
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.71	0.56
6:1G:115:ARG:HG2	6:1G:136:ARG:HH22	1.71	0.56
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.41	0.56
38:1g:27:ILE:HD13	38:1g:40:ALA:HA	1.88	0.56
21:2Z:141:VAL:HG11	21:2Z:174:VAL:HG21	1.88	0.56
32:2a:560:U:H5'	32:2a:566:G:N2	2.21	0.56
32:2a:1313:U:P	50:2s:5:LEU:HD12	2.46	0.56
34:2c:131:ARG:NH2	36:2e:50:GLU:HG3	2.21	0.56
35:2d:104:VAL:HG21	35:2d:140:VAL:HG21	1.88	0.56
50:2s:20:LEU:HA	50:2s:23:ASN:HB2	1.87	0.56
13:1R:56:LYS:NZ	13:1R:87:TYR:O	2.38	0.55
49:1r:37:VAL:HG22	49:1r:78:LEU:HB3	1.89	0.55
1:2A:2183:C:H2'	1:2A:2184:G:C8	2.39	0.55
4:2E:9:VAL:HG13	15:2T:3:ARG:HG2	1.88	0.55
23:21:2:SER:HB3	23:21:46:LEU:HD12	1.87	0.55
32:2a:403:C:O2'	35:2d:122:ARG:NH2	2.27	0.55
55:2x:40:C:H2'	55:2x:41:C:H6	1.71	0.55
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.87	0.55
32:1a:308:C:H2'	32:1a:309:G:H8	1.71	0.55
50:1s:19:VAL:O	50:1s:23:ASN:ND2	2.39	0.55
54:1w:54:5MU:O2	54:1w:58:A:N7	2.39	0.55
1:2A:892:G:H3'	1:2A:893:C:C5'	2.36	0.55
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.42	0.55
9:2N:38:HIS:CE1	9:2N:39:ARG:HG3	2.40	0.55
23:21:72:GLU:OE2	23:21:76:ARG:NH2	2.39	0.55
32:2a:434:U:H2'	32:2a:435:C:C6	2.40	0.55
32:2a:1288:A:N1	32:2a:1371:G:H1'	2.21	0.55
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.41	0.55
54:2w:8:4SU:HN3	54:2w:14:A:H62	1.55	0.55
1:1A:879:G:N1	1:1A:899:A:H1'	2.21	0.55
1:1A:2716:U:O2'	63:1A:4132:HOH:O	2.18	0.55
1:1A:2810:A:N6	1:1A:2891:G:O2'	2.33	0.55
32:1a:673:G:H2'	32:1a:674:G:C8	2.42	0.55
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.06	0.55
38:1g:74:GLU:HG2	38:1g:91:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:28:VAL:HG22	40:1i:63:ILE:HB	1.89	0.55
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.42	0.55
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.21	0.55
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.41	0.55
14:2S:10:ARG:NE	14:2S:91:PRO:O	2.37	0.55
26:24:61:ARG:HA	26:24:61:ARG:NE	2.19	0.55
32:2a:1142:G:H2'	32:2a:1143:G:O4'	2.06	0.55
1:1A:1223:G:N2	1:1A:1226:A:OP2	2.37	0.55
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.88	0.55
39:1h:25:ASP:OD2	39:1h:60:ARG:HG3	2.06	0.55
1:2A:2143:C:N4	1:2A:2148:G:H1	2.03	0.55
32:2a:866:C:O2'	32:2a:919:A:OP1	2.23	0.55
32:2a:1271:G:C2	32:2a:1272:G:N7	2.74	0.55
33:2b:16:HIS:HB2	33:2b:204:ASN:HD22	1.72	0.55
34:2c:34:LEU:HD21	34:2c:38:ARG:HH21	1.71	0.55
50:2s:13:ASP:HA	50:2s:16:LEU:HB3	1.88	0.55
1:1A:2106:G:H1	1:1A:2183:C:N4	2.05	0.55
32:1a:848:C:H2'	32:1a:849:C:H6	1.72	0.55
35:1d:119:GLN:HG2	35:1d:123:HIS:CD2	2.41	0.55
1:2A:1651:G:OP1	13:2R:40:LYS:NZ	2.40	0.55
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.39	0.55
7:2H:26:VAL:N	7:2H:33:LEU:O	2.37	0.55
34:2c:47:LEU:O	34:2c:51:GLY:N	2.36	0.55
36:2e:42:GLY:HA2	36:2e:65:ASN:O	2.06	0.55
38:2g:111:ARG:NH2	38:2g:126:ASP:OD2	2.39	0.55
44:2m:57:ARG:C	44:2m:59:TYR:H	2.15	0.55
48:2q:22:LEU:HD11	48:2q:39:SER:HB2	1.88	0.55
32:1a:343:U:O2'	32:1a:346:G:O6	2.18	0.55
33:1b:112:VAL:HG12	33:1b:149:LEU:HD23	1.89	0.55
1:2A:884:C:H3'	1:2A:885:C:C6	2.42	0.55
4:2E:50:GLY:HA3	4:2E:75:VAL:HG21	1.88	0.55
8:2I:66:GLU:HA	8:2I:69:LYS:HB3	1.88	0.55
1:1A:195:A:OP1	11:1P:46:LYS:NZ	2.39	0.55
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.42	0.55
32:1a:179:A:H2'	32:1a:180:U:H6	1.71	0.55
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.42	0.55
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.89	0.55
32:2a:737:A:H1'	37:2f:73:ASN:HD21	1.72	0.55
32:2a:911:U:O4	63:2a:1916:HOH:O	2.16	0.55
53:2v:23:A:H4'	53:2v:24:A:H5'	1.89	0.55
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:79:ASN:OD1	6:1G:79:ASN:N	2.39	0.55
21:1Z:72:ARG:NH2	21:1Z:97:GLU:O	2.39	0.55
32:1a:278:G:OP2	48:1q:92:ARG:NH2	2.39	0.55
32:1a:486:U:H2'	32:1a:487:A:H8	1.72	0.55
1:2A:879:G:H3'	1:2A:880:G:C8	2.41	0.55
1:2A:2060:A:N3	63:2A:4012:HOH:O	2.33	0.55
32:2a:572:A:OP1	63:2a:1921:HOH:O	2.18	0.55
32:2a:624:C:H2'	32:2a:625:G:C8	2.42	0.55
32:2a:1084:G:H5'	32:2a:1102:A:OP2	2.07	0.55
1:1A:2759:G:N7	63:1A:4203:HOH:O	2.33	0.55
32:1a:152:A:N6	32:1a:169:C:N3	2.55	0.55
48:1q:26:GLN:OE1	48:1q:37:LYS:NZ	2.28	0.55
1:2A:1340:U:OP1	19:2X:16:LYS:NZ	2.39	0.55
1:2A:2811:G:N2	1:2A:2891:G:H1'	2.21	0.55
32:2a:977:A:O2'	32:2a:980:C:N4	2.39	0.55
32:2a:1119:C:OP2	40:2i:9:ARG:NH2	2.40	0.55
32:2a:1263:C:C4	32:2a:1272:G:O6	2.59	0.55
33:2b:58:ILE:HA	33:2b:61:LEU:HB3	1.89	0.55
33:2b:187:LEU:HA	33:2b:201:ILE:HB	1.89	0.55
34:2c:44:GLU:HA	34:2c:52:LEU:HD23	1.89	0.55
39:2h:36:LEU:HA	39:2h:39:LEU:HB2	1.89	0.55
40:2i:9:ARG:HG2	40:2i:14:VAL:HG12	1.88	0.55
43:2l:77:LEU:HD21	43:2l:107:ALA:HB2	1.89	0.55
1:1A:271(J):C:O3'	1:1A:271(K):U:H3'	2.07	0.55
1:1A:1047:G:H2'	1:1A:1110:G:N2	2.21	0.55
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.89	0.55
1:2A:2751:G:H8	7:2H:2:SER:HB3	1.72	0.55
32:2a:920:U:H2'	32:2a:921:U:C6	2.42	0.55
32:2a:1151:A:O2'	32:2a:1152:A:H8	1.90	0.55
42:2k:18:ARG:NH2	42:2k:35:PRO:O	2.40	0.55
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.88	0.54
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.04	0.54
32:1a:376:G:H5''	47:1p:5:ARG:HB3	1.89	0.54
54:1w:63:C:H2'	54:1w:64:U:C6	2.42	0.54
1:2A:2471:C:N4	1:2A:2476:A:O2'	2.40	0.54
40:2i:3:GLN:HE21	40:2i:20:ARG:CZ	2.20	0.54
1:1A:1054:A:N1	1:1A:1105:U:O2	2.40	0.54
1:1A:2422:A:O4'	57:1y:76:A:N6	2.39	0.54
15:1T:112:ARG:HG3	15:1T:115:ARG:NH2	2.22	0.54
1:2A:125:G:O2'	29:27:48:LYS:HD2	2.07	0.54
1:2A:531:C:OP1	1:2A:561:G:N1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1026:U:OP1	63:2A:3914:HOH:O	2.17	0.54
26:24:61:ARG:HH11	26:24:61:ARG:HG3	1.71	0.54
32:2a:1003:G:H2'	32:2a:1004:A:O4'	2.07	0.54
32:2a:1029:C:C2	32:2a:1032:G:N2	2.70	0.54
38:2g:54:THR:O	38:2g:56:GLN:N	2.41	0.54
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.88	0.54
36:1e:6:PHE:HB3	36:1e:34:VAL:HG22	1.89	0.54
1:2A:890:A:H2'	1:2A:892:G:C8	2.42	0.54
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.43	0.54
15:2T:85:LYS:NZ	15:2T:87:ASP:OD2	2.40	0.54
1:1A:1671:U:O4	63:1A:4105:HOH:O	2.18	0.54
1:1A:2254:C:OP2	63:1A:4135:HOH:O	2.18	0.54
29:17:5:TRP:NE1	29:17:7:PRO:HG3	2.22	0.54
32:1a:376:G:O3'	47:1p:5:ARG:NH1	2.40	0.54
32:1a:559:A:P	36:1e:126:ARG:HH22	2.30	0.54
1:2A:500:G:N1	1:2A:503:A:OP2	2.41	0.54
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.43	0.54
1:2A:2396:G:O2'	63:2A:3946:HOH:O	2.19	0.54
32:2a:1126:U:H3	41:2j:40:LEU:HD11	1.73	0.54
38:2g:27:ILE:HA	38:2g:30:ILE:HD12	1.89	0.54
1:1A:1054:A:H3'	1:1A:1055:G:H8	1.73	0.54
1:1A:1076:C:O2'	1:1A:1077:A:N7	2.36	0.54
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.42	0.54
32:1a:576:G:O6	32:1a:880:C:O2'	2.22	0.54
32:1a:1109:C:OP2	34:1c:176:HIS:ND1	2.41	0.54
32:1a:1129:C:O2'	32:1a:1139:G:N7	2.35	0.54
39:1h:81:HIS:N	39:1h:138:TRP:O	2.40	0.54
40:1i:42:ARG:NH1	40:1i:71:SER:OG	2.39	0.54
44:1m:3:ARG:HD2	44:1m:9:ILE:HG12	1.89	0.54
1:2A:1226:A:OP1	17:2V:84:LYS:NZ	2.29	0.54
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.07	0.54
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.40	0.54
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.40	0.54
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.42	0.54
9:2N:12:ARG:HH21	9:2N:38:HIS:HE2	1.54	0.54
12:2Q:63:LYS:HG2	12:2Q:65:PHE:CE2	2.42	0.54
15:2T:30:VAL:HG22	15:2T:86:ILE:HG12	1.89	0.54
31:29:10:ILE:HD12	31:29:32:HIS:HA	1.89	0.54
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.21	0.54
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.73	0.54
33:2b:120:ALA:O	33:2b:122:PHE:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:13:LYS:HA	44:2m:44:ARG:CZ	2.37	0.54
1:2A:795:C:H2'	1:2A:796:C:C6	2.43	0.54
1:2A:1359:A:H2	1:2A:1372:U:O4	1.89	0.54
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.23	0.54
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.89	0.54
32:2a:570:G:H1'	32:2a:820:U:C4	2.42	0.54
32:2a:1456:G:N1	51:2t:51:GLU:OE2	2.40	0.54
1:1A:2155:G:H2'	1:1A:2155:G:N3	2.22	0.54
1:1A:2849:U:OP2	15:1T:95:ARG:NH1	2.41	0.54
39:1h:17:THR:O	39:1h:78:GLN:NE2	2.35	0.54
5:2F:40:GLN:HE22	5:2F:182:ASN:HB2	1.73	0.54
32:2a:540:G:H2'	32:2a:541:G:O4'	2.08	0.54
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.43	0.54
32:2a:1077:G:N2	32:2a:1080:A:OP2	2.36	0.54
32:2a:1239:A:H4'	32:2a:1240:U:H5''	1.89	0.54
57:2y:61:C:H2'	57:2y:62:C:C6	2.43	0.54
1:1A:897:C:N3	1:1A:898:C:N4	2.56	0.54
1:1A:2483:C:N3	12:1Q:124:LYS:NZ	2.52	0.54
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.41	0.54
1:2A:2136:C:O2'	1:2A:2137:C:H6	1.91	0.54
11:2P:55:ARG:HA	63:2P:201:HOH:O	2.06	0.54
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.41	0.54
32:2a:448:A:OP2	32:2a:485:G:N2	2.29	0.54
32:2a:539:A:H2'	32:2a:540:G:C8	2.43	0.54
32:2a:1239:A:H62	32:2a:1299:A:N6	2.05	0.54
35:2d:60:GLU:HG3	35:2d:202:LEU:HD12	1.90	0.54
1:1A:1701:A:OP2	63:1A:4134:HOH:O	2.18	0.54
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.42	0.54
1:1A:2406:U:H2'	1:1A:2406:U:OP2	2.07	0.54
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.21	0.54
6:1G:4:ASP:OD2	6:1G:9:ARG:NH1	2.41	0.54
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.43	0.54
32:2a:1347:G:H5''	40:2i:107:ARG:HB3	1.90	0.54
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.90	0.54
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.08	0.54
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.90	0.54
32:1a:161:A:H2'	32:1a:162:A:C8	2.43	0.54
57:1y:21:A:H2'	57:1y:22:G:C8	2.42	0.54
1:2A:855:G:H2'	1:2A:856:C:C6	2.42	0.54
6:2G:103:LEU:HA	6:2G:106:LEU:HB3	1.90	0.54
17:2V:64:HIS:ND1	17:2V:92:THR:OG1	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1071:C:H2'	32:2a:1072:G:H8	1.73	0.54
33:2b:82:ARG:HB3	33:2b:94:ASN:OD1	2.09	0.54
63:1A:5002:HOH:O	11:1P:44:GLY:HA2	2.08	0.53
32:1a:328:C:H4'	32:1a:329:A:H5''	1.90	0.53
35:1d:63:LYS:HD2	35:1d:198:VAL:HG12	1.90	0.53
35:1d:172:PRO:C	35:1d:174:LEU:H	2.15	0.53
49:1r:38:GLU:OE2	49:1r:41:LYS:NZ	2.33	0.53
1:2A:579:G:H2'	1:2A:580:C:C6	2.43	0.53
1:2A:744:G:OP1	4:2E:132:HIS:ND1	2.39	0.53
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.43	0.53
32:2a:7:G:H21	36:2e:121:LYS:HG2	1.73	0.53
32:2a:936:C:H2'	32:2a:937:A:O4'	2.08	0.53
32:2a:1065:U:H3	32:2a:1109:C:H5''	1.72	0.53
32:2a:1512:U:H2'	32:2a:1513:A:C8	2.43	0.53
32:1a:62:U:OP1	32:1a:385:C:O2'	2.25	0.53
32:1a:1086:U:H3	32:1a:1099:G:N2	2.06	0.53
32:1a:1262:C:H2'	32:1a:1263:C:H6	1.73	0.53
36:1e:105:VAL:HG21	36:1e:128:PRO:HB3	1.90	0.53
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.44	0.53
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.90	0.53
32:2a:1067:A:N3	32:2a:1068:G:H1'	2.23	0.53
44:2m:4:ILE:HG22	44:2m:57:ARG:HB2	1.89	0.53
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.41	0.53
32:1a:343:U:H1'	32:1a:347:G:N2	2.24	0.53
35:1d:110:PHE:CD2	35:1d:148:VAL:HG23	2.44	0.53
41:1j:11:PHE:HB3	45:1n:55:GLY:HA3	1.91	0.53
6:2G:111:LEU:HD21	6:2G:120:LEU:HD21	1.89	0.53
10:2O:71:ARG:NE	10:2O:105:GLU:OE2	2.41	0.53
32:2a:141:A:H1'	32:2a:182:U:O2	2.09	0.53
32:2a:1328:C:O2'	44:2m:29:ARG:NE	2.39	0.53
36:2e:84:PHE:O	36:2e:86:ALA:N	2.41	0.53
57:2y:42:C:H2'	57:2y:43:U:C6	2.43	0.53
36:1e:77:PRO:HD2	36:1e:142:LEU:HD13	1.91	0.53
1:2A:94(A):G:O3'	24:22:45:SER:OG	2.27	0.53
1:2A:212:G:H2'	1:2A:213:A:O4'	2.08	0.53
1:2A:2438:U:O2'	1:2A:2440:C:OP1	2.23	0.53
2:2B:7:G:N2	14:2S:38:GLN:HE22	1.99	0.53
26:14:58:ARG:NH2	50:1s:68:GLY:HA3	2.23	0.53
6:2G:19:LEU:HD22	6:2G:23:PHE:HE2	1.73	0.53
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.89	0.53
17:2V:8:GLY:O	17:2V:10:LYS:NZ	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:9:LEU:HD23	26:24:27:THR:HG23	1.89	0.53
32:2a:1135:U:H2'	32:2a:1137:C:N3	2.24	0.53
32:2a:1346:A:N1	32:2a:1374:A:H5''	2.24	0.53
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.43	0.53
1:1A:1721:G:H1'	1:1A:1741:A:H61	1.74	0.53
8:1I:101:LEU:HG	8:1I:107:VAL:HB	1.91	0.53
20:1Y:14:LEU:HB2	20:1Y:75:ILE:HD11	1.90	0.53
26:14:40:HIS:HB3	26:14:43:TYR:HD2	1.74	0.53
32:1a:456:C:H2'	32:1a:457:C:C6	2.43	0.53
34:1c:62:ASP:O	34:1c:97:LYS:HB3	2.08	0.53
42:1k:21:ILE:HB	42:1k:84:VAL:HG12	1.91	0.53
1:2A:731:C:OP1	63:2A:3945:HOH:O	2.19	0.53
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.07	0.53
26:24:46:GLN:C	26:24:48:ARG:H	2.16	0.53
32:2a:222:U:H2'	32:2a:223:U:C6	2.43	0.53
32:2a:1029:C:N4	32:2a:1032:G:C6	2.77	0.53
32:2a:1049:U:C5	32:2a:1201:A:H5'	2.44	0.53
32:2a:1323:G:O2'	32:2a:1362:C:O2'	2.27	0.53
35:2d:111:ALA:HB2	35:2d:120:LEU:HD22	1.90	0.53
36:2e:71:LEU:HD22	36:2e:115:VAL:HG23	1.90	0.53
1:1A:882:G:H4'	54:1w:18:G:C6	2.43	0.53
1:1A:889:C:O2'	1:1A:890:A:O4'	2.27	0.53
1:1A:1173:G:O2'	1:1A:1174:A:O4'	2.25	0.53
1:1A:1315:C:OP2	63:1A:4103:HOH:O	2.19	0.53
21:1Z:150:LEU:HD12	21:1Z:151:HIS:H	1.73	0.53
39:1h:119:LEU:HB3	39:1h:123:GLU:HB2	1.90	0.53
1:2A:981:A:N1	1:2A:2027:G:O2'	2.37	0.53
1:2A:2803:C:H5''	1:2A:2804:C:OP2	2.08	0.53
32:2a:619:U:N3	35:2d:134:ASP:OD1	2.32	0.53
32:2a:1371:G:N2	63:2a:1955:HOH:O	2.41	0.53
6:1G:145:THR:HG22	6:1G:147:ASP:H	1.74	0.53
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.40	0.53
37:1f:27:GLN:HA	37:1f:30:LEU:HD12	1.90	0.53
1:2A:184:C:H2'	1:2A:185:U:C6	2.44	0.53
1:2A:2136:C:N4	1:2A:2155:G:H1	2.05	0.53
8:2I:126:TYR:HB2	8:2I:142:VAL:HG23	1.91	0.53
31:29:2:LYS:HE2	31:29:31:LYS:O	2.09	0.53
32:2a:6:G:H4'	32:2a:298:A:H4'	1.91	0.53
1:1A:625:G:N7	11:1P:107:LYS:NZ	2.56	0.53
1:1A:2106:G:H1	1:1A:2183:C:H42	1.56	0.53
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.91	0.53
32:1a:160:A:H1'	32:1a:344:A:C5	2.44	0.53
32:1a:1293:G:H2'	32:1a:1294:G:C8	2.43	0.53
33:1b:126:GLU:HG3	33:1b:127:ILE:N	2.22	0.53
1:2A:586:A:N1	1:2A:809:G:O2'	2.37	0.53
1:2A:839:U:H2'	1:2A:840:C:C6	2.44	0.53
14:2S:25:ARG:NH1	14:2S:42:ASP:OD1	2.41	0.53
21:2Z:97:GLU:HB3	21:2Z:125:LEU:HD21	1.91	0.53
21:2Z:121:HIS:N	21:2Z:171:ILE:O	2.42	0.53
32:2a:157:G:H1	32:2a:164:U:H3	1.57	0.53
32:2a:728:A:H2'	32:2a:729:A:C8	2.44	0.53
41:2j:40:LEU:HB2	41:2j:69:ASN:HB2	1.91	0.53
42:2k:98:LEU:O	42:2k:101:SER:OG	2.26	0.53
47:2p:25:ARG:HH11	47:2p:25:ARG:HG3	1.74	0.53
57:2y:18:G:C2	57:2y:56:C:C4	2.97	0.53
57:2y:48:C:O2'	57:2y:49:G:OP2	2.17	0.53
1:1A:2105:C:H2'	1:1A:2106:G:C8	2.44	0.53
32:1a:977:A:H1'	32:1a:982:U:O4	2.09	0.53
32:1a:1228:C:OP1	44:1m:115:LYS:NZ	2.42	0.53
32:1a:1323:G:H2'	32:1a:1324:A:C8	2.44	0.53
53:1v:14:A:H3'	53:1v:15:A:H8	1.74	0.53
1:2A:489:G:N7	18:2W:49:LYS:NZ	2.57	0.53
32:2a:474:G:H2'	32:2a:475:G:H8	1.74	0.53
33:2b:76:GLN:NE2	33:2b:76:GLN:H	2.07	0.53
33:2b:121:LEU:HD21	33:2b:130:ARG:NH2	2.24	0.53
9:2N:35:ARG:O	9:2N:42:TRP:NE1	2.42	0.52
11:2P:138:LEU:HD23	11:2P:145:PRO:HB3	1.91	0.52
32:2a:742:G:P	46:2o:35:ARG:HH22	2.32	0.52
39:2h:42:GLU:HG3	39:2h:109:ILE:HD12	1.90	0.52
45:2n:23:ARG:NH1	45:2n:30:ALA:HB2	2.24	0.52
7:1H:97:ARG:NE	7:1H:104:GLU:OE1	2.36	0.52
32:2a:984:C:H2'	32:2a:985:C:H6	1.73	0.52
32:2a:986:A:H1'	50:2s:55:LYS:HA	1.92	0.52
32:2a:1251:A:H2'	32:2a:1252:A:C8	2.44	0.52
32:2a:1330:U:H4'	44:2m:23:TYR:CZ	2.45	0.52
33:2b:76:GLN:HB2	33:2b:208:ILE:HD11	1.91	0.52
34:2c:42:LEU:HA	34:2c:45:LYS:NZ	2.23	0.52
1:1A:907:U:HO2'	12:1Q:101:ARG:HH22	1.57	0.52
1:1A:1448:G:H4'	1:1A:1542:A:OP1	2.09	0.52
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.36	0.52
1:2A:271(D):G:H1	1:2A:271(T):C:H42	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.44	0.52
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.09	0.52
1:2A:2163:C:OP1	1:2A:2165:G:N2	2.43	0.52
1:2A:2277:G:OP2	22:20:10:THR:HG21	2.10	0.52
21:2Z:31:ARG:HH11	21:2Z:94:GLU:HG2	1.75	0.52
21:2Z:51:ALA:O	21:2Z:52:SER:HB3	2.09	0.52
26:24:14:ILE:HB	26:24:22:ILE:HD13	1.91	0.52
32:2a:157:G:H2'	32:2a:158:G:H8	1.74	0.52
32:2a:999:C:N4	32:2a:1042:G:H1	2.06	0.52
32:2a:1006:C:H2'	32:2a:1007:C:C6	2.43	0.52
32:2a:1235:U:O2'	32:2a:1305:G:O5'	2.27	0.52
33:2b:134:GLU:O	33:2b:138:LEU:HD22	2.09	0.52
41:2j:63:PHE:HE1	45:2n:58:LYS:HG2	1.73	0.52
1:1A:247:G:H4'	1:1A:386:G:C5	2.44	0.52
1:1A:639:U:H2'	1:1A:640:C:C6	2.45	0.52
1:1A:1069:A:O2'	1:1A:1072:C:OP1	2.24	0.52
1:1A:1769:G:O2'	1:1A:1958:C:OP1	2.23	0.52
26:14:53:GLU:HB2	26:14:55:ARG:O	2.09	0.52
1:2A:302:C:OP2	20:2Y:73:ARG:NH1	2.40	0.52
1:2A:324:A:N6	1:2A:338:G:O2'	2.42	0.52
1:2A:890:A:H2'	1:2A:892:G:H8	1.74	0.52
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.26	0.52
1:2A:1721:G:H8	1:2A:1741:A:H62	1.57	0.52
1:2A:2360:A:H2'	1:2A:2361:A:O4'	2.08	0.52
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.45	0.52
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.91	0.52
32:2a:1316:G:N2	32:2a:1318:A:H3'	2.23	0.52
34:2c:155:GLY:O	34:2c:157:ILE:N	2.43	0.52
48:2q:45:HIS:CD2	48:2q:47:PRO:HG3	2.44	0.52
1:1A:1359:A:H2'	1:1A:1360:A:H5'	1.90	0.52
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.45	0.52
18:1W:18:ARG:HG3	18:1W:76:VAL:HB	1.90	0.52
20:1Y:6:HIS:H	20:1Y:6:HIS:CD2	2.25	0.52
32:1a:953:G:H2'	32:1a:954:G:O4'	2.10	0.52
32:1a:1037:C:H2'	32:1a:1038:C:C6	2.45	0.52
33:1b:24:TRP:HZ3	33:1b:29:ALA:HB2	1.73	0.52
44:1m:19:LEU:HD11	44:1m:56:LEU:HD21	1.92	0.52
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.74	0.52
1:2A:455:C:N3	1:2A:472:A:H2'	2.23	0.52
1:2A:2189:U:H2'	1:2A:2190:G:H8	1.73	0.52
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:58:ARG:NH1	63:2E:402:HOH:O	2.43	0.52
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.45	0.52
32:2a:1518:MA6:H8	32:2a:1518:MA6:O5'	2.08	0.52
35:2d:187:ARG:NH1	35:2d:190:ASP:OD2	2.43	0.52
36:2e:106:PRO:O	36:2e:110:LEU:HG	2.09	0.52
38:2g:38:LEU:O	38:2g:42:ILE:HG12	2.10	0.52
1:1A:952:G:OP1	12:1Q:16:ARG:NH2	2.42	0.52
11:1P:39:LYS:HB2	11:1P:45:LEU:HD13	1.91	0.52
40:1i:4:TYR:CD1	40:1i:88:TYR:HA	2.45	0.52
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.45	0.52
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.44	0.52
1:2A:2252:G:H2'	1:2A:2253:G:O4'	2.10	0.52
32:2a:1352:C:H2'	32:2a:1353:G:C8	2.45	0.52
32:2a:1360:A:OP2	45:2n:35:ARG:NH2	2.42	0.52
36:2e:20:GLN:HE21	36:2e:21:ALA:N	2.08	0.52
49:2r:63:GLN:HE21	49:2r:63:GLN:HA	1.75	0.52
1:1A:185:U:H4'	1:1A:218:A:H4'	1.92	0.52
23:11:23:LYS:HB2	57:1y:74:C:H4'	1.91	0.52
32:1a:676:A:H1'	42:1k:115:PRO:HB3	1.92	0.52
36:1e:41:VAL:HG23	36:1e:67:VAL:HG13	1.91	0.52
36:1e:85:GLY:C	36:1e:87:SER:H	2.18	0.52
37:1f:89:MET:HE1	49:1r:72:ARG:HB3	1.92	0.52
1:2A:878:A:H61	1:2A:899:A:H1'	1.75	0.52
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.45	0.52
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.44	0.52
32:2a:110:C:O2'	47:2p:25:ARG:O	2.25	0.52
36:2e:83:GLU:HA	36:2e:88:LYS:HA	1.92	0.52
39:2h:124:ALA:O	39:2h:128:GLY:N	2.42	0.52
57:2y:2:C:H2'	57:2y:3:G:C8	2.45	0.52
1:1A:593:G:H4'	30:18:4:MET:HE2	1.91	0.52
32:1a:1148:U:H2'	32:1a:1149:C:O4'	2.10	0.52
32:1a:1239:A:H62	32:1a:1299:A:N6	2.08	0.52
35:1d:8:VAL:HG22	35:1d:21:LEU:HD13	1.90	0.52
1:2A:2131:G:OP2	1:2A:2131:G:N2	2.39	0.52
6:2G:15:VAL:HG13	6:2G:175:LEU:HD23	1.92	0.52
16:2U:52:ARG:HA	16:2U:55:ARG:HD3	1.92	0.52
32:2a:1002:G:C6	32:2a:1003:G:H8	2.28	0.52
32:2a:1010:G:H2'	32:2a:1011:G:C8	2.45	0.52
35:2d:8:VAL:HG22	35:2d:21:LEU:HD13	1.92	0.52
47:2p:58:TYR:O	47:2p:61:SER:OG	2.20	0.52
55:2x:50:U:H2'	55:2x:51:C:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:232:G:H1'	32:1a:262:A:N1	2.25	0.52
32:1a:877:C:OP1	39:1h:88:LYS:NZ	2.28	0.52
32:1a:1152:A:OP1	41:1j:68:HIS:ND1	2.43	0.52
35:1d:178:VAL:C	35:1d:180:GLY:H	2.17	0.52
8:2I:78:THR:HA	8:2I:143:SER:HB3	1.92	0.52
21:2Z:5:LEU:HB2	21:2Z:47:VAL:HG21	1.92	0.52
32:2a:6:G:N1	36:2e:98:THR:HG21	2.25	0.52
32:2a:108:G:C6	51:2t:15:ARG:HG2	2.45	0.52
32:2a:890:G:O2'	32:2a:906:G:O6	2.27	0.52
32:2a:1295:G:O2'	44:2m:14:ARG:NH1	2.43	0.52
32:2a:1328:C:OP1	52:2u:21:TYR:OH	2.14	0.52
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.78	0.52
33:2b:44:LEU:O	33:2b:47:THR:HG22	2.10	0.52
34:2c:13:GLY:HA3	45:2n:57:ARG:HH12	1.75	0.52
47:2p:28:ARG:HG2	47:2p:29:ASP:OD1	2.10	0.52
7:1H:20:ALA:HB3	7:1H:23:ARG:HG3	1.91	0.52
28:16:12:GLU:OE1	28:16:52:VAL:HG11	2.10	0.52
32:1a:1402:4OC:HM22	32:1a:1403:C:H5'	1.92	0.52
32:1a:1456:G:O3'	51:1t:39:LYS:NZ	2.43	0.52
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.92	0.52
33:1b:98:LEU:HD22	33:1b:101:MET:HE3	1.92	0.52
33:1b:109:SER:O	33:1b:112:VAL:HG22	2.10	0.52
1:2A:2188:C:H5'	1:2A:2189:U:OP2	2.10	0.52
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.73	0.52
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.44	0.52
19:2X:94:GLY:H	19:2X:95:LEU:HB2	1.75	0.52
25:23:4:LEU:N	25:23:37:LEU:O	2.42	0.52
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.92	0.52
47:2p:22:THR:HA	47:2p:33:ILE:HG13	1.92	0.52
55:2x:58:A:H4'	55:2x:59:A:OP1	2.10	0.52
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.10	0.51
32:1a:219:C:H2'	32:1a:220:G:O4'	2.10	0.51
32:1a:903:G:OP1	63:1a:1912:HOH:O	2.19	0.51
34:1c:7:PRO:O	34:1c:11:ARG:NH1	2.41	0.51
39:1h:73:ASP:OD1	39:1h:75:ARG:NE	2.42	0.51
33:2b:120:ALA:O	33:2b:125:PRO:HD2	2.10	0.51
39:2h:28:ALA:HB3	39:2h:57:PRO:HB2	1.91	0.51
40:2i:18:PHE:HD2	40:2i:62:TYR:HD2	1.58	0.51
43:2l:117:ARG:NE	43:2l:123:LYS:O	2.42	0.51
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.45	0.51
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.45	0.51
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.91	0.51
7:1H:101:ARG:HH22	7:1H:122:THR:HA	1.72	0.51
21:1Z:156:LYS:HD2	21:1Z:158:PRO:HD3	1.92	0.51
26:14:15:ILE:HG13	26:14:21:VAL:HG22	1.92	0.51
32:1a:183:G:N7	63:1a:1931:HOH:O	2.34	0.51
32:1a:783:C:OP1	32:1a:1515:C:O2'	2.27	0.51
1:2A:910:A:N3	1:2A:2264:C:O2'	2.36	0.51
32:2a:196:A:OP1	51:2t:68:LYS:NZ	2.27	0.51
32:2a:696:A:N1	32:2a:797:C:O2'	2.38	0.51
32:2a:719:C:N4	49:2r:71:LYS:HE2	2.25	0.51
32:2a:1292:U:H2'	32:2a:1293:G:H8	1.73	0.51
39:2h:12:ARG:HD3	39:2h:26:VAL:HG12	1.93	0.51
41:2j:31:GLY:HA3	41:2j:81:THR:OG1	2.10	0.51
1:1A:630:G:OP1	30:18:47:LYS:NZ	2.33	0.51
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.45	0.51
5:1F:185:ASP:OD1	5:1F:188:ARG:NH1	2.35	0.51
32:1a:458:C:H2'	32:1a:460:G:O4'	2.11	0.51
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.45	0.51
34:1c:21:ARG:HG3	34:1c:58:GLU:HG3	1.93	0.51
44:1m:78:ILE:HG22	44:1m:82:MET:HE2	1.91	0.51
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.92	0.51
1:2A:2108:C:O2	1:2A:2182:G:N2	2.44	0.51
1:2A:2126:A:N3	1:2A:2127:G:H1'	2.25	0.51
7:2H:80:SER:OG	7:2H:81:GLU:N	2.42	0.51
22:20:63:VAL:HG21	22:20:83:PRO:HG3	1.92	0.51
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.92	0.51
32:2a:1264:C:N4	32:2a:1265:G:O6	2.44	0.51
32:2a:1323:G:HO2'	32:2a:1362:C:HO2'	1.55	0.51
33:2b:16:HIS:CB	33:2b:210:SER:HB2	2.39	0.51
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.45	0.51
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.11	0.51
32:1a:222:U:H2'	32:1a:223:U:C6	2.46	0.51
34:1c:148:GLY:HA3	34:1c:172:ARG:H	1.75	0.51
37:1f:2:ARG:HD2	37:1f:69:GLU:HB3	1.93	0.51
57:1y:48:C:HO2'	57:1y:49:G:P	2.34	0.51
1:2A:61:G:H5'	24:22:50:ILE:HG21	1.92	0.51
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.74	0.51
4:2E:48:GLN:NE2	4:2E:78:LEU:HD13	2.26	0.51
26:24:13:ARG:HG3	26:24:23:GLU:HA	1.92	0.51
33:2b:80:ILE:HD12	33:2b:84:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:156:ARG:NE	34:2c:160:ALA:O	2.36	0.51
40:2i:18:PHE:O	40:2i:61:ALA:HA	2.11	0.51
40:2i:55:ALA:HA	40:2i:58:HIS:HD2	1.74	0.51
43:2l:32:PHE:HB3	43:2l:84:LEU:HD21	1.92	0.51
51:2t:50:GLU:HB2	51:2t:99:LEU:HD22	1.93	0.51
57:2y:58:A:H1'	57:2y:60:U:OP2	2.10	0.51
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.09	0.51
2:1B:66:A:H61	2:1B:108:U:H2'	1.75	0.51
21:1Z:132:ASN:N	21:1Z:132:ASN:OD1	2.43	0.51
28:16:26:ASN:HD21	28:16:28:ARG:NH2	2.08	0.51
32:1a:45:U:H2'	32:1a:46:G:C8	2.46	0.51
32:1a:877:C:H5''	39:1h:88:LYS:HD3	1.92	0.51
32:1a:1243:C:H2'	32:1a:1244:C:C6	2.46	0.51
36:1e:16:THR:OG1	36:1e:17:ALA:N	2.44	0.51
51:1t:71:THR:HG22	51:1t:72:LEU:HD13	1.92	0.51
1:2A:774:A:H2'	1:2A:774:A:N3	2.25	0.51
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.10	0.51
1:2A:2334:G:H5'	14:2S:9:ARG:HG2	1.92	0.51
1:2A:2336:A:H61	22:20:43:THR:HG22	1.75	0.51
6:2G:138:GLN:OE1	6:2G:153:ARG:N	2.41	0.51
19:2X:1:MET:N	24:22:29:LYS:HE3	2.25	0.51
32:2a:129(A):G:C6	32:2a:189(E):U:H4'	2.46	0.51
34:2c:148:GLY:HA3	34:2c:172:ARG:O	2.11	0.51
34:2c:173:VAL:HG12	34:2c:175:LEU:HD21	1.93	0.51
35:2d:119:GLN:HG2	35:2d:123:HIS:HD2	1.71	0.51
49:2r:58:LEU:HD22	49:2r:62:GLU:HB3	1.93	0.51
57:2y:40:C:H2'	57:2y:41:U:C6	2.45	0.51
1:1A:295:G:H4'	20:1Y:1:MET:HE3	1.93	0.51
1:1A:1041:C:H42	1:1A:1114:G:H1	1.57	0.51
1:1A:1093:G:H3'	1:1A:1094:U:H5''	1.92	0.51
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.25	0.51
8:1I:93:THR:H	8:1I:96:ASP:HB2	1.76	0.51
9:1N:73:THR:HB	9:1N:82:LEU:HD11	1.92	0.51
12:1Q:78:PRO:HG2	12:1Q:81:VAL:HG11	1.93	0.51
12:1Q:89:ASN:HB2	55:1x:1:C:N3	2.25	0.51
21:1Z:136:PHE:O	21:1Z:137:ILE:HG13	2.11	0.51
28:16:14:THR:HB	28:16:48:VAL:O	2.10	0.51
32:1a:1529:G:H4'	32:1a:1530:G:OP2	2.10	0.51
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.46	0.51
1:2A:2127:G:N2	1:2A:2161:C:C2	2.79	0.51
3:2D:133:LEU:HB3	3:2D:173:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:33:VAL:HG22	26:24:34:GLU:H	1.75	0.51
32:2a:448:A:P	32:2a:485:G:H22	2.31	0.51
32:2a:473:G:H2'	32:2a:474:G:H8	1.75	0.51
32:2a:1517:G:H2'	32:2a:1518:MA6:H8	1.92	0.51
33:2b:146:GLN:O	33:2b:150:SER:HB3	2.11	0.51
34:2c:30:ARG:HH21	45:2n:38:GLY:HA2	1.75	0.51
40:2i:5:TYR:O	40:2i:87:GLN:NE2	2.44	0.51
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.10	0.51
40:1i:50:LEU:HD13	40:1i:56:LEU:HA	1.92	0.51
44:1m:75:ALA:O	44:1m:79:LYS:HB2	2.11	0.51
47:1p:20:VAL:HG21	47:1p:32:TYR:CD2	2.45	0.51
1:2A:271(A):A:N1	1:2A:272(D):G:O2'	2.43	0.51
1:2A:800:A:H8	1:2A:800:A:OP1	1.94	0.51
1:2A:1241:A:OP2	63:2A:3949:HOH:O	2.19	0.51
1:2A:2136:C:N4	1:2A:2155:G:N1	2.59	0.51
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.11	0.51
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	1.91	0.51
21:2Z:54:HIS:HB3	21:2Z:101:PRO:HD3	1.91	0.51
32:2a:975:A:H5''	32:2a:1363(A):A:N6	2.25	0.51
32:2a:1005:A:H1'	32:2a:1025:U:H3	1.75	0.51
34:2c:6:HIS:HB3	45:2n:49:HIS:ND1	2.26	0.51
34:2c:70:VAL:O	34:2c:106:VAL:N	2.40	0.51
1:1A:800:A:H8	1:1A:800:A:OP1	1.94	0.51
6:1G:77:ILE:HD12	6:1G:82:LEU:HD12	1.92	0.51
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.44	0.51
45:1n:21:TYR:OH	45:1n:23:ARG:NH2	2.42	0.51
57:1y:4:G:C2	57:1y:5:G:H1'	2.46	0.51
1:2A:479:A:N3	1:2A:481:G:H5''	2.26	0.51
1:2A:2507:C:H5''	1:2A:2573:C:N4	2.26	0.51
5:2F:116:ASP:O	5:2F:120:GLU:HG2	2.11	0.51
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.76	0.51
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.93	0.51
26:24:64:GLY:C	26:24:66:SER:H	2.18	0.51
26:14:20:ASN:OD1	26:14:21:VAL:N	2.44	0.51
32:1a:377:G:OP1	47:1p:3:LYS:HD3	2.11	0.51
32:1a:828:A:H2'	32:1a:829:G:O4'	2.11	0.51
32:1a:1179:A:H4'	40:1i:103:THR:HA	1.93	0.51
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.46	0.51
35:1d:15:GLU:OE2	35:1d:66:ARG:NH1	2.44	0.51
1:2A:709:U:H2'	1:2A:710:G:C8	2.46	0.51
1:2A:881:G:C2	1:2A:882:G:H1'	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1300:U:H4'	1:2A:1301:A:H5'	1.93	0.51
1:2A:2122:U:H3	1:2A:2176:A:H61	1.59	0.51
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.43	0.51
12:2Q:34:LEU:HD11	12:2Q:129:THR:HB	1.93	0.51
32:2a:1037:C:H2'	32:2a:1038:C:C6	2.45	0.51
32:2a:1208:C:H2'	32:2a:1209:C:H6	1.75	0.51
32:2a:1376:U:OP1	38:2g:98:SER:OG	2.23	0.51
49:2r:52:PRO:HB2	49:2r:54:ARG:HG2	1.93	0.51
57:2y:14:A:H3'	57:2y:15:A:H5''	1.93	0.51
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.46	0.51
32:1a:1194:U:H4'	36:1e:22:GLY:HA2	1.93	0.51
32:1a:1367:C:H5'	41:1j:60:ARG:NH1	2.26	0.51
1:2A:84:A:H5''	20:2Y:8:LYS:HE3	1.92	0.51
1:2A:602:G:O2'	1:2A:655:A:N6	2.43	0.51
1:2A:1446:C:H42	1:2A:1465:G:H1	1.58	0.51
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.11	0.51
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.25	0.51
5:2F:156:LEU:HA	5:2F:193:VAL:HG23	1.91	0.51
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.50	0.51
19:2X:53:LYS:HB2	19:2X:82:GLN:HB3	1.92	0.51
32:2a:1479:C:H2'	32:2a:1480:G:C8	2.45	0.51
33:2b:74:LYS:HG2	33:2b:75:LYS:H	1.76	0.51
35:2d:173:TRP:CD2	35:2d:189:PRO:HB3	2.46	0.51
40:2i:9:ARG:HG2	40:2i:14:VAL:HA	1.93	0.51
44:2m:10:PRO:HB2	44:2m:13:LYS:HD2	1.93	0.51
44:2m:23:TYR:O	44:2m:67:GLU:N	2.36	0.51
57:2y:6:C:H2'	57:2y:7:G:C8	2.46	0.51
1:1A:579:G:OP1	63:1A:4137:HOH:O	2.19	0.50
1:1A:1012:U:C5	9:1N:28:THR:HG21	2.46	0.50
16:1U:104:GLN:HE21	16:1U:105:VAL:HG23	1.76	0.50
44:1m:34:LEU:HD13	44:1m:41:PRO:HA	1.93	0.50
54:1w:50:A:H61	54:1w:64:U:H3	1.60	0.50
1:2A:446:G:OP1	16:2U:3:ARG:NH1	2.44	0.50
1:2A:1664:A:H2	10:2O:1:MET:HE1	1.75	0.50
1:2A:2724:C:OP1	4:2E:118:LYS:NZ	2.36	0.50
16:2U:85:LYS:HD3	16:2U:117:GLN:HB3	1.92	0.50
1:1A:2122:U:O4	1:1A:2176:A:N1	2.44	0.50
3:1D:71:ASP:HB3	3:1D:103:ARG:HH22	1.77	0.50
6:1G:56:ALA:HA	6:1G:59:GLU:HG2	1.91	0.50
32:1a:501:C:H2'	32:1a:502:G:C8	2.47	0.50
35:1d:155:LEU:H	35:1d:158:ILE:HD11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1f:100:ASN:HB2	49:1r:28:GLU:HA	1.93	0.50
41:1j:7:LYS:HE3	41:1j:40:LEU:HD13	1.93	0.50
3:2D:121:PRO:HB3	3:2D:135:PHE:CE2	2.46	0.50
16:2U:79:PHE:CZ	16:2U:83:LEU:HD11	2.47	0.50
32:2a:189(C):C:H2'	32:2a:189(D):C:O4'	2.11	0.50
32:2a:736:C:H2'	32:2a:737:A:C8	2.46	0.50
32:2a:755:G:OP2	46:2o:65:ARG:HD2	2.11	0.50
32:2a:1064:G:O6	32:2a:1191:A:N6	2.43	0.50
1:1A:870:A:OP1	12:1Q:6:ARG:NH1	2.45	0.50
1:1A:1474:C:H2'	1:1A:1475:G:H8	1.76	0.50
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.10	0.50
11:1P:38:GLN:O	11:1P:39:LYS:HB3	2.11	0.50
17:1V:60:GLU:HB2	17:1V:97:LYS:HE2	1.93	0.50
35:1d:108:LEU:HD13	35:1d:183:GLY:HA3	1.93	0.50
49:1r:63:GLN:HA	49:1r:63:GLN:HE21	1.77	0.50
1:2A:307:G:N1	1:2A:310:A:OP2	2.39	0.50
9:2N:30:ILE:O	9:2N:34:LEU:HG	2.12	0.50
15:2T:91:ARG:HB2	15:2T:121:ILE:HG13	1.93	0.50
21:2Z:28:MET:HE1	21:2Z:61:LEU:HD11	1.92	0.50
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.26	0.50
32:2a:203:U:H2'	32:2a:203:U:OP2	2.11	0.50
32:2a:779:C:H2'	32:2a:780:A:O4'	2.12	0.50
32:2a:967:5MC:H2'	32:2a:968:A:C8	2.46	0.50
32:2a:1159:U:O4'	32:2a:1182:G:N2	2.45	0.50
36:2e:71:LEU:O	36:2e:72:GLN:NE2	2.41	0.50
1:1A:887:A:H2	1:1A:889:C:H3'	1.77	0.50
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.12	0.50
1:1A:2101:G:H1	1:1A:2188:C:N4	2.08	0.50
1:1A:2627:G:O2'	1:1A:2781:A:N1	2.38	0.50
5:1F:129:PHE:CD2	5:1F:163:VAL:HG21	2.47	0.50
19:1X:60:ARG:HH12	29:17:47:ARG:HH22	1.58	0.50
32:1a:507:C:OP2	32:1a:508:C:O2'	2.24	0.50
48:1q:58:GLU:HG3	48:1q:77:VAL:HG21	1.92	0.50
1:2A:657:U:H2'	1:2A:658:C:C6	2.47	0.50
1:2A:1012:U:H5	9:2N:28:THR:HG21	1.74	0.50
1:2A:1019:U:OP1	1:2A:1035:U:O2'	2.19	0.50
32:2a:179:A:H2'	32:2a:180:U:C6	2.46	0.50
32:2a:246:A:N1	32:2a:278:G:O2'	2.42	0.50
32:2a:974:A:P	45:2n:41:ARG:HH21	2.35	0.50
8:1I:38:LEU:H	8:1I:38:LEU:CD2	2.23	0.50
32:1a:13:U:OP1	63:1a:1913:HOH:O	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:22:TRP:CZ2	45:1n:54:PRO:HG2	2.46	0.50
49:1r:43:PHE:C	49:1r:51:LEU:HD12	2.36	0.50
1:2A:811:U:H2'	11:2P:21:ARG:HA	1.94	0.50
1:2A:2099:U:H3	1:2A:2190:G:H1	1.60	0.50
7:2H:88:LEU:HD22	7:2H:165:ALA:HA	1.92	0.50
15:2T:96:ARG:HG2	15:2T:98:LYS:O	2.12	0.50
19:2X:26:TYR:HB3	19:2X:92:LEU:HD12	1.93	0.50
22:20:14:ARG:NH1	63:20:201:HOH:O	2.45	0.50
24:22:25:VAL:HG13	24:22:57:ILE:HG23	1.92	0.50
32:2a:1040:U:H2'	32:2a:1041:A:C8	2.42	0.50
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.46	0.50
33:2b:68:ILE:HG22	33:2b:90:MET:HG3	1.92	0.50
1:1A:1045:A:OP1	1:1A:1045:A:H4'	2.11	0.50
1:1A:2136:C:C2	1:1A:2155:G:N2	2.79	0.50
7:1H:88:LEU:HD12	7:1H:130:ARG:HG3	1.92	0.50
21:1Z:45:ASP:O	21:1Z:49:ARG:HB2	2.12	0.50
24:12:65:ASN:ND2	24:12:69:ARG:HH11	2.08	0.50
32:1a:757:U:H2'	32:1a:758:G:O4'	2.12	0.50
32:1a:1521:G:N3	63:1a:1942:HOH:O	2.35	0.50
36:1e:52:PRO:HG2	36:1e:53:LEU:HD12	1.93	0.50
1:2A:323:G:O2'	1:2A:1205:U:N3	2.38	0.50
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.11	0.50
1:2A:2540:C:O2'	1:2A:2740:A:N3	2.43	0.50
4:2E:5:LEU:HD21	4:2E:79:ARG:HB2	1.92	0.50
8:2I:3:VAL:HG12	8:2I:38:LEU:HA	1.93	0.50
26:24:61:ARG:NH2	26:24:62:ARG:O	2.45	0.50
32:2a:23:C:H5	32:2a:561:U:O4	1.95	0.50
32:2a:1089:G:H1	32:2a:1096:C:H42	1.59	0.50
40:2i:4:TYR:HB2	40:2i:19:LEU:HB2	1.92	0.50
40:2i:15:ALA:HB2	40:2i:65:VAL:HG23	1.92	0.50
1:1A:272(G):C:H42	1:1A:363(C):G:H1	1.59	0.50
1:1A:2134:A:O2'	1:1A:2135:A:OP1	2.27	0.50
32:1a:972:C:O2'	41:1j:55:LYS:O	2.29	0.50
32:1a:974:A:OP2	45:1n:29:ARG:NH2	2.42	0.50
1:2A:2165:G:H2'	1:2A:2166:G:H5''	1.93	0.50
5:2F:126:VAL:HG21	5:2F:129:PHE:CZ	2.47	0.50
10:2O:2:ILE:HB	10:2O:33:ALA:HB3	1.94	0.50
11:2P:81:GLN:NE2	11:2P:105:LEU:O	2.42	0.50
28:26:13:CYS:SG	28:26:47:THR:HG21	2.52	0.50
32:2a:444:C:H2'	32:2a:445:G:H8	1.77	0.50
32:2a:728:A:N7	46:2o:54:ARG:HD3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:913:A:OP1	43:2l:46:LYS:NZ	2.42	0.50
54:2w:29:A:H2'	54:2w:30:G:C8	2.47	0.50
1:1A:1039:G:H1	1:1A:1116:C:H42	1.60	0.50
34:1c:19:GLU:HG2	34:1c:54:ARG:CZ	2.42	0.50
35:1d:10:ARG:HB2	35:1d:40:PRO:HG3	1.94	0.50
35:1d:118:ARG:HG3	35:1d:136:PRO:HB3	1.93	0.50
36:1e:142:LEU:O	36:1e:143:ARG:NH1	2.43	0.50
37:1f:69:GLU:H	37:1f:69:GLU:CD	2.20	0.50
38:1g:106:GLN:O	38:1g:110:GLN:HG2	2.11	0.50
51:1t:43:LEU:HA	51:1t:46:GLU:HB2	1.92	0.50
1:2A:1038:C:H42	1:2A:1117:G:H1	1.59	0.50
1:2A:2127:G:N2	1:2A:2161:C:N3	2.60	0.50
1:2A:2130:U:H3	1:2A:2159:G:H1	1.60	0.50
4:2E:48:GLN:HE21	4:2E:78:LEU:HD22	1.76	0.50
19:2X:5:TYR:CE1	24:22:30:ARG:HG3	2.46	0.50
32:2a:376:G:H5''	47:2p:5:ARG:HB2	1.93	0.50
38:2g:113:GLU:HB3	38:2g:118:VAL:HG23	1.92	0.50
40:2i:17:VAL:HG11	40:2i:81:ILE:HG13	1.92	0.50
1:1A:668:G:H5'	1:1A:669:G:OP2	2.11	0.50
1:1A:1065:U:H5''	1:1A:1066:U:OP2	2.11	0.50
1:1A:1421:G:N2	1:1A:1495:A:N1	2.58	0.50
1:1A:1474:C:H2'	1:1A:1475:G:C8	2.46	0.50
15:1T:127:ALA:C	15:1T:129:ARG:H	2.20	0.50
1:2A:55:G:O2'	1:2A:127:A:N1	2.40	0.50
1:2A:1364:G:P	23:21:3:LYS:HG3	2.52	0.50
1:2A:1506:C:H2'	1:2A:1507:A:H5'	1.94	0.50
1:2A:2112:G:O6	57:2y:18:G:N2	2.44	0.50
8:2I:75:LEU:HD13	8:2I:105:HIS:CD2	2.47	0.50
32:2a:15:G:H21	36:2e:18:ARG:HA	1.77	0.50
32:2a:1194:U:H2'	32:2a:1195:C:C6	2.47	0.50
32:2a:1279:A:O2'	32:2a:1281:U:OP2	2.24	0.50
35:2d:22:LYS:O	35:2d:113:SER:HB3	2.12	0.50
1:1A:1226:A:OP1	17:1V:84:LYS:NZ	2.40	0.49
1:1A:2097:C:H2'	1:1A:2098:U:C6	2.47	0.49
1:1A:2417:C:OP1	11:1P:65:ARG:NH2	2.45	0.49
1:1A:2791:C:H2'	1:1A:2792:G:H8	1.76	0.49
32:1a:8:A:N7	35:1d:208:SER:OG	2.45	0.49
32:1a:501:C:H2'	32:1a:502:G:H8	1.77	0.49
32:1a:983:A:H1'	32:1a:1049:U:O2	2.12	0.49
33:1b:145:LEU:HD23	33:1b:149:LEU:HD13	1.93	0.49
35:1d:81:GLU:O	35:1d:85:LYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.12	0.49
1:2A:2136:C:N3	1:2A:2155:G:N2	2.53	0.49
2:2B:24:G:H4'	2:2B:25:A:C8	2.46	0.49
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.42	0.49
7:2H:87:LEU:N	7:2H:131:VAL:O	2.40	0.49
11:2P:118:GLY:O	11:2P:137:LYS:NZ	2.42	0.49
32:2a:1058:G:OP1	34:2c:199:LYS:NZ	2.45	0.49
51:2t:16:HIS:O	51:2t:19:SER:OG	2.20	0.49
1:1A:764:A:H5'	3:1D:210:GLY:CA	2.41	0.49
1:1A:910:A:N1	1:1A:2277:G:H1'	2.27	0.49
1:1A:1074:G:C2	1:1A:1075:C:H1'	2.47	0.49
1:1A:1721:G:H1'	1:1A:1741:A:N6	2.27	0.49
1:1A:2611:U:C4	27:15:3:LYS:HG2	2.47	0.49
25:13:26:LEU:O	25:13:35:ARG:NE	2.35	0.49
32:1a:190:U:H2'	32:1a:191:G:H8	1.76	0.49
54:1w:4:G:H2'	54:1w:5:G:H5'	1.94	0.49
4:2E:18:ASP:HB3	15:2T:82:LEU:HD21	1.94	0.49
6:2G:11:TYR:HB2	6:2G:176:LEU:HD21	1.93	0.49
32:2a:1132:C:N4	32:2a:1133:G:O6	2.44	0.49
36:2e:105:VAL:HB	36:2e:106:PRO:HD3	1.93	0.49
37:2f:44:GLY:HA2	37:2f:59:TYR:CE1	2.47	0.49
42:2k:61:ALA:HB1	42:2k:94:ALA:HB2	1.92	0.49
1:1A:671:C:N4	63:1A:4310:HOH:O	2.45	0.49
1:1A:1092:C:C2'	1:1A:1093:G:H5'	2.43	0.49
1:1A:2712:U:OP1	1:1A:2714:G:H4'	2.11	0.49
1:1A:2751:G:H4'	7:1H:4:ILE:HD11	1.93	0.49
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.76	0.49
32:1a:1262:C:H2'	32:1a:1263:C:C6	2.48	0.49
33:1b:134:GLU:O	33:1b:138:LEU:HD12	2.12	0.49
42:1k:98:LEU:O	42:1k:101:SER:OG	2.23	0.49
47:1p:47:ASP:OD1	47:1p:47:ASP:N	2.45	0.49
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.46	0.49
1:2A:1031:G:H5''	31:29:8:LYS:HE3	1.93	0.49
1:2A:1169:G:H1	1:2A:1180:C:H42	1.60	0.49
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.93	0.49
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	1.94	0.49
9:2N:110:GLY:O	9:2N:114:ARG:HG3	2.12	0.49
32:2a:15:G:H2'	32:2a:16:A:H8	1.78	0.49
32:2a:165:C:H2'	32:2a:166:G:C8	2.46	0.49
32:2a:280:C:N3	48:2q:39:SER:OG	2.43	0.49
32:2a:446:G:O6	63:2a:1923:HOH:O	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:685:G:C2	32:2a:686:U:C4	3.01	0.49
32:2a:815:A:N7	32:2a:1509:C:O2'	2.37	0.49
32:2a:922:G:N3	32:2a:1398:A:H2	2.10	0.49
32:2a:1053:G:N2	32:2a:1058:G:O6	2.45	0.49
32:2a:1226:C:OP2	44:2m:91:ARG:NH1	2.37	0.49
57:2y:19:U:H1'	57:2y:21:A:H5'	1.93	0.49
1:1A:271(G):C:H2'	1:1A:271(H):G:C8	2.47	0.49
1:1A:271(M):G:O2'	1:1A:271(N):U:H5''	2.13	0.49
1:1A:807:U:OP1	11:1P:36:LYS:NZ	2.45	0.49
1:1A:1364:G:P	23:11:3:LYS:HG3	2.52	0.49
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.11	0.49
1:1A:2361:A:OP2	30:18:26:LYS:NZ	2.43	0.49
8:1I:54:GLN:HG3	8:1I:55:ALA:N	2.28	0.49
32:1a:973:G:OP1	41:1j:57:LYS:NZ	2.31	0.49
34:1c:82:GLU:OE1	34:1c:85:ARG:NH1	2.45	0.49
1:2A:849:A:H2	25:23:24:LYS:HB3	1.76	0.49
1:2A:2839:G:H5'	13:2R:46:GLY:CA	2.41	0.49
7:2H:3:ARG:HB3	7:2H:6:ARG:HG3	1.94	0.49
32:2a:671:G:H2'	32:2a:672:U:O4'	2.12	0.49
33:2b:178:ARG:HH22	39:2h:68:ARG:NH1	2.10	0.49
39:2h:21:LYS:O	39:2h:65:TYR:OH	2.28	0.49
44:2m:40:ASN:HD22	44:2m:41:PRO:HD2	1.77	0.49
1:1A:1062:G:P	1:1A:1070:A:H1'	2.53	0.49
1:1A:2126:A:N6	1:1A:2163:C:O4'	2.46	0.49
1:1A:2506:U:C2	1:1A:2585:U:O4	2.66	0.49
1:1A:2789:C:O2	1:1A:2894:G:N1	2.40	0.49
1:1A:2794:C:H42	1:1A:2802:G:H22	1.60	0.49
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.47	0.49
43:1l:70:ILE:HD13	43:1l:77:LEU:HD12	1.93	0.49
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.39	0.49
2:2B:17:C:H2'	2:2B:18:G:O4'	2.13	0.49
27:25:40:LYS:NZ	27:25:44:THR:O	2.38	0.49
32:2a:565:U:OP2	32:2a:566:G:O2'	2.21	0.49
35:2d:201:GLN:HE21	36:2e:99:GLY:HA2	1.76	0.49
44:2m:94:ARG:HH21	50:2s:81:ARG:HA	1.76	0.49
1:1A:579:G:H2'	1:1A:580:C:C6	2.48	0.49
3:1D:26:LYS:HE2	3:1D:28:GLU:O	2.13	0.49
26:14:46:GLN:O	26:14:48:ARG:N	2.45	0.49
32:1a:276:G:O3'	48:1q:68:ARG:NH1	2.46	0.49
32:1a:560:U:H5'	32:1a:566:G:N2	2.28	0.49
32:1a:1284:C:H3'	32:1a:1285:A:C8	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.46	0.49
39:1h:121:ASP:OD1	39:1h:121:ASP:N	2.45	0.49
41:1j:21:GLN:O	41:1j:25:GLU:HG2	2.13	0.49
1:2A:236:C:H2'	1:2A:237:C:C6	2.47	0.49
31:29:14:CYS:HA	31:29:27:CYS:HB2	1.93	0.49
32:2a:516:PSU:O2'	32:2a:519:C:N3	2.39	0.49
32:2a:921:U:O2	36:2e:19:MET:HB2	2.12	0.49
32:2a:1027:C:H2'	32:2a:1034:G:H22	1.77	0.49
32:2a:1274:G:N2	32:2a:1275:A:N7	2.60	0.49
33:2b:178:ARG:HH22	39:2h:68:ARG:HH22	1.59	0.49
38:2g:89:MET:SD	38:2g:155:ARG:HB2	2.52	0.49
1:1A:264:C:O2	63:1A:4136:HOH:O	2.19	0.49
1:1A:2596:U:OP1	63:1A:4138:HOH:O	2.20	0.49
1:1A:2615:U:H2'	1:1A:2616:C:H6	1.78	0.49
2:1B:40:U:H2'	26:14:2:LYS:HE3	1.95	0.49
7:1H:7:LEU:HD22	7:1H:69:ARG:NH2	2.28	0.49
32:1a:60:A:H4'	32:1a:61:G:H5'	1.95	0.49
32:1a:244:U:OP2	48:1q:100:LYS:NZ	2.45	0.49
32:1a:975:A:H5'	32:1a:975:A:H8	1.78	0.49
32:1a:1239:A:H62	32:1a:1299:A:H62	1.60	0.49
33:1b:115:LEU:HD13	33:1b:145:LEU:HB3	1.94	0.49
34:1c:34:LEU:O	34:1c:38:ARG:HG3	2.13	0.49
36:1e:37:ARG:HH12	36:1e:111:GLU:HB3	1.76	0.49
37:1f:33:TYR:CD2	37:1f:75:LEU:HD23	2.47	0.49
4:2E:178:GLU:CD	4:2E:178:GLU:H	2.21	0.49
13:2R:98:LEU:HB2	13:2R:113:LEU:HD11	1.94	0.49
32:2a:328:C:H4'	32:2a:329:A:H5'	1.95	0.49
32:2a:1014:A:H2'	32:2a:1015:A:C8	2.48	0.49
32:2a:1053:G:H4'	32:2a:1054:C:H3'	1.94	0.49
1:1A:871:U:OP1	12:1Q:5:ARG:HD3	2.12	0.49
1:1A:2131:G:H5'	1:1A:2133:G:C8	2.48	0.49
33:1b:204:ASN:OD1	33:1b:206:ASP:N	2.36	0.49
40:1i:79:LEU:HG	40:1i:83:ARG:HD2	1.94	0.49
52:1u:18:TYR:CZ	52:1u:24:ARG:HD3	2.48	0.49
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.48	0.49
1:2A:1411:C:H2'	1:2A:1412:A:C8	2.47	0.49
1:2A:1837:C:OP1	32:2a:784:C:H4'	2.13	0.49
1:2A:2127:G:H1	1:2A:2161:C:N4	2.10	0.49
5:2F:32:LEU:HD22	5:2F:112:MET:HE2	1.93	0.49
32:2a:103:C:O2'	32:2a:172:A:N1	2.44	0.49
39:2h:51:VAL:HG12	39:2h:52:ASP:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:50:GLU:HA	44:2m:53:VAL:HG22	1.95	0.49
1:1A:1053:C:N4	1:1A:1106:G:H1	2.10	0.49
1:1A:1173:G:OP2	1:1A:1173:G:H2'	2.13	0.49
1:1A:2189:U:H2'	1:1A:2190:G:C8	2.48	0.49
21:1Z:33:LEU:HD11	21:1Z:90:VAL:HG21	1.95	0.49
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.96	0.49
36:1e:83:GLU:HG2	36:1e:88:LYS:HG3	1.93	0.49
1:2A:397:G:N7	63:2A:4026:HOH:O	2.35	0.49
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.12	0.49
1:2A:2319:G:N2	14:2S:3:ARG:HD2	2.28	0.49
12:2Q:17:LEU:HD13	12:2Q:39:PRO:HB2	1.95	0.49
32:2a:458:C:H2'	32:2a:460:G:O4'	2.13	0.49
32:2a:1026:G:O6	32:2a:1036:G:N2	2.44	0.49
32:2a:1092:A:H5''	38:2g:4:ARG:NH1	2.28	0.49
35:2d:79:PHE:HE1	35:2d:204:ILE:HD13	1.77	0.49
52:2u:5:ASP:O	52:2u:11:GLY:HA3	2.13	0.49
53:2v:23:A:H4'	53:2v:24:A:C5'	2.43	0.49
1:1A:875:G:H2'	1:1A:876:C:O4'	2.13	0.49
1:1A:1069:A:H5'	1:1A:1070:A:C8	2.39	0.49
1:1A:2291:U:OP1	1:1A:2380:C:O2'	2.30	0.49
1:1A:2492:U:H2'	1:1A:2493:U:C6	2.48	0.49
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.46	0.49
14:1S:71:ARG:HH11	14:1S:107:GLU:CD	2.20	0.49
21:1Z:132:ASN:HD22	21:1Z:160:GLY:HA3	1.78	0.49
32:1a:486:U:H2'	32:1a:487:A:C8	2.48	0.49
32:1a:718:G:C8	42:1k:116:HIS:HB3	2.48	0.49
33:1b:15:VAL:HG12	33:1b:210:SER:HA	1.94	0.49
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.46	0.49
57:1y:28:G:H2'	57:1y:29:A:C8	2.48	0.49
1:2A:892:G:H3'	1:2A:893:C:H5''	1.95	0.49
1:2A:956:G:H2'	1:2A:957:A:H2'	1.95	0.49
1:2A:1913:A:H4'	1:2A:1914:C:C5'	2.42	0.49
1:2A:2522:U:O2'	1:2A:2647:U:OP1	2.27	0.49
32:2a:811:C:O2'	32:2a:901:A:N1	2.46	0.49
32:2a:1111:A:H2	34:2c:179:ARG:HH21	1.61	0.49
32:2a:1261:A:H3'	32:2a:1262:C:C6	2.48	0.49
54:2w:8:4SU:S4	54:2w:14:A:C8	3.06	0.49
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.13	0.48
22:10:16:SER:OG	63:10:202:HOH:O	2.20	0.48
32:1a:35:G:O2'	43:1l:118:SER:O	2.29	0.48
32:1a:195:A:OP1	51:1t:68:LYS:NZ	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:26:VAL:HG22	40:1i:61:ALA:HB3	1.94	0.48
50:1s:40:ILE:HA	50:1s:44:MET:SD	2.52	0.48
51:1t:18:GLN:O	51:1t:22:ARG:HG3	2.13	0.48
54:1w:63:C:H2'	54:1w:64:U:H6	1.78	0.48
1:2A:217:G:OP2	63:2A:3947:HOH:O	2.19	0.48
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.45	0.48
1:2A:1580:A:H8	1:2A:1580:A:OP2	1.96	0.48
1:2A:2387:U:H1'	22:20:41:ARG:HE	1.77	0.48
32:2a:263:A:OP1	51:2t:79:ARG:NH1	2.46	0.48
43:2l:70:ILE:HG12	43:2l:100:ILE:HD12	1.94	0.48
57:2y:35:C:H3'	57:2y:36:C:C6	2.48	0.48
1:1A:184:C:H2'	1:1A:185:U:C6	2.47	0.48
4:1E:6:GLY:O	4:1E:195:LEU:HD22	2.13	0.48
7:1H:124:GLU:OE1	7:1H:134:SER:OG	2.29	0.48
33:1b:178:ARG:HH22	39:1h:68:ARG:HH12	1.61	0.48
38:1g:26:PHE:CE2	38:1g:30:ILE:HD11	2.48	0.48
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.49	0.48
1:2A:2135:A:H2'	1:2A:2136:C:C5	2.48	0.48
7:2H:121:ILE:HD11	7:2H:140:LYS:HG2	1.95	0.48
32:2a:45:U:H2'	32:2a:46:G:C8	2.48	0.48
32:2a:130:A:N3	32:2a:263:A:O2'	2.37	0.48
32:2a:875:C:O2'	39:2h:14:ARG:HD2	2.13	0.48
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.29	0.48
42:2k:85:ARG:HG2	42:2k:112:THR:HA	1.94	0.48
44:2m:91:ARG:HH11	44:2m:96:LEU:HD13	1.78	0.48
48:2q:95:TYR:HA	48:2q:98:LEU:HD12	1.95	0.48
54:2w:33:U:N3	54:2w:36:C:OP2	2.43	0.48
1:1A:205:G:O6	23:11:39:LYS:NZ	2.36	0.48
1:1A:1584:C:O2'	1:1A:1586:A:H5'	2.13	0.48
6:1G:7:LEU:N	6:1G:104:GLU:OE1	2.40	0.48
32:1a:194:C:O3'	51:1t:68:LYS:HD2	2.13	0.48
33:1b:91:PRO:HG2	33:1b:155:LEU:HD13	1.95	0.48
33:1b:143:GLU:O	33:1b:147:LYS:HG2	2.13	0.48
45:1n:3:ARG:HA	45:1n:3:ARG:HE	1.78	0.48
1:2A:184:C:H2'	1:2A:185:U:H6	1.78	0.48
1:2A:888:C:OP1	44:2m:93:ARG:NE	2.45	0.48
2:2B:19:G:H2'	2:2B:20:C:O4'	2.14	0.48
2:2B:90:A:N7	2:2B:91:C:H1'	2.27	0.48
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.48	0.48
16:2U:49:HIS:HA	16:2U:52:ARG:HB2	1.95	0.48
26:24:46:GLN:NE2	26:24:48:ARG:HG2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:88:A:H5''	32:2a:89:C:C6	2.48	0.48
32:2a:880:C:H2'	32:2a:881:G:H8	1.78	0.48
54:2w:29:A:H2'	54:2w:30:G:H8	1.78	0.48
1:1A:880:G:H2'	1:1A:881:G:H8	1.77	0.48
1:1A:2218:U:O4'	23:11:52:ARG:NH2	2.46	0.48
32:1a:950:U:H2'	32:1a:951:G:C8	2.49	0.48
32:1a:1131:G:H5'	40:1i:3:GLN:NE2	2.28	0.48
32:1a:1367:C:H5'	41:1j:60:ARG:HH12	1.78	0.48
40:1i:85:LEU:O	40:1i:88:TYR:HB3	2.14	0.48
1:2A:272:G:H4'	1:2A:272(A):U:H5''	1.94	0.48
1:2A:597:U:H2'	1:2A:598:G:C8	2.49	0.48
32:2a:1063:C:H3'	32:2a:1064:G:H2'	1.95	0.48
32:2a:1273:G:H3'	32:2a:1274:G:C8	2.46	0.48
33:2b:53:ARG:HB3	33:2b:53:ARG:NH1	2.28	0.48
37:2f:17:SER:O	37:2f:21:LEU:HD22	2.13	0.48
38:2g:22:LEU:HG	38:2g:62:PHE:CE2	2.46	0.48
44:2m:92:HIS:HD2	44:2m:110:ARG:HH21	1.61	0.48
48:2q:53:LEU:HD23	48:2q:82:MET:HE1	1.95	0.48
1:1A:2789:C:O2'	1:1A:2790:A:H4'	2.14	0.48
4:1E:13:ARG:HD2	4:1E:20:ALA:HB1	1.95	0.48
7:1H:25:LYS:HE3	7:1H:27:LYS:HE3	1.95	0.48
10:1O:64:ARG:NH2	10:1O:99:PHE:O	2.47	0.48
32:1a:41:G:H2'	32:1a:42:G:C8	2.48	0.48
32:1a:345:C:H5'	32:1a:346:G:C4	2.48	0.48
54:1w:4:G:C2'	54:1w:5:G:H5'	2.43	0.48
1:2A:286:C:H2'	1:2A:287:C:C6	2.49	0.48
1:2A:956:G:H5''	12:2Q:77:LYS:HD2	1.94	0.48
1:2A:1503:U:H2'	1:2A:1504:C:C6	2.48	0.48
1:2A:1857:G:O6	1:2A:1858:G:N1	2.46	0.48
1:2A:2238:G:H5''	63:2A:4279:HOH:O	2.13	0.48
32:2a:9:G:H2'	32:2a:10:A:H8	1.78	0.48
32:2a:1145:C:H4'	32:2a:1146:A:H8	1.78	0.48
32:2a:1299:A:H2'	32:2a:1299:A:N3	2.29	0.48
34:2c:83:ARG:HA	34:2c:87:LEU:HD23	1.94	0.48
39:2h:9:MET:HB2	39:2h:32:LYS:HE3	1.95	0.48
48:2q:68:ARG:H	48:2q:70:ARG:NH1	2.12	0.48
1:1A:2572:A:C8	4:1E:144:ARG:HD3	2.48	0.48
1:1A:2778:A:OP2	63:1A:4139:HOH:O	2.20	0.48
32:1a:472:A:OP1	47:1p:75:ARG:NH2	2.42	0.48
32:1a:1531:A:H8	32:1a:1531:A:O5'	1.97	0.48
33:1b:59:GLU:HB2	33:1b:221:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1e:78:HIS:CD2	39:1h:104:ARG:HD2	2.49	0.48
42:1k:15:ALA:HA	42:1k:77:MET:N	2.28	0.48
43:1l:38:THR:OG1	43:1l:39:VAL:N	2.46	0.48
1:2A:1297:C:OP1	1:2A:2710:C:H4'	2.13	0.48
23:21:64:ALA:HA	23:21:67:ILE:HG13	1.95	0.48
32:2a:1225:A:OP1	44:2m:103:THR:OG1	2.30	0.48
32:2a:1427:U:H2'	32:2a:1428:A:C8	2.48	0.48
40:2i:5:TYR:CD1	40:2i:18:PHE:HE1	2.31	0.48
40:2i:105:ASP:HB2	40:2i:107:ARG:HG3	1.96	0.48
42:2k:16:SER:O	42:2k:35:PRO:HD3	2.14	0.48
57:2y:48:C:H4'	57:2y:49:G:H5''	1.95	0.48
1:1A:289:A:N6	1:1A:351:G:O2'	2.45	0.48
1:1A:363(A):A:H2'	1:1A:363(B):G:C8	2.49	0.48
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.13	0.48
1:1A:879:G:H1	1:1A:899:A:H1'	1.78	0.48
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.96	0.48
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.95	0.48
32:1a:200:G:H1	32:1a:217:C:H42	1.61	0.48
32:1a:339:C:H2'	32:1a:340:U:C6	2.49	0.48
33:1b:122:PHE:HE2	33:1b:139:LYS:HB2	1.78	0.48
35:1d:122:ARG:NH1	35:1d:134:ASP:OD2	2.47	0.48
37:1f:91:VAL:HG11	49:1r:72:ARG:NH1	2.29	0.48
42:1k:45:GLY:O	42:1k:50:TYR:HB2	2.14	0.48
55:1x:16:C:OP1	55:1x:17:C:N4	2.46	0.48
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.44	0.48
21:2Z:51:ALA:HB1	21:2Z:57:ILE:HD11	1.95	0.48
31:29:29:ASN:HD22	31:29:32:HIS:CE1	2.31	0.48
32:2a:509:A:O2'	32:2a:510:A:OP1	2.26	0.48
32:2a:946:A:O2'	32:2a:1333:A:N3	2.39	0.48
32:2a:1105:A:H2'	32:2a:1106:G:C8	2.48	0.48
32:2a:1226:C:H4'	50:2s:80:TYR:CZ	2.49	0.48
36:2e:6:PHE:HB3	36:2e:34:VAL:HG22	1.95	0.48
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	1.95	0.48
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.29	0.48
6:1G:32:PRO:HB3	6:1G:163:ALA:HB2	1.95	0.48
32:1a:236:G:H5''	48:1q:42:TYR:OH	2.13	0.48
32:1a:431:A:H2'	32:1a:432:A:O4'	2.14	0.48
32:1a:1137:C:H4'	32:1a:1138:G:C2	2.49	0.48
42:1k:91:ARG:NH2	42:1k:110:ASP:OD1	2.46	0.48
45:1n:8:GLU:HA	45:1n:11:LYS:HD3	1.95	0.48
1:2A:645:C:H5''	1:2A:646:A:OP2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:952:G:OP1	12:2Q:16:ARG:NH2	2.47	0.48
1:2A:1697:G:OP2	1:2A:1698:A:O2'	2.25	0.48
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.48	0.48
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.48	0.48
3:2D:206:LEU:HD22	3:2D:211:ARG:HG2	1.95	0.48
7:2H:96:ALA:N	7:2H:128:PRO:O	2.47	0.48
28:26:11:LEU:HB2	28:26:21:TYR:HB2	1.94	0.48
32:2a:674:G:H2'	32:2a:675:A:H8	1.78	0.48
32:2a:989:C:H2'	32:2a:990:C:C6	2.49	0.48
32:2a:1104:G:O3'	33:2b:111:ARG:NH2	2.46	0.48
32:2a:1109:C:H2'	32:2a:1110:A:O4'	2.14	0.48
33:2b:216:SER:OG	33:2b:217:ARG:N	2.46	0.48
1:1A:299:A:N1	1:1A:322:A:O2'	2.39	0.48
1:1A:2140:C:H2'	1:1A:2141:G:C8	2.47	0.48
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.49	0.48
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.49	0.48
32:1a:234:C:H5''	48:1q:70:ARG:HH21	1.78	0.48
32:1a:404:U:H2'	32:1a:405:U:C6	2.49	0.48
33:1b:12:GLU:HA	33:1b:15:VAL:HG23	1.96	0.48
40:1i:23:ASN:OD1	40:1i:23:ASN:N	2.40	0.48
40:1i:99:LEU:HD12	40:1i:99:LEU:H	1.79	0.48
1:2A:27:G:N2	1:2A:512:G:H1'	2.29	0.48
1:2A:493:G:H2'	1:2A:494:G:O4'	2.14	0.48
1:2A:646:A:H2'	1:2A:647:G:O4'	2.14	0.48
1:2A:1141:U:OP2	9:2N:63:THR:OG1	2.30	0.48
15:2T:18:ASP:OD1	15:2T:18:ASP:N	2.47	0.48
18:2W:11:ARG:HD3	18:2W:82:LEU:HD12	1.94	0.48
32:2a:1060:C:H2'	32:2a:1061:G:H8	1.77	0.48
32:2a:1446:U:H2'	32:2a:1452:C:C5	2.48	0.48
1:1A:1068:G:C8	1:1A:1096:A:H1'	2.49	0.48
1:1A:1939:5MU:OP1	1:1A:2604:U:O2'	2.31	0.48
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.49	0.48
32:1a:308:C:H2'	32:1a:309:G:C8	2.49	0.48
32:1a:625:G:H2'	32:1a:626:U:C6	2.49	0.48
32:1a:834:C:H2'	32:1a:835:U:C6	2.48	0.48
32:1a:964:A:O2'	41:1j:55:LYS:NZ	2.25	0.48
33:1b:33:TYR:HB2	33:1b:43:ASP:HB2	1.96	0.48
33:1b:97:TRP:HZ2	33:1b:102:LEU:HD13	1.78	0.48
1:2A:236:C:H2'	1:2A:237:C:H6	1.79	0.48
1:2A:1022:G:N2	1:2A:1023:U:O4	2.46	0.48
12:2Q:137:TYR:O	12:2Q:141:GLN:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:575:G:O2'	32:2a:821:G:H5'	2.14	0.48
32:2a:1112:C:N3	34:2c:178:LEU:HD12	2.29	0.48
33:2b:102:LEU:HD13	33:2b:182:ILE:HD12	1.96	0.48
37:2f:62:TRP:CH2	37:2f:64:GLN:HB2	2.49	0.48
39:2h:121:ASP:N	39:2h:121:ASP:OD1	2.46	0.48
1:1A:2615:U:H2'	1:1A:2616:C:C6	2.49	0.47
11:1P:126:VAL:HG12	11:1P:148:LEU:HD22	1.96	0.47
21:1Z:150:LEU:O	21:1Z:171:ILE:HG12	2.13	0.47
42:1k:99:GLN:HG3	42:1k:105:VAL:HG21	1.95	0.47
1:2A:118:A:N3	1:2A:178:G:H1'	2.29	0.47
1:2A:2335:A:C8	1:2A:2337:G:C5	3.02	0.47
8:2I:117:GLU:OE1	8:2I:118:LYS:N	2.34	0.47
12:2Q:78:PRO:HD3	55:2x:1:C:N3	2.29	0.47
21:2Z:30:ASN:HA	21:2Z:89:PHE:HE1	1.79	0.47
32:2a:1412:C:H2'	32:2a:1413:A:H8	1.77	0.47
33:2b:109:SER:O	33:2b:112:VAL:HG12	2.14	0.47
43:2l:69:TYR:HE2	43:2l:71:PRO:HA	1.79	0.47
1:1A:1069:A:O4'	1:1A:1096:A:O2'	2.30	0.47
1:1A:2127:G:H2'	1:1A:2128:C:H6	1.78	0.47
5:1F:123:LEU:HD13	5:1F:192:LEU:HD13	1.96	0.47
32:1a:266:G:O3'	48:1q:67:LYS:HB2	2.14	0.47
32:1a:1124:G:OP1	41:1j:36:GLY:N	2.46	0.47
32:1a:1299:A:N3	32:1a:1299:A:H5''	2.29	0.47
33:1b:84:GLU:O	33:1b:219:VAL:HG21	2.14	0.47
33:1b:201:ILE:HG21	33:1b:214:ILE:HG21	1.96	0.47
34:1c:121:ALA:HB2	34:1c:198:VAL:HG11	1.96	0.47
1:2A:637:A:OP1	11:2P:133:SER:OG	2.23	0.47
1:2A:1742:G:O6	63:2A:3941:HOH:O	2.17	0.47
5:2F:18:ARG:NH1	5:2F:127:GLU:OE2	2.39	0.47
20:2Y:6:HIS:H	20:2Y:6:HIS:CD2	2.32	0.47
32:2a:718:G:H5'	42:2k:117:ASN:CG	2.38	0.47
32:2a:794:A:OP1	63:2a:1919:HOH:O	2.20	0.47
32:2a:973:G:H3'	32:2a:974:A:H5''	1.95	0.47
32:2a:975:A:N1	41:2j:48:THR:HB	2.28	0.47
33:2b:15:VAL:HG23	33:2b:16:HIS:HD2	1.79	0.47
33:2b:149:LEU:HD22	33:2b:152:PHE:CD2	2.49	0.47
33:2b:212:GLN:O	33:2b:216:SER:N	2.37	0.47
35:2d:57:ARG:H	35:2d:57:ARG:HD2	1.78	0.47
35:2d:121:VAL:O	35:2d:134:ASP:HA	2.14	0.47
41:2j:47:PHE:N	41:2j:63:PHE:O	2.32	0.47
49:2r:73:ALA:HB3	49:2r:79:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:271(G):C:H2'	1:1A:271(H):G:H8	1.78	0.47
1:1A:1045:A:OP1	1:1A:1046:A:H3'	2.14	0.47
1:1A:1508:A:H4'	1:1A:1509:C:OP1	2.14	0.47
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.95	0.47
2:1B:75:G:H22	21:1Z:73:GLN:HE22	1.62	0.47
8:1I:4:ILE:HB	8:1I:37:VAL:HG23	1.95	0.47
23:11:72:GLU:OE2	23:11:76:ARG:NH2	2.47	0.47
50:1s:18:LYS:O	50:1s:22:LEU:HD23	2.14	0.47
1:2A:272(B):G:H2'	1:2A:272(C):G:H8	1.79	0.47
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.13	0.47
14:2S:78:LEU:HD21	14:2S:109:GLY:HA3	1.96	0.47
32:2a:397:A:H3'	32:2a:397:A:N3	2.29	0.47
32:2a:909:A:N3	32:2a:1413:A:O2'	2.39	0.47
32:2a:1048:G:OP1	45:2n:3:ARG:HB3	2.14	0.47
32:2a:1218:C:OP2	45:2n:9:LYS:NZ	2.46	0.47
38:2g:86:GLN:HE21	57:2y:39:G:N2	2.12	0.47
41:2j:23:ILE:HA	41:2j:26:ALA:HB3	1.95	0.47
50:2s:66:MET:HB2	50:2s:74:PHE:CZ	2.49	0.47
55:2x:23:C:H2'	55:2x:24:U:C6	2.48	0.47
1:1A:286:C:H2'	1:1A:287:C:H6	1.80	0.47
1:1A:2794:C:N4	1:1A:2802:G:H22	2.12	0.47
4:1E:2:LYS:NZ	4:1E:95:ILE:O	2.40	0.47
5:1F:29:ASN:HB3	5:1F:112:MET:HE1	1.96	0.47
12:1Q:65:PHE:HB2	12:1Q:105:GLU:HB2	1.97	0.47
34:1c:20:SER:HB3	45:1n:54:PRO:HG3	1.96	0.47
38:1g:78:ARG:HG2	38:1g:79:ARG:H	1.79	0.47
44:1m:50:GLU:HA	44:1m:53:VAL:HG22	1.96	0.47
46:1o:7:GLU:O	46:1o:11:VAL:HG23	2.14	0.47
57:1y:63:C:H2'	57:1y:64:U:O4'	2.15	0.47
1:2A:171:G:H2'	1:2A:172:C:C6	2.49	0.47
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.13	0.47
1:2A:2118:U:C4	1:2A:2149:G:H1'	2.49	0.47
1:2A:2166:G:O6	1:2A:2171:A:N6	2.47	0.47
32:2a:597:G:OP2	63:2a:1903:HOH:O	2.20	0.47
32:2a:920:U:H2'	32:2a:921:U:H6	1.79	0.47
32:2a:1002:G:C2	32:2a:1003:G:H1'	2.49	0.47
32:2a:1075:C:H5''	33:2b:179:LYS:HE3	1.97	0.47
33:2b:185:ILE:HG22	33:2b:199:TYR:CD2	2.49	0.47
33:2b:185:ILE:HG22	33:2b:199:TYR:HB2	1.96	0.47
41:2j:45:ARG:HG2	41:2j:47:PHE:CZ	2.49	0.47
44:2m:17:VAL:O	44:2m:20:THR:OG1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2y:32:U:H2'	57:2y:33:U:O2	2.14	0.47
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.48	0.47
1:1A:1992:G:H5'	1:1A:1994:C:H41	1.79	0.47
1:1A:2255:G:N7	63:1A:4213:HOH:O	2.35	0.47
1:1A:2319:G:H22	14:1S:3:ARG:NE	2.11	0.47
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.97	0.47
32:1a:79:G:C6	32:1a:90:U:O2	2.68	0.47
32:1a:714:G:H2'	32:1a:715:A:C8	2.50	0.47
32:1a:1376:U:H2'	32:1a:1377:A:H8	1.79	0.47
33:1b:102:LEU:HB3	33:1b:180:LEU:HD12	1.96	0.47
34:1c:52:LEU:HD13	34:1c:68:VAL:HG13	1.96	0.47
44:1m:73:GLU:O	44:1m:76:ALA:N	2.46	0.47
44:1m:84:ILE:HD11	44:1m:86:CYS:HB2	1.95	0.47
47:1p:6:LEU:HB3	47:1p:17:TYR:CD1	2.50	0.47
1:2A:601:C:O2	1:2A:605:C:H4'	2.14	0.47
1:2A:1714:G:H1	1:2A:1745(A):C:H42	1.62	0.47
1:2A:1913:A:H4'	1:2A:1914:C:O5'	2.12	0.47
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.96	0.47
1:2A:2250:G:OP1	12:2Q:85:LYS:NZ	2.47	0.47
2:2B:1:U:O2'	2:2B:2:C:O5'	2.28	0.47
4:2E:56:PRO:HA	4:2E:59:VAL:HG22	1.97	0.47
26:24:24:THR:OG1	26:24:25:TYR:N	2.33	0.47
28:26:10:LEU:HG	28:26:54:ILE:HG13	1.96	0.47
32:2a:662:G:H2'	32:2a:663:A:H8	1.76	0.47
32:2a:793:U:O2	32:2a:1516:G:H4'	2.15	0.47
34:2c:136:GLN:O	34:2c:140:ARG:HG3	2.14	0.47
36:2e:107:ARG:O	36:2e:110:LEU:N	2.46	0.47
40:2i:5:TYR:HB3	40:2i:87:GLN:HE22	1.80	0.47
40:2i:17:VAL:HG11	40:2i:81:ILE:CG1	2.45	0.47
54:2w:27:A:H2'	54:2w:28:G:H8	1.79	0.47
15:1T:125:ARG:HD3	15:1T:129:ARG:NH2	2.29	0.47
26:14:48:ARG:HD3	26:14:48:ARG:HA	1.67	0.47
32:1a:343:U:H2'	32:1a:345:C:C5	2.49	0.47
32:1a:452:A:H4'	47:1p:72:ARG:NH1	2.30	0.47
32:1a:524:G:H2'	32:1a:525:C:C6	2.50	0.47
32:1a:662:G:H2'	32:1a:663:A:C8	2.48	0.47
32:1a:834:C:H2'	32:1a:835:U:H6	1.80	0.47
33:1b:8:LYS:HB3	33:1b:48:MET:HE1	1.96	0.47
33:1b:20:GLU:HB2	33:1b:190:THR:OG1	2.14	0.47
35:1d:178:VAL:HG12	35:1d:179:GLU:H	1.80	0.47
36:1e:89:ILE:HG12	36:1e:135:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:127:LYS:NZ	55:1x:34:C:OP2	2.45	0.47
45:1n:48:ALA:HB2	45:1n:53:LEU:HD12	1.97	0.47
46:1o:8:LYS:O	46:1o:12:ILE:HG13	2.15	0.47
47:1p:56:ALA:O	47:1p:60:LEU:HB2	2.14	0.47
1:2A:910:A:C5	12:2Q:13:GLN:HG3	2.50	0.47
1:2A:1889:A:N1	1:2A:2234:G:H1'	2.29	0.47
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.50	0.47
20:2Y:43:ASN:OD1	20:2Y:65:ALA:HB3	2.14	0.47
32:2a:971:G:H1'	32:2a:1365:G:O2'	2.13	0.47
33:2b:79:ASP:O	33:2b:82:ARG:HG2	2.14	0.47
33:2b:218:ALA:O	33:2b:222:ILE:HG13	2.14	0.47
34:2c:69:HIS:CD2	34:2c:104:GLN:HG2	2.50	0.47
41:2j:68:HIS:CD2	41:2j:68:HIS:H	2.31	0.47
1:1A:428:A:H8	1:1A:428:A:OP2	1.98	0.47
1:1A:2051:A:H5'	1:1A:2578:G:O4'	2.14	0.47
1:1A:2206:G:H5''	1:1A:2207:G:C5	2.50	0.47
19:1X:11:PRO:HB3	19:1X:92:LEU:HD21	1.97	0.47
32:1a:78:G:O2'	32:1a:79:G:H8	1.97	0.47
32:1a:159:G:H2'	32:1a:161:A:OP2	2.15	0.47
32:1a:1402:4OC:O5'	32:1a:1402:4OC:H6	2.14	0.47
37:1f:35:ALA:HB2	37:1f:67:MET:HE2	1.96	0.47
40:1i:127:LYS:O	40:1i:128:ARG:HB3	2.15	0.47
44:1m:2:ALA:N	44:1m:8:GLU:OE1	2.48	0.47
54:1w:27:A:H2'	54:1w:28:G:C8	2.49	0.47
57:1y:48:C:O2'	57:1y:49:G:OP2	2.33	0.47
1:2A:192:C:O2'	1:2A:802:A:N3	2.46	0.47
1:2A:263:C:H2'	1:2A:264:C:O4'	2.14	0.47
1:2A:1183:G:H2'	1:2A:1184:G:H8	1.79	0.47
1:2A:1384:A:N3	1:2A:1405:U:H1'	2.30	0.47
1:2A:1441:G:H2'	1:2A:1442:G:H8	1.79	0.47
1:2A:2110:G:H1	1:2A:2179:C:H42	1.63	0.47
1:2A:2331:G:O2'	1:2A:2336:A:N1	2.41	0.47
1:2A:2336:A:H61	22:20:43:THR:CG2	2.27	0.47
1:2A:2572:A:N7	4:2E:145:LYS:HB2	2.30	0.47
1:2A:2666:C:O2	7:2H:152:ARG:NH1	2.37	0.47
6:2G:68:PRO:HB2	6:2G:90:LEU:HB3	1.96	0.47
8:2I:59:ALA:HA	8:2I:62:LYS:HB2	1.96	0.47
21:2Z:159:PRO:HA	21:2Z:161:VAL:H	1.78	0.47
32:2a:181:G:O2'	32:2a:183:G:O6	2.30	0.47
32:2a:892:A:O2'	32:2a:1415:G:H4'	2.15	0.47
32:2a:1002:G:N3	32:2a:1003:G:H1'	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1192:C:OP2	34:2c:4:LYS:NZ	2.39	0.47
32:2a:1308:U:H3'	44:2m:99:ARG:HH21	1.80	0.47
34:2c:7:PRO:HB2	34:2c:182:ILE:CD1	2.44	0.47
44:2m:59:TYR:CD2	44:2m:60:VAL:HG23	2.49	0.47
48:2q:66:SER:OG	48:2q:69:LYS:HB2	2.13	0.47
54:2w:8:4SU:HN3	54:2w:14:A:N6	2.13	0.47
57:2y:2:C:H2'	57:2y:3:G:H8	1.80	0.47
57:2y:60:U:OP1	57:2y:61:C:N4	2.39	0.47
1:1A:1418:G:N7	63:1A:4216:HOH:O	2.35	0.47
1:1A:1814:G:C4'	3:1D:51:VAL:HG21	2.44	0.47
1:1A:2161:C:O2'	1:1A:2162:G:H5''	2.15	0.47
1:1A:2203:U:H4'	3:1D:151:LYS:HG2	1.97	0.47
8:1I:77:LEU:HD23	8:1I:97:ILE:HG23	1.97	0.47
8:1I:129:THR:HG22	8:1I:139:GLN:NE2	2.27	0.47
10:1O:48:PRO:CB	32:1a:1422:G:H5''	2.42	0.47
36:1e:53:LEU:HD12	36:1e:53:LEU:H	1.79	0.47
43:1l:56:ALA:HB3	43:1l:100:ILE:HD11	1.97	0.47
2:2B:11:C:H3'	2:2B:12:C:H6	1.80	0.47
2:2B:55:U:H1'	6:2G:29:TRP:CD1	2.50	0.47
5:2F:118:ALA:HB2	5:2F:123:LEU:HD23	1.96	0.47
8:2I:130:TYR:HD2	8:2I:138:ILE:HD12	1.80	0.47
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.15	0.47
14:2S:24:LEU:HB2	14:2S:85:VAL:HG12	1.97	0.47
32:2a:9:G:H2'	32:2a:10:A:C8	2.50	0.47
32:2a:58:C:O2'	32:2a:388:G:N7	2.34	0.47
36:2e:93:PRO:HG2	39:2h:105:ARG:NE	2.30	0.47
40:2i:108:VAL:HG22	40:2i:109:VAL:H	1.79	0.47
51:2t:90:GLN:O	51:2t:93:GLU:HG2	2.15	0.47
51:2t:100:ILE:HG22	51:2t:101:GLY:H	1.80	0.47
32:1a:688:G:H2'	32:1a:689:C:H6	1.79	0.47
32:1a:1026:G:H3'	32:1a:1027:C:C6	2.50	0.47
32:1a:1175:G:H2'	32:1a:1176:A:C8	2.50	0.47
33:1b:55:PHE:CD1	33:1b:221:LEU:HD22	2.50	0.47
51:1t:50:GLU:HG3	51:1t:100:ILE:HG23	1.96	0.47
1:2A:492:A:H2'	1:2A:493:G:O4'	2.15	0.47
1:2A:863:A:H2'	1:2A:864:G:C8	2.50	0.47
1:2A:887:A:H4'	1:2A:888:C:C5	2.50	0.47
1:2A:2127:G:N1	1:2A:2161:C:N4	2.63	0.47
1:2A:2506:U:C2	1:2A:2585:U:O4	2.68	0.47
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.95	0.47
15:2T:26:ASP:OD1	15:2T:120:ARG:NH2	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:99:TYR:CZ	21:2Z:125:LEU:HD12	2.49	0.47
32:2a:108:G:N1	51:2t:15:ARG:HG2	2.30	0.47
32:2a:1010:G:C2	32:2a:1020:U:H1'	2.50	0.47
32:2a:1320:C:H2'	32:2a:1321:C:O4'	2.15	0.47
32:2a:1411:C:H2'	32:2a:1412:C:H6	1.80	0.47
33:2b:212:GLN:NE2	33:2b:234:PRO:O	2.48	0.47
35:2d:57:ARG:HB3	35:2d:206:PHE:HB2	1.96	0.47
41:2j:81:THR:C	41:2j:83:GLU:N	2.73	0.47
48:2q:22:LEU:HD13	48:2q:41:LYS:HG2	1.97	0.47
57:2y:11:U:H2'	57:2y:12:U:H6	1.79	0.47
1:1A:2127:G:H2'	1:1A:2128:C:C6	2.50	0.47
32:1a:444:C:H2'	32:1a:445:G:H8	1.80	0.47
32:1a:473:G:H2'	32:1a:474:G:H8	1.79	0.47
57:1y:38:A:H2'	57:1y:39:G:O4'	2.14	0.47
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.50	0.47
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.15	0.47
5:2F:158:THR:O	5:2F:164:ARG:NH1	2.41	0.47
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.14	0.47
9:2N:4:TYR:HB2	16:2U:101:ARG:NH1	2.29	0.47
12:2Q:89:ASN:HB2	55:2x:1:C:C4	2.50	0.47
21:2Z:104:PHE:HD2	21:2Z:139:VAL:HG11	1.80	0.47
26:24:53:GLU:N	26:24:53:GLU:OE2	2.48	0.47
32:2a:19:C:H5''	36:2e:86:ALA:HB1	1.97	0.47
32:2a:583:A:H2'	32:2a:584:G:O4'	2.15	0.47
32:2a:741:G:H2'	32:2a:742:G:O4'	2.14	0.47
32:2a:935:A:N6	38:2g:3:ARG:HG3	2.30	0.47
32:2a:1129:C:H2'	32:2a:1139:G:N7	2.30	0.47
57:2y:46:A:O2'	57:2y:48:C:OP2	2.27	0.47
1:1A:1021:A:H3'	1:1A:1021:A:N3	2.29	0.46
1:1A:2747:G:O6	1:1A:2755:C:H5''	2.15	0.46
63:1A:5352:HOH:O	5:1F:74:ARG:HD2	2.14	0.46
7:1H:11:VAL:HG21	7:1H:50:VAL:HG23	1.97	0.46
13:1R:2:ARG:HA	13:1R:5:LYS:HD2	1.96	0.46
40:1i:23:ASN:CG	40:1i:25:LYS:HE3	2.40	0.46
45:1n:45:ARG:O	45:1n:49:HIS:HD2	1.98	0.46
52:1u:5:ASP:O	52:1u:11:GLY:HA3	2.15	0.46
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.48	0.46
1:2A:1991:U:H2'	1:2A:1992:G:H5''	1.97	0.46
6:2G:122:PRO:HB3	6:2G:170:ARG:HH21	1.79	0.46
6:2G:150:ASP:OD1	6:2G:150:ASP:N	2.48	0.46
7:2H:35:VAL:HG11	7:2H:71:LEU:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:20:49:LYS:HG2	22:20:50:ASN:ND2	2.30	0.46
23:21:24:ALA:HB3	23:21:27:GLU:HG3	1.97	0.46
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.15	0.46
32:2a:953:G:H5'	32:2a:965:A:N6	2.27	0.46
32:2a:1051:C:H2'	32:2a:1052:U:C6	2.50	0.46
32:2a:1157:A:H5'	32:2a:1158:C:C6	2.50	0.46
32:2a:1380:U:C4	38:2g:3:ARG:HG2	2.50	0.46
33:2b:158:LEU:HD23	33:2b:182:ILE:HD11	1.97	0.46
38:2g:132:GLY:O	38:2g:136:LYS:HG2	2.16	0.46
41:2j:6:ILE:HA	41:2j:98:ILE:HG12	1.96	0.46
54:2w:18:G:N2	54:2w:57:G:H1'	2.30	0.46
55:2x:37:A:H2'	55:2x:38:A:O4'	2.15	0.46
1:1A:1311:G:O2'	29:17:47:ARG:NH2	2.49	0.46
1:1A:2031:A:C6	1:1A:2498:C:H1'	2.50	0.46
32:1a:79:G:O6	32:1a:90:U:O2	2.33	0.46
32:1a:688:G:O2'	32:1a:704:A:N1	2.37	0.46
32:1a:1353:G:OP1	52:1u:10:ARG:NH1	2.48	0.46
32:1a:1504:G:OP1	32:1a:1507:A:H4'	2.15	0.46
41:1j:7:LYS:HE2	41:1j:9:ARG:HH12	1.79	0.46
1:2A:422:A:H2'	1:2A:423:A:C8	2.51	0.46
1:2A:1032:A:H2	1:2A:1122:G:H22	1.63	0.46
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.50	0.46
1:2A:1845:G:OP1	3:2D:258:LYS:NZ	2.42	0.46
32:2a:343:U:O2'	32:2a:344:A:H2'	2.15	0.46
34:2c:127:ARG:NH1	34:2c:190:ARG:HH22	2.13	0.46
35:2d:50:ARG:NH2	36:2e:9:LYS:HE2	2.30	0.46
35:2d:187:ARG:NH1	35:2d:190:ASP:H	2.12	0.46
38:2g:108:ALA:HA	38:2g:111:ARG:HD2	1.97	0.46
39:2h:121:ASP:HB2	39:2h:125:ARG:NH2	2.30	0.46
55:2x:72:A:H2'	55:2x:73:A:H8	1.80	0.46
1:1A:222:A:H5''	1:1A:421:U:OP1	2.15	0.46
1:1A:1173:G:H22	1:1A:1177:A:P	2.38	0.46
1:1A:1358:G:O2'	1:1A:1373:A:N6	2.48	0.46
1:1A:1859:A:N6	1:1A:1883:G:O2'	2.49	0.46
21:1Z:69:THR:HG22	21:1Z:90:VAL:HA	1.96	0.46
32:1a:358:U:H2'	32:1a:359:U:H6	1.79	0.46
32:1a:946:A:O2'	32:1a:1333:A:N3	2.46	0.46
32:1a:973:G:H3'	32:1a:974:A:H5''	1.97	0.46
42:1k:87:THR:O	42:1k:87:THR:OG1	2.27	0.46
50:1s:22:LEU:HD12	50:1s:27:GLU:HA	1.98	0.46
57:1y:42:C:H2'	57:1y:43:U:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1116:C:H2'	1:2A:1117:G:H8	1.80	0.46
2:2B:66:A:N6	2:2B:108:U:H3'	2.30	0.46
8:2I:77:LEU:O	8:2I:143:SER:N	2.28	0.46
26:24:53:GLU:C	26:24:55:ARG:H	2.23	0.46
32:2a:707:C:H2'	32:2a:708:C:C6	2.50	0.46
32:2a:1133:G:H2'	32:2a:1134:G:H8	1.79	0.46
36:2e:102:ALA:HB2	36:2e:120:THR:HG21	1.98	0.46
37:2f:99:ALA:HB1	49:2r:23:LYS:NZ	2.30	0.46
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.96	0.46
1:1A:721:C:H2'	1:1A:722:A:C8	2.51	0.46
32:1a:119:A:H4'	32:1a:120:A:C8	2.50	0.46
32:1a:1027:C:N3	32:1a:1034:G:N2	2.62	0.46
32:1a:1293:G:H2'	32:1a:1294:G:H8	1.80	0.46
35:1d:88:VAL:O	35:1d:92:VAL:HG23	2.16	0.46
35:1d:173:TRP:HB3	35:1d:187:ARG:HG3	1.98	0.46
39:1h:87:SER:HB2	39:1h:93:VAL:H	1.80	0.46
41:1j:11:PHE:CE1	41:1j:67:THR:HG22	2.50	0.46
50:1s:27:GLU:HB2	50:1s:28:LYS:HA	1.96	0.46
1:2A:272(B):G:H2'	1:2A:272(C):G:C8	2.50	0.46
1:2A:1029:A:N1	1:2A:2465:C:O2'	2.38	0.46
1:2A:1814:G:H4'	3:2D:51:VAL:HG21	1.96	0.46
7:2H:91:GLY:HA3	7:2H:160:LYS:HG3	1.98	0.46
10:2O:66:LYS:HA	10:2O:79:PHE:O	2.16	0.46
32:2a:67:C:H2'	32:2a:68:G:C8	2.50	0.46
32:2a:201:C:H5'	32:2a:202:U:OP2	2.16	0.46
32:2a:628:G:H2'	32:2a:629:G:C8	2.51	0.46
32:2a:737:A:H2'	32:2a:738:C:H6	1.79	0.46
32:2a:999:C:H2'	32:2a:1000:U:C6	2.50	0.46
32:2a:1208:C:H2'	32:2a:1209:C:C6	2.51	0.46
32:2a:1327:C:H2'	32:2a:1328:C:H6	1.80	0.46
33:2b:87:ARG:HH11	33:2b:219:VAL:HG13	1.80	0.46
35:2d:61:LYS:HD3	35:2d:206:PHE:CE2	2.51	0.46
1:1A:752:A:H3'	29:17:1:MET:HE1	1.97	0.46
1:1A:1113:U:H2'	1:1A:1114:G:H8	1.79	0.46
1:1A:1799:G:O2'	3:1D:181:GLU:OE2	2.25	0.46
1:1A:1930:G:O2'	1:1A:1968:G:O6	2.30	0.46
1:1A:2165:G:H1	1:1A:2171:A:H2'	1.81	0.46
4:1E:7:VAL:HG23	4:1E:51:PHE:HE2	1.81	0.46
6:1G:135:LEU:HD13	6:1G:140:ILE:HD11	1.97	0.46
21:1Z:158:PRO:HG2	21:1Z:161:VAL:HG21	1.98	0.46
28:16:6:ARG:HD3	28:16:24:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:258:G:H2'	32:1a:259:G:C8	2.43	0.46
32:1a:473:G:H2'	32:1a:474:G:C8	2.50	0.46
32:1a:666:G:H5'	32:1a:726:C:H1'	1.97	0.46
32:1a:994:A:N1	32:1a:1047:G:H4'	2.31	0.46
32:1a:1280:A:OP1	41:1j:7:LYS:NZ	2.48	0.46
34:1c:8:ILE:HG13	34:1c:9:GLY:N	2.30	0.46
36:1e:105:VAL:HB	36:1e:106:PRO:HD3	1.97	0.46
44:1m:121:LYS:HE3	44:1m:121:LYS:HB3	1.77	0.46
1:2A:1027:A:C2	1:2A:2488:A:H5'	2.51	0.46
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.50	0.46
1:2A:2769:C:H2'	1:2A:2770:G:O4'	2.15	0.46
7:2H:140:LYS:HB2	7:2H:140:LYS:HE3	1.68	0.46
32:2a:202:U:H3'	32:2a:203:U:C6	2.50	0.46
32:2a:1346:A:H61	32:2a:1374:A:H3'	1.80	0.46
40:2i:4:TYR:CE1	40:2i:88:TYR:HA	2.50	0.46
40:2i:28:VAL:N	40:2i:31:GLN:O	2.42	0.46
46:2o:11:VAL:HG21	46:2o:34:LEU:HD22	1.96	0.46
57:2y:34:C:H2'	57:2y:35:C:C6	2.50	0.46
1:1A:747:U:O2	1:1A:2014:A:H1'	2.15	0.46
3:1D:108:PRO:HD2	3:1D:111:LEU:HD22	1.97	0.46
28:16:38:LYS:HE3	28:16:38:LYS:HB3	1.69	0.46
32:1a:748:C:H4'	32:1a:749:C:O5'	2.16	0.46
32:1a:942:G:H21	40:1i:124:GLN:NE2	2.13	0.46
50:1s:63:THR:OG1	50:1s:65:ASN:OD1	2.29	0.46
1:2A:1434:A:H61	1:2A:1558:A:H62	1.64	0.46
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.40	0.46
1:2A:2107:C:H2'	1:2A:2108:C:O4'	2.15	0.46
1:2A:2612:C:OP2	27:25:2:ALA:N	2.49	0.46
3:2D:132:PRO:HD3	3:2D:190:TYR:CZ	2.50	0.46
4:2E:48:GLN:HA	4:2E:80:GLU:HA	1.98	0.46
32:2a:1054:C:C4	54:2w:34:C:H1'	2.50	0.46
32:2a:1070:U:H2'	32:2a:1071:C:C6	2.50	0.46
32:2a:1318:A:H5''	50:2s:3:ARG:NH2	2.31	0.46
33:2b:121:LEU:HA	33:2b:125:PRO:HB2	1.97	0.46
33:2b:172:ILE:HD12	33:2b:172:ILE:H	1.81	0.46
40:2i:3:GLN:HE21	40:2i:20:ARG:NH2	2.13	0.46
40:2i:34:ASN:O	40:2i:38:GLN:HB3	2.15	0.46
43:2l:10:LEU:O	43:2l:14:GLY:N	2.45	0.46
54:2w:76:L3X:N	55:2x:76:8AN:O2'	2.49	0.46
1:1A:774:A:N3	1:1A:774:A:H2'	2.30	0.46
1:1A:1064:C:H1'	1:1A:1076:C:H5	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2629:A:HO2'	1:1A:2630:G:P	2.35	0.46
1:1A:2649:U:H2'	1:1A:2650:U:C6	2.50	0.46
23:11:2:SER:HB3	23:11:46:LEU:HD12	1.98	0.46
32:1a:625:G:H2'	32:1a:626:U:H6	1.80	0.46
32:1a:685:G:O2'	32:1a:686:U:H5'	2.16	0.46
32:1a:950:U:H2'	32:1a:951:G:H8	1.81	0.46
44:1m:11:ARG:C	44:1m:13:LYS:H	2.23	0.46
1:2A:315:G:H2'	1:2A:316:C:C6	2.51	0.46
1:2A:2889:C:H2'	1:2A:2891:G:O4'	2.15	0.46
25:23:43:ILE:O	25:23:47:VAL:HG23	2.16	0.46
32:2a:12:U:H4'	32:2a:526:C:O2'	2.16	0.46
32:2a:316:G:OP2	32:2a:351:G:O2'	2.28	0.46
32:2a:407:G:H5''	35:2d:115:ARG:HB3	1.98	0.46
38:2g:77:SER:HA	38:2g:85:TYR:O	2.16	0.46
1:1A:1030:G:OP2	12:1Q:128:LYS:NZ	2.49	0.46
1:1A:2350:C:OP2	63:1A:4142:HOH:O	2.21	0.46
7:1H:35:VAL:O	7:1H:37:VAL:HG23	2.15	0.46
7:1H:98:LEU:HG	7:1H:125:VAL:HG23	1.97	0.46
26:14:63:TYR:N	26:14:64:GLY:HA2	2.29	0.46
32:1a:457:C:H2'	32:1a:458:C:C6	2.50	0.46
32:1a:922:G:H4'	36:1e:20:GLN:HA	1.98	0.46
38:1g:51:GLN:O	38:1g:55:GLY:HA2	2.16	0.46
1:2A:90:U:H1'	1:2A:92:A:C8	2.51	0.46
1:2A:795:C:H2'	1:2A:796:C:H6	1.81	0.46
1:2A:1885:A:H2'	1:2A:1886:C:O4'	2.16	0.46
1:2A:1902:C:H5'	3:2D:246:PRO:HD3	1.96	0.46
1:2A:2138:C:H2'	1:2A:2139:C:O4'	2.14	0.46
1:2A:2171:A:C4	1:2A:2172:U:C4	3.03	0.46
1:2A:2245:U:O2'	1:2A:2436:G:OP2	2.29	0.46
2:2B:24:G:N7	2:2B:56:G:H2'	2.31	0.46
4:2E:51:PHE:HB3	4:2E:77:ILE:HG23	1.98	0.46
7:2H:25:LYS:HD3	7:2H:27:LYS:HE3	1.98	0.46
8:2I:48:GLU:O	8:2I:51:ILE:HG22	2.15	0.46
30:28:28:GLY:O	30:28:36:LYS:NZ	2.44	0.46
32:2a:1176:A:H2'	32:2a:1177:G:C8	2.51	0.46
32:2a:1512:U:H2'	32:2a:1513:A:H8	1.80	0.46
35:2d:150:GLU:CD	35:2d:150:GLU:H	2.24	0.46
41:2j:46:ARG:HG3	41:2j:64:GLU:HB3	1.98	0.46
44:2m:60:VAL:HA	44:2m:63:THR:HB	1.97	0.46
1:1A:1174:A:H1'	1:1A:1175:U:O5'	2.16	0.46
1:1A:1429:G:H2'	1:1A:1430:C:H6	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1506:C:H2'	1:1A:1507:A:C8	2.50	0.46
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.51	0.46
2:1B:2:C:H2'	2:1B:3:C:C6	2.50	0.46
5:1F:136:THR:HA	5:1F:166:ALA:O	2.15	0.46
6:1G:126:ASP:HB3	6:1G:128:ARG:H	1.80	0.46
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.69	0.46
15:1T:98:LYS:NZ	63:1T:301:HOH:O	2.22	0.46
32:1a:731:G:OP1	32:1a:766:A:H1'	2.16	0.46
32:1a:750:G:N3	46:1o:23:GLY:HA3	2.31	0.46
32:1a:1192:C:OP2	34:1c:4:LYS:NZ	2.32	0.46
32:1a:1318:A:H5''	50:1s:3:ARG:NH1	2.31	0.46
34:1c:113:ALA:N	34:1c:183:ASP:OD2	2.44	0.46
1:2A:1354:A:H2'	1:2A:1355:G:O4'	2.16	0.46
1:2A:1412:A:H2'	1:2A:1413:G:H8	1.81	0.46
1:2A:1587:A:H2'	1:2A:1588:C:C6	2.51	0.46
3:2D:141:VAL:HG13	3:2D:162:SER:HB2	1.96	0.46
4:2E:181:LEU:HD12	4:2E:181:LEU:HA	1.80	0.46
7:2H:102:ALA:HB2	7:2H:116:GLU:HG2	1.98	0.46
10:2O:20:MET:HE3	10:2O:44:LYS:HE3	1.97	0.46
32:2a:15:G:H2'	32:2a:16:A:C8	2.51	0.46
32:2a:1030(A):G:N2	32:2a:1030(D):A:OP2	2.49	0.46
32:2a:1240:U:C2	38:2g:32:ARG:HG3	2.51	0.46
32:2a:1291:G:C6	32:2a:1292:U:C4	3.04	0.46
33:2b:97:TRP:HE1	33:2b:172:ILE:HG22	1.81	0.46
45:2n:24:CYS:HB2	45:2n:40:CYS:HB3	1.98	0.46
1:1A:1430:C:H2'	1:1A:1431:U:C6	2.51	0.46
1:1A:1557:C:H5''	1:1A:1558:A:OP2	2.16	0.46
6:1G:122:PRO:HB3	6:1G:170:ARG:HH12	1.81	0.46
8:1I:27:ARG:HG2	23:11:71:TYR:CZ	2.50	0.46
32:1a:110:C:H2'	32:1a:111:G:O4'	2.15	0.46
32:1a:130:A:N3	32:1a:263:A:O2'	2.45	0.46
32:1a:250:A:H4'	32:1a:251:G:O5'	2.15	0.46
32:1a:472:A:P	47:1p:75:ARG:HH22	2.39	0.46
32:1a:501:C:OP1	43:1l:117:ARG:NH2	2.38	0.46
32:1a:1241:G:H2'	32:1a:1242:C:C6	2.51	0.46
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.16	0.46
46:1o:5:LYS:O	46:1o:9:GLN:HG2	2.15	0.46
46:1o:87:ILE:HG22	46:1o:88:ARG:H	1.81	0.46
50:1s:32:LYS:HB3	50:1s:32:LYS:HE2	1.68	0.46
57:1y:17:G:H4'	57:1y:18:G:OP1	2.16	0.46
1:2A:887:A:H1'	1:2A:889:C:H5	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.51	0.46
1:2A:1866:C:H2'	1:2A:1876:A:O4'	2.16	0.46
1:2A:2538:C:H2'	1:2A:2539:C:H6	1.81	0.46
5:2F:110:LEU:HD11	5:2F:181:LEU:HG	1.98	0.46
32:2a:20:U:H2'	32:2a:21:G:O4'	2.16	0.46
32:2a:560:U:OP2	63:2a:1926:HOH:O	2.20	0.46
32:2a:857:C:H2'	32:2a:858:G:O4'	2.16	0.46
32:2a:1102:A:O3'	33:2b:96:ARG:NH2	2.48	0.46
40:2i:50:LEU:HD13	40:2i:56:LEU:HA	1.98	0.46
1:1A:536:A:H2'	1:1A:537:C:C6	2.51	0.45
1:1A:796:C:H2'	1:1A:797:C:C6	2.50	0.45
1:1A:858:U:O2	1:1A:2268:A:H2'	2.16	0.45
1:1A:1203:G:H5'	11:1P:3:LEU:HD12	1.98	0.45
1:1A:2112:G:H1'	57:1y:18:G:O2'	2.15	0.45
1:1A:2336:A:H61	22:10:43:THR:CG2	2.29	0.45
1:1A:2404:C:O3'	11:1P:77:ARG:NH2	2.47	0.45
2:1B:23:G:O6	63:1B:303:HOH:O	2.18	0.45
10:1O:122:LEU:HD13	15:1T:72:VAL:HG11	1.98	0.45
32:1a:736:C:H2'	32:1a:737:A:C8	2.51	0.45
32:1a:848:C:H2'	32:1a:849:C:C6	2.51	0.45
32:1a:1310:G:OP2	44:1m:88:ARG:NH2	2.49	0.45
32:1a:1530:G:H4'	32:1a:1530:G:OP1	2.16	0.45
36:1e:152:ARG:NH2	39:1h:107:LEU:O	2.49	0.45
51:1t:10:LEU:HD22	51:1t:10:LEU:HA	1.69	0.45
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.51	0.45
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.52	0.45
1:2A:1243:G:O2'	11:2P:7:ARG:NH2	2.50	0.45
1:2A:1417:C:H2'	1:2A:1418:G:O4'	2.16	0.45
1:2A:2112:G:H1'	57:2y:18:G:O2'	2.16	0.45
4:2E:77:ILE:HG13	4:2E:78:LEU:N	2.31	0.45
6:2G:20:ILE:HA	6:2G:25:TYR:HD2	1.80	0.45
7:2H:24:VAL:HG21	7:2H:72:ILE:HD13	1.97	0.45
12:2Q:18:LYS:HE2	12:2Q:18:LYS:HB2	1.86	0.45
13:2R:8:ARG:HE	13:2R:43:GLU:HG2	1.80	0.45
32:2a:89:C:H2'	32:2a:90:U:O4'	2.16	0.45
32:2a:762:C:H2'	32:2a:763:G:C8	2.51	0.45
32:2a:955:U:H2'	32:2a:956:U:O4'	2.17	0.45
32:2a:1271:G:N1	32:2a:1272:G:N7	2.63	0.45
33:2b:185:ILE:O	33:2b:185:ILE:HG12	2.16	0.45
34:2c:51:GLY:O	34:2c:70:VAL:HG13	2.16	0.45
55:2x:15:G:H2'	55:2x:59:A:N1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2y:8:4SU:H2'	57:2y:46:A:H2	1.24	0.45
57:2y:48:C:C4'	57:2y:49:G:H5''	2.46	0.45
1:1A:880:G:N2	1:1A:898:C:N3	2.60	0.45
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.81	0.45
1:1A:2029:G:H2'	1:1A:2031:A:OP1	2.16	0.45
2:1B:73:A:N1	21:1Z:34:ASN:ND2	2.64	0.45
32:1a:457:C:H2'	32:1a:458:C:H6	1.82	0.45
32:1a:664:G:N2	32:1a:741:G:H1	2.10	0.45
32:1a:738:C:H2'	32:1a:739:C:H6	1.82	0.45
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.98	0.45
33:1b:24:TRP:CZ3	33:1b:26:PRO:HA	2.51	0.45
33:1b:167:PRO:HG3	33:1b:188:ALA:HB2	1.98	0.45
35:1d:99:SER:O	35:1d:140:VAL:HG23	2.16	0.45
36:1e:10:MET:H	36:1e:10:MET:HG2	1.63	0.45
42:1k:33:THR:HA	42:1k:39:PRO:HA	1.97	0.45
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.79	0.45
1:2A:2378:A:H4'	14:2S:23:ARG:HE	1.81	0.45
2:2B:51:G:OP2	14:2S:61:ASN:HA	2.16	0.45
5:2F:176:LEU:HD23	5:2F:176:LEU:HA	1.85	0.45
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.52	0.45
32:2a:1004:A:N1	32:2a:1037:C:C2	2.84	0.45
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.52	0.45
34:2c:6:HIS:CG	45:2n:49:HIS:HB3	2.51	0.45
38:2g:71:PRO:HG3	38:2g:103:TRP:CH2	2.51	0.45
57:2y:60:U:O5'	57:2y:61:C:H5	1.99	0.45
1:1A:484:C:H2'	1:1A:485:C:C6	2.51	0.45
1:1A:1815:A:P	3:1D:54:ARG:HH22	2.39	0.45
8:1I:31:LEU:HD21	8:1I:38:LEU:HD22	1.98	0.45
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.51	0.45
32:1a:193:C:H2'	32:1a:194:C:C6	2.51	0.45
32:1a:353:A:H5'	32:1a:353:A:H8	1.81	0.45
32:1a:922:G:C6	32:1a:923:A:C6	3.05	0.45
32:1a:946:A:H2'	32:1a:947:G:C8	2.52	0.45
32:1a:955:U:O2'	50:1s:83:HIS:HD2	2.00	0.45
35:1d:60:GLU:OE1	35:1d:199:ASN:N	2.43	0.45
50:1s:31:ILE:O	50:1s:50:ALA:N	2.48	0.45
1:2A:880:G:C2	1:2A:881:G:C8	3.04	0.45
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.17	0.45
1:2A:2143:C:N3	1:2A:2148:G:N2	2.54	0.45
1:2A:2773:C:OP1	4:2E:166:THR:OG1	2.34	0.45
3:2D:24:ILE:HD13	3:2D:84:TYR:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:77:ASP:CG	21:2Z:80:ARG:HH11	2.25	0.45
25:23:6:VAL:HG12	25:23:35:ARG:O	2.16	0.45
32:2a:1030(A):G:N2	32:2a:1030(C):G:H3'	2.31	0.45
35:2d:22:LYS:HB2	35:2d:26:CYS:SG	2.56	0.45
36:2e:145:LYS:O	36:2e:149:GLU:N	2.48	0.45
43:2l:6:THR:OG1	43:2l:9:GLN:OE1	2.29	0.45
44:2m:79:LYS:HB3	44:2m:79:LYS:HE3	1.70	0.45
50:2s:49:ILE:HG12	50:2s:50:ALA:N	2.31	0.45
1:1A:2128:C:N4	1:1A:2160:G:C6	2.84	0.45
2:1B:24:G:N7	2:1B:56:G:H2'	2.31	0.45
26:14:63:TYR:N	26:14:63:TYR:CD1	2.83	0.45
31:19:17:ILE:HD13	31:19:26:ILE:HD13	1.98	0.45
32:1a:7:G:H5'	32:1a:298:A:O4'	2.16	0.45
32:1a:1023:G:H3'	32:1a:1024:G:H8	1.81	0.45
32:1a:1279:A:H5''	32:1a:1280:A:OP1	2.17	0.45
34:1c:150:LYS:HD3	34:1c:152:ILE:HD11	1.98	0.45
34:1c:172:ARG:HG3	34:1c:174:PRO:HD3	1.99	0.45
51:1t:30:LYS:O	51:1t:34:LYS:HG3	2.15	0.45
57:1y:4:G:H5'	57:1y:5:G:OP2	2.16	0.45
1:2A:458:G:O2'	1:2A:469:G:O6	2.34	0.45
1:2A:747:U:H1'	18:2W:92:ARG:HH22	1.82	0.45
1:2A:922:U:H2'	1:2A:923:C:C6	2.51	0.45
1:2A:1015:G:H2'	1:2A:1016:G:C8	2.51	0.45
25:23:59:VAL:HG12	25:23:60:GLU:H	1.82	0.45
32:2a:353:A:H5'	32:2a:353:A:H8	1.81	0.45
32:2a:473:G:H2'	32:2a:474:G:C8	2.51	0.45
32:2a:866:C:H4'	32:2a:919:A:H5'	1.99	0.45
32:2a:1148:U:H2'	32:2a:1149:C:O4'	2.17	0.45
32:2a:1276:G:C2'	32:2a:1277:C:H5'	2.46	0.45
54:2w:14:A:H2'	54:2w:15:A:H8	1.82	0.45
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.51	0.45
32:1a:96:U:H2'	32:1a:97:G:H8	1.80	0.45
32:1a:277:C:P	48:1q:68:ARG:HH12	2.40	0.45
35:1d:18:LYS:HD3	62:1d:302:SF4:S1	2.56	0.45
35:1d:100:ARG:HE	35:1d:137:SER:HA	1.82	0.45
1:2A:68:G:N2	1:2A:74:A:OP2	2.48	0.45
1:2A:143(A):C:O2'	19:2X:2:LYS:NZ	2.37	0.45
1:2A:284:U:H2'	1:2A:285:C:C6	2.52	0.45
1:2A:945:A:C4	1:2A:2448:A:C2	3.05	0.45
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.52	0.45
1:2A:1423:G:OP1	1:2A:1492:G:O2'	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.33	0.45
7:2H:71:LEU:HD23	7:2H:71:LEU:HA	1.80	0.45
10:2O:24:VAL:HG22	10:2O:33:ALA:HB2	1.98	0.45
20:2Y:35:TYR:CE2	20:2Y:69:ALA:HB3	2.51	0.45
32:2a:149:A:H2'	32:2a:150:C:C6	2.52	0.45
32:2a:972:C:H4'	41:2j:57:LYS:HB2	1.99	0.45
45:2n:24:CYS:HB3	45:2n:29:ARG:H	1.81	0.45
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.51	0.45
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.50	0.45
1:1A:1227:G:OP2	16:1U:16:LYS:NZ	2.42	0.45
1:1A:2336:A:H61	22:10:43:THR:HG22	1.81	0.45
1:1A:2810:A:H61	1:1A:2891:G:HO2'	1.61	0.45
8:1I:85:GLU:HG3	8:1I:86:THR:HG23	1.98	0.45
32:1a:352:C:OP2	63:1a:1914:HOH:O	2.21	0.45
32:1a:1048:G:OP1	45:1n:3:ARG:HB3	2.16	0.45
32:1a:1066:C:O2'	32:1a:1067:A:H5'	2.16	0.45
34:1c:16:ARG:HE	34:1c:16:ARG:HB3	1.60	0.45
35:1d:112:VAL:H	35:1d:116:GLN:NE2	2.15	0.45
36:1e:151:LEU:HD22	39:1h:79:VAL:HG22	1.99	0.45
38:1g:65:ALA:HB1	38:1g:127:ALA:HB3	1.99	0.45
39:1h:87:SER:HB2	39:1h:93:VAL:HB	1.99	0.45
51:1t:86:ARG:HB3	51:1t:90:GLN:HE22	1.82	0.45
1:2A:458:G:C8	29:27:37:LYS:HG2	2.51	0.45
1:2A:1264:G:H2'	1:2A:2014:A:N6	2.31	0.45
1:2A:2100:G:N2	1:2A:2189:U:O2	2.38	0.45
1:2A:2128:C:H6	1:2A:2128:C:O5'	1.99	0.45
5:2F:10:PRO:HB3	5:2F:17:ARG:NH1	2.31	0.45
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	1.98	0.45
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.98	0.45
31:29:1:MET:HE2	31:29:33:LYS:HD2	1.99	0.45
32:2a:509:A:H5''	35:2d:55:ALA:HB2	1.99	0.45
32:2a:757:U:H2'	32:2a:758:G:O4'	2.17	0.45
32:2a:1426:C:H2'	32:2a:1427:U:H6	1.81	0.45
33:2b:40:HIS:HB3	33:2b:190:THR:HG21	1.99	0.45
34:2c:129:ALA:O	34:2c:133:ALA:N	2.41	0.45
36:2e:80:ILE:HG22	36:2e:91:LEU:HB2	1.98	0.45
42:2k:40:ILE:HG13	42:2k:41:THR:HG22	1.99	0.45
48:2q:45:HIS:HB3	48:2q:72:ARG:HG2	1.99	0.45
50:2s:49:ILE:H	50:2s:62:ILE:HD11	1.82	0.45
1:1A:236:C:H2'	1:1A:237:C:C6	2.52	0.45
1:1A:880:G:H8	1:1A:880:G:OP2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1800:C:OP2	3:1D:183:ARG:NH2	2.49	0.45
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.32	0.45
19:1X:92:LEU:O	19:1X:94:GLY:N	2.49	0.45
32:1a:741:G:H2'	32:1a:742:G:O4'	2.17	0.45
32:1a:1149:C:P	40:1i:9:ARG:HH21	2.40	0.45
33:1b:222:ILE:O	33:1b:226:ARG:HG2	2.17	0.45
37:1f:76:ALA:O	37:1f:80:ARG:HG3	2.17	0.45
39:1h:11:THR:HG22	39:1h:15:ASN:HD21	1.81	0.45
1:2A:746:A:H2'	1:2A:2612:C:H5''	1.98	0.45
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.98	0.45
6:2G:97:ASP:HA	6:2G:100:TRP:HD1	1.81	0.45
20:2Y:5:MET:HB2	20:2Y:5:MET:HE2	1.74	0.45
32:2a:951:G:N3	32:2a:970:C:O2'	2.42	0.45
32:2a:1498:UR3:O2'	53:2v:17:U:OP1	2.33	0.45
33:2b:86:GLU:C	33:2b:89:GLY:H	2.25	0.45
33:2b:223:ILE:O	33:2b:226:ARG:HG2	2.16	0.45
39:2h:33:GLU:HG2	39:2h:48:TYR:CE1	2.51	0.45
40:2i:50:LEU:HA	40:2i:53:VAL:HG22	1.98	0.45
44:2m:29:ARG:HD3	44:2m:64:TRP:CE2	2.52	0.45
50:2s:30:LEU:HA	50:2s:48:THR:O	2.17	0.45
55:2x:10:G:N2	55:2x:26:G:H1'	2.32	0.45
1:1A:1045:A:H1'	1:1A:1047:G:N3	2.31	0.45
1:1A:2320:A:H2'	1:1A:2320:A:N3	2.32	0.45
1:1A:2630:G:H2'	1:1A:2631:G:C8	2.52	0.45
4:1E:7:VAL:HG23	4:1E:51:PHE:CE2	2.51	0.45
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.51	0.45
21:1Z:31:ARG:HG3	21:1Z:32:HIS:CE1	2.52	0.45
32:1a:434:U:H2'	32:1a:435:C:C6	2.52	0.45
32:1a:448:A:C4	32:1a:487:A:C2	3.05	0.45
32:1a:718:G:H5'	42:1k:117:ASN:HB2	1.99	0.45
32:1a:1140:C:H2'	32:1a:1141:C:C6	2.50	0.45
32:1a:1212:U:H4'	32:1a:1213:A:C8	2.52	0.45
35:1d:140:VAL:HG12	35:1d:144:ASP:OD1	2.17	0.45
1:2A:127:A:H5''	1:2A:128:C:C6	2.51	0.45
1:2A:190:A:OP2	23:21:39:LYS:HE3	2.17	0.45
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.31	0.45
1:2A:1418:G:H2'	1:2A:1579:A:H62	1.82	0.45
1:2A:1771:C:OP1	63:2A:3952:HOH:O	2.21	0.45
1:2A:2106:G:H2'	1:2A:2107:C:O4'	2.16	0.45
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.17	0.45
5:2F:157:VAL:HA	5:2F:176:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2N:42:TRP:CH2	9:2N:44:PRO:HB3	2.52	0.45
21:2Z:163:LEU:HD21	21:2Z:165:VAL:HG22	1.99	0.45
32:2a:947:G:H1	32:2a:1234:C:H42	1.63	0.45
32:2a:1178:G:N2	32:2a:1180:A:H3'	2.32	0.45
34:2c:47:LEU:HD22	34:2c:52:LEU:HD13	1.99	0.45
49:2r:53:ARG:HA	49:2r:56:THR:OG1	2.17	0.45
50:2s:27:GLU:HB2	50:2s:28:LYS:HG3	1.99	0.45
1:1A:284:U:H2'	1:1A:285:C:C6	2.51	0.45
1:1A:2124:G:H3'	1:1A:2125:G:C8	2.52	0.45
8:1I:61:ARG:HD3	8:1I:61:ARG:HA	1.72	0.45
32:1a:815:A:N7	32:1a:1509:C:O2'	2.45	0.45
34:1c:33:LEU:HD11	45:1n:53:LEU:HD22	1.98	0.45
35:1d:114:ARG:HA	35:1d:117:ALA:HB3	1.99	0.45
35:1d:117:ALA:O	35:1d:121:VAL:HG23	2.17	0.45
37:1f:12:PRO:HG3	37:1f:57:GLN:O	2.17	0.45
41:1j:50:ILE:HB	45:1n:41:ARG:HD2	1.99	0.45
1:2A:208:C:H2'	1:2A:209:C:C6	2.52	0.45
1:2A:747:U:O2'	18:2W:92:ARG:NH2	2.42	0.45
1:2A:764:A:H5'	3:2D:210:GLY:HA2	1.99	0.45
1:2A:2141:G:H2'	1:2A:2142:C:O4'	2.16	0.45
1:2A:2563:U:O2	1:2A:2565:A:H8	1.99	0.45
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.80	0.45
1:2A:2823:A:OP1	4:2E:159:HIS:NE2	2.46	0.45
21:2Z:95:PRO:HA	21:2Z:129:SER:HA	1.98	0.45
32:2a:1016:A:HO2'	32:2a:1217:C:HO2'	1.61	0.45
32:2a:1271:G:C2	32:2a:1272:G:C8	3.04	0.45
32:2a:1324:A:H4'	32:2a:1362:C:O3'	2.17	0.45
33:2b:8:LYS:HG3	33:2b:51:LEU:HD13	1.98	0.45
33:2b:163:PHE:HA	33:2b:185:ILE:HG12	1.99	0.45
33:2b:167:PRO:HG3	33:2b:188:ALA:HB2	1.99	0.45
34:2c:121:ALA:HB1	34:2c:188:LEU:O	2.17	0.45
36:2e:20:GLN:HE21	36:2e:20:GLN:C	2.25	0.45
48:2q:41:LYS:NZ	48:2q:92:ARG:HH21	2.14	0.45
50:2s:42:PRO:HG3	50:2s:67:VAL:HG11	1.98	0.45
51:2t:50:GLU:OE1	51:2t:100:ILE:HD11	2.17	0.45
54:2w:54:5MU:C4	54:2w:55:PSU:C2	3.04	0.45
57:2y:66:C:H2'	57:2y:67:G:O4'	2.17	0.45
1:1A:674:G:O2'	5:1F:74:ARG:HD3	2.17	0.45
1:1A:784:A:C8	1:1A:792:G:C5	3.05	0.45
1:1A:1876:A:H2'	1:1A:1877:A:C8	2.51	0.45
1:1A:2482:G:O3'	54:1w:64:U:H4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:32:TYR:HD1	15:1T:83:ILE:HG12	1.82	0.45
21:1Z:150:LEU:HD11	21:1Z:154:ASP:HB2	1.98	0.45
32:1a:79:G:O6	32:1a:90:U:C2	2.70	0.45
32:1a:160:A:H3'	32:1a:161:A:C8	2.52	0.45
32:1a:202:U:H3'	32:1a:203:U:C5	2.52	0.45
32:1a:993:G:H2'	32:1a:995:C:H41	1.81	0.45
32:1a:1101:A:H4'	32:1a:1102:A:O5'	2.17	0.45
33:1b:16:HIS:CD2	33:1b:17:PHE:N	2.85	0.45
36:1e:90:VAL:O	36:1e:120:THR:HA	2.16	0.45
57:1y:50:A:H2'	57:1y:51:G:O4'	2.17	0.45
1:2A:141:A:C8	1:2A:1408:C:O2'	2.69	0.45
1:2A:1001:A:H2'	1:2A:1002:G:O4'	2.17	0.45
1:2A:1509(B):A:H2'	1:2A:1510:G:C8	2.51	0.45
1:2A:1721:G:H2'	1:2A:1740:G:O6	2.16	0.45
1:2A:2318:G:H21	14:2S:3:ARG:NE	2.15	0.45
2:2B:13:A:N1	2:2B:69:G:O2'	2.44	0.45
6:2G:115:ARG:HH21	6:2G:136:ARG:NH2	2.14	0.45
21:2Z:150:LEU:HG	21:2Z:154:ASP:OD2	2.17	0.45
32:2a:165:C:H2'	32:2a:166:G:H8	1.81	0.45
32:2a:410:G:OP1	35:2d:30:LYS:NZ	2.25	0.45
32:2a:1216:G:H5''	45:2n:5:ALA:HB2	1.98	0.45
32:2a:1221:G:H4'	50:2s:53:ASN:O	2.17	0.45
32:2a:1490:C:H2'	32:2a:1491:G:C8	2.52	0.45
41:2j:50:ILE:HA	41:2j:60:ARG:HD3	1.99	0.45
43:2l:51:ALA:O	43:2l:52:LEU:HD23	2.17	0.45
44:2m:90:LEU:HD12	44:2m:93:ARG:HD2	1.99	0.45
1:1A:1266:G:O4'	18:1W:15:ARG:NH2	2.46	0.44
1:1A:1365:A:O2'	23:11:11:ARG:NH1	2.49	0.44
1:1A:1779:U:H2'	63:1A:4413:HOH:O	2.17	0.44
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	1.99	0.44
7:1H:3:ARG:HD2	7:1H:3:ARG:HA	1.46	0.44
9:1N:96:GLU:H	9:1N:96:GLU:CD	2.25	0.44
26:14:50:VAL:HG11	44:1m:64:TRP:HA	1.99	0.44
32:1a:645:C:H2'	32:1a:646:U:C6	2.52	0.44
32:1a:1223:C:P	50:1s:78:ARG:HH21	2.40	0.44
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.52	0.44
55:1x:2:G:H2'	55:1x:2:G:N3	2.31	0.44
1:2A:686:G:H21	1:2A:788:A:H61	1.65	0.44
1:2A:1183:G:H5''	25:23:30:ARG:NH2	2.31	0.44
1:2A:2812:G:H2'	1:2A:2813:A:C8	2.52	0.44
5:2F:108:LYS:O	5:2F:112:MET:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:35:ILE:HD13	14:2S:66:ALA:HB2	1.99	0.44
32:2a:8:A:H5'	36:2e:101:ILE:HG22	1.99	0.44
32:2a:620:C:H2'	32:2a:621:A:O4'	2.17	0.44
32:2a:1227:A:O3'	44:2m:115:LYS:HE2	2.17	0.44
33:2b:111:ARG:HH11	33:2b:111:ARG:HA	1.82	0.44
33:2b:215:LEU:O	33:2b:219:VAL:HG12	2.17	0.44
33:2b:217:ARG:HA	33:2b:220:ASP:HB2	1.99	0.44
34:2c:119:ARG:HE	34:2c:140:ARG:CZ	2.30	0.44
34:2c:159:GLY:HA2	34:2c:193:TYR:CZ	2.52	0.44
38:2g:72:ARG:HH22	38:2g:138:LYS:NZ	2.15	0.44
41:2j:16:LEU:HB3	41:2j:70:ARG:HG3	1.98	0.44
48:2q:67:LYS:O	48:2q:68:ARG:HB2	2.17	0.44
1:1A:1999:C:H4'	1:1A:2723:C:O2	2.16	0.44
1:1A:2080:G:OP1	23:11:35:THR:HG21	2.18	0.44
1:1A:2165:G:H2'	1:1A:2166:G:C5	2.52	0.44
1:1A:2277:G:OP2	22:10:10:THR:HG21	2.18	0.44
2:1B:92:C:H5''	21:1Z:79:ARG:NH1	2.32	0.44
8:1I:62:LYS:HA	8:1I:133:HIS:HE1	1.83	0.44
11:1P:38:GLN:O	11:1P:40:SER:N	2.49	0.44
32:1a:620:C:H2'	32:1a:621:A:O4'	2.17	0.44
1:2A:307:G:H21	1:2A:330:A:N6	2.13	0.44
1:2A:1183:G:H5''	25:23:30:ARG:HH21	1.82	0.44
1:2A:1478:G:O2'	1:2A:1558:A:N1	2.48	0.44
1:2A:2117:A:H1'	1:2A:2119:A:OP2	2.18	0.44
6:2G:135:LEU:HD11	6:2G:157:ILE:HD11	1.98	0.44
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.18	0.44
17:2V:2:PHE:CZ	17:2V:41:GLY:HA3	2.52	0.44
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.53	0.44
21:2Z:122:ARG:H	21:2Z:122:ARG:HD2	1.82	0.44
23:21:59:THR:O	23:21:91:LYS:NZ	2.45	0.44
23:21:82:LEU:HA	23:21:85:LEU:HD12	1.99	0.44
32:2a:429:U:H1'	32:2a:430:A:H5''	1.99	0.44
32:2a:1333:A:H2'	32:2a:1334:G:O4'	2.18	0.44
32:2a:1403:C:H2'	32:2a:1404:5MC:HM53	1.98	0.44
32:2a:1517:G:N7	32:2a:1518:MA6:H103	2.32	0.44
36:2e:11:ILE:HD11	36:2e:33:VAL:HG12	1.99	0.44
39:2h:20:TYR:CE1	39:2h:76:PRO:HG2	2.51	0.44
1:1A:218:A:C2	1:1A:235:U:H4'	2.52	0.44
1:1A:576:U:H2'	1:1A:577:G:C8	2.53	0.44
1:1A:1239:G:H2'	1:1A:1240:U:O4'	2.17	0.44
1:1A:2544:G:H1'	1:1A:2646:C:H4'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.18	0.44
26:14:59:PHE:CD2	50:1s:64:GLU:HB3	2.52	0.44
31:19:25:VAL:HB	31:19:34:GLN:HB2	1.99	0.44
32:1a:674:G:H2'	32:1a:675:A:H8	1.82	0.44
32:1a:1456:G:H22	51:1t:51:GLU:CD	2.20	0.44
36:1e:66:MET:HE3	36:1e:66:MET:HB3	1.85	0.44
41:1j:11:PHE:HE1	41:1j:67:THR:HG22	1.82	0.44
1:2A:320:A:H4'	1:2A:322:A:C8	2.52	0.44
1:2A:829:A:N7	1:2A:2248:C:H5'	2.32	0.44
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.29	0.44
1:2A:2320:A:H1'	1:2A:2321:G:N1	2.31	0.44
6:2G:70:VAL:HA	6:2G:90:LEU:HD23	1.99	0.44
6:2G:179:PRO:HG3	26:24:43:TYR:CZ	2.52	0.44
21:2Z:40:ASP:OD2	21:2Z:42:VAL:HG13	2.17	0.44
32:2a:434:U:H2'	32:2a:435:C:H6	1.80	0.44
32:2a:1206:G:C6	32:2a:1207:2MG:C5	3.05	0.44
33:2b:103:THR:HA	33:2b:180:LEU:HD11	1.99	0.44
1:1A:1698:A:C8	1:1A:1700:A:O4'	2.70	0.44
16:1U:19:LYS:O	16:1U:22:LYS:HG3	2.18	0.44
21:1Z:7:ALA:O	21:1Z:62:PRO:HD3	2.17	0.44
36:1e:145:LYS:HA	36:1e:148:VAL:HG22	2.00	0.44
41:1j:6:ILE:O	41:1j:71:LEU:HD12	2.17	0.44
1:2A:740:U:H2'	1:2A:741:G:C8	2.53	0.44
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.52	0.44
1:2A:2533:A:OP1	1:2A:2665:A:O2'	2.34	0.44
1:2A:2647:U:H2'	1:2A:2648:C:C6	2.53	0.44
2:2B:59:A:H2'	2:2B:60:C:O4'	2.17	0.44
6:2G:56:ALA:HA	6:2G:59:GLU:HG2	1.98	0.44
32:2a:1220:G:O3'	50:2s:36:ARG:HD3	2.17	0.44
41:2j:32:ALA:HB1	41:2j:33:GLN:HA	1.98	0.44
57:2y:7:G:H8	57:2y:7:G:OP2	2.01	0.44
1:1A:2074:U:H2'	1:1A:2075:U:C6	2.52	0.44
1:1A:2206:G:OP2	1:1A:2206:G:H4'	2.17	0.44
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.17	0.44
8:1I:69:LYS:HA	8:1I:138:ILE:HD12	2.00	0.44
32:1a:909:A:H2'	32:1a:910:C:O4'	2.17	0.44
32:1a:986:A:H1'	50:1s:54:GLY:O	2.17	0.44
32:1a:1298:C:H4'	32:1a:1299:A:C4	2.53	0.44
32:1a:1518:MA6:H93	32:1a:1519:MA6:C9	2.47	0.44
33:1b:24:TRP:CD1	33:1b:24:TRP:H	2.36	0.44
1:2A:68:G:H2'	1:2A:69:C:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:196:A:N3	1:2A:196:A:H2'	2.33	0.44
1:2A:952:G:C6	1:2A:966:G:C6	3.06	0.44
1:2A:2375:G:O2'	1:2A:2377:A:N7	2.40	0.44
1:2A:2788:C:O2'	1:2A:2809:A:N3	2.46	0.44
6:2G:5:VAL:HG22	6:2G:8:LYS:H	1.82	0.44
6:2G:42:GLY:O	6:2G:44:GLY:N	2.51	0.44
6:2G:91:ARG:CZ	6:2G:91:ARG:HB3	2.48	0.44
16:2U:27:LEU:HD23	16:2U:27:LEU:HA	1.83	0.44
32:2a:677:U:H3	32:2a:713:G:H22	1.65	0.44
32:2a:1142:G:H3'	32:2a:1143:G:H8	1.81	0.44
44:2m:4:ILE:HG13	44:2m:5:ALA:H	1.82	0.44
50:2s:12:ASP:OD1	50:2s:37:ARG:NH2	2.50	0.44
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.43	0.44
1:1A:228:A:H2'	1:1A:230:U:O4'	2.18	0.44
1:1A:286:C:H2'	1:1A:287:C:C6	2.53	0.44
1:1A:2278:A:OP2	22:10:12:ASN:ND2	2.44	0.44
7:1H:11:VAL:HG13	7:1H:15:VAL:HG22	1.99	0.44
10:1O:73:ASP:HB2	15:1T:82:LEU:HD13	2.00	0.44
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.17	0.44
32:1a:271:C:H2'	32:1a:272:C:C6	2.52	0.44
35:1d:162:LEU:HD13	35:1d:181:MET:HG2	1.99	0.44
36:1e:85:GLY:O	36:1e:87:SER:N	2.51	0.44
37:1f:4:TYR:HD1	37:1f:92:LYS:HA	1.83	0.44
37:1f:19:LEU:HD21	37:1f:59:TYR:CE1	2.53	0.44
40:1i:17:VAL:HG21	40:1i:81:ILE:HG12	1.99	0.44
55:1x:8:4SU:O2	55:1x:21:A:H2	2.00	0.44
1:2A:370:G:N7	63:2A:4036:HOH:O	2.36	0.44
1:2A:2065:C:H4'	1:2A:2251:OMG:HM22	2.00	0.44
1:2A:2203:U:O4'	3:2D:151:LYS:HE2	2.17	0.44
1:2A:2611:U:H6	1:2A:2611:U:H5'	1.83	0.44
19:2X:11:PRO:HB3	19:2X:92:LEU:HD21	2.00	0.44
21:2Z:126:VAL:HG13	21:2Z:161:VAL:HG23	2.00	0.44
26:24:41:PRO:HG3	26:24:49:PHE:CE1	2.53	0.44
28:26:38:LYS:HB3	28:26:38:LYS:HE3	1.67	0.44
32:2a:1027:C:C2	32:2a:1034:G:N2	2.86	0.44
45:2n:23:ARG:CZ	45:2n:30:ALA:HB2	2.47	0.44
55:2x:53:G:H2'	55:2x:54:5MU:H6	1.83	0.44
57:2y:9:A:H4'	57:2y:45:U:O2'	2.17	0.44
1:1A:264:C:O2'	1:1A:265:A:H2'	2.18	0.44
1:1A:1641:A:H2'	1:1A:1642:G:O4'	2.17	0.44
1:1A:1800:C:OP1	3:1D:260:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2319:G:H22	14:1S:3:ARG:CD	2.30	0.44
10:1O:19:ILE:HB	10:1O:41:ALA:HB1	2.00	0.44
10:1O:49:ARG:HH12	32:1a:1423:G:P	2.40	0.44
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.17	0.44
26:14:46:GLN:HB3	26:14:48:ARG:NH2	2.32	0.44
32:1a:418:C:H1'	32:1a:540:G:O2'	2.18	0.44
32:1a:1012:U:H3	32:1a:1017:G:H1	1.65	0.44
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	1.98	0.44
36:1e:95:ALA:HB1	36:1e:96:PRO:HD2	2.00	0.44
1:2A:287:C:H2'	1:2A:288:C:H6	1.82	0.44
1:2A:937:U:H2'	1:2A:938:G:O4'	2.18	0.44
1:2A:1003:G:N2	1:2A:1153:C:C2	2.85	0.44
1:2A:2134:A:H2'	1:2A:2134:A:N3	2.32	0.44
1:2A:2155:G:N7	1:2A:2156:G:H1'	2.32	0.44
1:2A:2389:G:H5''	1:2A:2390:U:O4'	2.18	0.44
4:2E:101:ARG:NH2	4:2E:171:GLU:HB2	2.33	0.44
5:2F:11:VAL:HB	5:2F:18:ARG:HB2	2.00	0.44
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.43	0.44
9:2N:62:VAL:HG11	9:2N:87:LEU:HD21	2.00	0.44
12:2Q:38:GLU:HB2	12:2Q:127:ILE:HG22	2.00	0.44
15:2T:127:ALA:C	15:2T:129:ARG:H	2.24	0.44
21:2Z:150:LEU:HD12	21:2Z:150:LEU:HA	1.74	0.44
24:22:17:SER:N	24:22:20:GLU:OE1	2.34	0.44
32:2a:422:C:H5'	32:2a:423:G:C5	2.53	0.44
32:2a:1401:G:H2'	32:2a:1402:4OC:O4'	2.18	0.44
33:2b:9:GLU:HB3	33:2b:10:LEU:H	1.58	0.44
33:2b:178:ARG:HH12	39:2h:68:ARG:HH22	1.64	0.44
34:2c:137:ALA:HA	34:2c:140:ARG:NH1	2.32	0.44
57:2y:9:A:O2'	57:2y:11:U:O4	2.32	0.44
57:2y:14:A:H2'	57:2y:15:A:C8	2.53	0.44
1:1A:322:A:OP1	5:1F:168:ARG:HD3	2.18	0.44
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.52	0.44
1:1A:2059:A:H2'	1:1A:2503:2MA:HM23	2.00	0.44
1:1A:2849:U:O4	15:1T:23:ARG:NH2	2.40	0.44
2:1B:48:A:H2'	2:1B:49:C:C6	2.52	0.44
4:1E:52:LEU:O	4:1E:76:ARG:N	2.46	0.44
9:1N:4:TYR:CE2	16:1U:100:VAL:HG11	2.53	0.44
10:1O:16:ALA:HB2	10:1O:52:VAL:HG21	1.99	0.44
21:1Z:152:ALA:HB1	21:1Z:163:LEU:HD21	2.00	0.44
32:1a:358:U:H2'	32:1a:359:U:C6	2.52	0.44
32:1a:985:C:H2'	32:1a:986:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1224:G:OP1	63:1a:1915:HOH:O	2.21	0.44
32:1a:1410:G:H2'	32:1a:1411:C:C6	2.53	0.44
46:1o:29:VAL:HG11	46:1o:67:LEU:HD21	2.00	0.44
1:2A:224:G:H2'	1:2A:225:A:O4'	2.17	0.44
1:2A:330:A:H2	1:2A:1210:A:O2'	1.98	0.44
1:2A:579:G:H2'	1:2A:580:C:H6	1.82	0.44
1:2A:667:U:O2	30:28:2:PRO:HD2	2.18	0.44
1:2A:1198:U:H2'	1:2A:1199:U:C6	2.53	0.44
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.18	0.44
1:2A:1411:C:H2'	1:2A:1412:A:H8	1.83	0.44
1:2A:2741:A:H2'	1:2A:2742:C:O4'	2.17	0.44
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.51	0.44
6:2G:11:TYR:HA	6:2G:15:VAL:HB	2.00	0.44
8:2I:134:PRO:C	8:2I:136:VAL:H	2.26	0.44
9:2N:96:GLU:CD	9:2N:96:GLU:H	2.25	0.44
21:2Z:130:PRO:HG2	21:2Z:131:ARG:HD2	1.99	0.44
22:20:29:GLN:HE21	22:20:29:GLN:HB3	1.64	0.44
32:2a:7:G:O2'	36:2c:120:THR:O	2.35	0.44
32:2a:833:U:H2'	32:2a:834:C:C6	2.53	0.44
32:2a:1004:A:C8	32:2a:1005:A:H4'	2.53	0.44
32:2a:1051:C:H2'	32:2a:1052:U:H6	1.83	0.44
32:2a:1379:G:O6	38:2g:2:ALA:HB3	2.18	0.44
33:2b:19:HIS:ND1	33:2b:206:ASP:OD2	2.51	0.44
34:2c:129:ALA:HB3	34:2c:132:ARG:HB3	1.99	0.44
42:2k:21:ILE:HD12	42:2k:95:ILE:HG12	1.99	0.44
44:2m:33:ALA:HA	44:2m:59:TYR:HE2	1.82	0.44
45:2n:9:LYS:HB2	45:2n:9:LYS:HE3	1.82	0.44
51:2t:98:PRO:O	51:2t:99:LEU:HB2	2.18	0.44
1:1A:375:C:H2'	1:1A:376:C:C6	2.53	0.44
1:1A:602:G:O2'	1:1A:655:A:N6	2.49	0.44
1:1A:655:A:H2'	1:1A:656:G:O4'	2.17	0.44
1:1A:1071:G:OP1	1:1A:1071:G:H3'	2.18	0.44
1:1A:1312:U:OP2	19:1X:63:LYS:HE2	2.18	0.44
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.32	0.44
8:1I:109:ILE:HD12	8:1I:109:ILE:HA	1.88	0.44
36:1e:137:GLU:HA	36:1e:140:ARG:HH11	1.82	0.44
50:1s:27:GLU:H	50:1s:27:GLU:CD	2.21	0.44
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.43	0.44
1:2A:868:U:C4	1:2A:869:G:N7	2.85	0.44
1:2A:1830:C:OP2	63:2A:3953:HOH:O	2.21	0.44
1:2A:2125:G:H1	1:2A:2172:U:P	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2O:1:MET:HE3	10:2O:32:TYR:CE1	2.52	0.44
14:2S:34:HIS:C	14:2S:35:ILE:HG13	2.43	0.44
21:2Z:128:VAL:HG12	21:2Z:161:VAL:HA	1.99	0.44
26:24:45:GLY:C	26:24:47:GLN:H	2.26	0.44
32:2a:109:A:C6	32:2a:326:G:C6	3.06	0.44
32:2a:678:U:H2'	32:2a:679:C:C6	2.52	0.44
32:2a:779:C:O2'	42:2k:120:ARG:HD3	2.18	0.44
32:2a:1261:A:H3'	32:2a:1262:C:H6	1.82	0.44
32:2a:1266:G:N2	32:2a:1268:A:H3'	2.32	0.44
35:2d:33:MET:O	35:2d:37:PRO:HB3	2.18	0.44
1:1A:863:A:OP1	12:1Q:22:LYS:HG3	2.18	0.43
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.50	0.43
8:1I:47:LEU:HD23	8:1I:47:LEU:HA	1.80	0.43
9:1N:58:ASP:OD1	9:1N:58:ASP:N	2.43	0.43
32:1a:186:C:H2'	32:1a:187:C:C6	2.53	0.43
32:1a:841:U:C2	32:1a:848:C:H1'	2.53	0.43
34:1c:9:GLY:HA2	34:1c:12:LEU:HG	2.00	0.43
51:1t:36:LEU:HD13	51:1t:58:LYS:HG3	2.00	0.43
1:2A:1916:A:H2'	1:2A:1917:PSU:O4'	2.16	0.43
32:2a:1253:G:H2'	32:2a:1254:C:C6	2.53	0.43
33:2b:185:ILE:HG22	33:2b:199:TYR:HD2	1.81	0.43
1:1A:1405:U:H2'	1:1A:1406:U:H6	1.78	0.43
1:1A:2163:C:H5''	1:1A:2164:C:OP2	2.17	0.43
6:1G:20:ILE:O	6:1G:24:GLY:N	2.43	0.43
32:1a:418:C:H2'	32:1a:419:C:C6	2.53	0.43
32:1a:693:G:H2'	32:1a:694:A:C8	2.53	0.43
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.54	0.43
32:1a:1039:C:H2'	32:1a:1040:U:C6	2.53	0.43
36:1e:51:VAL:O	36:1e:55:VAL:HG23	2.18	0.43
38:1g:20:ASP:HB3	38:1g:23:VAL:HG23	1.99	0.43
39:1h:11:THR:HG22	39:1h:15:ASN:ND2	2.34	0.43
43:1l:69:TYR:HB2	43:1l:96:VAL:HG11	2.00	0.43
54:1w:76:L3X:N	55:1x:76:8AN:N3'	2.65	0.43
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.53	0.43
1:2A:643:A:C8	28:26:44:ARG:NH1	2.86	0.43
1:2A:748:G:C8	18:2W:89:ALA:HB1	2.53	0.43
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.16	0.43
4:2E:54:GLN:NE2	4:2E:76:ARG:HG2	2.33	0.43
8:2I:84:GLY:C	8:2I:86:THR:H	2.26	0.43
10:2O:48:PRO:CB	32:2a:1422:G:H5''	2.44	0.43
14:2S:87:PHE:CE1	14:2S:102:ALA:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:20:5:LYS:NZ	55:2x:2:G:OP2	2.51	0.43
32:2a:60:A:H4'	32:2a:61:G:O5'	2.18	0.43
32:2a:580:U:H2'	32:2a:581:G:O4'	2.17	0.43
32:2a:859:A:H2'	32:2a:860:A:O4'	2.18	0.43
32:2a:957:U:H2'	32:2a:959:A:OP2	2.18	0.43
32:2a:1272:G:N2	32:2a:1273:G:C8	2.87	0.43
32:2a:1323:G:H4'	32:2a:1363:C:N3	2.32	0.43
32:2a:1326:C:H2'	32:2a:1327:C:C6	2.54	0.43
34:2c:20:SER:HB3	34:2c:22:TRP:HE1	1.82	0.43
37:2f:36:ARG:HH12	37:2f:38:GLU:HG2	1.83	0.43
1:1A:113:G:H5'	63:1A:4495:HOH:O	2.18	0.43
1:1A:586:A:N1	1:1A:809:G:O2'	2.42	0.43
1:1A:897:C:H4'	54:1w:55:PSU:O3'	2.17	0.43
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.18	0.43
1:1A:1744:C:H2'	1:1A:1745:C:C6	2.53	0.43
2:1B:43:C:H5''	26:14:1:MET:HG2	2.00	0.43
5:1F:9:ILE:HG12	5:1F:123:LEU:HD23	1.99	0.43
19:1X:94:GLY:CA	19:1X:95:LEU:HB2	2.48	0.43
32:1a:192:U:O3'	51:1t:57:ARG:HD2	2.18	0.43
32:1a:445:G:H2'	32:1a:446:G:O4'	2.18	0.43
35:1d:18:LYS:NZ	35:1d:26:CYS:O	2.50	0.43
36:1e:78:HIS:CE1	36:1e:142:LEU:HD23	2.54	0.43
55:1x:17:C:OP2	55:1x:17(A):U:O2'	2.33	0.43
1:2A:1782:C:O2	1:2A:2608:G:O2'	2.32	0.43
1:2A:2365:G:OP1	22:20:55:ARG:N	2.43	0.43
1:2A:2735:G:H2'	1:2A:2736:G:H8	1.84	0.43
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.27	0.43
7:2H:68:THR:O	7:2H:72:ILE:HG13	2.17	0.43
12:2Q:59:ARG:C	12:2Q:61:GLY:H	2.25	0.43
21:2Z:5:LEU:O	21:2Z:59:LEU:HA	2.18	0.43
32:2a:1410:G:H2'	32:2a:1411:C:H6	1.84	0.43
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.26	0.43
48:2q:67:LYS:HA	48:2q:70:ARG:HH12	1.83	0.43
54:2w:76:L3X:N	55:2x:76:8AN:N3'	2.66	0.43
1:1A:251:A:C5	1:1A:252:G:H1'	2.53	0.43
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.33	0.43
1:1A:1065:U:H1'	1:1A:1074:G:C2	2.53	0.43
10:1O:7:TYR:OH	10:1O:44:LYS:HG3	2.17	0.43
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.54	0.43
26:14:13:ARG:HB2	26:14:30:GLU:HG2	2.00	0.43
32:1a:690:G:C6	32:1a:691:G:C6	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1157:A:H5'	32:1a:1158:C:C6	2.52	0.43
32:1a:1252:A:H2'	32:1a:1253:G:O4'	2.18	0.43
34:1c:175:LEU:HD23	34:1c:182:ILE:HD13	1.99	0.43
35:1d:105:VAL:HG13	35:1d:110:PHE:HB2	2.00	0.43
37:1f:100:ASN:HD21	49:1r:23:LYS:HE3	1.84	0.43
39:1h:14:ARG:NH2	39:1h:83:ILE:O	2.32	0.43
44:1m:108:ARG:HD3	44:1m:108:ARG:HA	1.72	0.43
50:1s:70:LYS:HB2	50:1s:73:GLU:HG3	2.00	0.43
53:1v:19:G:N2	54:1w:37:A:H1'	2.33	0.43
1:2A:764:A:H5'	3:2D:210:GLY:CA	2.48	0.43
1:2A:1309:G:H4'	29:27:7:PRO:HB2	2.00	0.43
1:2A:1336:A:H2'	1:2A:1337:G:H8	1.82	0.43
1:2A:2472:G:N1	1:2A:2477:C:OP1	2.45	0.43
9:2N:12:ARG:NH2	9:2N:50:ASP:OD2	2.51	0.43
9:2N:29:LYS:HD2	9:2N:140:VAL:HB	1.99	0.43
26:24:35:VAL:HG12	26:24:36:CYS:H	1.83	0.43
32:2a:404:U:H2'	32:2a:405:U:C6	2.53	0.43
32:2a:1064:G:H1'	32:2a:1190:G:N2	2.34	0.43
32:2a:1236:A:O2'	32:2a:1304:G:H4'	2.18	0.43
32:2a:1427:U:H2'	32:2a:1428:A:H8	1.82	0.43
33:2b:144:ARG:HE	33:2b:148:TYR:HE2	1.65	0.43
34:2c:20:SER:HB3	34:2c:22:TRP:NE1	2.33	0.43
34:2c:104:GLN:HG3	34:2c:105:GLU:O	2.18	0.43
38:2g:136:LYS:HA	38:2g:139:GLU:HB2	2.01	0.43
40:2i:99:LEU:HB3	40:2i:101:PHE:CE2	2.53	0.43
42:2k:27:ASN:OD1	42:2k:28:THR:N	2.47	0.43
1:1A:1924:C:H4'	55:1x:13:C:O2'	2.18	0.43
1:1A:2135:A:H2'	1:1A:2135:A:N3	2.33	0.43
1:1A:2406:U:H2'	1:1A:2406:U:H6	1.68	0.43
6:1G:77:ILE:HB	6:1G:82:LEU:HB2	2.01	0.43
11:1P:67:MET:HE3	11:1P:67:MET:HB2	1.94	0.43
32:1a:523:A:H61	43:1l:92:0TD:CG	2.31	0.43
32:1a:1126:U:HO2'	32:1a:1127:G:H8	1.65	0.43
32:1a:1244:C:H42	32:1a:1293:G:H1	1.67	0.43
33:1b:139:LYS:O	33:1b:143:GLU:HG3	2.19	0.43
42:1k:48:ILE:O	42:1k:48:ILE:HG12	2.18	0.43
1:2A:271(D):G:H2'	1:2A:271(E):U:H6	1.83	0.43
1:2A:271(K):U:O2	8:2I:50:ARG:HD3	2.18	0.43
1:2A:710:G:H2'	1:2A:711:G:C8	2.52	0.43
1:2A:2171:A:O2'	1:2A:2172:U:OP2	2.35	0.43
1:2A:2843:G:N7	63:2A:4043:HOH:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2U:109:LEU:HD23	16:2U:109:LEU:HA	1.88	0.43
19:2X:9:LEU:HB2	19:2X:29:TRP:O	2.19	0.43
25:23:19:GLN:OE1	25:23:52:HIS:NE2	2.47	0.43
32:2a:954:G:H2'	32:2a:955:U:C6	2.54	0.43
32:2a:994:A:C5	32:2a:1216:G:H4'	2.53	0.43
32:2a:1276:G:H2'	32:2a:1277:C:H5'	2.00	0.43
32:2a:1305:G:H5'	52:2u:4:GLY:HA3	2.00	0.43
34:2c:188:LEU:HD12	34:2c:188:LEU:HA	1.85	0.43
38:2g:74:GLU:HG2	38:2g:91:VAL:HG22	2.00	0.43
44:2m:3:ARG:N	44:2m:8:GLU:HA	2.33	0.43
44:2m:54:VAL:HG23	44:2m:57:ARG:HH21	1.84	0.43
54:2w:2:C:H2'	54:2w:3:G:C8	2.53	0.43
1:1A:658:C:H2'	1:1A:659:C:C6	2.53	0.43
1:1A:2203:U:O4'	3:1D:151:LYS:HE2	2.19	0.43
21:1Z:63:ASP:OD1	21:1Z:65:GLN:HB2	2.19	0.43
29:17:24:THR:O	29:17:28:ARG:HG3	2.19	0.43
32:1a:532:A:H2	32:1a:1206:G:H21	1.66	0.43
41:1j:50:ILE:HA	41:1j:60:ARG:HD3	2.01	0.43
44:1m:15:VAL:HG23	44:1m:43:THR:O	2.18	0.43
1:2A:893:C:H5'	1:2A:894:C:C5	2.53	0.43
1:2A:1640:C:H5'	1:2A:1641:A:OP2	2.19	0.43
1:2A:2112:G:C6	1:2A:2113:U:H1'	2.54	0.43
1:2A:2439:A:H5'	1:2A:2439:A:C8	2.53	0.43
6:2G:7:LEU:HD22	6:2G:104:GLU:N	2.34	0.43
25:23:39:ASP:OD1	25:23:44:ARG:HD2	2.18	0.43
25:23:46:ASN:O	25:23:50:VAL:HG22	2.19	0.43
32:2a:714:G:H2'	32:2a:715:A:C8	2.54	0.43
32:2a:751:U:H4'	46:2o:24:SER:HA	2.00	0.43
32:2a:1128:C:O2'	32:2a:1129:C:OP1	2.37	0.43
32:2a:1312:G:H5'	50:2s:5:LEU:HD11	2.00	0.43
32:2a:1530:G:OP1	32:2a:1530:G:H4'	2.18	0.43
33:2b:87:ARG:NH1	33:2b:219:VAL:HG13	2.33	0.43
38:2g:75:VAL:HG13	38:2g:145:ALA:HA	2.00	0.43
43:2l:92:0TD:H4	43:2l:92:0TD:H8	1.76	0.43
49:2r:33:ASP:OD2	49:2r:36:ASN:HB2	2.17	0.43
50:2s:64:GLU:H	50:2s:64:GLU:CD	2.27	0.43
54:2w:49:G:O6	54:2w:65:U:O4	2.36	0.43
57:2y:8:4SU:H6	57:2y:8:4SU:O5'	2.18	0.43
1:1A:191:A:H2'	1:1A:192:C:C6	2.53	0.43
1:1A:1095:A:C8	1:1A:1096:A:C8	3.06	0.43
3:1D:92:ILE:HD12	3:1D:104:TYR:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:270:A:H2'	32:1a:271:C:C6	2.54	0.43
32:1a:310:G:OP2	47:1p:27:LYS:HE2	2.18	0.43
32:1a:643:C:H5'	39:1h:31:PHE:CD1	2.53	0.43
33:1b:156:LYS:HB2	33:1b:156:LYS:HE2	1.75	0.43
45:1n:9:LYS:HG3	45:1n:12:ARG:HH21	1.84	0.43
50:1s:20:LEU:HA	50:1s:23:ASN:HD22	1.83	0.43
1:2A:570:G:H2'	1:2A:2030:A:C5	2.54	0.43
1:2A:981:A:OP1	63:2A:3955:HOH:O	2.22	0.43
1:2A:1777:U:H2'	1:2A:1778:U:C6	2.53	0.43
1:2A:1843:C:H5'	3:2D:253:GLN:OE1	2.18	0.43
1:2A:2224:G:H4'	1:2A:2226:C:C2	2.54	0.43
1:2A:2331:G:O2'	22:20:43:THR:HG22	2.19	0.43
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.18	0.43
2:2B:75:G:H1	21:2Z:73:GLN:HE22	1.66	0.43
6:2G:124:SER:OG	6:2G:132:ASN:O	2.37	0.43
12:2Q:24:GLY:HA2	12:2Q:67:ARG:NH2	2.34	0.43
14:2S:52:SER:HB2	14:2S:55:ALA:H	1.84	0.43
17:2V:48:GLY:HA3	17:2V:52:VAL:HG22	2.00	0.43
26:24:61:ARG:HG3	26:24:61:ARG:NH1	2.33	0.43
32:2a:299:G:O6	63:2a:1924:HOH:O	2.20	0.43
1:1A:657:U:H2'	1:1A:658:C:C6	2.54	0.43
1:1A:879:G:H1	1:1A:899:A:H8	1.65	0.43
1:1A:1614:A:N1	18:1W:87:PRO:HB3	2.33	0.43
1:1A:2309:A:N6	1:1A:2310:A:N1	2.67	0.43
1:1A:2756:U:H1'	1:1A:2757:A:H5''	2.00	0.43
5:1F:65:TRP:CZ2	5:1F:75:HIS:HD2	2.36	0.43
11:1P:37:GLY:C	11:1P:38:GLN:O	2.62	0.43
18:1W:92:ARG:HB3	18:1W:92:ARG:HH21	1.84	0.43
21:1Z:153:SER:HA	21:1Z:167:PRO:HB3	2.01	0.43
32:1a:114:U:O2'	32:1a:115:G:H5'	2.19	0.43
32:1a:568:G:O2'	32:1a:574:A:N1	2.46	0.43
32:1a:688:G:H2'	32:1a:689:C:C6	2.53	0.43
35:1d:39:PRO:O	35:1d:44:GLY:HA3	2.19	0.43
44:1m:20:THR:HA	44:1m:25:ILE:O	2.19	0.43
47:1p:74:LEU:HB3	47:1p:79:VAL:HG21	2.01	0.43
57:1y:6:C:N4	57:1y:7:G:O6	2.52	0.43
1:2A:910:A:N1	1:2A:2277:G:H1'	2.33	0.43
1:2A:987:G:OP2	63:2A:3954:HOH:O	2.21	0.43
1:2A:1441:G:H2'	1:2A:1442:G:C8	2.54	0.43
1:2A:2330:G:O2'	22:20:41:ARG:O	2.23	0.43
5:2F:36:VAL:O	5:2F:40:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:122:LYS:HA	5:2F:191:ARG:NH1	2.34	0.43
9:2N:34:LEU:O	9:2N:49:GLY:HA3	2.18	0.43
12:2Q:54:MET:HE1	12:2Q:104:PHE:HB3	2.00	0.43
14:2S:4:LEU:HD23	14:2S:4:LEU:HA	1.88	0.43
26:24:64:GLY:C	26:24:66:SER:N	2.77	0.43
32:2a:257:G:H2'	32:2a:258:G:O4'	2.19	0.43
42:2k:43:SER:HB3	42:2k:68:ALA:HB2	2.00	0.43
1:1A:271(K):U:H1'	8:1I:50:ARG:CZ	2.48	0.43
1:1A:957:A:N1	1:1A:2458:G:H4'	2.33	0.43
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.53	0.43
1:1A:2182:G:H2'	1:1A:2183:C:C6	2.54	0.43
1:1A:2347:C:H2'	1:1A:2348:U:C6	2.54	0.43
32:1a:540:G:H2'	32:1a:541:G:O4'	2.19	0.43
32:1a:820:U:H4'	32:1a:821:G:OP2	2.19	0.43
32:1a:985:C:H2'	32:1a:986:A:H8	1.83	0.43
34:1c:116:VAL:HG21	34:1c:202:ILE:HD11	2.01	0.43
36:1e:31:LEU:HD23	36:1e:45:PHE:CD1	2.54	0.43
43:1l:70:ILE:HG12	43:1l:100:ILE:HD12	2.01	0.43
51:1t:56:MET:HE3	51:1t:85:MET:HE2	2.00	0.43
1:2A:30:G:H2'	1:2A:31:C:C6	2.54	0.43
1:2A:2299:G:H2'	1:2A:2300:G:H8	1.84	0.43
2:2B:6:C:H42	2:2B:115:G:H1	1.66	0.43
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.49	0.43
6:2G:38:VAL:HG12	6:2G:93:THR:HG22	2.00	0.43
7:2H:125:VAL:HG22	7:2H:131:VAL:HG22	2.01	0.43
8:2I:26:ALA:O	8:2I:31:LEU:HB2	2.18	0.43
16:2U:102:GLU:HG3	17:2V:2:PHE:CZ	2.53	0.43
18:2W:65:LEU:HD12	18:2W:68:ARG:HE	1.84	0.43
20:2Y:87:LYS:HB3	20:2Y:95:LYS:HD2	1.99	0.43
25:23:8:LEU:HB2	25:23:28:LEU:HD13	2.01	0.43
26:24:3:GLU:H	26:24:3:GLU:HG2	1.61	0.43
32:2a:153:C:H2'	32:2a:154:C:C6	2.53	0.43
32:2a:237:C:H5''	48:2q:25:ARG:CZ	2.49	0.43
32:2a:509:A:N3	32:2a:543:C:O2'	2.47	0.43
32:2a:582:U:C2	32:2a:760:G:C6	3.07	0.43
32:2a:762:C:H2'	32:2a:763:G:H8	1.83	0.43
34:2c:125:GLU:HG2	34:2c:190:ARG:H	1.83	0.43
1:1A:118:A:C8	1:1A:119:A:C8	3.07	0.43
1:1A:224:G:H2'	1:1A:225:A:O4'	2.17	0.43
1:1A:1006:C:C2	1:1A:1138:G:N2	2.87	0.43
1:1A:1528:A:OP2	63:1A:4141:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.54	0.43
3:1D:71:ASP:CB	3:1D:103:ARG:HH12	2.28	0.43
32:1a:79:G:H1'	32:1a:91:C:O2	2.19	0.43
32:1a:1090:U:H2'	32:1a:1091:U:H6	1.84	0.43
32:1a:1239:A:C4	32:1a:1298:C:N4	2.86	0.43
32:1a:1346:A:O3'	32:1a:1347:G:H4'	2.19	0.43
32:1a:1508:G:H2'	32:1a:1509:C:O4'	2.19	0.43
55:1x:18:G:C2	55:1x:58:A:C5	3.07	0.43
1:2A:272(G):C:H42	1:2A:363(C):G:H1	1.66	0.43
1:2A:652(B):A:H3'	1:2A:652(B):A:N3	2.34	0.43
1:2A:862:G:O2'	2:2B:78:A:N3	2.52	0.43
1:2A:1013:C:H2'	1:2A:1014:U:H6	1.84	0.43
1:2A:1167:U:H2'	1:2A:1168:G:H8	1.83	0.43
1:2A:2119:A:C2	1:2A:2171:A:H5'	2.54	0.43
1:2A:2280:G:O6	22:20:14:ARG:HD2	2.19	0.43
1:2A:2286:A:H4'	1:2A:2287:A:O5'	2.18	0.43
1:2A:2294:C:P	14:2S:89:ARG:HH22	2.41	0.43
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.33	0.43
1:2A:2572:A:OP1	1:2A:2574:G:O2'	2.33	0.43
5:2F:172:TRP:CD1	5:2F:172:TRP:H	2.37	0.43
7:2H:3:ARG:NH1	7:2H:4:ILE:H	2.17	0.43
7:2H:117:PRO:HA	7:2H:118:PRO:HD3	1.93	0.43
21:2Z:23:LYS:HA	21:2Z:23:LYS:HD3	1.85	0.43
23:21:53:VAL:HG22	23:21:74:VAL:HG13	2.01	0.43
30:28:62:LEU:HB3	30:28:65:GLU:HG2	2.01	0.43
32:2a:143:A:O3'	32:2a:144:G:H8	2.02	0.43
32:2a:157:G:H2'	32:2a:158:G:C8	2.53	0.43
32:2a:403:C:HO2'	35:2d:122:ARG:HH21	1.58	0.43
32:2a:976:G:C8	32:2a:1358:U:C2	3.06	0.43
32:2a:1150:U:O4	32:2a:1151:A:N6	2.51	0.43
32:2a:1151:A:O2'	32:2a:1152:A:O5'	2.35	0.43
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.18	0.43
34:2c:142:MET:HE3	34:2c:146:ALA:O	2.19	0.43
37:2f:69:GLU:O	37:2f:72:VAL:HG12	2.18	0.43
40:2i:111:ARG:HE	40:2i:111:ARG:HB2	1.71	0.43
43:2l:37:CYS:HB2	43:2l:81:SER:H	1.84	0.43
1:1A:119:A:H4'	1:1A:120:U:OP1	2.19	0.42
1:1A:207:A:H2'	1:1A:208:C:O4'	2.18	0.42
1:1A:647:G:H2'	1:1A:648:G:O4'	2.19	0.42
6:1G:114:ILE:HG23	6:1G:136:ARG:HH12	1.84	0.42
10:1O:7:TYR:CZ	10:1O:44:LYS:HG3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:121:LYS:O	11:1P:123:LEU:N	2.52	0.42
13:1R:71:GLN:NE2	63:1R:304:HOH:O	2.52	0.42
26:14:61:ARG:O	26:14:62:ARG:C	2.62	0.42
32:1a:97:G:H2'	32:1a:98:G:O4'	2.18	0.42
32:1a:925:G:H1'	32:1a:1502:A:C4	2.54	0.42
41:1j:35:SER:CB	41:1j:73:ASP:HB2	2.45	0.42
1:2A:83:G:N1	1:2A:102:G:O2'	2.41	0.42
1:2A:866:A:N3	1:2A:866:A:H2'	2.33	0.42
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.53	0.42
1:2A:1815:A:P	3:2D:54:ARG:HH22	2.41	0.42
1:2A:2082:A:H2'	1:2A:2083:G:O4'	2.18	0.42
1:2A:2164:C:C5	1:2A:2165:G:H1'	2.54	0.42
1:2A:2320:A:H1'	1:2A:2321:G:C2	2.54	0.42
1:2A:2390:U:P	30:28:35:GLN:HE22	2.39	0.42
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.70	0.42
21:2Z:53:ILE:HG22	21:2Z:71:VAL:O	2.19	0.42
29:27:24:THR:O	29:27:28:ARG:HG3	2.18	0.42
32:2a:202:U:H3'	32:2a:203:U:C5	2.54	0.42
32:2a:957:U:O2'	32:2a:959:A:N7	2.43	0.42
32:2a:1309:G:OP2	44:2m:99:ARG:NH2	2.50	0.42
32:2a:1330:U:H4'	44:2m:23:TYR:CE1	2.54	0.42
33:2b:187:LEU:HD12	33:2b:214:ILE:HG21	2.01	0.42
35:2d:58:LEU:HD22	35:2d:62:GLN:HG2	1.99	0.42
36:2e:68:GLU:OE2	36:2e:70:PRO:HG3	2.19	0.42
36:2e:84:PHE:N	36:2e:87:SER:O	2.50	0.42
36:2e:93:PRO:HG2	39:2h:105:ARG:HE	1.83	0.42
37:2f:76:ALA:O	37:2f:80:ARG:HG3	2.19	0.42
40:2i:4:TYR:O	40:2i:19:LEU:N	2.49	0.42
40:2i:65:VAL:HG21	40:2i:73:GLN:HB3	2.01	0.42
40:2i:88:TYR:HD2	40:2i:89:ASN:HB2	1.84	0.42
44:2m:4:ILE:HA	44:2m:57:ARG:HD3	2.01	0.42
44:2m:117:VAL:HG22	44:2m:118:ALA:H	1.83	0.42
1:1A:813:U:H2'	1:1A:814:C:C6	2.54	0.42
1:1A:1062:G:C8	1:1A:1088:A:H2'	2.54	0.42
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.54	0.42
1:1A:1946:U:H2'	1:1A:1947:C:C6	2.53	0.42
12:1Q:16:ARG:HG2	12:1Q:18:LYS:HG3	2.00	0.42
25:13:3:ARG:HB2	25:13:59:VAL:HG23	2.01	0.42
32:1a:839:U:H3'	32:1a:840:C:H5'	2.01	0.42
32:1a:1278:U:H5'	32:1a:1279:A:C5'	2.49	0.42
35:1d:126:ILE:HG22	35:1d:127:THR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1j:11:PHE:HA	41:1j:66:ARG:O	2.19	0.42
1:2A:847:U:H5'	1:2A:848:G:OP2	2.19	0.42
1:2A:882:G:H2'	1:2A:883:G:C8	2.54	0.42
1:2A:884:C:H5'	1:2A:885:C:OP2	2.19	0.42
1:2A:921:G:C6	1:2A:922:U:C4	3.08	0.42
1:2A:1019:U:H2'	1:2A:1020:A:H8	1.83	0.42
1:2A:1589:C:H2'	1:2A:1590:U:H6	1.85	0.42
1:2A:2249:U:N3	1:2A:2253:G:OP2	2.51	0.42
1:2A:2280:G:N7	63:2A:4045:HOH:O	2.36	0.42
1:2A:2303:G:O2'	6:2G:132:ASN:HB2	2.18	0.42
18:2W:34:ASN:OD1	18:2W:37:ARG:NH2	2.44	0.42
19:2X:72:LYS:NZ	19:2X:75:ASP:OD1	2.52	0.42
32:2a:99:U:H2'	32:2a:100:C:C6	2.54	0.42
32:2a:745:C:H2'	32:2a:746:A:C8	2.53	0.42
32:2a:748:C:H4'	32:2a:749:C:O5'	2.19	0.42
32:2a:947:G:O3'	44:2m:109:THR:OG1	2.36	0.42
32:2a:1087:G:N2	32:2a:1099:G:H1'	2.35	0.42
32:2a:1201:A:H4'	32:2a:1202:G:O5'	2.19	0.42
32:2a:1316:G:H22	32:2a:1318:A:H3'	1.84	0.42
35:2d:101:LEU:HA	35:2d:104:VAL:HG22	2.00	0.42
47:2p:21:VAL:HG13	47:2p:34:GLU:HB3	2.01	0.42
50:2s:80:TYR:C	50:2s:82:GLY:H	2.26	0.42
1:1A:1048:A:N1	1:1A:1112:G:O2'	2.35	0.42
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.19	0.42
1:1A:2139:C:H2'	1:1A:2140:C:O4'	2.19	0.42
28:16:10:LEU:HG	28:16:54:ILE:HG13	2.00	0.42
32:1a:371:G:O2'	32:1a:373:A:N7	2.48	0.42
32:1a:538:G:H5''	43:1l:114:LYS:HB2	2.00	0.42
32:1a:859:A:H2'	32:1a:860:A:O4'	2.19	0.42
32:1a:1396:A:H2	36:1e:19:MET:HG3	1.83	0.42
33:1b:163:PHE:HA	33:1b:185:ILE:HG13	2.01	0.42
34:1c:66:VAL:HG11	34:1c:91:LEU:HD23	2.01	0.42
36:1e:135:THR:H	36:1e:135:THR:HG1	1.51	0.42
39:1h:17:THR:HG22	39:1h:63:LEU:HD13	2.01	0.42
46:1o:15:PHE:CZ	46:1o:84:LYS:HG3	2.54	0.42
47:1p:60:LEU:HA	47:1p:60:LEU:HD12	1.76	0.42
1:2A:871:U:OP1	12:2Q:5:ARG:HD3	2.19	0.42
1:2A:2151:G:H2'	1:2A:2152:G:C8	2.51	0.42
1:2A:2564:A:OP1	1:2A:2648:C:H4'	2.19	0.42
63:2A:4566:HOH:O	13:2R:3:HIS:HD2	2.02	0.42
3:2D:6:PHE:HE2	3:2D:18:VAL:HG13	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:164:ARG:O	5:2F:168:ARG:HB2	2.19	0.42
8:2I:120:ILE:HG21	8:2I:126:TYR:CE2	2.54	0.42
12:2Q:43:THR:HG22	12:2Q:94:VAL:HG12	2.00	0.42
21:2Z:106:GLY:HA3	21:2Z:141:VAL:H	1.84	0.42
32:2a:554:C:H2'	32:2a:555:C:C6	2.54	0.42
32:2a:620:C:C2	35:2d:135:LEU:HG	2.53	0.42
32:2a:730:G:O6	46:2o:51:HIS:NE2	2.47	0.42
32:2a:772:U:H2'	32:2a:773:G:O4'	2.18	0.42
32:2a:1272:G:H5'	32:2a:1273:G:OP2	2.19	0.42
32:2a:1438:G:H2'	32:2a:1439:C:C6	2.53	0.42
32:2a:1517:G:H2'	32:2a:1518:MA6:C8	2.49	0.42
33:2b:119:GLU:OE1	33:2b:153:ARG:NH2	2.49	0.42
1:1A:34:C:N4	1:1A:447:A:H61	2.18	0.42
1:1A:1354:A:H2'	1:1A:1355:G:O4'	2.19	0.42
1:1A:2118:U:O4	1:1A:2149:G:H1'	2.18	0.42
12:1Q:137:TYR:O	12:1Q:141:GLN:HG2	2.19	0.42
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	2.01	0.42
32:1a:178:C:H2'	32:1a:179:A:C8	2.55	0.42
32:1a:341:C:H2'	32:1a:342:C:C6	2.54	0.42
32:1a:403:C:H5''	35:1d:136:PRO:HD2	2.02	0.42
32:1a:1070:U:H2'	32:1a:1071:C:H6	1.84	0.42
33:1b:55:PHE:HD1	33:1b:221:LEU:HD22	1.84	0.42
38:1g:23:VAL:HG13	38:1g:43:PHE:CZ	2.55	0.42
42:1k:84:VAL:HG23	42:1k:110:ASP:HA	2.01	0.42
1:2A:247:G:OP2	1:2A:249:C:N4	2.45	0.42
1:2A:271(S):G:C6	1:2A:271(T):C:C4	3.07	0.42
1:2A:813:U:H2'	1:2A:814:C:C6	2.55	0.42
1:2A:882:G:OP2	1:2A:882:G:H8	2.02	0.42
1:2A:1022:G:N7	9:2N:66:LYS:HE2	2.35	0.42
1:2A:1908:C:O2	55:2x:12:G:H4'	2.20	0.42
2:2B:11:C:H3'	2:2B:12:C:C6	2.54	0.42
23:21:35:THR:OG1	23:21:35:THR:O	2.38	0.42
24:22:13:ALA:HB1	24:22:21:LEU:HD21	2.02	0.42
24:22:51:ARG:O	24:22:55:ARG:HG3	2.19	0.42
33:2b:224:GLN:HA	33:2b:228:GLY:O	2.19	0.42
34:2c:6:HIS:CD2	34:2c:8:ILE:H	2.32	0.42
42:2k:48:ILE:H	42:2k:48:ILE:HD12	1.84	0.42
45:2n:4:LYS:O	45:2n:8:GLU:HG2	2.20	0.42
46:2o:4:THR:C	46:2o:6:GLU:H	2.27	0.42
46:2o:54:ARG:O	46:2o:58:MET:HG3	2.19	0.42
50:2s:69:HIS:HB2	50:2s:74:PHE:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:2y:18:G:N2	57:2y:56:C:N1	2.67	0.42
1:1A:272(J):C:H2'	1:1A:274:G:H8	1.85	0.42
1:1A:868:U:C4	1:1A:869:G:N7	2.87	0.42
1:1A:880:G:H2'	1:1A:881:G:C8	2.53	0.42
1:1A:1750:G:O2'	1:1A:2860:A:N1	2.44	0.42
1:1A:2846:G:H2'	1:1A:2847:U:O4'	2.20	0.42
8:1I:130:TYR:O	8:1I:138:ILE:N	2.41	0.42
11:1P:1:MET:HE2	11:1P:1:MET:HB2	1.91	0.42
20:1Y:55:TYR:CE1	20:1Y:61:ILE:HG21	2.54	0.42
32:1a:528:C:H5'	32:1a:529:G:OP2	2.19	0.42
32:1a:1131:G:H5'	40:1i:3:GLN:HE22	1.83	0.42
35:1d:190:ASP:OD1	35:1d:190:ASP:N	2.52	0.42
39:1h:23:SER:OG	39:1h:60:ARG:HG2	2.19	0.42
57:1y:37:A:H2'	57:1y:38:A:C8	2.45	0.42
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.54	0.42
1:2A:2552:OMU:H6	1:2A:2552:OMU:O5'	2.19	0.42
3:2D:146:GLU:HG2	3:2D:152:GLY:C	2.44	0.42
5:2F:165:ARG:HG2	5:2F:168:ARG:NH2	2.34	0.42
8:2I:79:ILE:N	8:2I:143:SER:O	2.35	0.42
10:2O:120:GLU:OE2	10:2O:122:LEU:HD21	2.20	0.42
11:2P:63:PRO:HD3	30:28:27:THR:HG22	2.02	0.42
17:2V:24:LYS:HE2	17:2V:24:LYS:HB3	1.89	0.42
21:2Z:98:MET:O	21:2Z:126:VAL:N	2.52	0.42
32:2a:532:A:N1	34:2c:156:ARG:NH1	2.65	0.42
32:2a:828:A:H5''	32:2a:859:A:C2	2.55	0.42
33:2b:15:VAL:HG21	33:2b:213:LEU:HD13	2.01	0.42
1:1A:2887:U:H2'	1:1A:2888:C:H6	1.85	0.42
3:1D:141:VAL:HG13	3:1D:162:SER:HB2	2.02	0.42
3:1D:159:ALA:HB1	3:1D:198:ASN:O	2.20	0.42
5:1F:152:GLU:OE1	5:1F:191:ARG:HD2	2.19	0.42
15:1T:28:VAL:O	15:1T:46:GLU:HA	2.20	0.42
32:1a:1057:G:H2'	32:1a:1058:G:O4'	2.20	0.42
38:1g:26:PHE:O	38:1g:30:ILE:HG13	2.18	0.42
1:2A:2134:A:H1'	1:2A:2158:A:C2	2.54	0.42
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.37	0.42
1:2A:2682:U:O2'	15:2T:58:ASN:ND2	2.52	0.42
1:2A:2756:U:H1'	1:2A:2757:A:H5''	2.00	0.42
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	2.01	0.42
6:2G:116:ASP:CG	44:2m:68:GLY:HA3	2.44	0.42
6:2G:120:LEU:HB3	6:2G:131:TYR:OH	2.19	0.42
12:2Q:48:GLU:O	12:2Q:52:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:216:G:H2'	32:2a:217:C:C6	2.54	0.42
32:2a:562:C:H4'	32:2a:563:A:O5'	2.19	0.42
32:2a:1080:A:OP1	36:2e:47:LYS:HD2	2.20	0.42
32:2a:1241:G:H2'	32:2a:1242:C:C6	2.54	0.42
33:2b:28:PHE:CD2	33:2b:31:TYR:HB2	2.55	0.42
33:2b:32:ILE:HD11	33:2b:190:THR:HB	2.02	0.42
35:2d:20:TYR:HD1	35:2d:26:CYS:HB3	1.84	0.42
36:2e:24:ARG:HD2	53:2v:24:A:OP2	2.20	0.42
36:2e:128:PRO:O	36:2e:131:ILE:HG13	2.19	0.42
38:2g:138:LYS:O	38:2g:142:GLU:HG3	2.20	0.42
1:1A:271(F):C:N4	63:1A:4398:HOH:O	2.53	0.42
1:1A:1062:G:N2	1:1A:1088:A:C6	2.88	0.42
1:1A:1649:G:O2'	13:1R:107:ASP:OD2	2.27	0.42
1:1A:1812:A:O2'	3:1D:45:ASN:N	2.43	0.42
1:1A:1851:U:H2'	1:1A:1852:C:O4'	2.20	0.42
1:1A:2306:C:O2	63:1G:301:HOH:O	2.19	0.42
6:1G:126:ASP:HB2	6:1G:130:ASN:H	1.85	0.42
17:1V:1:MET:CE	17:1V:44:LYS:H	2.32	0.42
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.66	0.42
23:11:64:ALA:HA	23:11:67:ILE:HG13	2.01	0.42
32:1a:392:G:H2'	32:1a:393:A:H8	1.83	0.42
32:1a:404:U:H2'	32:1a:405:U:H6	1.84	0.42
32:1a:660:G:OP1	46:1o:5:LYS:HE2	2.19	0.42
32:1a:1346:A:H5''	40:1i:120:ARG:NH1	2.35	0.42
33:1b:92:TYR:CE1	33:1b:94:ASN:HB2	2.54	0.42
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	2.01	0.42
45:1n:6:LEU:HB3	45:1n:23:ARG:NH2	2.34	0.42
54:1w:5:G:H2'	54:1w:6:C:C6	2.54	0.42
57:1y:8:4SU:O2'	57:1y:48:C:H1'	2.20	0.42
1:2A:111:A:O2'	24:22:65:ASN:ND2	2.50	0.42
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.20	0.42
1:2A:721:C:H2'	1:2A:722:A:C8	2.55	0.42
1:2A:807:U:OP2	11:2P:41:ARG:NH2	2.52	0.42
1:2A:1580:A:H3'	1:2A:1581:G:H8	1.83	0.42
1:2A:2134:A:H1'	1:2A:2158:A:C6	2.55	0.42
1:2A:2353:G:H2'	1:2A:2354:G:O4'	2.18	0.42
6:2G:67:LYS:H	26:24:6:HIS:CE1	2.37	0.42
6:2G:140:ILE:HD12	6:2G:140:ILE:HA	1.86	0.42
7:2H:59:ARG:O	7:2H:63:SER:OG	2.37	0.42
8:2I:57:ARG:HA	8:2I:61:ARG:HH21	1.83	0.42
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:344:A:H5''	32:2a:345:C:C5	2.41	0.42
32:2a:1005:A:H62	32:2a:1024:G:H1'	1.84	0.42
32:2a:1150:U:H4'	41:2j:41:PRO:HG3	2.01	0.42
32:2a:1263:C:H3'	32:2a:1263:C:H6	1.85	0.42
32:2a:1320:C:H1'	50:2s:73:GLU:HA	2.01	0.42
38:2g:67:GLU:OE2	38:2g:70:LYS:NZ	2.31	0.42
39:2h:85:ARG:NH1	39:2h:134:ILE:HG23	2.35	0.42
41:2j:78:ASN:O	41:2j:80:LYS:N	2.52	0.42
42:2k:45:GLY:O	42:2k:50:TYR:HB2	2.20	0.42
43:2l:23:LYS:C	43:2l:25:PRO:HD3	2.45	0.42
54:2w:2:C:H2'	54:2w:3:G:O4'	2.20	0.42
1:1A:362:U:H6	1:1A:362:U:H2'	1.56	0.42
1:1A:479:A:N3	1:1A:481:G:H5''	2.34	0.42
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.20	0.42
1:1A:1959:G:N7	63:1A:4239:HOH:O	2.37	0.42
1:1A:2167:U:O2	1:1A:2167:U:H2'	2.20	0.42
1:1A:2304:G:O2'	6:1G:156:ASP:OD1	2.34	0.42
1:1A:2492:U:H2'	1:1A:2493:U:H6	1.84	0.42
1:1A:2853:C:H2'	1:1A:2854:G:C8	2.54	0.42
14:1S:68:GLN:NE2	14:1S:71:ARG:HE	2.18	0.42
32:1a:742:G:OP2	46:1o:35:ARG:NH2	2.45	0.42
32:1a:1203:C:H2'	32:1a:1204:A:O4'	2.20	0.42
35:1d:122:ARG:HD2	35:1d:122:ARG:HA	1.73	0.42
41:1j:81:THR:C	41:1j:83:GLU:N	2.77	0.42
54:1w:48:C:C2	54:1w:59:U:H1'	2.54	0.42
1:2A:815:C:H2'	1:2A:816:C:C6	2.55	0.42
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.55	0.42
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.31	0.42
1:2A:1448:G:H2'	1:2A:1449:A:C8	2.55	0.42
3:2D:35:LYS:HD3	3:2D:64:ILE:HD11	2.01	0.42
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.45	0.42
18:2W:4:LYS:HD3	18:2W:6:ILE:HD11	2.01	0.42
26:24:13:ARG:HA	26:24:22:ILE:O	2.19	0.42
28:26:34:LEU:H	28:26:51:GLU:HB2	1.83	0.42
32:2a:547:A:H4'	32:2a:548:G:O5'	2.20	0.42
32:2a:1278:U:H5'	32:2a:1279:A:C5'	2.50	0.42
32:2a:1410:G:H2'	32:2a:1411:C:C6	2.54	0.42
32:2a:1466:C:H2'	32:2a:1467:G:O4'	2.20	0.42
33:2b:149:LEU:HA	33:2b:152:PHE:HB3	2.02	0.42
36:2e:99:GLY:O	36:2e:117:ASP:HA	2.20	0.42
40:2i:38:GLN:H	40:2i:38:GLN:HG3	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:2p:28:ARG:HG2	47:2p:28:ARG:HH11	1.85	0.42
1:1A:945:A:C4	1:1A:2448:A:C2	3.07	0.42
1:1A:1092:C:H2'	1:1A:1093:G:H5'	2.01	0.42
1:1A:1164:G:H2'	1:1A:1165:U:C6	2.55	0.42
1:1A:1166:C:H2'	1:1A:1167:U:C6	2.55	0.42
1:1A:1843:C:H5'	3:1D:253:GLN:OE1	2.20	0.42
1:1A:2572:A:N7	4:1E:145:LYS:HB2	2.35	0.42
1:1A:2864:G:OP1	15:1T:119:LYS:HD2	2.20	0.42
3:1D:145:VAL:HG12	3:1D:146:GLU:O	2.19	0.42
11:1P:27:HIS:HB2	63:1P:306:HOH:O	2.19	0.42
11:1P:94:GLU:CD	11:1P:124:LYS:HD3	2.45	0.42
13:1R:8:ARG:HB2	13:1R:43:GLU:CD	2.45	0.42
32:1a:262:A:H2'	32:1a:263:A:C8	2.55	0.42
32:1a:975:A:N1	41:1j:48:THR:OG1	2.52	0.42
32:1a:1036:G:H5''	32:1a:1037:C:H5	1.85	0.42
32:1a:1248:A:N3	40:1i:70:LYS:HE2	2.34	0.42
32:1a:1347:G:N7	40:1i:11:LYS:HE2	2.35	0.42
32:1a:1350:A:O2'	38:1g:33:ASP:OD1	2.37	0.42
33:1b:21:ARG:O	33:1b:23:ARG:HG2	2.20	0.42
33:1b:118:LEU:HB2	33:1b:142:LEU:HD12	2.01	0.42
38:1g:90:GLU:H	38:1g:90:GLU:HG2	1.62	0.42
49:1r:52:PRO:O	49:1r:56:THR:HG23	2.20	0.42
1:2A:581:C:H2'	1:2A:582:G:C8	2.55	0.42
1:2A:900:A:C4	1:2A:901:A:C8	3.08	0.42
1:2A:1815:A:OP2	3:2D:54:ARG:NH2	2.53	0.42
1:2A:2408:U:H2'	1:2A:2409:G:C8	2.55	0.42
1:2A:2872:G:O2'	1:2A:2873:A:H5'	2.20	0.42
2:2B:1:U:H2'	2:2B:2:C:C6	2.55	0.42
3:2D:132:PRO:HG3	3:2D:190:TYR:CE2	2.55	0.42
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.55	0.42
7:2H:33:LEU:HD21	7:2H:136:ILE:HG13	2.02	0.42
10:2O:49:ARG:HH12	32:2a:1423:G:P	2.42	0.42
23:21:3:LYS:O	23:21:12:PRO:HD3	2.20	0.42
30:28:48:PHE:H	30:28:48:PHE:HD2	1.68	0.42
33:2b:94:ASN:HD22	33:2b:94:ASN:HA	1.63	0.42
34:2c:23:TYR:CG	34:2c:24:ALA:N	2.88	0.42
36:2e:6:PHE:HB2	36:2e:63:ARG:NH2	2.33	0.42
36:2e:71:LEU:C	36:2e:72:GLN:HE21	2.27	0.42
39:2h:123:GLU:O	39:2h:127:LEU:HB2	2.19	0.42
1:1A:274:G:H2'	1:1A:275:G:C8	2.54	0.42
1:1A:857:C:N4	1:1A:858:U:O4	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:C4	1:1A:1086:A:N1	2.79	0.42
1:1A:1550:C:OP1	1:1A:1720:U:O2'	2.34	0.42
1:1A:1991:U:H2'	1:1A:1992:G:H5''	2.01	0.42
1:1A:2102:U:H3	1:1A:2187:G:H1	1.67	0.42
1:1A:2506:U:O4'	60:1A:4087:CLM:H8	2.20	0.42
1:1A:2611:U:H6	1:1A:2611:U:H5'	1.85	0.42
2:1B:99:G:OP2	63:1B:304:HOH:O	2.21	0.42
6:1G:146:TYR:HD1	44:1m:8:GLU:HG2	1.84	0.42
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	2.01	0.42
13:1R:38:VAL:HB	13:1R:39:PRO:HD3	2.02	0.42
25:13:44:ARG:O	25:13:48:GLU:HG3	2.20	0.42
28:16:19:ARG:NH1	28:16:52:VAL:HG21	2.35	0.42
32:1a:109:A:C6	32:1a:326:G:C6	3.07	0.42
32:1a:632:A:H2'	32:1a:633:G:O4'	2.20	0.42
32:1a:1349:A:OP2	40:1i:118:LYS:HE2	2.20	0.42
35:1d:108:LEU:HB2	35:1d:110:PHE:CD1	2.55	0.42
44:1m:9:ILE:HG21	44:1m:22:ILE:HD11	2.02	0.42
51:1t:37:SER:O	51:1t:41:ILE:HG13	2.19	0.42
1:2A:251:A:C5	1:2A:252:G:H1'	2.55	0.42
1:2A:302:C:P	20:2Y:73:ARG:HH12	2.42	0.42
1:2A:311:A:C6	1:2A:328:U:C4	3.08	0.42
1:2A:1171:G:H1	1:2A:1178:C:N4	2.16	0.42
1:2A:2171:A:N3	1:2A:2172:U:N3	2.68	0.42
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.33	0.42
2:2B:89:G:C6	2:2B:90:A:C6	3.07	0.42
8:2I:87:LYS:HA	8:2I:122:GLU:HA	2.02	0.42
25:23:8:LEU:O	25:23:32:GLN:N	2.49	0.42
26:24:50:VAL:HG21	44:2m:65:LYS:N	2.34	0.42
32:2a:818:G:O2'	32:2a:819:A:H5'	2.20	0.42
32:2a:918:A:H2'	32:2a:919:A:O4'	2.20	0.42
32:2a:1139:G:N2	32:2a:1142:G:O6	2.43	0.42
32:2a:1268:A:H2'	32:2a:1269:A:C8	2.55	0.42
32:2a:1396:A:O4'	32:2a:1398:A:H1'	2.20	0.42
32:2a:1424:C:H2'	32:2a:1425:U:H6	1.84	0.42
33:2b:34:ALA:HB3	33:2b:41:ILE:HD11	2.02	0.42
33:2b:74:LYS:O	33:2b:78:GLN:NE2	2.52	0.42
45:2n:4:LYS:HA	45:2n:7:ILE:HG22	2.01	0.42
47:2p:43:LYS:HG2	47:2p:48:TRP:CE2	2.54	0.42
48:2q:45:HIS:NE2	48:2q:47:PRO:HG3	2.35	0.42
57:2y:56:C:H2'	57:2y:57:G:C8	2.55	0.42
1:1A:305:U:H2'	1:1A:306:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:864:G:O2'	1:1A:865:C:H5'	2.20	0.41
1:1A:1045:A:O2'	1:1A:1047:G:C4	2.68	0.41
1:1A:1712:C:H2'	1:1A:1713:U:O4'	2.19	0.41
1:1A:1826:G:H4'	3:1D:242:ARG:CZ	2.50	0.41
1:1A:2151:G:C6	1:1A:2152:G:C6	3.08	0.41
1:1A:2788:C:P	4:1E:61:ARG:HH21	2.43	0.41
2:1B:117:G:N7	63:1B:307:HOH:O	2.37	0.41
5:1F:101:LEU:O	5:1F:106:ARG:NH1	2.53	0.41
6:1G:34:LEU:HD23	6:1G:34:LEU:HA	1.90	0.41
9:1N:13:TRP:CE2	9:1N:133:GLN:HG2	2.55	0.41
32:1a:721:G:H4'	32:1a:722:A:O4'	2.20	0.41
32:1a:735:C:H2'	32:1a:736:C:H6	1.85	0.41
32:1a:1085:U:C2	32:1a:1094:G:O6	2.73	0.41
32:1a:1168:A:H2'	32:1a:1169:A:C8	2.55	0.41
32:1a:1255:G:O2'	32:1a:1258:G:O2'	2.37	0.41
33:1b:148:TYR:HB2	33:1b:149:LEU:HD12	2.02	0.41
38:1g:78:ARG:NH1	38:1g:156:TRP:HB3	2.35	0.41
42:1k:91:ARG:O	42:1k:95:ILE:HD12	2.20	0.41
1:2A:298:G:H1'	1:2A:340:A:H61	1.84	0.41
1:2A:503:A:H4'	1:2A:504:U:H5''	2.02	0.41
1:2A:1263:U:C4	1:2A:1264:G:C6	3.07	0.41
1:2A:1703:G:H2'	1:2A:1704:G:C8	2.55	0.41
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.54	0.41
1:2A:2627:G:O2'	1:2A:2781:A:N1	2.47	0.41
5:2F:95:ARG:NH1	5:2F:97:TYR:OH	2.53	0.41
6:2G:67:LYS:HD3	26:24:5:ILE:HD12	2.01	0.41
32:2a:224:C:H2'	32:2a:225:C:C6	2.55	0.41
32:2a:865:A:H5'	32:2a:1078:U:C5	2.55	0.41
32:2a:1265:G:C4	32:2a:1271:G:N2	2.88	0.41
32:2a:1478:C:H2'	32:2a:1479:C:H6	1.85	0.41
39:2h:32:LYS:HA	39:2h:35:ILE:HD12	2.00	0.41
44:2m:80:ARG:O	44:2m:84:ILE:HG23	2.19	0.41
49:2r:65:ILE:H	49:2r:65:ILE:HG12	1.52	0.41
1:1A:603:A:N1	1:1A:625:G:O2'	2.50	0.41
1:1A:764:A:O4'	3:1D:213:ARG:HG3	2.20	0.41
1:1A:969:U:H2'	1:1A:970:C:C6	2.56	0.41
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.20	0.41
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	2.01	0.41
2:1B:78:A:C2	2:1B:100:A:C4	3.07	0.41
8:1I:48:GLU:O	8:1I:52:ARG:HB2	2.20	0.41
32:1a:316:G:OP2	32:1a:351:G:O2'	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:719:C:H1'	49:1r:49:LYS:HB3	2.02	0.41
32:1a:826:C:H4'	39:1h:12:ARG:HG2	2.01	0.41
32:1a:875:C:O2'	39:1h:14:ARG:HD2	2.20	0.41
32:1a:922:G:N3	32:1a:1398:A:H2	2.18	0.41
32:1a:958:A:C6	32:1a:959:A:N1	2.88	0.41
32:1a:1070:U:H2'	32:1a:1071:C:C6	2.55	0.41
32:1a:1370:G:C2	32:1a:1371:G:C8	3.08	0.41
32:1a:1504:G:H4'	32:1a:1505:G:C4	2.55	0.41
34:1c:116:VAL:O	34:1c:120:VAL:HG22	2.21	0.41
38:1g:91:VAL:O	38:1g:96:GLN:NE2	2.44	0.41
44:1m:98:VAL:HG12	44:1m:99:ARG:HG3	2.01	0.41
48:1q:56:VAL:HB	48:1q:78:GLU:HB3	2.01	0.41
1:2A:710:G:H2'	1:2A:711:G:H8	1.85	0.41
1:2A:1167:U:H2'	1:2A:1168:G:C8	2.55	0.41
12:2Q:36:ALA:HB1	12:2Q:127:ILE:HD12	2.01	0.41
17:2V:58:VAL:HB	17:2V:98:GLU:HG3	2.02	0.41
32:2a:189(D):C:H2'	32:2a:189(E):U:O4'	2.20	0.41
32:2a:545:C:OP1	35:2d:61:LYS:NZ	2.53	0.41
32:2a:1261:A:H5'	32:2a:1284:C:OP1	2.18	0.41
32:2a:1411:C:H2'	32:2a:1412:C:C6	2.54	0.41
33:2b:9:GLU:O	33:2b:11:LEU:N	2.54	0.41
40:2i:114:TYR:N	40:2i:114:TYR:CD1	2.88	0.41
43:2l:28:LYS:HD3	43:2l:62:SER:HB3	2.01	0.41
44:2m:81:LEU:H	44:2m:81:LEU:HG	1.62	0.41
46:2o:18:PHE:CE2	46:2o:21:ASP:HB2	2.55	0.41
51:2t:92:LEU:HD23	51:2t:92:LEU:HA	1.87	0.41
1:1A:768:G:O2'	1:1A:1379:A:N1	2.47	0.41
1:1A:1503:U:H2'	1:1A:1504:C:C6	2.55	0.41
13:1R:118:GLU:H	13:1R:118:GLU:CD	2.28	0.41
20:1Y:11:ASP:O	20:1Y:26:LYS:HD3	2.19	0.41
32:1a:1030(A):G:O2'	32:1a:1031:G:N2	2.52	0.41
34:1c:130:VAL:HG11	34:1c:153:VAL:HG11	2.02	0.41
35:1d:86:LYS:HE3	35:1d:86:LYS:HB2	1.93	0.41
39:1h:4:ASP:CG	39:1h:85:ARG:HH21	2.28	0.41
1:2A:608:A:H2'	1:2A:609:A:C8	2.54	0.41
9:2N:67:LEU:O	9:2N:88:GLU:HG3	2.19	0.41
17:2V:29:PRO:HA	17:2V:61:VAL:HG12	2.01	0.41
24:22:35:LEU:HD23	24:22:35:LEU:HA	1.83	0.41
25:23:18:ASP:N	25:23:18:ASP:OD1	2.51	0.41
32:2a:745:C:H2'	32:2a:746:A:H8	1.86	0.41
32:2a:838:G:N2	32:2a:840:C:H5''	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:957:U:H2'	32:2a:958:A:H3'	2.02	0.41
32:2a:1005:A:H5''	32:2a:1006:C:C5	2.53	0.41
32:2a:1014:A:H2	32:2a:1219:U:H1'	1.85	0.41
32:2a:1095:U:H2'	32:2a:1096:C:O4'	2.21	0.41
32:2a:1277:C:O2'	32:2a:1278:U:O5'	2.38	0.41
32:2a:1291:G:O3'	40:2i:39:GLY:HA3	2.21	0.41
32:2a:1413:A:H2'	32:2a:1414:U:O4'	2.20	0.41
32:2a:1526:G:H4'	63:2a:1902:HOH:O	2.21	0.41
34:2c:32:LEU:O	34:2c:36:ASP:HB2	2.20	0.41
34:2c:153:VAL:O	34:2c:165:THR:HA	2.20	0.41
40:2i:18:PHE:CD2	40:2i:62:TYR:HD2	2.38	0.41
41:2j:24:VAL:O	41:2j:34:VAL:HG11	2.19	0.41
42:2k:48:ILE:HG21	42:2k:63:LEU:HD12	2.02	0.41
47:2p:21:VAL:HG22	47:2p:33:ILE:HB	2.03	0.41
51:2t:10:LEU:HG	51:2t:12:ALA:H	1.85	0.41
57:2y:69:C:H3'	57:2y:70:C:H5''	2.03	0.41
1:1A:590:A:H2'	1:1A:591:C:O4'	2.20	0.41
1:1A:1394:U:H2'	1:1A:1395:A:O4'	2.19	0.41
1:1A:1815:A:N1	63:1A:4238:HOH:O	2.37	0.41
1:1A:1899:G:H2'	1:1A:1899:G:N3	2.35	0.41
1:1A:2156:G:H2'	1:1A:2157:G:N3	2.35	0.41
1:1A:2533:A:H2'	1:1A:2534:A:O4'	2.20	0.41
1:1A:2576:G:H1'	63:1A:4632:HOH:O	2.20	0.41
5:1F:108:LYS:O	5:1F:112:MET:HG3	2.21	0.41
8:1I:87:LYS:HD3	8:1I:87:LYS:H	1.83	0.41
26:14:50:VAL:HG22	44:1m:62:ASN:O	2.21	0.41
32:1a:189(C):C:H2'	32:1a:189(D):C:O4'	2.21	0.41
32:1a:503:C:H2'	32:1a:504:C:H6	1.86	0.41
32:1a:1273:G:C2	32:1a:1274:G:H1'	2.56	0.41
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.54	0.41
38:1g:78:ARG:HD2	38:1g:156:TRP:CE3	2.54	0.41
39:1h:124:ALA:O	39:1h:128:GLY:N	2.53	0.41
41:1j:16:LEU:HD22	41:1j:68:HIS:HB2	2.03	0.41
44:1m:33:ALA:HA	44:1m:59:TYR:CE2	2.55	0.41
46:1o:61:GLY:O	46:1o:65:ARG:HG3	2.20	0.41
54:1w:15:A:N6	54:1w:59:U:O2	2.53	0.41
1:2A:298:G:O2'	1:2A:322:A:N1	2.46	0.41
1:2A:1002:G:H2'	1:2A:1003:G:O4'	2.20	0.41
1:2A:1664:A:C2	10:2O:1:MET:HE1	2.55	0.41
14:2S:14:VAL:HG11	14:2S:89:ARG:HG2	2.02	0.41
27:25:35:GLU:HG3	27:25:51:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:300:A:H1'	32:2a:565:U:O2	2.21	0.41
32:2a:335:C:H2'	32:2a:336:C:C6	2.56	0.41
32:2a:565:U:H3'	32:2a:566:G:H2'	2.02	0.41
32:2a:603:U:H2'	32:2a:604:G:C8	2.56	0.41
32:2a:949:A:O2'	32:2a:971:G:O6	2.37	0.41
32:2a:1187:G:H4'	40:2i:111:ARG:HH11	1.85	0.41
32:2a:1287:A:N6	32:2a:1371:G:O4'	2.47	0.41
32:2a:1327:C:H2'	32:2a:1328:C:C6	2.55	0.41
33:2b:178:ARG:NH2	39:2h:68:ARG:HH22	2.17	0.41
37:2f:99:ALA:HB1	49:2r:23:LYS:HZ2	1.84	0.41
40:2i:85:LEU:HB3	40:2i:92:TYR:CD2	2.54	0.41
41:2j:74:ILE:O	63:2j:301:HOH:O	2.22	0.41
48:2q:76:LEU:HD12	48:2q:77:VAL:H	1.85	0.41
49:2r:84:LYS:H	49:2r:84:LYS:HG3	1.63	0.41
54:2w:8:4SU:H1'	54:2w:21:A:H61	1.84	0.41
54:2w:63:C:H2'	54:2w:64:U:C6	2.56	0.41
1:1A:2078:C:C4	1:1A:2079:U:C4	3.08	0.41
1:1A:2283:C:H2'	1:1A:2284:C:O4'	2.21	0.41
1:1A:2820:A:O2'	1:1A:2821:A:OP1	2.37	0.41
8:1I:140:LEU:HD12	8:1I:140:LEU:HA	1.84	0.41
15:1T:41:ARG:NH2	15:1T:43:GLN:HE21	2.19	0.41
32:1a:271:C:H2'	32:1a:272:C:H6	1.85	0.41
32:1a:345:C:H5'	32:1a:346:G:C5	2.55	0.41
32:1a:551:U:H2'	32:1a:552:U:C6	2.54	0.41
32:1a:983:A:H5''	32:1a:984:C:OP2	2.19	0.41
32:1a:1388:C:H2'	32:1a:1389:C:C6	2.55	0.41
33:1b:78:GLN:HE22	33:1b:95:GLN:HA	1.84	0.41
35:1d:101:LEU:HB2	35:1d:138:TYR:HB3	2.03	0.41
35:1d:173:TRP:CD1	35:1d:173:TRP:N	2.87	0.41
38:1g:89:MET:HE2	38:1g:89:MET:HA	2.02	0.41
54:1w:54:5MU:C4	54:1w:55:PSU:C2	3.07	0.41
1:2A:86:C:H4'	1:2A:104:U:H1'	2.02	0.41
1:2A:271(Q):G:H2'	1:2A:271(R):G:H8	1.85	0.41
1:2A:2127:G:H22	1:2A:2160:G:H1	1.67	0.41
1:2A:2516:G:C6	1:2A:2517:C:C4	3.08	0.41
1:2A:2591:C:H2'	1:2A:2592:G:C8	2.55	0.41
5:2F:116:ASP:OD2	11:2P:1:MET:N	2.38	0.41
9:2N:38:HIS:NE2	9:2N:50:ASP:OD2	2.54	0.41
10:2O:108:GLU:H	10:2O:108:GLU:HG2	1.69	0.41
32:2a:1181:G:O2'	32:2a:1182:G:C5	2.72	0.41
33:2b:101:MET:HA	33:2b:108:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:2p:25:ARG:NH1	47:2p:25:ARG:HG3	2.36	0.41
47:2p:53:VAL:HB	47:2p:79:VAL:HG22	2.01	0.41
48:2q:41:LYS:HZ1	48:2q:92:ARG:HH21	1.68	0.41
51:2t:43:LEU:HD23	51:2t:43:LEU:HA	1.85	0.41
55:2x:61:C:H2'	55:2x:62:C:H6	1.85	0.41
1:1A:548:A:H1'	1:1A:549:G:OP1	2.21	0.41
1:1A:1057:A:H62	1:1A:1087:G:P	2.44	0.41
1:1A:1745(A):C:H2'	1:1A:1746:G:O4'	2.21	0.41
1:1A:2158:A:H1'	1:1A:2159:G:O4'	2.20	0.41
1:1A:2359:C:H2'	1:1A:2360:A:O4'	2.20	0.41
1:1A:2405:G:O2'	1:1A:2406:U:OP1	2.27	0.41
2:1B:14:U:O2	2:1B:108:U:H4'	2.21	0.41
17:1V:1:MET:HG2	17:1V:43:GLU:OE1	2.20	0.41
32:1a:148:G:H2'	32:1a:149:A:C8	2.50	0.41
32:1a:167:G:H2'	32:1a:168:G:C8	2.56	0.41
39:1h:6:ILE:HD11	39:1h:31:PHE:HD2	1.86	0.41
44:1m:23:TYR:CE2	44:1m:71:ARG:HG3	2.56	0.41
1:2A:815:C:H2'	1:2A:816:C:H6	1.84	0.41
1:2A:1187:G:O6	63:2A:3950:HOH:O	2.20	0.41
1:2A:1589:C:H2'	1:2A:1590:U:C6	2.55	0.41
1:2A:2153:G:H2'	1:2A:2154:G:H8	1.86	0.41
1:2A:2474:C:OP2	1:2A:2475:C:H5	2.03	0.41
1:2A:2484:G:C2	1:2A:2485:G:C8	3.08	0.41
11:2P:19:VAL:HB	11:2P:31:ALA:HA	2.02	0.41
11:2P:37:GLY:O	11:2P:40:SER:OG	2.35	0.41
12:2Q:75:THR:HA	12:2Q:89:ASN:O	2.20	0.41
26:24:16:CYS:SG	26:24:17:GLY:N	2.93	0.41
32:2a:537:G:H2'	32:2a:538:G:C8	2.55	0.41
32:2a:977:A:HO2'	32:2a:981:U:H3	1.67	0.41
32:2a:1133:G:H2'	32:2a:1134:G:C8	2.56	0.41
32:2a:1203:C:H2'	32:2a:1204:A:O4'	2.21	0.41
32:2a:1426:C:H2'	32:2a:1427:U:C6	2.56	0.41
33:2b:16:HIS:HB2	33:2b:204:ASN:ND2	2.33	0.41
45:2n:13:THR:HA	45:2n:14:PRO:HD3	1.87	0.41
51:2t:72:LEU:HA	51:2t:72:LEU:HD12	1.84	0.41
1:1A:876:C:H2'	1:1A:877:U:O4'	2.20	0.41
1:1A:882:G:N2	1:1A:895:U:H1'	2.35	0.41
1:1A:958:U:H4'	63:1A:4161:HOH:O	2.21	0.41
1:1A:1075:C:O2	1:1A:1076:C:H2'	2.20	0.41
1:1A:2584:U:O2	1:1A:2585:U:C4	2.74	0.41
4:1E:72:VAL:HG12	4:1E:73:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:116:ASP:OD2	11:1P:1:MET:N	2.38	0.41
11:1P:135:LEU:HD23	11:1P:135:LEU:HA	1.83	0.41
12:1Q:135:ASP:N	12:1Q:138:ASP:OD2	2.53	0.41
15:1T:8:LYS:HE3	15:1T:8:LYS:HB3	1.90	0.41
32:1a:1152:A:H5'	41:1j:13:HIS:CG	2.56	0.41
32:1a:1237:C:N4	32:1a:1336:C:O2	2.54	0.41
32:1a:1346:A:N1	32:1a:1374:A:H5''	2.36	0.41
32:1a:1366:C:H2'	32:1a:1367:C:C6	2.56	0.41
32:1a:1513:A:H2'	32:1a:1514:C:C6	2.55	0.41
35:1d:88:VAL:HA	36:1e:97:GLY:HA3	2.03	0.41
35:1d:158:ILE:H	35:1d:158:ILE:HG13	1.50	0.41
37:1f:8:ILE:HD11	37:1f:79:LEU:HD13	2.01	0.41
40:1i:61:ALA:HB1	40:1i:63:ILE:HD11	2.02	0.41
57:1y:2:C:H2'	57:1y:3:G:C8	2.55	0.41
1:2A:271(M):G:H4'	1:2A:271(N):U:OP1	2.21	0.41
1:2A:438:G:H2'	1:2A:440:G:C8	2.56	0.41
1:2A:933:A:P	25:23:24:LYS:HZ1	2.44	0.41
1:2A:1005:C:H2'	1:2A:1006:C:H6	1.84	0.41
1:2A:1857:G:C6	1:2A:1858:G:N1	2.89	0.41
1:2A:1913:A:C8	32:2a:1494:G:H4'	2.56	0.41
1:2A:2469:A:O2'	12:2Q:56:ARG:HD3	2.20	0.41
1:2A:2516:G:C6	1:2A:2517:C:N4	2.88	0.41
5:2F:155:LEU:HB2	5:2F:189:THR:HG21	2.02	0.41
11:2P:63:PRO:HG2	30:28:25:MET:HB2	2.03	0.41
13:2R:38:VAL:HG22	13:2R:112:ALA:HB2	2.03	0.41
18:2W:86:LEU:HB2	18:2W:96:ILE:HG13	2.02	0.41
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.21	0.41
26:24:67:TYR:HD2	50:2s:9:VAL:HB	1.85	0.41
32:2a:1318:A:N3	50:2s:37:ARG:HD2	2.36	0.41
44:2m:96:LEU:C	44:2m:110:ARG:HG2	2.46	0.41
54:2w:8:4SU:H1'	54:2w:21:A:N1	2.36	0.41
57:2y:27:A:H61	57:2y:43:U:H3	1.69	0.41
1:1A:819:A:C4	1:1A:1189:A:C2	3.08	0.41
1:1A:1059:G:H2'	1:1A:1060:U:C5	2.55	0.41
1:1A:1078:U:H5'	1:1A:1079:C:OP1	2.21	0.41
1:1A:1094:U:H1'	1:1A:1097:U:C5	2.55	0.41
4:1E:79:ARG:HA	4:1E:79:ARG:HD3	1.89	0.41
25:13:18:ASP:OD1	25:13:18:ASP:N	2.54	0.41
32:1a:254:G:O2'	48:1q:16:GLN:O	2.38	0.41
32:1a:373:A:C2	32:1a:482:A:C6	3.09	0.41
32:1a:1073:U:H2'	32:1a:1074:G:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1179:A:H2'	32:1a:1180:A:O4'	2.20	0.41
33:1b:16:HIS:HB2	33:1b:204:ASN:CB	2.51	0.41
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.85	0.41
44:1m:59:TYR:O	44:1m:63:THR:OG1	2.38	0.41
53:1v:12:A:N3	53:1v:12:A:H2'	2.36	0.41
1:2A:191:A:H2'	1:2A:192:C:C6	2.56	0.41
1:2A:322:A:C5	1:2A:340:A:C2	3.08	0.41
1:2A:699:A:H2'	1:2A:700:G:O4'	2.21	0.41
1:2A:764:A:O4'	3:2D:213:ARG:HG3	2.20	0.41
1:2A:911:A:H2'	12:2Q:9:TYR:OH	2.21	0.41
1:2A:958:U:OP2	12:2Q:14:ARG:NE	2.43	0.41
1:2A:1529:G:C5	1:2A:1530:C:C4	3.09	0.41
5:2F:40:GLN:NE2	5:2F:182:ASN:HB2	2.34	0.41
6:2G:125:PHE:HB3	6:2G:166:ASP:OD1	2.21	0.41
7:2H:70:THR:HG22	7:2H:74:ASN:OD1	2.21	0.41
32:2a:381:C:H2'	32:2a:382:A:O4'	2.20	0.41
32:2a:501:C:H2'	32:2a:502:G:C8	2.56	0.41
32:2a:572:A:H5'	63:2a:1913:HOH:O	2.20	0.41
32:2a:952:U:H2'	32:2a:953:G:C8	2.56	0.41
32:2a:1168:A:C6	32:2a:1169:A:C6	3.09	0.41
33:2b:97:TRP:CH2	33:2b:101:MET:HB2	2.55	0.41
33:2b:118:LEU:HG	33:2b:142:LEU:HB2	2.03	0.41
42:2k:18:ARG:O	42:2k:32:ILE:HA	2.21	0.41
44:2m:82:MET:O	44:2m:93:ARG:NH2	2.52	0.41
44:2m:84:ILE:HG13	44:2m:86:CYS:H	1.86	0.41
47:2p:3:LYS:O	47:2p:21:VAL:HA	2.21	0.41
51:2t:58:LYS:HE3	51:2t:62:LEU:HD11	2.03	0.41
1:1A:1062:G:C5	1:1A:1088:A:H2'	2.56	0.41
1:1A:2066:C:O2'	1:1A:2067:G:H5'	2.21	0.41
1:1A:2705:A:O2'	1:1A:2852:G:OP1	2.25	0.41
1:1A:2854:G:H2'	1:1A:2855:C:C6	2.56	0.41
19:1X:31:HIS:CD2	19:1X:33:LYS:HB2	2.56	0.41
21:1Z:4:ARG:NE	21:1Z:60:GLU:OE2	2.38	0.41
23:11:59:THR:O	23:11:91:LYS:NZ	2.30	0.41
24:12:2:LYS:HB2	24:12:5:GLU:HG3	2.03	0.41
32:1a:193:C:H2'	32:1a:194:C:H6	1.86	0.41
32:1a:487:A:H2'	32:1a:488:C:O4'	2.21	0.41
32:1a:738:C:H2'	32:1a:739:C:C6	2.55	0.41
32:1a:1032:G:H2'	32:1a:1033:G:O4'	2.21	0.41
32:1a:1145:C:H4'	32:1a:1146:A:H8	1.86	0.41
32:1a:1157:A:C6	32:1a:1180:A:C6	3.09	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:C6	2.55	0.41
32:1a:1333:A:H2'	32:1a:1334:G:O4'	2.21	0.41
32:1a:1503:A:C2	53:1v:12:A:H2	2.39	0.41
33:1b:97:TRP:CZ2	33:1b:102:LEU:HD13	2.55	0.41
35:1d:13:ARG:HB3	35:1d:38:TYR:O	2.21	0.41
35:1d:65:ARG:NH1	35:1d:72:GLU:HB2	2.36	0.41
35:1d:98:GLU:HG3	35:1d:189:PRO:HG2	2.02	0.41
36:1e:78:HIS:HE1	36:1e:142:LEU:HD23	1.86	0.41
37:1f:61:LEU:HB3	37:1f:63:TYR:HE2	1.86	0.41
37:1f:68:PRO:HG2	37:1f:71:ARG:HD2	2.02	0.41
41:1j:31:GLY:HA3	41:1j:32:ALA:HA	1.75	0.41
41:1j:38:ILE:CG1	41:1j:71:LEU:HB3	2.50	0.41
47:1p:49:LEU:HD22	47:1p:49:LEU:HA	1.93	0.41
50:1s:48:THR:HG22	50:1s:61:TYR:HA	2.03	0.41
53:1v:15:A:H5''	53:1v:16:A:OP1	2.21	0.41
54:1w:60:U:H5''	54:1w:61:C:H5	1.86	0.41
1:2A:93:G:H2'	1:2A:94:C:C6	2.56	0.41
1:2A:443:A:H5''	1:2A:444:C:OP1	2.21	0.41
1:2A:864:G:C6	1:2A:865:C:N4	2.88	0.41
1:2A:1539:G:H2'	1:2A:1540:U:O4'	2.21	0.41
1:2A:1591:G:H2'	1:2A:1592:C:H6	1.86	0.41
1:2A:1754:C:OP2	15:2T:113:LYS:NZ	2.52	0.41
1:2A:2134:A:H2'	1:2A:2135:A:H5'	2.03	0.41
1:2A:2318:G:H21	14:2S:3:ARG:CD	2.34	0.41
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.85	0.41
4:2E:76:ARG:NH1	63:2E:402:HOH:O	2.54	0.41
4:2E:143:ASN:HD22	4:2E:147:PRO:HD3	1.85	0.41
6:2G:39:ILE:HG13	6:2G:92:VAL:HG13	2.02	0.41
6:2G:58:GLN:HA	6:2G:61:ALA:HB3	2.02	0.41
8:2I:75:LEU:HD13	8:2I:105:HIS:CG	2.55	0.41
8:2I:87:LYS:HE3	8:2I:87:LYS:HB2	1.82	0.41
10:2O:34:THR:OG1	10:2O:35:VAL:N	2.54	0.41
16:2U:104:GLN:NE2	16:2U:105:VAL:HG23	2.36	0.41
17:2V:4:ILE:HD12	17:2V:39:LEU:HB3	2.02	0.41
23:21:98:LEU:HD23	23:21:98:LEU:HA	1.81	0.41
32:2a:7:G:H2'	36:2e:119:LEU:HD22	2.03	0.41
32:2a:243:A:H4'	32:2a:244:U:H5''	2.03	0.41
32:2a:502:G:H2'	32:2a:503:C:O4'	2.21	0.41
32:2a:524:G:H2'	32:2a:525:C:C6	2.56	0.41
32:2a:553:A:H5''	43:2l:24:VAL:HG21	2.02	0.41
32:2a:630:G:H2'	32:2a:631:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1010:G:N2	32:2a:1020:U:H1'	2.36	0.41
32:2a:1122:U:C4	32:2a:1123:A:N7	2.88	0.41
32:2a:1422:G:H2'	32:2a:1423:G:H8	1.86	0.41
32:2a:1441:G:H1'	32:2a:1461:G:N2	2.36	0.41
33:2b:92:TYR:CE2	33:2b:151:GLY:HA3	2.55	0.41
33:2b:100:GLY:N	33:2b:176:GLU:OE2	2.52	0.41
35:2d:180:GLY:O	35:2d:182:LYS:HG3	2.20	0.41
40:2i:99:LEU:HB3	40:2i:101:PHE:CD2	2.55	0.41
42:2k:17:GLY:O	42:2k:80:VAL:HA	2.20	0.41
47:2p:8:ARG:HG3	47:2p:17:TYR:CE1	2.56	0.41
51:2t:67:ALA:HA	51:2t:72:LEU:O	2.21	0.41
1:1A:412:A:O5'	1:1A:412:A:H8	2.04	0.41
1:1A:1826:G:H2'	1:1A:1827:C:O4'	2.20	0.41
5:1F:28:ILE:O	5:1F:30:PRO:HD3	2.21	0.41
9:1N:12:ARG:HH12	9:1N:138:LEU:HD21	1.86	0.41
12:1Q:57:HIS:CD2	12:1Q:117:ALA:HB2	2.56	0.41
15:1T:108:ARG:HA	15:1T:111:ARG:NH1	2.36	0.41
28:16:13:CYS:SG	28:16:47:THR:HG21	2.61	0.41
28:16:47:THR:HG22	28:16:48:VAL:O	2.20	0.41
32:1a:160:A:H61	32:1a:347:G:H21	1.69	0.41
32:1a:406:G:N3	35:1d:119:GLN:NE2	2.67	0.41
32:1a:447:G:H2'	32:1a:485:G:N2	2.35	0.41
33:1b:184:VAL:N	33:1b:198:ASP:OD2	2.33	0.41
1:2A:271(O):C:H2'	1:2A:271(P):C:C6	2.56	0.41
1:2A:271(X):G:C2	1:2A:271(Y):U:O4	2.73	0.41
1:2A:614(B):G:H2'	5:2F:44:ARG:HH11	1.86	0.41
1:2A:820:A:H1'	1:2A:943:U:H1'	2.03	0.41
1:2A:2305:A:H2'	1:2A:2306:C:O4'	2.20	0.41
18:2W:92:ARG:HG3	18:2W:93:ALA:N	2.36	0.41
22:20:33:ALA:N	22:20:64:ASP:OD1	2.33	0.41
32:2a:114:U:O2'	32:2a:115:G:H5'	2.21	0.41
32:2a:302:G:N3	32:2a:556:C:H4'	2.36	0.41
33:2b:19:HIS:HB2	33:2b:204:ASN:HB2	2.03	0.41
33:2b:28:PHE:CG	33:2b:190:THR:HA	2.56	0.41
33:2b:188:ALA:HB1	33:2b:192:SER:HB2	2.02	0.41
34:2c:162:GLN:NE2	53:2v:24:A:O3'	2.54	0.41
39:2h:6:ILE:O	39:2h:10:LEU:HG	2.20	0.41
40:2i:4:TYR:O	40:2i:18:PHE:HA	2.21	0.41
48:2q:32:TYR:O	48:2q:34:LYS:N	2.51	0.41
50:2s:37:ARG:O	50:2s:70:LYS:HE3	2.20	0.41
50:2s:40:ILE:HB	50:2s:67:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:278:A:H2'	1:1A:279:C:C6	2.56	0.40
1:1A:2066:C:H5''	63:1A:5244:HOH:O	2.21	0.40
1:1A:2126:A:H4'	1:1A:2127:G:OP1	2.20	0.40
1:1A:2126:A:H62	1:1A:2163:C:C4'	2.34	0.40
1:1A:2298:A:H2'	1:1A:2299:G:O4'	2.21	0.40
2:1B:75:G:O2'	21:1Z:85:HIS:NE2	2.47	0.40
3:1D:206:LEU:HD22	3:1D:211:ARG:HG2	2.03	0.40
3:1D:232:PRO:HB3	3:1D:244:ARG:CZ	2.50	0.40
4:1E:181:LEU:HD12	4:1E:181:LEU:HA	1.78	0.40
6:1G:109:VAL:C	6:1G:112:PRO:HD2	2.47	0.40
9:1N:73:THR:HA	9:1N:83:LYS:O	2.20	0.40
19:1X:57:LEU:HA	63:1X:202:HOH:O	2.21	0.40
32:1a:196:A:OP1	51:1t:68:LYS:NZ	2.53	0.40
32:1a:767:A:H2'	32:1a:768:A:O4'	2.21	0.40
32:1a:890:G:O2'	32:1a:906:G:O6	2.35	0.40
32:1a:1305:G:C2	32:1a:1331:G:N3	2.89	0.40
32:1a:1316:G:N2	32:1a:1318:A:H3'	2.36	0.40
50:1s:18:LYS:H	50:1s:18:LYS:HG3	1.69	0.40
50:1s:52:TYR:HA	50:1s:56:GLN:O	2.20	0.40
54:1w:60:U:H3'	54:1w:61:C:H6	1.86	0.40
57:1y:19:U:H2'	57:1y:19:U:OP2	2.21	0.40
1:2A:42:G:H2'	1:2A:43:A:O4'	2.21	0.40
1:2A:234:C:H2'	1:2A:235:U:C6	2.56	0.40
1:2A:363:G:H2'	1:2A:363(A):A:H8	1.86	0.40
1:2A:530:G:N3	1:2A:530:G:O4'	2.54	0.40
1:2A:704:G:N3	1:2A:726:G:C2	2.89	0.40
1:2A:947:G:H2'	1:2A:948:G:C8	2.56	0.40
1:2A:2287:A:C8	1:2A:2289:G:C8	3.10	0.40
1:2A:2494:G:C4	1:2A:2495:G:C8	3.09	0.40
2:2B:55:U:H1'	6:2G:29:TRP:HD1	1.86	0.40
2:2B:61:G:C6	2:2B:62:C:C4	3.09	0.40
21:2Z:36:LYS:HE3	21:2Z:36:LYS:HB2	1.78	0.40
21:2Z:74:VAL:HB	21:2Z:86:VAL:HG23	2.02	0.40
32:2a:736:C:H2'	32:2a:737:A:H8	1.85	0.40
32:2a:1312:G:N7	50:2s:2:PRO:HD3	2.35	0.40
32:2a:1459:C:OP1	51:2t:31:SER:OG	2.35	0.40
40:2i:5:TYR:CE1	40:2i:18:PHE:HE1	2.39	0.40
40:2i:33:PHE:CE2	40:2i:43:ALA:HB1	2.56	0.40
47:2p:1:MET:HE2	47:2p:1:MET:N	2.36	0.40
1:1A:573:G:O2'	1:1A:574:C:H3'	2.22	0.40
1:1A:706:A:H2'	1:1A:707:G:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:760:G:H2'	1:1A:761:A:O4'	2.21	0.40
1:1A:1094:U:H1'	1:1A:1097:U:C4	2.57	0.40
1:1A:1142(A):A:C4	1:1A:1144:G:N7	2.89	0.40
1:1A:1665:A:H2'	1:1A:1666:G:O4'	2.21	0.40
1:1A:2161:C:O2'	1:1A:2162:G:H8	2.04	0.40
1:1A:2319:G:C2	14:1S:3:ARG:HA	2.56	0.40
3:1D:5:LYS:HE3	3:1D:5:LYS:HB3	1.79	0.40
6:1G:23:PHE:HB2	6:1G:25:TYR:CE2	2.56	0.40
6:1G:34:LEU:HD23	6:1G:161:THR:HG22	2.03	0.40
21:1Z:28:MET:HE2	21:1Z:35:ARG:HB2	2.01	0.40
32:1a:946:A:C6	32:1a:947:G:C6	3.09	0.40
40:1i:70:LYS:O	40:1i:74:ILE:HG13	2.21	0.40
43:1l:39:VAL:HG11	43:1l:41:ARG:NH1	2.29	0.40
47:1p:18:ARG:NH1	47:1p:32:TYR:OH	2.55	0.40
1:2A:392:C:H5''	1:2A:409:C:H5''	2.03	0.40
1:2A:854:G:H2'	1:2A:855:G:H8	1.86	0.40
1:2A:2135:A:H2'	1:2A:2136:C:C6	2.57	0.40
1:2A:2171:A:H1'	1:2A:2172:U:C6	2.56	0.40
4:2E:127:ASP:OD2	63:2E:401:HOH:O	2.22	0.40
6:2G:60:LEU:HD23	6:2G:60:LEU:O	2.22	0.40
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.56	0.40
14:2S:19:LYS:C	14:2S:21:THR:H	2.29	0.40
14:2S:93:LYS:HB2	14:2S:93:LYS:HE3	1.64	0.40
30:28:22:VAL:HG12	30:28:50:LEU:HD12	2.04	0.40
32:2a:520:A:C2	32:2a:536:C:H1'	2.56	0.40
32:2a:1120:G:C6	32:2a:1121:U:C4	3.09	0.40
32:2a:1256:A:H61	32:2a:1278:U:C2'	2.34	0.40
32:2a:1469:G:H2'	32:2a:1470:G:C8	2.56	0.40
34:2c:12:LEU:HA	34:2c:16:ARG:O	2.21	0.40
34:2c:18:TRP:HB2	34:2c:21:ARG:HG3	2.02	0.40
39:2h:116:LYS:HE3	39:2h:127:LEU:HD22	2.03	0.40
40:2i:28:VAL:HA	40:2i:63:ILE:O	2.22	0.40
43:2l:59:ARG:HA	43:2l:65:GLU:HA	2.04	0.40
43:2l:82:VAL:O	43:2l:106:ASP:HB2	2.21	0.40
46:2o:47:LYS:HE3	46:2o:47:LYS:HB2	1.96	0.40
60:2w:103:CLM:CL1	56:2z:2:ALA:HB2	2.58	0.40
1:1A:84:A:OP2	20:1Y:8:LYS:NZ	2.32	0.40
1:1A:548:A:N6	17:1V:19:LYS:H	2.19	0.40
1:1A:1794:U:H2'	1:1A:1795:C:H6	1.86	0.40
1:1A:1914:C:H3'	1:1A:1915:5MU:H73	2.04	0.40
1:1A:2040:C:H2'	1:1A:2041:U:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2133:G:C6	1:1A:2157:G:C4	3.10	0.40
1:1A:2331:G:O2'	22:10:43:THR:HG22	2.22	0.40
1:1A:2484:G:H1'	12:1Q:124:LYS:HD2	2.03	0.40
1:1A:2537:U:H2'	1:1A:2538:C:C6	2.56	0.40
63:1A:5743:HOH:O	9:1N:28:THR:HG23	2.20	0.40
6:1G:32:PRO:HB2	6:1G:172:LEU:HD22	2.04	0.40
20:1Y:6:HIS:H	20:1Y:6:HIS:HD2	1.69	0.40
32:1a:421:U:O2'	32:1a:423:G:N7	2.55	0.40
32:1a:1095:U:P	32:1a:1108:G:H1	2.44	0.40
32:1a:1356:G:H2'	32:1a:1357:A:H8	1.83	0.40
32:1a:1442:G:O2'	32:1a:1442(A):G:H5'	2.21	0.40
33:1b:220:ASP:O	33:1b:223:ILE:HG22	2.21	0.40
34:1c:132:ARG:HE	34:1c:136:GLN:NE2	2.19	0.40
50:1s:48:THR:HA	50:1s:60:VAL:O	2.21	0.40
1:2A:1630:G:H2'	1:2A:1631:C:C6	2.56	0.40
1:2A:1865:G:N2	1:2A:1877:A:OP2	2.52	0.40
1:2A:1973:G:OP1	63:2A:3957:HOH:O	2.22	0.40
1:2A:2497:A:H5''	63:2A:4248:HOH:O	2.21	0.40
1:2A:2802:G:C2	1:2A:2803:C:H1'	2.57	0.40
1:2A:2822:G:O2'	1:2A:2825:C:N4	2.51	0.40
3:2D:70:TRP:CE2	3:2D:150:LYS:HD3	2.57	0.40
6:2G:41:GLN:O	6:2G:43:LEU:HB2	2.21	0.40
9:2N:58:ASP:OD1	9:2N:58:ASP:N	2.54	0.40
15:2T:105:LEU:HD22	15:2T:109:GLU:HB3	2.03	0.40
21:2Z:104:PHE:HA	21:2Z:139:VAL:HB	2.03	0.40
32:2a:926:G:H5''	32:2a:927:G:O5'	2.20	0.40
32:2a:1004:A:N6	32:2a:1037:C:H1'	2.35	0.40
32:2a:1012:U:H2'	32:2a:1013:G:C8	2.57	0.40
32:2a:1064:G:OP1	32:2a:1386:G:H4'	2.22	0.40
32:2a:1070:U:H2'	32:2a:1071:C:H6	1.84	0.40
32:2a:1103:C:P	33:2b:96:ARG:HH22	2.44	0.40
32:2a:1320:C:H42	50:2s:36:ARG:HE	1.68	0.40
33:2b:98:LEU:HB2	33:2b:101:MET:HE3	2.02	0.40
41:2j:65:LEU:HD12	45:2n:55:GLY:O	2.21	0.40
44:2m:92:HIS:NE2	44:2m:98:VAL:HG21	2.36	0.40
55:2x:19:G:H5''	55:2x:60:U:O4	2.21	0.40
1:1A:817:C:O2'	1:1A:839:U:H5''	2.20	0.40
1:1A:2206:G:H8	1:1A:2207:G:N7	2.19	0.40
1:1A:2335:A:C8	1:1A:2337:G:C5	3.10	0.40
1:1A:2774:C:H2'	1:1A:2775:A:O4'	2.21	0.40
3:1D:148:GLU:CB	3:1D:151:LYS:HD2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:10:ARG:HH11	12:1Q:11:LYS:HE3	1.86	0.40
19:1X:60:ARG:HH22	29:17:47:ARG:NH2	2.20	0.40
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.59	0.40
32:1a:352:C:O2'	32:1a:354:G:OP1	2.30	0.40
32:1a:672:U:O2'	32:1a:673:G:O5'	2.39	0.40
32:1a:1302:U:OP2	44:1m:21:TYR:OH	2.33	0.40
33:1b:63:MET:HE2	33:1b:63:MET:HB3	1.92	0.40
33:1b:155:LEU:HD21	33:1b:159:PRO:HD3	2.02	0.40
34:1c:19:GLU:O	34:1c:40:ARG:NH2	2.53	0.40
35:1d:165:MET:HE3	35:1d:165:MET:HB3	1.89	0.40
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.21	0.40
50:1s:15:LEU:O	50:1s:19:VAL:HG23	2.22	0.40
51:1t:47:GLY:N	51:1t:48:LYS:HB2	2.37	0.40
1:2A:556:G:C6	1:2A:557:U:C4	3.09	0.40
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.56	0.40
6:2G:148:MET:HE3	6:2G:148:MET:HB2	1.90	0.40
7:2H:38:SER:HB3	7:2H:41:MET:HG2	2.02	0.40
10:2O:7:TYR:CE2	10:2O:20:MET:HB2	2.56	0.40
10:2O:47:ILE:HB	10:2O:48:PRO:HD2	2.03	0.40
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	2.04	0.40
32:2a:1212:U:H5'	32:2a:1213:A:C8	2.57	0.40
32:2a:1375:A:H4'	38:2g:29:LYS:NZ	2.37	0.40
34:2c:18:TRP:NE1	45:2n:55:GLY:H	2.19	0.40
38:2g:65:ALA:O	38:2g:69:VAL:HG23	2.21	0.40
39:2h:48:TYR:HA	39:2h:60:ARG:O	2.22	0.40
41:2j:47:PHE:CE2	45:2n:37:PHE:HE2	2.39	0.40
41:2j:81:THR:O	41:2j:84:GLN:N	2.50	0.40
46:2o:4:THR:C	46:2o:6:GLU:N	2.80	0.40
56:2z:1:FME:HE3	56:2z:1:FME:HB2	1.87	0.40
1:1A:173:G:C6	1:1A:174:C:C4	3.10	0.40
1:1A:1087:G:H2'	1:1A:1089:G:C8	2.56	0.40
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.52	0.40
8:1I:102:SER:O	8:1I:106:GLY:HA2	2.21	0.40
15:1T:96:ARG:CZ	15:1T:96:ARG:HB3	2.50	0.40
32:1a:580:U:H2'	32:1a:581:G:O4'	2.22	0.40
32:1a:926:G:H5''	32:1a:927:G:O5'	2.21	0.40
32:1a:987:G:H2'	32:1a:988:G:C8	2.57	0.40
32:1a:1004:A:H8	32:1a:1005:A:O4'	2.04	0.40
32:1a:1260:C:OP1	32:1a:1284:C:O2'	2.38	0.40
33:1b:141:GLU:HG2	33:1b:145:LEU:HD12	2.02	0.40
35:1d:196:LEU:HB3	35:1d:198:VAL:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1g:92:SER:O	38:1g:96:GLN:HG3	2.20	0.40
40:1i:48:GLU:N	40:1i:49:PRO:CD	2.85	0.40
49:1r:58:LEU:HB3	49:1r:62:GLU:HB2	2.04	0.40
50:1s:27:GLU:HB2	50:1s:28:LYS:CA	2.51	0.40
51:1t:99:LEU:HA	51:1t:100:ILE:C	2.47	0.40
1:2A:253:C:O2'	63:2A:3956:HOH:O	2.22	0.40
1:2A:571:A:H5'	1:2A:2030:A:N7	2.37	0.40
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.38	0.40
1:2A:647:G:H8	1:2A:647:G:O5'	2.04	0.40
1:2A:1288:U:O4	13:2R:106:GLY:HA3	2.21	0.40
1:2A:1826:G:H2'	1:2A:1827:C:O4'	2.22	0.40
1:2A:2116:G:O6	1:2A:2162:G:H5''	2.21	0.40
1:2A:2118:U:N3	1:2A:2149:G:H1'	2.37	0.40
1:2A:2305:A:H1'	6:2G:136:ARG:HG2	2.03	0.40
19:2X:5:TYR:CZ	24:22:30:ARG:HG3	2.57	0.40
19:2X:60:ARG:HH22	29:27:47:ARG:NH1	2.19	0.40
32:2a:359:U:H2'	32:2a:360:A:C8	2.57	0.40
32:2a:841:U:H6	32:2a:841:U:OP2	2.03	0.40
32:2a:926:G:C6	32:2a:1505:G:C5	3.10	0.40
32:2a:959:A:O2'	32:2a:984:C:O2'	2.22	0.40
32:2a:1252:A:H2'	32:2a:1253:G:O4'	2.22	0.40
32:2a:1256:A:H61	32:2a:1278:U:H2'	1.87	0.40
34:2c:136:GLN:HA	34:2c:139:GLN:HB3	2.03	0.40
37:2f:12:PRO:HG3	37:2f:57:GLN:O	2.22	0.40
41:2j:38:ILE:HG13	41:2j:71:LEU:HB3	2.04	0.40
55:2x:53:G:H2'	55:2x:54:5MU:C6	2.56	0.40
57:2y:6:C:O2'	57:2y:7:G:H5'	2.22	0.40
57:2y:22:G:C8	57:2y:46:A:N6	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	259 (95%)	14 (5%)	0	100	100
3	2D	273/276 (99%)	257 (94%)	16 (6%)	0	100	100
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	34
4	2E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	24	34
5	1F	200/210 (95%)	195 (98%)	4 (2%)	1 (0%)	24	34
5	2F	200/210 (95%)	191 (96%)	7 (4%)	2 (1%)	12	17
6	1G	179/182 (98%)	165 (92%)	13 (7%)	1 (1%)	21	29
6	2G	179/182 (98%)	160 (89%)	17 (10%)	2 (1%)	11	15
7	1H	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	21	29
7	2H	172/180 (96%)	158 (92%)	11 (6%)	3 (2%)	7	8
8	1I	144/148 (97%)	130 (90%)	14 (10%)	0	100	100
8	2I	144/148 (97%)	125 (87%)	17 (12%)	2 (1%)	9	11
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	131 (95%)	5 (4%)	2 (1%)	9	11
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16	22
11	1P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	9	11
11	2P	147/150 (98%)	130 (88%)	16 (11%)	1 (1%)	18	25
12	1Q	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
12	2Q	139/141 (99%)	128 (92%)	10 (7%)	1 (1%)	18	25
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	9 (8%)	0	100	100
14	2S	108/112 (96%)	97 (90%)	8 (7%)	3 (3%)	4	3
15	1T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
15	2T	129/146 (88%)	119 (92%)	9 (7%)	1 (1%)	16	22
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	12	17
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11	15
19	2X	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
20	1Y	105/110 (96%)	98 (93%)	6 (6%)	1 (1%)	12	17
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
21	1Z	148/206 (72%)	134 (90%)	13 (9%)	1 (1%)	18	25
21	2Z	156/206 (76%)	130 (83%)	25 (16%)	1 (1%)	21	29
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	76 (94%)	5 (6%)	0	100	100
23	11	95/98 (97%)	94 (99%)	0	1 (1%)	11	15
23	21	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	14	67/71 (94%)	54 (81%)	9 (13%)	4 (6%)	1	0
26	24	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	0
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%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	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%)	189 (82%)	34 (15%)	6 (3%)	4	3
33	2b	229/256 (90%)	180 (79%)	41 (18%)	8 (4%)	3	1
34	1c	204/239 (85%)	184 (90%)	19 (9%)	1 (0%)	24	34
34	2c	204/239 (85%)	173 (85%)	27 (13%)	4 (2%)	6	6
35	1d	206/209 (99%)	189 (92%)	15 (7%)	2 (1%)	12	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/209 (99%)	192 (93%)	13 (6%)	1 (0%)	24	34
36	1e	146/162 (90%)	128 (88%)	15 (10%)	3 (2%)	5	5
36	2e	146/162 (90%)	129 (88%)	13 (9%)	4 (3%)	4	3
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	141 (92%)	12 (8%)	0	100	100
38	2g	153/156 (98%)	137 (90%)	13 (8%)	3 (2%)	6	6
39	1h	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
39	2h	135/138 (98%)	125 (93%)	10 (7%)	0	100	100
40	1i	125/128 (98%)	105 (84%)	18 (14%)	2 (2%)	7	9
40	2i	125/128 (98%)	105 (84%)	20 (16%)	0	100	100
41	1j	95/105 (90%)	84 (88%)	8 (8%)	3 (3%)	3	2
41	2j	94/105 (90%)	80 (85%)	12 (13%)	2 (2%)	5	5
42	1k	112/129 (87%)	103 (92%)	7 (6%)	2 (2%)	6	7
42	2k	112/129 (87%)	105 (94%)	5 (4%)	2 (2%)	6	7
43	1l	119/132 (90%)	110 (92%)	8 (7%)	1 (1%)	16	22
43	2l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	16	22
44	1m	121/126 (96%)	109 (90%)	11 (9%)	1 (1%)	16	22
44	2m	120/126 (95%)	105 (88%)	12 (10%)	3 (2%)	4	4
45	1n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	2o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
47	1p	80/88 (91%)	65 (81%)	15 (19%)	0	100	100
47	2p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	9	12
48	1q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
48	2q	97/105 (92%)	91 (94%)	5 (5%)	1 (1%)	12	17
49	1r	66/88 (75%)	56 (85%)	10 (15%)	0	100	100
49	2r	66/88 (75%)	62 (94%)	3 (4%)	1 (2%)	8	10
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
50	2s	81/93 (87%)	66 (82%)	12 (15%)	3 (4%)	2	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1t	94/106 (89%)	85 (90%)	6 (6%)	3 (3%)	3	2
51	2t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	5	5
52	1u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
56	1z	1/3 (33%)	0	1 (100%)	0	100	100
56	2z	1/3 (33%)	1 (100%)	0	0	100	100
All	All	11370/12134 (94%)	10453 (92%)	817 (7%)	100 (1%)	14	20

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
26	14	47	GLN
26	14	62	ARG
33	1b	17	PHE
33	1b	22	LYS
35	1d	173	TRP
42	1k	49	GLY
44	1m	67	GLU
5	2F	130	ALA
6	2G	51	ARG
33	2b	17	PHE
33	2b	121	LEU
38	2g	55	GLY
38	2g	80	VAL
6	1G	43	LEU
19	1X	93	GLU
21	1Z	52	SER
23	11	3	LYS
33	1b	227	GLY
36	1e	85	GLY
40	1i	54	ASP
51	1t	47	GLY
6	2G	47	LYS
7	2H	47	GLU
10	2O	5	GLN
26	24	45	GLY
26	24	54	GLY
33	2b	21	ARG
33	2b	123	ALA

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Mol	Chain	Res	Type
34	2c	156	ARG
34	2c	181	ASN
36	2e	65	ASN
36	2e	85	GLY
42	2k	49	GLY
44	2m	5	ALA
44	2m	67	GLU
51	2t	47	GLY
7	1H	159	GLU
26	14	49	PHE
35	1d	172	PRO
42	1k	77	MET
4	2E	52	LEU
7	2H	126	PRO
14	2S	20	ARG
21	2Z	52	SER
33	2b	9	GLU
33	2b	20	GLU
50	2s	81	ARG
4	1E	52	LEU
11	1P	45	LEU
33	1b	20	GLU
33	1b	231	GLU
41	1j	78	ASN
43	1l	105	TYR
8	2I	49	ALA
9	2N	2	LYS
9	2N	23	LEU
14	2S	84	GLN
14	2S	96	GLY
26	24	50	VAL
34	2c	91	LEU
34	2c	95	THR
35	2d	179	GLU
41	2j	79	ARG
43	2l	105	TYR
44	2m	58	GLU
48	2q	68	ARG
50	2s	13	ASP
50	2s	70	LYS
51	2t	95	ALA
20	1Y	54	LYS

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Mol	Chain	Res	Type
26	14	53	GLU
33	1b	125	PRO
36	1e	69	VAL
41	1j	29	ARG
41	1j	77	PRO
8	2I	10	GLU
11	2P	45	LEU
26	24	49	PHE
33	2b	120	ALA
33	2b	125	PRO
38	2g	4	ARG
41	2j	78	ASN
49	2r	25	THR
36	1e	86	ALA
51	1t	102	GLY
12	2Q	60	ARG
15	2T	127	ALA
26	24	65	ASP
36	2e	37	ARG
36	2e	77	PRO
5	2F	206	ILE
34	1c	81	GLY
40	1i	53	VAL
11	1P	122	PRO
7	2H	21	PRO
42	2k	105	VAL
47	2p	78	GLY
51	1t	100	ILE
17	2V	50	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	205 (95%)	10 (5%)	23	36
3	2D	215/218 (99%)	208 (97%)	7 (3%)	33	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	1E	164/166 (99%)	156 (95%)	8 (5%)	22	34
4	2E	164/166 (99%)	156 (95%)	8 (5%)	22	34
5	1F	160/166 (96%)	146 (91%)	14 (9%)	9	12
5	2F	159/166 (96%)	153 (96%)	6 (4%)	29	44
6	1G	143/156 (92%)	130 (91%)	13 (9%)	9	11
6	2G	143/156 (92%)	120 (84%)	23 (16%)	2	2
7	1H	144/148 (97%)	135 (94%)	9 (6%)	16	23
7	2H	144/148 (97%)	130 (90%)	14 (10%)	8	9
8	1I	113/124 (91%)	100 (88%)	13 (12%)	5	6
8	2I	105/124 (85%)	89 (85%)	16 (15%)	3	2
9	1N	118/119 (99%)	111 (94%)	7 (6%)	18	27
9	2N	118/119 (99%)	109 (92%)	9 (8%)	12	17
10	1O	100/100 (100%)	97 (97%)	3 (3%)	36	53
10	2O	100/100 (100%)	96 (96%)	4 (4%)	28	42
11	1P	115/116 (99%)	109 (95%)	6 (5%)	21	32
11	2P	115/116 (99%)	111 (96%)	4 (4%)	32	48
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	39	58
12	2Q	111/111 (100%)	103 (93%)	8 (7%)	13	18
13	1R	101/101 (100%)	97 (96%)	4 (4%)	28	42
13	2R	101/101 (100%)	99 (98%)	2 (2%)	48	67
14	1S	86/88 (98%)	82 (95%)	4 (5%)	23	36
14	2S	85/88 (97%)	79 (93%)	6 (7%)	13	19
15	1T	115/127 (91%)	111 (96%)	4 (4%)	32	48
15	2T	113/127 (89%)	111 (98%)	2 (2%)	51	70
16	1U	93/94 (99%)	89 (96%)	4 (4%)	26	39
16	2U	93/94 (99%)	87 (94%)	6 (6%)	15	22
17	1V	80/82 (98%)	78 (98%)	2 (2%)	42	60
17	2V	80/82 (98%)	74 (92%)	6 (8%)	12	17
18	1W	90/92 (98%)	83 (92%)	7 (8%)	11	16
18	2W	90/92 (98%)	87 (97%)	3 (3%)	33	50
19	1X	77/78 (99%)	75 (97%)	2 (3%)	40	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40	59
20	1Y	85/91 (93%)	76 (89%)	9 (11%)	6	7
20	2Y	85/91 (93%)	74 (87%)	11 (13%)	4	4
21	1Z	135/179 (75%)	120 (89%)	15 (11%)	6	6
21	2Z	137/179 (76%)	123 (90%)	14 (10%)	7	8
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	62 (95%)	3 (5%)	24	36
23	11	80/83 (96%)	77 (96%)	3 (4%)	29	44
23	21	80/83 (96%)	77 (96%)	3 (4%)	29	44
24	12	65/67 (97%)	62 (95%)	3 (5%)	24	36
24	22	65/67 (97%)	62 (95%)	3 (5%)	24	36
25	13	51/52 (98%)	48 (94%)	3 (6%)	18	27
25	23	50/52 (96%)	46 (92%)	4 (8%)	11	15
26	14	59/63 (94%)	53 (90%)	6 (10%)	7	8
26	24	53/63 (84%)	48 (91%)	5 (9%)	8	10
27	15	50/52 (96%)	46 (92%)	4 (8%)	11	15
27	25	50/52 (96%)	48 (96%)	2 (4%)	28	42
28	16	51/52 (98%)	48 (94%)	3 (6%)	18	27
28	26	50/52 (96%)	44 (88%)	6 (12%)	5	5
29	17	41/42 (98%)	35 (85%)	6 (15%)	3	2
29	27	41/42 (98%)	38 (93%)	3 (7%)	13	18
30	18	54/55 (98%)	51 (94%)	3 (6%)	19	29
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	29
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	31 (91%)	3 (9%)	9	12
33	1b	192/220 (87%)	167 (87%)	25 (13%)	4	4
33	2b	187/220 (85%)	160 (86%)	27 (14%)	3	2
34	1c	142/188 (76%)	122 (86%)	20 (14%)	3	3
34	2c	140/188 (74%)	122 (87%)	18 (13%)	4	4
35	1d	169/181 (93%)	155 (92%)	14 (8%)	10	14
35	2d	173/181 (96%)	158 (91%)	15 (9%)	9	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	1e	113/123 (92%)	105 (93%)	8 (7%)	13	19
36	2e	114/123 (93%)	94 (82%)	20 (18%)	2	1
37	1f	84/90 (93%)	79 (94%)	5 (6%)	17	26
37	2f	85/90 (94%)	78 (92%)	7 (8%)	10	14
38	1g	119/127 (94%)	106 (89%)	13 (11%)	6	7
38	2g	120/127 (94%)	113 (94%)	7 (6%)	18	27
39	1h	114/119 (96%)	103 (90%)	11 (10%)	8	9
39	2h	114/119 (96%)	104 (91%)	10 (9%)	9	12
40	1i	90/99 (91%)	77 (86%)	13 (14%)	3	2
40	2i	89/99 (90%)	77 (86%)	12 (14%)	4	3
41	1j	66/92 (72%)	55 (83%)	11 (17%)	2	2
41	2j	69/92 (75%)	61 (88%)	8 (12%)	5	6
42	1k	82/99 (83%)	77 (94%)	5 (6%)	17	25
42	2k	83/99 (84%)	75 (90%)	8 (10%)	8	9
43	1l	96/108 (89%)	92 (96%)	4 (4%)	26	40
43	2l	96/108 (89%)	84 (88%)	12 (12%)	4	4
44	1m	93/101 (92%)	86 (92%)	7 (8%)	12	17
44	2m	92/101 (91%)	81 (88%)	11 (12%)	5	5
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	4
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	8
46	1o	78/80 (98%)	77 (99%)	1 (1%)	61	76
46	2o	78/80 (98%)	75 (96%)	3 (4%)	29	44
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5	6
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7	8
48	1q	94/97 (97%)	85 (90%)	9 (10%)	8	9
48	2q	94/97 (97%)	90 (96%)	4 (4%)	26	39
49	1r	59/77 (77%)	54 (92%)	5 (8%)	10	13
49	2r	59/77 (77%)	54 (92%)	5 (8%)	10	13
50	1s	69/80 (86%)	63 (91%)	6 (9%)	9	13
50	2s	67/80 (84%)	58 (87%)	9 (13%)	4	3
51	1t	70/82 (85%)	67 (96%)	3 (4%)	26	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	2t	70/82 (85%)	67 (96%)	3 (4%)	26	39
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
56	1z	1/1 (100%)	1 (100%)	0	100	100
56	2z	1/1 (100%)	1 (100%)	0	100	100
All	All	9305/10066 (92%)	8586 (92%)	719 (8%)	12	17

All (719) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	37	LEU
3	1D	39	LYS
3	1D	122	ASP
3	1D	126	GLN
3	1D	131	LEU
3	1D	181	GLU
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
4	1E	21	VAL
4	1E	59	VAL
4	1E	73	GLU
4	1E	89	ASP
4	1E	93	VAL
4	1E	116	VAL
4	1E	181	LEU
4	1E	184	VAL
5	1F	9	ILE
5	1F	24	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	70	THR
5	1F	74	ARG
5	1F	106	ARG
5	1F	144	LYS
5	1F	162	LEU
5	1F	168	ARG
5	1F	175	THR
5	1F	183	VAL

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Mol	Chain	Res	Type
5	1F	192	LEU
5	1F	201	VAL
6	1G	7	LEU
6	1G	22	ARG
6	1G	31	VAL
6	1G	33	ARG
6	1G	43	LEU
6	1G	64	THR
6	1G	70	VAL
6	1G	79	ASN
6	1G	139	LEU
6	1G	148	MET
6	1G	150	ASP
6	1G	159	VAL
6	1G	174	GLU
7	1H	3	ARG
7	1H	13	LYS
7	1H	15	VAL
7	1H	88	LEU
7	1H	119	GLU
7	1H	122	THR
7	1H	124	GLU
7	1H	134	SER
7	1H	172	LYS
8	1I	20	ASP
8	1I	38	LEU
8	1I	41	GLU
8	1I	45	LYS
8	1I	47	LEU
8	1I	57	ARG
8	1I	61	ARG
8	1I	78	THR
8	1I	85	GLU
8	1I	86	THR
8	1I	87	LYS
8	1I	92	VAL
8	1I	109	ILE
9	1N	1	MET
9	1N	14	VAL
9	1N	22	THR
9	1N	28	THR
9	1N	71	ILE

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Mol	Chain	Res	Type
9	1N	83	LYS
9	1N	89	LYS
10	1O	20	MET
10	1O	28	SER
10	1O	113	LYS
11	1P	3	LEU
11	1P	45	LEU
11	1P	75	ILE
11	1P	95	VAL
11	1P	126	VAL
11	1P	133	SER
12	1Q	1	MET
12	1Q	7	MET
12	1Q	75	THR
13	1R	6	SER
13	1R	8	ARG
13	1R	67	LEU
13	1R	114	VAL
14	1S	14	VAL
14	1S	36	TYR
14	1S	46	VAL
14	1S	69	VAL
15	1T	28	VAL
15	1T	51	ARG
15	1T	96	ARG
15	1T	128	GLU
16	1U	17	ILE
16	1U	27	LEU
16	1U	74	LEU
16	1U	108	GLU
17	1V	28	GLU
17	1V	56	SER
18	1W	4	LYS
18	1W	11	ARG
18	1W	18	ARG
18	1W	50	VAL
18	1W	60	ASN
18	1W	63	ASP
18	1W	92	ARG
19	1X	81	VAL
19	1X	92	LEU
20	1Y	1	MET

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Mol	Chain	Res	Type
20	1Y	7	VAL
20	1Y	8	LYS
20	1Y	31	LEU
20	1Y	43	ASN
20	1Y	55	TYR
20	1Y	67	LEU
20	1Y	91	GLU
20	1Y	99	CYS
21	1Z	18	LEU
21	1Z	46	LYS
21	1Z	49	ARG
21	1Z	61	LEU
21	1Z	66	SER
21	1Z	70	LEU
21	1Z	72	ARG
21	1Z	96	VAL
21	1Z	132	ASN
21	1Z	136	PHE
21	1Z	138	GLU
21	1Z	139	VAL
21	1Z	146	ILE
21	1Z	163	LEU
21	1Z	170	THR
23	11	40	ARG
23	11	57	GLU
23	11	83	GLU
24	12	40	SER
24	12	50	ILE
24	12	69	ARG
25	13	23	LEU
25	13	54	VAL
25	13	60	GLU
26	14	49	PHE
26	14	53	GLU
26	14	59	PHE
26	14	61	ARG
26	14	63	TYR
26	14	67	TYR
27	15	6	VAL
27	15	40	LYS
27	15	57	VAL
27	15	58	LEU

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Mol	Chain	Res	Type
28	16	9	LEU
28	16	14	THR
28	16	19	ARG
29	17	14	LYS
29	17	24	THR
29	17	41	ARG
29	17	43	THR
29	17	46	VAL
29	17	48	LYS
30	18	14	VAL
30	18	15	LYS
30	18	29	LYS
33	1b	7	VAL
33	1b	11	LEU
33	1b	21	ARG
33	1b	35	GLU
33	1b	39	ILE
33	1b	45	GLN
33	1b	48	MET
33	1b	53	ARG
33	1b	54	THR
33	1b	67	THR
33	1b	78	GLN
33	1b	83	MET
33	1b	107	THR
33	1b	108	ILE
33	1b	112	VAL
33	1b	118	LEU
33	1b	126	GLU
33	1b	127	ILE
33	1b	138	LEU
33	1b	185	ILE
33	1b	196	LEU
33	1b	197	VAL
33	1b	215	LEU
33	1b	219	VAL
33	1b	230	VAL
34	1c	3	ASN
34	1c	8	ILE
34	1c	16	ARG
34	1c	17	ASP
34	1c	20	SER

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Mol	Chain	Res	Type
34	1c	26	LYS
34	1c	28	GLN
34	1c	33	LEU
34	1c	66	VAL
34	1c	67	THR
34	1c	70	VAL
34	1c	89	GLU
34	1c	101	LEU
34	1c	103	VAL
34	1c	118	GLN
34	1c	119	ARG
34	1c	126	ARG
34	1c	151	VAL
34	1c	165	THR
34	1c	195	VAL
35	1d	3	ARG
35	1d	5	ILE
35	1d	19	LEU
35	1d	31	CYS
35	1d	112	VAL
35	1d	127	THR
35	1d	135	LEU
35	1d	140	VAL
35	1d	146	ILE
35	1d	158	ILE
35	1d	170	VAL
35	1d	177	ASP
35	1d	178	VAL
35	1d	181	MET
36	1e	16	THR
36	1e	31	LEU
36	1e	41	VAL
36	1e	51	VAL
36	1e	78	HIS
36	1e	79	GLU
36	1e	135	THR
36	1e	151	LEU
37	1f	43	LEU
37	1f	55	ASP
37	1f	64	GLN
37	1f	72	VAL
37	1f	75	LEU

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Mol	Chain	Res	Type
38	1g	12	LEU
38	1g	22	LEU
38	1g	24	THR
38	1g	32	ARG
38	1g	50	ILE
38	1g	61	VAL
38	1g	80	VAL
38	1g	89	MET
38	1g	91	VAL
38	1g	104	LEU
38	1g	106	GLN
38	1g	113	GLU
38	1g	139	GLU
39	1h	13	ILE
39	1h	24	THR
39	1h	25	ASP
39	1h	26	VAL
39	1h	39	LEU
39	1h	51	VAL
39	1h	52	ASP
39	1h	60	ARG
39	1h	109	ILE
39	1h	112	LEU
39	1h	127	LEU
40	1i	17	VAL
40	1i	23	ASN
40	1i	51	ARG
40	1i	53	VAL
40	1i	60	ASP
40	1i	75	ASP
40	1i	83	ARG
40	1i	92	TYR
40	1i	97	LYS
40	1i	103	THR
40	1i	105	ASP
40	1i	121	ARG
40	1i	128	ARG
41	1j	9	ARG
41	1j	23	ILE
41	1j	34	VAL
41	1j	43	ARG
41	1j	44	VAL

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Mol	Chain	Res	Type
41	1j	72	VAL
41	1j	81	THR
41	1j	92	THR
41	1j	94	VAL
41	1j	97	GLU
41	1j	98	ILE
42	1k	48	ILE
42	1k	87	THR
42	1k	114	VAL
42	1k	117	ASN
42	1k	120	ARG
43	1l	18	VAL
43	1l	33	ARG
43	1l	36	VAL
43	1l	40	VAL
44	1m	4	ILE
44	1m	17	VAL
44	1m	43	THR
44	1m	70	LEU
44	1m	98	VAL
44	1m	109	THR
44	1m	122	LYS
45	1n	7	ILE
45	1n	11	LYS
45	1n	18	VAL
45	1n	33	VAL
45	1n	41	ARG
45	1n	56	VAL
46	1o	76	GLU
47	1p	1	MET
47	1p	19	ILE
47	1p	20	VAL
47	1p	27	LYS
47	1p	49	LEU
47	1p	62	VAL
47	1p	67	THR
47	1p	73	LEU
48	1q	7	THR
48	1q	9	VAL
48	1q	14	LYS
48	1q	34	LYS
48	1q	53	LEU

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Mol	Chain	Res	Type
48	1q	60	ILE
48	1q	79	SER
48	1q	93	GLN
48	1q	99	SER
49	1r	42	ARG
49	1r	47	THR
49	1r	51	LEU
49	1r	63	GLN
49	1r	65	ILE
50	1s	12	ASP
50	1s	28	LYS
50	1s	32	LYS
50	1s	39	THR
50	1s	62	ILE
50	1s	66	MET
51	1t	10	LEU
51	1t	53	LEU
51	1t	62	LEU
3	2D	37	LEU
3	2D	38	LYS
3	2D	39	LYS
3	2D	127	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
4	2E	7	VAL
4	2E	21	VAL
4	2E	73	GLU
4	2E	77	ILE
4	2E	90	THR
4	2E	92	THR
4	2E	116	VAL
4	2E	181	LEU
5	2F	33	LEU
5	2F	60	SER
5	2F	70	THR
5	2F	154	VAL
5	2F	165	ARG
5	2F	170	LEU
6	2G	5	VAL
6	2G	7	LEU
6	2G	18	GLU

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Mol	Chain	Res	Type
6	2G	28	VAL
6	2G	31	VAL
6	2G	39	ILE
6	2G	41	GLN
6	2G	45	GLU
6	2G	49	ASP
6	2G	91	ARG
6	2G	111	LEU
6	2G	124	SER
6	2G	126	ASP
6	2G	135	LEU
6	2G	140	ILE
6	2G	148	MET
6	2G	149	VAL
6	2G	152	LEU
6	2G	157	ILE
6	2G	161	THR
6	2G	165	THR
6	2G	170	ARG
6	2G	173	LEU
7	2H	7	LEU
7	2H	15	VAL
7	2H	24	VAL
7	2H	40	GLU
7	2H	43	VAL
7	2H	45	VAL
7	2H	47	GLU
7	2H	63	SER
7	2H	68	THR
7	2H	72	ILE
7	2H	88	LEU
7	2H	106	THR
7	2H	119	GLU
7	2H	124	GLU
8	2I	7	GLU
8	2I	15	VAL
8	2I	31	LEU
8	2I	38	LEU
8	2I	44	LEU
8	2I	51	ILE
8	2I	79	ILE
8	2I	85	GLU

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Mol	Chain	Res	Type
8	2I	86	THR
8	2I	87	LYS
8	2I	101	LEU
8	2I	108	THR
8	2I	117	GLU
8	2I	129	THR
8	2I	142	VAL
8	2I	144	VAL
9	2N	1	MET
9	2N	22	THR
9	2N	28	THR
9	2N	32	THR
9	2N	43	THR
9	2N	46	VAL
9	2N	48	MET
9	2N	60	ILE
9	2N	83	LYS
10	2O	28	SER
10	2O	52	VAL
10	2O	69	ILE
10	2O	113	LYS
11	2P	30	THR
11	2P	39	LYS
11	2P	45	LEU
11	2P	77	ARG
12	2Q	18	LYS
12	2Q	22	LYS
12	2Q	54	MET
12	2Q	56	ARG
12	2Q	75	THR
12	2Q	85	LYS
12	2Q	109	VAL
12	2Q	110	THR
13	2R	67	LEU
13	2R	114	VAL
14	2S	25	ARG
14	2S	53	SER
14	2S	58	LEU
14	2S	63	THR
14	2S	75	GLU
14	2S	78	LEU
15	2T	28	VAL

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Mol	Chain	Res	Type
15	2T	107	ASP
16	2U	5	LYS
16	2U	60	LEU
16	2U	74	LEU
16	2U	77	SER
16	2U	100	VAL
16	2U	108	GLU
17	2V	7	THR
17	2V	15	GLU
17	2V	38	LEU
17	2V	52	VAL
17	2V	73	SER
17	2V	98	GLU
18	2W	11	ARG
18	2W	63	ASP
18	2W	92	ARG
19	2X	38	GLU
19	2X	45	THR
20	2Y	3	VAL
20	2Y	7	VAL
20	2Y	9	LYS
20	2Y	28	LYS
20	2Y	40	GLU
20	2Y	45	VAL
20	2Y	91	GLU
20	2Y	97	ARG
20	2Y	98	VAL
20	2Y	99	CYS
20	2Y	101	LYS
21	2Z	5	LEU
21	2Z	33	LEU
21	2Z	35	ARG
21	2Z	42	VAL
21	2Z	71	VAL
21	2Z	72	ARG
21	2Z	74	VAL
21	2Z	98	MET
21	2Z	121	HIS
21	2Z	126	VAL
21	2Z	154	ASP
21	2Z	161	VAL
21	2Z	171	ILE

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Mol	Chain	Res	Type
21	2Z	174	VAL
22	20	10	THR
22	20	11	ARG
22	20	74	ARG
23	21	35	THR
23	21	40	ARG
23	21	83	GLU
24	22	28	LYS
24	22	54	LYS
24	22	70	GLN
25	23	24	LYS
25	23	31	LEU
25	23	34	GLU
25	23	54	VAL
26	24	20	ASN
26	24	37	SER
26	24	48	ARG
26	24	50	VAL
26	24	61	ARG
27	25	6	VAL
27	25	40	LYS
28	26	6	ARG
28	26	13	CYS
28	26	19	ARG
28	26	20	ASN
28	26	34	LEU
28	26	48	VAL
29	27	24	THR
29	27	43	THR
29	27	46	VAL
30	28	14	VAL
30	28	37	SER
30	28	48	PHE
31	29	7	VAL
31	29	26	ILE
31	29	28	GLU
33	2b	7	VAL
33	2b	8	LYS
33	2b	9	GLU
33	2b	11	LEU
33	2b	16	HIS
33	2b	28	PHE

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Mol	Chain	Res	Type
33	2b	35	GLU
33	2b	49	GLU
33	2b	67	THR
33	2b	68	ILE
33	2b	71	VAL
33	2b	76	GLN
33	2b	80	ILE
33	2b	94	ASN
33	2b	107	THR
33	2b	111	ARG
33	2b	112	VAL
33	2b	138	LEU
33	2b	146	GLN
33	2b	157	ARG
33	2b	164	VAL
33	2b	168	THR
33	2b	185	ILE
33	2b	189	ASP
33	2b	195	ASP
33	2b	220	ASP
33	2b	229	VAL
34	2c	4	LYS
34	2c	15	THR
34	2c	35	GLU
34	2c	47	LEU
34	2c	57	ILE
34	2c	70	VAL
34	2c	89	GLU
34	2c	105	GLU
34	2c	120	VAL
34	2c	142	MET
34	2c	143	GLU
34	2c	152	ILE
34	2c	153	VAL
34	2c	178	LEU
34	2c	182	ILE
34	2c	191	THR
34	2c	192	THR
34	2c	207	VAL
35	2d	8	VAL
35	2d	34	GLU
35	2d	45	GLN

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Mol	Chain	Res	Type
35	2d	47	ARG
35	2d	58	LEU
35	2d	86	LYS
35	2d	98	GLU
35	2d	135	LEU
35	2d	150	GLU
35	2d	155	LEU
35	2d	156	GLU
35	2d	169	LYS
35	2d	175	SER
35	2d	188	LEU
35	2d	201	GLN
36	2e	5	ASP
36	2e	9	LYS
36	2e	13	ILE
36	2e	20	GLN
36	2e	24	ARG
36	2e	25	ARG
36	2e	31	LEU
36	2e	41	VAL
36	2e	51	VAL
36	2e	55	VAL
36	2e	66	MET
36	2e	69	VAL
36	2e	75	THR
36	2e	82	VAL
36	2e	87	SER
36	2e	90	VAL
36	2e	115	VAL
36	2e	121	LYS
36	2e	125	SER
36	2e	151	LEU
37	2f	21	LEU
37	2f	31	GLU
37	2f	63	TYR
37	2f	69	GLU
37	2f	70	ASP
37	2f	72	VAL
37	2f	81	ILE
38	2g	6	ARG
38	2g	9	VAL
38	2g	75	VAL

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Mol	Chain	Res	Type
38	2g	78	ARG
38	2g	79	ARG
38	2g	85	TYR
38	2g	146	GLU
39	2h	24	THR
39	2h	25	ASP
39	2h	39	LEU
39	2h	51	VAL
39	2h	103	VAL
39	2h	109	ILE
39	2h	112	LEU
39	2h	116	LYS
39	2h	127	LEU
39	2h	137	VAL
40	2i	17	VAL
40	2i	29	ASN
40	2i	31	GLN
40	2i	32	ASP
40	2i	54	ASP
40	2i	63	ILE
40	2i	65	VAL
40	2i	92	TYR
40	2i	99	LEU
40	2i	102	LEU
40	2i	114	TYR
40	2i	128	ARG
41	2j	13	HIS
41	2j	33	GLN
41	2j	35	SER
41	2j	46	ARG
41	2j	67	THR
41	2j	68	HIS
41	2j	74	ILE
41	2j	95	GLU
42	2k	14	VAL
42	2k	25	TYR
42	2k	28	THR
42	2k	33	THR
42	2k	57	THR
42	2k	62	GLN
42	2k	71	LYS
42	2k	107	SER

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Mol	Chain	Res	Type
43	2l	6	THR
43	2l	18	VAL
43	2l	33	ARG
43	2l	36	VAL
43	2l	40	VAL
43	2l	53	ARG
43	2l	54	LYS
43	2l	57	LYS
43	2l	62	SER
43	2l	79	GLU
43	2l	81	SER
43	2l	116	SER
44	2m	4	ILE
44	2m	11	ARG
44	2m	20	THR
44	2m	32	GLU
44	2m	44	ARG
44	2m	48	LEU
44	2m	49	THR
44	2m	73	GLU
44	2m	102	ARG
44	2m	105	THR
44	2m	106	ASN
45	2n	11	LYS
45	2n	32	SER
45	2n	33	VAL
45	2n	41	ARG
45	2n	56	VAL
46	2o	3	ILE
46	2o	76	GLU
46	2o	87	ILE
47	2p	1	MET
47	2p	2	VAL
47	2p	11	SER
47	2p	20	VAL
47	2p	21	VAL
47	2p	72	ARG
47	2p	73	LEU
48	2q	5	VAL
48	2q	53	LEU
48	2q	83	ASP
48	2q	99	SER

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Mol	Chain	Res	Type
49	2r	25	THR
49	2r	37	VAL
49	2r	63	GLN
49	2r	65	ILE
49	2r	84	LYS
50	2s	12	ASP
50	2s	20	LEU
50	2s	27	GLU
50	2s	31	ILE
50	2s	37	ARG
50	2s	41	VAL
50	2s	48	THR
50	2s	49	ILE
50	2s	79	THR
51	2t	9	ASN
51	2t	45	GLN
51	2t	53	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	48	GLN
5	1F	203	GLN
6	1G	26	GLN
6	1G	123	ASN
7	1H	74	ASN
8	1I	105	HIS
8	1I	133	HIS
9	1N	56	ASN
12	1Q	12	GLN
12	1Q	57	HIS
12	1Q	113	GLN
12	1Q	123	HIS
13	1R	50	HIS
13	1R	71	GLN
14	1S	38	GLN
14	1S	68	GLN
14	1S	84	GLN
14	1S	95	HIS
15	1T	58	ASN
15	1T	84	GLN
16	1U	81	HIS

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Mol	Chain	Res	Type
16	1U	94	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	32	HIS
21	1Z	34	ASN
24	12	65	ASN
30	18	35	GLN
33	1b	37	ASN
33	1b	45	GLN
33	1b	76	GLN
33	1b	78	GLN
33	1b	212	GLN
34	1c	6	HIS
34	1c	28	GLN
34	1c	69	HIS
34	1c	98	ASN
34	1c	104	GLN
34	1c	162	GLN
35	1d	77	ASN
35	1d	116	GLN
35	1d	123	HIS
35	1d	160	GLN
36	1e	78	HIS
37	1f	13	ASN
37	1f	18	GLN
37	1f	73	ASN
37	1f	100	ASN
38	1g	28	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	124	GLN
41	1j	56	HIS
42	1k	62	GLN
42	1k	93	GLN
42	1k	116	HIS
44	1m	92	HIS
44	1m	106	ASN
46	1o	46	HIS
47	1p	13	HIS
48	1q	93	GLN

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Mol	Chain	Res	Type
49	1r	63	GLN
50	1s	23	ASN
50	1s	47	HIS
50	1s	57	HIS
50	1s	83	HIS
51	1t	90	GLN
4	2E	48	GLN
4	2E	121	ASN
4	2E	169	ASN
4	2E	180	ASN
5	2F	69	HIS
6	2G	26	GLN
6	2G	40	ASN
8	2I	11	ASN
8	2I	139	GLN
10	2O	3	GLN
11	2P	128	HIS
12	2Q	12	GLN
13	2R	13	HIS
13	2R	24	GLN
14	2S	38	GLN
15	2T	58	ASN
15	2T	84	GLN
16	2U	94	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	32	HIS
22	20	29	GLN
22	20	35	ASN
22	20	50	ASN
24	22	9	GLN
24	22	65	ASN
25	23	32	GLN
26	24	20	ASN
33	2b	45	GLN
33	2b	94	ASN
33	2b	95	GLN
33	2b	135	GLN
33	2b	146	GLN
33	2b	212	GLN
34	2c	98	ASN
34	2c	162	GLN

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Mol	Chain	Res	Type
34	2c	181	ASN
35	2d	77	ASN
35	2d	116	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	201	GLN
36	2e	20	GLN
37	2f	73	ASN
37	2f	100	ASN
38	2g	28	ASN
38	2g	68	ASN
38	2g	86	GLN
38	2g	97	GLN
38	2g	106	GLN
38	2g	148	ASN
40	2i	3	GLN
40	2i	58	HIS
40	2i	87	GLN
41	2j	13	HIS
41	2j	33	GLN
42	2k	22	HIS
42	2k	38	ASN
42	2k	78	GLN
42	2k	104	GLN
43	2l	99	HIS
44	2m	40	ASN
47	2p	13	HIS
48	2q	26	GLN
48	2q	93	GLN
49	2r	63	GLN
50	2s	69	HIS
51	2t	18	GLN
51	2t	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	432 (15%)	27 (0%)
1	2A	2791/2915 (95%)	450 (16%)	24 (0%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	118/121 (97%)	25 (21%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	1a	1497/1521 (98%)	250 (16%)	0
32	2a	1501/1521 (98%)	276 (18%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	70/74 (94%)	25 (35%)	0
54	2w	68/74 (91%)	27 (39%)	0
55	1x	75/77 (97%)	7 (9%)	0
55	2x	75/77 (97%)	7 (9%)	0
57	1y	71/74 (95%)	28 (39%)	0
57	2y	71/74 (95%)	33 (46%)	0
All	All	9344/9612 (97%)	1576 (16%)	51 (0%)

All (1576) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	11	G
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	182	A
1	1A	196	A
1	1A	197	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	225	A
1	1A	229	A
1	1A	232	G
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(C)	C

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Mol	Chain	Res	Type
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(S)	G
1	1A	272(B)	G
1	1A	272(G)	C
1	1A	272(H)	C
1	1A	272(I)	U
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	370	G
1	1A	380	U
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	421	U
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	455	C
1	1A	456	C
1	1A	457	A
1	1A	467	G
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	512	G
1	1A	528	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G

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Mol	Chain	Res	Type
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	586	A
1	1A	587	C
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	616	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(D)	C
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	740	U
1	1A	746	A
1	1A	747	U
1	1A	764	A
1	1A	774	A
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U

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Mol	Chain	Res	Type
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	880	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	907	U
1	1A	910	A
1	1A	931	G
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	959	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1041	C
1	1A	1044	G
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A

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Mol	Chain	Res	Type
1	1A	1055	G
1	1A	1058	G
1	1A	1063	G
1	1A	1066	U
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1083	U
1	1A	1087	G
1	1A	1088	A
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1096	A
1	1A	1097	U
1	1A	1098	A
1	1A	1101	U
1	1A	1109	C
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1115	G
1	1A	1116	C
1	1A	1128	A
1	1A	1135	C
1	1A	1136	G
1	1A	1170	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1220	A
1	1A	1244	G
1	1A	1253	A

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Mol	Chain	Res	Type
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1308	A
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1370	C
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1437	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1467	C
1	1A	1482	G
1	1A	1490	A
1	1A	1493	C
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1532	C
1	1A	1543	C
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G

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Mol	Chain	Res	Type
1	1A	1582	C
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1610	A
1	1A	1647	G
1	1A	1648	C
1	1A	1654	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1756	G
1	1A	1758	G
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1828	G
1	1A	1829	A
1	1A	1847	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1927	A
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A

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Mol	Chain	Res	Type
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2093	G
1	1A	2102	U
1	1A	2113	U
1	1A	2114	A
1	1A	2116	G
1	1A	2118	U
1	1A	2119	A
1	1A	2120	G
1	1A	2121	G
1	1A	2123	G
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2147	G
1	1A	2148	G
1	1A	2150	U

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Mol	Chain	Res	Type
1	1A	2151	G
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2161	C
1	1A	2162	G
1	1A	2165	G
1	1A	2166	G
1	1A	2167	U
1	1A	2169	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2181	G
1	1A	2182	G
1	1A	2183	C
1	1A	2184	G
1	1A	2189	U
1	1A	2190	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2267	A
1	1A	2268	A
1	1A	2269	A
1	1A	2283	C
1	1A	2286	A
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C

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Mol	Chain	Res	Type
1	1A	2350	C
1	1A	2354	G
1	1A	2361	A
1	1A	2372	G
1	1A	2379	G
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2407	G
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2440	C
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2476	A
1	1A	2478	A
1	1A	2490	G
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2602	A
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2641	G
1	1A	2654	A
1	1A	2689	U
1	1A	2703	C

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Mol	Chain	Res	Type
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2757	A
1	1A	2758	A
1	1A	2764	A
1	1A	2765	A
1	1A	2766	G
1	1A	2769	C
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2805	G
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2858	C
1	1A	2872	G
1	1A	2880	C
1	1A	2893	G
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	13	A
2	1B	35	U
2	1B	45	A
2	1B	50	G
2	1B	56	G
2	1B	73	A
2	1B	84	C
2	1B	85	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	22	G
32	1a	32	A
32	1a	33	A

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Mol	Chain	Res	Type
32	1a	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	54	C
32	1a	61	G
32	1a	76	C
32	1a	78	G
32	1a	79	G
32	1a	91	C
32	1a	96	U
32	1a	97	G
32	1a	98	G
32	1a	101	A
32	1a	115	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	162	A
32	1a	163	C
32	1a	174	C
32	1a	180	U
32	1a	182	U
32	1a	189(F)	U
32	1a	189(H)	G
32	1a	195	A
32	1a	197	A
32	1a	203	U
32	1a	204	U
32	1a	222	U
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	279	A
32	1a	289	G
32	1a	306	G
32	1a	321	A
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	347	G

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Mol	Chain	Res	Type
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	480	U
32	1a	482	A
32	1a	483	C
32	1a	485	G
32	1a	493	G
32	1a	495	A
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	524	G
32	1a	531	U
32	1a	532	A
32	1a	533	A
32	1a	536	C
32	1a	547	A
32	1a	550	G

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Mol	Chain	Res	Type
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	592	G
32	1a	596	C
32	1a	627	G
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	672	U
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	695	A
32	1a	703	G
32	1a	723	U
32	1a	724	G
32	1a	731	G
32	1a	747	C
32	1a	749	C
32	1a	755	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	817	C
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	891	U
32	1a	902	G
32	1a	914	A
32	1a	922	G
32	1a	926	G
32	1a	927	G

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Mol	Chain	Res	Type
32	1a	934	C
32	1a	935	A
32	1a	942	G
32	1a	958	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	989	C
32	1a	992	U
32	1a	993	G
32	1a	996	A
32	1a	997	U
32	1a	1000	U
32	1a	1003	G
32	1a	1004	A
32	1a	1005	A
32	1a	1008	C
32	1a	1009	G
32	1a	1011	G
32	1a	1017	G
32	1a	1020	U
32	1a	1021	G
32	1a	1022	G
32	1a	1023	G
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1039	C
32	1a	1043	C
32	1a	1044	A
32	1a	1045	C

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Mol	Chain	Res	Type
32	1a	1065	U
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1123	A
32	1a	1125	U
32	1a	1127	G
32	1a	1132	C
32	1a	1134	G
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G
32	1a	1157	A
32	1a	1159	U
32	1a	1184	G
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1213	A
32	1a	1214	C
32	1a	1222	G
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1250	A
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A

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Mol	Chain	Res	Type
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1319	A
32	1a	1320	C
32	1a	1323	G
32	1a	1338	G
32	1a	1340	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1519	MA6
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	14	A
53	1v	15	A
54	1w	2	C
54	1w	5	G
54	1w	8	4SU
54	1w	9	A

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Mol	Chain	Res	Type
54	1w	14	A
54	1w	15	A
54	1w	18	G
54	1w	19	U
54	1w	21	A
54	1w	23	A
54	1w	24	A
54	1w	27	A
54	1w	45	U
54	1w	46	A
54	1w	48	C
54	1w	49	G
54	1w	50	A
54	1w	56	C
54	1w	62	C
54	1w	66	C
54	1w	67	G
54	1w	70	C
54	1w	71	G
54	1w	73	U
54	1w	74	C
55	1x	2	G
55	1x	9	G
55	1x	18	G
55	1x	19	G
55	1x	20	U
55	1x	47	U
55	1x	61	C
57	1y	4	G
57	1y	5	G
57	1y	7	G
57	1y	9	A
57	1y	14	A
57	1y	18	G
57	1y	19	U
57	1y	21	A
57	1y	33	U
57	1y	34	C
57	1y	35	C
57	1y	39	G
57	1y	41	U
57	1y	44	A

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Mol	Chain	Res	Type
57	1y	45	U
57	1y	46	A
57	1y	48	C
57	1y	49	G
57	1y	50	A
57	1y	51	G
57	1y	57	G
57	1y	58	A
57	1y	59	U
57	1y	65	U
57	1y	66	C
57	1y	69	C
57	1y	70	C
57	1y	71	G
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	140	G
1	2A	141	A
1	2A	154(A)	C
1	2A	157	U
1	2A	172	C
1	2A	173	G
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	215	G
1	2A	216	A
1	2A	222	A

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Mol	Chain	Res	Type
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	232	G
1	2A	233	A
1	2A	248	G
1	2A	250	G
1	2A	266	G
1	2A	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272	G
1	2A	272(B)	G
1	2A	274	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	312	G
1	2A	324	A
1	2A	326	G
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	396	G
1	2A	399	G
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	422	A
1	2A	443	A
1	2A	444	C
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G

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Mol	Chain	Res	Type
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	653	A
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	764	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	832	G
1	2A	847	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	867	C
1	2A	874	G
1	2A	879	G
1	2A	880	G
1	2A	882	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	892	G
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	897	C
1	2A	899	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1012	U
1	2A	1013	C

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Mol	Chain	Res	Type
1	2A	1017	G
1	2A	1020	A
1	2A	1022	G
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1117	G
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1169	G
1	2A	1170	G
1	2A	1171	G
1	2A	1188	U
1	2A	1195	G
1	2A	1211	U
1	2A	1219	G
1	2A	1220	A
1	2A	1236	G
1	2A	1240	U
1	2A	1244	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1321	A
1	2A	1342	A
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G

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Mol	Chain	Res	Type
1	2A	1370	C
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1416	G
1	2A	1417	C
1	2A	1421	G
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
1	2A	1460	A
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1478	G
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	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	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1608	A
1	2A	1609	A

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Mol	Chain	Res	Type
1	2A	1610	A
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1884	A
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A

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Mol	Chain	Res	Type
1	2A	1971	A
1	2A	1972	A
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2030	A
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	2099	U
1	2A	2102	U
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2120	G
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C

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Mol	Chain	Res	Type
1	2A	2143	C
1	2A	2145	C
1	2A	2146	C
1	2A	2148	G
1	2A	2149	G
1	2A	2150	U
1	2A	2151	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2176	A
1	2A	2178	C
1	2A	2188	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2234	G
1	2A	2238	G
1	2A	2239	G
1	2A	2268	A
1	2A	2269	A
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A

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Mol	Chain	Res	Type
1	2A	2311	A
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2329	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2406	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2460	U
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A
1	2A	2478	A
1	2A	2487	G
1	2A	2491	U
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	2529	G
1	2A	2535	G
1	2A	2549	G
1	2A	2554	U
1	2A	2555	U

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Mol	Chain	Res	Type
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2585	U
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
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	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2748	A
1	2A	2751	G
1	2A	2757	A
1	2A	2758	A
1	2A	2760	C
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
1	2A	2802	G
1	2A	2803	C
1	2A	2804	C
1	2A	2805	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G
1	2A	2880	C

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Mol	Chain	Res	Type
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	12	C
2	2B	13	A
2	2B	17	C
2	2B	19	G
2	2B	20	C
2	2B	25	A
2	2B	29	A
2	2B	34	U
2	2B	41	U
2	2B	42	C
2	2B	51	G
2	2B	53	A
2	2B	56	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	88	C
2	2B	89	G
2	2B	91	C
2	2B	108	U
2	2B	110	G
2	2B	120	A
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	52	G
32	2a	65	U
32	2a	66	G
32	2a	73	G
32	2a	80	G
32	2a	88	A
32	2a	89	C

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Mol	Chain	Res	Type
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	143	A
32	2a	144	G
32	2a	159	G
32	2a	162	A
32	2a	163	C
32	2a	182	U
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	217	C
32	2a	231	G
32	2a	247	G
32	2a	249	U
32	2a	250	A
32	2a	251	G
32	2a	266	G
32	2a	267	C
32	2a	270	A
32	2a	289	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	344	A
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C

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Mol	Chain	Res	Type
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	470	C
32	2a	471	G
32	2a	484	G
32	2a	485	G
32	2a	487	A
32	2a	496	A
32	2a	498	U
32	2a	499	A
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	545	C
32	2a	547	A
32	2a	559	A
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	597	G
32	2a	607	A
32	2a	619	U
32	2a	630	G
32	2a	653	A

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Mol	Chain	Res	Type
32	2a	665	A
32	2a	666	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	705	U
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	733	A
32	2a	749	C
32	2a	755	G
32	2a	774	G
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	834	C
32	2a	836	G
32	2a	840	C
32	2a	841	U
32	2a	853	G
32	2a	859	A
32	2a	874	G
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	933	G
32	2a	934	C
32	2a	935	A
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A

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Mol	Chain	Res	Type
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	978	A
32	2a	989	C
32	2a	991	U
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	996	A
32	2a	997	U
32	2a	999	C
32	2a	1000	U
32	2a	1001	A
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1020	U
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1030(D)	A
32	2a	1032	G
32	2a	1033	G
32	2a	1034	G
32	2a	1035	A
32	2a	1039	C
32	2a	1040	U
32	2a	1051	C

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Mol	Chain	Res	Type
32	2a	1053	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1078	U
32	2a	1079	G
32	2a	1081	G
32	2a	1086	U
32	2a	1092	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1108	G
32	2a	1109	C
32	2a	1113	C
32	2a	1122	U
32	2a	1125	U
32	2a	1126	U
32	2a	1127	G
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1135	U
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1142	G
32	2a	1147	C
32	2a	1152	A
32	2a	1154	G
32	2a	1157	A
32	2a	1159	U
32	2a	1172	C
32	2a	1181	G
32	2a	1182	G
32	2a	1184	G
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G

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Mol	Chain	Res	Type
32	2a	1211	U
32	2a	1213	A
32	2a	1227	A
32	2a	1228	C
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1255	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1261	A
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1277	C
32	2a	1279	A
32	2a	1280	A
32	2a	1286	A
32	2a	1287	A
32	2a	1299	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1312	G
32	2a	1320	C
32	2a	1323	G
32	2a	1346	A
32	2a	1347	G
32	2a	1358	U
32	2a	1363	C
32	2a	1364	U
32	2a	1368	G
32	2a	1398	A
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A

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Mol	Chain	Res	Type
32	2a	1497	G
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	14	A
53	2v	15	A
54	2w	6	C
54	2w	8	4SU
54	2w	9	A
54	2w	10	G
54	2w	12	U
54	2w	13	C
54	2w	14	A
54	2w	18	G
54	2w	22	G
54	2w	23	A
54	2w	24	A
54	2w	25	C
54	2w	26	G
54	2w	36	C
54	2w	46	A
54	2w	48	C
54	2w	49	G
54	2w	50	A
54	2w	56	C
54	2w	57	G
54	2w	61	C
54	2w	62	C
54	2w	64	U
54	2w	69	C
54	2w	70	C
54	2w	72	C
54	2w	74	C
55	2x	3	C
55	2x	9	G
55	2x	19	G

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Mol	Chain	Res	Type
55	2x	20	U
55	2x	21	A
55	2x	47	U
55	2x	48	C
57	2y	4	G
57	2y	5	G
57	2y	7	G
57	2y	8	4SU
57	2y	9	A
57	2y	15	A
57	2y	18	G
57	2y	19	U
57	2y	21	A
57	2y	22	G
57	2y	26	G
57	2y	27	A
57	2y	33	U
57	2y	34	C
57	2y	37	A
57	2y	45	U
57	2y	46	A
57	2y	48	C
57	2y	49	G
57	2y	52	G
57	2y	53	G
57	2y	55	PSU
57	2y	57	G
57	2y	58	A
57	2y	59	U
57	2y	60	U
57	2y	61	C
57	2y	66	C
57	2y	67	G
57	2y	69	C
57	2y	70	C
57	2y	73	U
57	2y	75	C

All (51) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A

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Mol	Chain	Res	Type
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	746	A
1	1A	774	A
1	1A	974	G
1	1A	1067	A
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1176	G
1	1A	1379	A
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1762	A
1	1A	1992	G
1	1A	2126	A
1	1A	2134	A
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2439	A
1	1A	2629	A
1	1A	2756	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1530	C
1	2A	1913	A

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Mol	Chain	Res	Type
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2156	G
1	2A	2406	U
1	2A	2439	A
1	2A	2689	U
1	2A	2756	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
55	5MC	2x	32	55	19,22,23	1.62	3 (15%)	26,32,35	1.22	3 (11%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	2.18	5 (23%)
55	5MC	1x	32	55	19,22,23	1.66	3 (15%)	26,32,35	1.26	3 (11%)
1	OMG	1A	2251	1,58,55	23,26,27	1.26	3 (13%)	32,38,41	1.88	6 (18%)
32	G7M	1a	527	58,32	23,26,27	1.55	3 (13%)	34,39,42	1.66	5 (14%)
55	4SU	2x	8	55	18,21,22	2.00	7 (38%)	25,30,33	1.43	4 (16%)
1	OMG	2A	2251	1,55	23,26,27	1.22	3 (13%)	32,38,41	2.08	6 (18%)
54	4SU	2w	8	54	18,21,22	1.83	5 (27%)	25,30,33	2.90	6 (24%)
55	4SU	1x	8	55	18,21,22	2.37	5 (27%)	25,30,33	1.86	6 (24%)
1	5MC	2A	1942	1	19,22,23	1.59	3 (15%)	26,32,35	1.07	2 (7%)
54	PSU	2w	55	58,54	18,21,22	1.37	2 (11%)	21,30,33	2.06	3 (14%)
55	5MU	1x	54	55	19,22,23	1.45	6 (31%)	27,32,35	1.89	5 (18%)
57	4SU	2y	8	57	18,21,22	1.73	5 (27%)	25,30,33	2.06	5 (20%)
1	PSU	1A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	2.03	4 (19%)
57	5MU	2y	54	57	19,22,23	1.49	5 (26%)	27,32,35	1.88	8 (29%)
1	PSU	2A	1917	1	18,21,22	1.38	2 (11%)	21,30,33	2.09	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	UR3	1a	1498	32	19,22,23	1.00	1 (5%)	26,32,35	1.67	3 (11%)
54	5MU	1w	54	54	19,22,23	1.39	4 (21%)	27,32,35	1.97	7 (25%)
57	4SU	1y	8	57	18,21,22	1.78	5 (27%)	25,30,33	1.74	4 (16%)
1	PSU	2A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	1.94	3 (14%)
1	PSU	2A	2605	1	18,21,22	1.34	3 (16%)	21,30,33	2.25	5 (23%)
57	5MU	1y	54	57	19,22,23	1.43	5 (26%)	27,32,35	2.01	6 (22%)
32	2MG	1a	1207	58,32	23,26,27	1.24	3 (13%)	33,38,41	2.20	7 (21%)
32	5MC	2a	1400	32	19,22,23	1.77	3 (15%)	26,32,35	1.18	3 (11%)
32	5MC	1a	1407	32	19,22,23	1.73	3 (15%)	26,32,35	1.11	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	0.95	1 (4%)
55	PSU	1x	55	58,55	18,21,22	1.33	2 (11%)	21,30,33	2.13	4 (19%)
32	PSU	1a	516	32	18,21,22	1.38	2 (11%)	21,30,33	2.06	4 (19%)
32	MA6	1a	1519	32	23,26,27	0.43	0	33,38,41	2.05	9 (27%)
32	5MC	1a	1400	32	19,22,23	1.66	3 (15%)	26,32,35	1.13	3 (11%)
32	4OC	2a	1402	58,32	20,23,24	0.77	0	25,32,35	0.96	2 (8%)
32	MA6	2a	1519	32	23,26,27	0.44	0	33,38,41	2.10	10 (30%)
54	4SU	1w	8	54	18,21,22	1.75	4 (22%)	25,30,33	2.24	5 (20%)
56	FME	1z	1	56	8,9,10	1.01	0	8,9,11	0.93	0
43	0TD	2l	92	43	8,9,10	4.73	2 (25%)	6,11,13	3.35	2 (33%)
32	5MC	2a	967	32	19,22,23	1.66	3 (15%)	26,32,35	1.14	3 (11%)
32	UR3	2a	1498	32	19,22,23	1.01	1 (5%)	26,32,35	1.73	4 (15%)
32	5MC	2a	1407	32	19,22,23	1.58	3 (15%)	26,32,35	1.24	3 (11%)
1	OMC	2A	1920	1	19,22,23	0.79	0	25,31,34	0.93	1 (4%)
1	PSU	1A	2605	1,58	18,21,22	1.36	3 (16%)	21,30,33	2.08	4 (19%)
43	0TD	1l	92	43	8,9,10	4.56	1 (12%)	6,11,13	4.49	2 (33%)
32	2MG	2a	1207	58,32	23,26,27	1.23	2 (8%)	33,38,41	2.21	7 (21%)
1	OMU	2A	2552	1,58	19,22,23	1.23	3 (15%)	25,31,34	1.87	5 (20%)
57	PSU	2y	55	57	18,21,22	1.42	2 (11%)	21,30,33	2.04	3 (14%)
32	M2G	1a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.87	6 (18%)
1	OMC	1A	1920	1	19,22,23	0.80	0	25,31,34	1.04	1 (4%)
1	2MA	1A	2503	1,58	22,25,26	1.44	4 (18%)	32,37,40	2.27	9 (28%)
32	M2G	2a	966	32	24,27,28	1.28	3 (12%)	33,40,43	1.89	6 (18%)
55	8AN	1x	76	56,58,55	21,24,25	1.42	3 (14%)	26,35,38	2.29	11 (42%)
1	2MA	2A	2503	1,58	22,25,26	1.53	5 (22%)	32,37,40	2.39	7 (21%)
1	5MC	1A	1942	1	19,22,23	1.75	3 (15%)	26,32,35	1.22	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	1A	1939	1,58	19,22,23	1.52	6 (31%)	27,32,35	2.02	5 (18%)
1	5MC	1A	1962	1,58	19,22,23	1.71	3 (15%)	26,32,35	1.16	3 (11%)
32	MA6	1a	1518	32	23,26,27	0.40	0	33,38,41	1.99	10 (30%)
1	5MU	2A	1939	1,58	19,22,23	1.42	5 (26%)	27,32,35	2.37	6 (22%)
32	5MC	1a	1404	32	19,22,23	1.61	3 (15%)	26,32,35	1.17	3 (11%)
32	G7M	2a	527	58,32	23,26,27	1.51	4 (17%)	34,39,42	1.66	4 (11%)
1	5MU	1A	1915	1	19,22,23	1.42	4 (21%)	27,32,35	2.06	7 (25%)
1	PSU	1A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	1.97	5 (23%)
1	5MC	2A	1962	1,58	19,22,23	1.69	3 (15%)	26,32,35	1.18	2 (7%)
54	L3X	1w	76	1,54	24,28,29	1.55	4 (16%)	27,40,43	1.74	4 (14%)
32	5MC	2a	1404	32	19,22,23	1.67	3 (15%)	26,32,35	1.17	3 (11%)
54	5MU	2w	54	54	19,22,23	1.40	4 (21%)	27,32,35	1.68	6 (22%)
55	5MU	2x	54	55	19,22,23	1.42	5 (26%)	27,32,35	1.97	6 (22%)
57	PSU	1y	55	57	18,21,22	1.39	2 (11%)	21,30,33	2.04	3 (14%)
56	FME	2z	1	56	8,9,10	1.00	0	8,9,11	0.97	1 (12%)
1	5MU	2A	1915	1	19,22,23	1.41	5 (26%)	27,32,35	2.17	7 (25%)
54	PSU	1w	55	58,54	18,21,22	1.44	2 (11%)	21,30,33	2.06	4 (19%)
55	8AN	2x	76	56,58,55	21,24,25	1.44	3 (14%)	26,35,38	2.34	10 (38%)
55	PSU	2x	55	55	18,21,22	1.37	2 (11%)	21,30,33	2.05	4 (19%)
32	MA6	2a	1518	32	23,26,27	0.43	0	33,38,41	1.97	9 (27%)
1	OMU	1A	2552	1,58	19,22,23	1.22	3 (15%)	25,31,34	1.89	6 (24%)
32	5MC	1a	967	32	19,22,23	1.68	3 (15%)	26,32,35	1.15	2 (7%)
54	L3X	2w	76	1,54,60	24,28,29	1.41	3 (12%)	27,40,43	2.11	9 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,58,55	-	0/9/27/28	0/3/3/3
32	G7M	1a	527	58,32	-	2/7/25/26	0/3/3/3
55	4SU	2x	8	55	-	1/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	58,54	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
57	4SU	2y	8	57	-	2/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
57	5MU	2y	54	57	-	3/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
57	4SU	1y	8	57	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
57	5MU	1y	54	57	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	58,32	-	1/9/27/28	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
55	PSU	1x	55	58,55	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	58,32	-	2/9/29/30	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
56	FME	1z	1	56	-	3/7/9/11	-
43	0TD	2l	92	43	-	3/7/12/14	-
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
1	PSU	1A	2605	1,58	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
32	2MG	2a	1207	58,32	-	1/9/27/28	0/3/3/3
1	OMU	2A	2552	1,58	-	0/9/27/28	0/2/2/2
57	PSU	2y	55	57	-	3/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	2MA	1A	2503	1,58	-	2/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
55	8AN	1x	76	56,58,55	-	3/7/25/26	0/3/3/3
1	2MA	2A	2503	1,58	-	1/7/25/26	0/3/3/3
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,58	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,58	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	5MU	2A	1939	1,58	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	58,32	-	2/7/25/26	0/3/3/3
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,58	-	0/7/25/26	0/2/2/2
54	L3X	1w	76	1,54	-	0/13/31/32	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
57	PSU	1y	55	57	-	2/7/25/26	0/2/2/2
56	FME	2z	1	56	-	0/7/9/11	-
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	58,54	-	0/7/25/26	0/2/2/2
55	8AN	2x	76	56,58,55	-	3/7/25/26	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
1	OMU	1A	2552	1,58	-	0/9/27/28	0/2/2/2
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
54	L3X	2w	76	1,54,60	-	2/13/31/32	0/3/3/3

All (210) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.83	1.69	1.82
43	1l	92	0TD	CB-SB	-12.51	1.69	1.82
32	2a	1400	5MC	C5-C4	6.58	1.49	1.44
1	1A	1942	5MC	C5-C4	6.44	1.49	1.44
32	1a	1407	5MC	C5-C4	6.34	1.48	1.44
1	1A	1962	5MC	C5-C4	6.34	1.48	1.44
1	2A	1962	5MC	C5-C4	6.14	1.48	1.44
32	2a	967	5MC	C5-C4	6.11	1.48	1.44
32	1a	967	5MC	C5-C4	6.04	1.48	1.44
32	1a	1400	5MC	C5-C4	6.00	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1404	5MC	C5-C4	5.96	1.48	1.44
55	1x	8	4SU	C4-N3	-5.93	1.31	1.37
55	1x	32	5MC	C5-C4	5.78	1.48	1.44
32	1a	1404	5MC	C5-C4	5.75	1.48	1.44
55	2x	32	5MC	C5-C4	5.66	1.48	1.44
32	2a	1407	5MC	C5-C4	5.61	1.48	1.44
1	2A	1942	5MC	C5-C4	5.55	1.48	1.44
54	2w	8	4SU	C4-S4	-4.99	1.59	1.68
55	1x	8	4SU	C4-S4	-4.92	1.60	1.68
32	1a	527	G7M	C5-N7	-4.88	1.33	1.39
54	1w	8	4SU	C4-S4	-4.78	1.60	1.68
57	2y	8	4SU	C4-S4	-4.69	1.60	1.68
57	1y	8	4SU	C4-S4	-4.61	1.60	1.68
55	2x	8	4SU	C4-S4	-4.50	1.60	1.68
1	2A	2503	2MA	C5-C4	4.48	1.47	1.39
55	2x	8	4SU	C4-N3	-4.42	1.33	1.37
54	1w	76	L3X	C5-C4	-4.34	1.31	1.39
1	1A	2503	2MA	C5-C4	4.28	1.46	1.39
57	2y	55	PSU	C6-C5	4.23	1.40	1.35
32	2a	527	G7M	C5-N7	-4.21	1.34	1.39
54	1w	76	L3X	C5-N7	-4.20	1.31	1.39
54	1w	55	PSU	C6-C5	4.13	1.39	1.35
55	1x	8	4SU	C2-N3	-4.05	1.30	1.38
57	1y	55	PSU	C6-C5	3.98	1.39	1.35
55	2x	76	8AN	C5-N7	-3.95	1.31	1.39
54	2w	76	L3X	C5-N7	-3.92	1.31	1.39
54	2w	55	PSU	C6-C5	3.83	1.39	1.35
55	1x	76	8AN	C5-N7	-3.80	1.32	1.39
32	1a	516	PSU	C6-C5	3.78	1.39	1.35
55	2x	55	PSU	C6-C5	3.67	1.39	1.35
1	2A	1911	PSU	C6-C5	3.66	1.39	1.35
1	2A	1917	PSU	C6-C5	3.55	1.39	1.35
1	1A	1911	PSU	C6-C5	3.51	1.39	1.35
55	1x	8	4SU	C5-C4	-3.51	1.38	1.42
55	1x	55	PSU	C6-C5	3.46	1.39	1.35
32	2a	516	PSU	C6-C5	3.34	1.39	1.35
32	2a	527	G7M	C5-C4	3.33	1.46	1.38
32	2a	1207	2MG	C5-C4	3.28	1.47	1.38
1	1A	1917	PSU	C6-C5	3.27	1.38	1.35
54	2w	8	4SU	C2-N1	3.21	1.43	1.38
32	2a	1404	5MC	C6-C5	3.21	1.39	1.34
57	1y	8	4SU	C4-N3	-3.20	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	527	G7M	C5-C4	3.17	1.46	1.38
32	1a	1207	2MG	C5-C4	3.14	1.47	1.38
54	2w	76	L3X	C5-C4	-3.13	1.33	1.39
32	1a	966	M2G	C5-C4	3.13	1.47	1.38
1	2A	2605	PSU	C6-C5	3.12	1.38	1.35
1	2A	2251	OMG	C5-C4	3.08	1.47	1.38
55	1x	76	8AN	C5-C4	-3.05	1.33	1.39
55	2x	76	8AN	C5-C4	-3.04	1.33	1.39
1	1A	1939	5MU	C4-N3	-3.04	1.33	1.38
55	1x	76	8AN	C5-C6	-3.03	1.32	1.41
1	2A	1939	5MU	C6-C5	3.00	1.39	1.34
1	1A	2605	PSU	C4-N3	-2.98	1.33	1.38
32	2a	966	M2G	C5-C4	2.98	1.46	1.38
1	1A	2251	OMG	C5-C4	2.98	1.46	1.38
1	2A	1942	5MC	C6-C5	2.97	1.39	1.34
55	2x	8	4SU	C5-C4	-2.95	1.39	1.42
55	1x	32	5MC	C6-C5	2.95	1.39	1.34
57	2y	54	5MU	C6-C5	2.95	1.39	1.34
55	2x	8	4SU	C2-N3	-2.94	1.32	1.38
32	1a	1407	5MC	C6-C5	2.93	1.39	1.34
32	1a	967	5MC	C6-C5	2.92	1.39	1.34
55	2x	54	5MU	C6-C5	2.92	1.39	1.34
55	1x	54	5MU	C6-C5	2.92	1.39	1.34
1	1A	2251	OMG	C6-N1	-2.88	1.33	1.38
57	1y	54	5MU	C6-C5	2.87	1.39	1.34
55	2x	32	5MC	C6-C5	2.87	1.39	1.34
1	1A	1915	5MU	C6-C5	2.86	1.39	1.34
54	1w	8	4SU	C5-C4	-2.86	1.39	1.42
1	2A	1939	5MU	C4-N3	-2.84	1.33	1.38
1	1A	1939	5MU	C6-C5	2.84	1.39	1.34
32	2a	966	M2G	C2-N2	2.84	1.40	1.35
57	2y	8	4SU	C4-N3	-2.81	1.34	1.37
32	1a	1400	5MC	C6-C5	2.80	1.39	1.34
1	2A	1915	5MU	C6-C5	2.80	1.39	1.34
55	1x	54	5MU	C4-N3	-2.80	1.33	1.38
1	1A	1942	5MC	C6-C5	2.77	1.39	1.34
1	1A	1962	5MC	C6-C5	2.77	1.39	1.34
1	1A	1915	5MU	C2-N1	2.75	1.42	1.38
57	2y	54	5MU	C2-N1	2.74	1.42	1.38
54	2w	54	5MU	C6-C5	2.74	1.39	1.34
54	2w	8	4SU	C5-C4	-2.70	1.39	1.42
32	2a	1400	5MC	C6-C5	2.69	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2605	PSU	C4-N3	-2.68	1.33	1.38
54	1w	54	5MU	C6-C5	2.67	1.39	1.34
57	2y	54	5MU	C4-N3	-2.67	1.33	1.38
32	1a	966	M2G	C2-N2	2.64	1.40	1.35
55	2x	76	8AN	C5-C6	-2.64	1.33	1.41
1	1A	1917	PSU	C4-N3	-2.64	1.33	1.38
32	2a	1407	5MC	C6-C5	2.64	1.38	1.34
1	2A	2503	2MA	C5-N7	-2.63	1.34	1.39
1	2A	1917	PSU	C4-N3	-2.63	1.33	1.38
54	1w	54	5MU	C2-N1	2.63	1.42	1.38
1	1A	1911	PSU	C4-N3	-2.63	1.33	1.38
54	2w	8	4SU	O2-C2	2.61	1.27	1.23
1	1A	1939	5MU	C4-C5	2.60	1.49	1.44
1	2A	1962	5MC	C6-C5	2.58	1.38	1.34
32	1a	1404	5MC	C6-C5	2.57	1.38	1.34
1	1A	2251	OMG	C5-N7	-2.56	1.33	1.39
1	1A	2605	PSU	C6-C5	2.55	1.38	1.35
32	1a	516	PSU	C4-N3	-2.55	1.34	1.38
57	2y	8	4SU	C5-C4	-2.55	1.39	1.42
54	1w	54	5MU	C4-C5	2.55	1.49	1.44
32	1a	966	M2G	C6-N1	-2.55	1.34	1.38
32	2a	527	G7M	C6-N1	-2.54	1.34	1.38
55	2x	54	5MU	C4-N3	-2.53	1.34	1.38
1	2A	2552	OMU	C4-N3	-2.53	1.34	1.38
32	2a	967	5MC	C6-C5	2.52	1.38	1.34
57	1y	54	5MU	C4-C5	2.51	1.48	1.44
54	2w	54	5MU	C2-N1	2.51	1.42	1.38
54	2w	76	L3X	C5-C6	-2.50	1.34	1.41
1	2A	1911	PSU	C4-N3	-2.50	1.34	1.38
32	2a	516	PSU	C4-N3	-2.49	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.49	1.33	1.38
1	2A	1915	5MU	C4-C5	2.48	1.48	1.44
32	1a	527	G7M	C6-N1	-2.48	1.34	1.38
57	2y	54	5MU	C4-C5	2.47	1.48	1.44
1	1A	1915	5MU	C4-N3	-2.47	1.34	1.38
1	2A	1915	5MU	C2-N1	2.46	1.42	1.38
54	1w	8	4SU	C4-N3	-2.46	1.35	1.37
57	1y	54	5MU	C2-N1	2.46	1.42	1.38
32	2a	966	M2G	C6-N1	-2.45	1.34	1.38
54	1w	55	PSU	C4-N3	-2.44	1.34	1.38
54	1w	8	4SU	C2-N1	2.44	1.42	1.38
1	2A	2251	OMG	C5-N7	-2.44	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2552	OMU	C4-N3	-2.43	1.34	1.38
1	2A	2251	OMG	C6-N1	-2.43	1.34	1.38
55	2x	54	5MU	C4-C5	2.43	1.48	1.44
54	2w	54	5MU	C4-N3	-2.43	1.34	1.38
1	2A	2503	2MA	C5-C6	2.43	1.47	1.41
1	1A	1942	5MC	C6-N1	-2.43	1.33	1.38
1	2A	1915	5MU	C4-N3	-2.42	1.34	1.38
55	1x	54	5MU	C2-N1	2.41	1.42	1.38
1	2A	1939	5MU	C2-N3	-2.41	1.33	1.38
55	2x	55	PSU	C4-N3	-2.41	1.34	1.38
57	1y	54	5MU	C4-N3	-2.40	1.34	1.38
54	2w	55	PSU	C4-N3	-2.39	1.34	1.38
54	2w	54	5MU	C4-C5	2.39	1.48	1.44
32	1a	1404	5MC	C6-N1	-2.37	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.36	1.34	1.38
57	1y	8	4SU	C5-C4	-2.36	1.39	1.42
1	1A	1939	5MU	C2-N3	-2.35	1.33	1.38
1	1A	1939	5MU	C6-N1	-2.35	1.34	1.38
1	1A	1915	5MU	C4-C5	2.34	1.48	1.44
1	1A	2503	2MA	C5-C6	2.34	1.47	1.41
32	1a	1207	2MG	C6-N1	-2.34	1.34	1.38
55	1x	8	4SU	O2-C2	2.34	1.27	1.23
55	1x	55	PSU	C4-N3	-2.34	1.34	1.38
1	2A	1939	5MU	C4-C5	2.34	1.48	1.44
57	1y	55	PSU	C4-N3	-2.33	1.34	1.38
55	2x	54	5MU	C2-N1	2.33	1.42	1.38
55	1x	32	5MC	C6-N1	-2.33	1.34	1.38
57	2y	55	PSU	C4-N3	-2.32	1.34	1.38
1	1A	1939	5MU	C2-N1	2.31	1.42	1.38
54	1w	54	5MU	C4-N3	-2.28	1.34	1.38
1	2A	2552	OMU	C5-C4	2.26	1.48	1.43
57	2y	8	4SU	C2-N1	2.25	1.42	1.38
32	1a	1400	5MC	C6-N1	-2.24	1.34	1.38
57	1y	8	4SU	C2-N1	2.23	1.42	1.38
32	1a	967	5MC	C6-N1	-2.23	1.34	1.38
1	1A	2503	2MA	C5-N7	-2.23	1.35	1.39
43	2l	92	0TD	CB-CA	2.22	1.55	1.54
54	2w	8	4SU	C4-N3	-2.22	1.35	1.37
1	1A	1962	5MC	C6-N1	-2.20	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.20	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.18	1.34	1.38
32	2a	527	G7M	C5-C6	2.17	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	967	5MC	C6-N1	-2.16	1.34	1.38
57	1y	8	4SU	C2-N3	-2.16	1.34	1.38
32	1a	1498	UR3	C2-N1	2.16	1.41	1.38
57	2y	54	5MU	C2-N3	-2.15	1.34	1.38
55	1x	54	5MU	C4-C5	2.15	1.48	1.44
32	1a	966	M2G	C5-N7	-2.14	1.34	1.39
1	2A	1942	5MC	C6-N1	-2.14	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.14	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.14	1.34	1.38
1	2A	2503	2MA	C4-N9	-2.13	1.33	1.37
1	1A	2503	2MA	C8-N7	2.13	1.35	1.31
1	1A	2605	PSU	C2-N3	-2.12	1.34	1.37
1	2A	1939	5MU	C6-N1	-2.11	1.34	1.38
57	1y	54	5MU	C6-N1	-2.11	1.34	1.38
1	1A	2552	OMU	C2-N3	-2.11	1.34	1.38
55	2x	32	5MC	C6-N1	-2.07	1.34	1.38
57	2y	8	4SU	C2-N3	-2.07	1.34	1.38
54	1w	76	L3X	O4'-C1'	2.07	1.46	1.42
1	1A	2552	OMU	C5-C4	2.06	1.48	1.43
55	2x	54	5MU	C2-N3	-2.06	1.34	1.38
55	1x	54	5MU	C2-N3	-2.06	1.34	1.38
55	2x	8	4SU	C6-C5	2.06	1.39	1.35
1	2A	2605	PSU	C2-N3	-2.04	1.34	1.37
55	1x	54	5MU	C6-N1	-2.04	1.34	1.38
32	1a	1207	2MG	C5-N7	-2.04	1.35	1.39
54	1w	76	L3X	C8-N9	-2.03	1.34	1.37
55	2x	8	4SU	C2-N1	2.02	1.41	1.38
1	2A	2552	OMU	C2-N3	-2.01	1.34	1.38
32	1a	1407	5MC	C6-N1	-2.01	1.34	1.38
55	2x	8	4SU	O2-C2	2.01	1.26	1.23
32	2a	1498	UR3	C2-N1	2.01	1.41	1.38
1	2A	2503	2MA	C8-N7	2.00	1.35	1.31

All (349) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-10.38	83.71	102.36
54	2w	8	4SU	C4-N3-C2	-8.61	119.06	127.31
1	2A	2503	2MA	C5-C4-N3	-8.32	118.42	127.18
1	1A	2503	2MA	C5-C4-N3	-7.60	119.18	127.18
43	2l	92	0TD	CSB-SB-CB	-7.26	89.32	102.36
54	2w	8	4SU	C5-C4-N3	7.04	121.30	114.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2503	2MA	N3-C4-N9	7.00	135.88	126.99
32	2a	1207	2MG	C2-N3-C4	6.95	120.69	112.00
1	2A	2605	PSU	N1-C2-N3	6.94	122.49	115.17
32	1a	1207	2MG	C2-N3-C4	6.90	120.64	112.00
32	2a	516	PSU	N1-C2-N3	6.81	122.35	115.17
54	2w	8	4SU	C5-C4-S4	-6.77	116.57	124.31
1	2A	1917	PSU	N1-C2-N3	6.65	122.19	115.17
32	2a	1498	UR3	C4-N3-C2	-6.64	119.23	124.58
32	1a	1498	UR3	C4-N3-C2	-6.61	119.26	124.58
55	2x	55	PSU	N1-C2-N3	6.51	122.03	115.17
32	1a	516	PSU	N1-C2-N3	6.43	121.95	115.17
1	1A	2503	2MA	N3-C4-N9	6.42	135.14	126.99
55	1x	55	PSU	N1-C2-N3	6.39	121.91	115.17
54	2w	55	PSU	N1-C2-N3	6.34	121.86	115.17
1	2A	2251	OMG	C5-C4-N3	-6.34	118.31	128.39
54	1w	8	4SU	C4-N3-C2	-6.32	121.25	127.31
57	1y	55	PSU	N1-C2-N3	6.31	121.82	115.17
54	1w	55	PSU	N1-C2-N3	6.29	121.80	115.17
32	1a	966	M2G	C5-C4-N3	-6.27	118.41	128.39
57	2y	55	PSU	N1-C2-N3	6.22	121.73	115.17
1	1A	1911	PSU	N1-C2-N3	6.20	121.71	115.17
1	1A	1917	PSU	N1-C2-N3	6.18	121.68	115.17
1	1A	2605	PSU	N1-C2-N3	6.17	121.68	115.17
1	2A	1911	PSU	N1-C2-N3	6.13	121.64	115.17
32	2a	966	M2G	C5-C4-N3	-6.02	118.82	128.39
1	2A	1939	5MU	C4-N3-C2	-5.95	119.53	127.34
32	1a	1207	2MG	C5-C4-N3	-5.93	118.95	128.39
1	2A	1939	5MU	N3-C2-N1	5.91	122.58	114.89
54	1w	8	4SU	C5-C4-N3	5.74	120.09	114.75
32	2a	1207	2MG	C5-C4-N3	-5.74	119.26	128.39
57	2y	8	4SU	C4-N3-C2	-5.73	121.82	127.31
54	2w	76	L3X	N1-C2-N3	-5.71	119.94	128.58
1	1A	2251	OMG	C5-C4-N3	-5.69	119.33	128.39
55	2x	76	8AN	N1-C2-N3	-5.68	119.99	128.58
54	1w	76	L3X	N1-C2-N3	-5.62	120.07	128.58
57	2y	8	4SU	C5-C4-N3	5.38	119.75	114.75
55	1x	76	8AN	N1-C2-N3	-5.36	120.47	128.58
1	2A	2251	OMG	N9-C4-N3	5.31	136.57	125.95
32	2a	527	G7M	C5-C4-N3	-5.26	118.21	128.15
32	2a	527	G7M	N9-C4-N3	5.26	136.47	125.95
1	1A	1915	5MU	N3-C2-N1	5.20	121.66	114.89
32	1a	527	G7M	N9-C4-N3	5.19	136.32	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1915	5MU	C4-N3-C2	-5.15	120.58	127.34
32	1a	527	G7M	C5-C4-N3	-5.10	118.51	128.15
1	1A	2552	OMU	N3-C2-N1	5.04	121.46	114.89
1	2A	2552	OMU	N3-C2-N1	5.03	121.44	114.89
57	1y	8	4SU	C5-C4-N3	5.03	119.43	114.75
1	2A	2251	OMG	C2-N3-C4	5.02	120.95	112.30
55	1x	76	8AN	C5-C4-N3	-5.01	119.82	126.72
1	2A	1915	5MU	C5-C4-N3	4.97	119.64	115.32
1	2A	2605	PSU	C4-N3-C2	-4.96	119.54	126.37
1	2A	1939	5MU	C5-C4-N3	4.95	119.62	115.32
54	2w	76	L3X	C5-C4-N3	-4.94	119.92	126.72
32	2a	1519	MA6	N1-C2-N3	-4.87	121.20	128.58
1	1A	1939	5MU	C4-N3-C2	-4.87	120.96	127.34
57	1y	54	5MU	N3-C2-N1	4.85	121.21	114.89
32	1a	1518	MA6	N1-C2-N3	-4.85	121.24	128.58
55	2x	76	8AN	C5-C4-N3	-4.85	120.04	126.72
57	1y	54	5MU	C4-N3-C2	-4.84	120.99	127.34
1	1A	2552	OMU	C4-N3-C2	-4.84	120.61	126.61
1	1A	1915	5MU	C4-N3-C2	-4.83	121.01	127.34
32	1a	1519	MA6	N1-C2-N3	-4.80	121.31	128.58
55	1x	8	4SU	C6-C5-C4	-4.79	115.80	119.95
54	1w	8	4SU	C5-C4-S4	-4.78	118.84	124.31
55	2x	54	5MU	N3-C2-N1	4.76	121.09	114.89
57	1y	8	4SU	C4-N3-C2	-4.74	122.77	127.31
54	1w	54	5MU	N3-C2-N1	4.73	121.05	114.89
32	1a	966	M2G	N9-C4-N3	4.73	135.40	125.95
32	2a	1518	MA6	C5-C4-N3	-4.70	120.24	126.72
1	2A	1915	5MU	N3-C2-N1	4.70	121.01	114.89
1	2A	1915	5MU	O4-C4-C5	-4.66	119.59	124.92
32	2a	1519	MA6	C5-C4-N3	-4.64	120.32	126.72
32	2a	527	G7M	C2-N3-C4	4.63	120.27	112.30
54	1w	54	5MU	C4-N3-C2	-4.62	121.28	127.34
1	1A	2251	OMG	N9-C4-N3	4.61	135.17	125.95
55	2x	54	5MU	C4-N3-C2	-4.58	121.33	127.34
1	1A	2605	PSU	C4-N3-C2	-4.57	120.08	126.37
1	2A	1939	5MU	C5-C6-N1	-4.56	118.36	123.31
32	2a	966	M2G	C2-N3-C4	4.54	120.91	112.51
1	1A	2251	OMG	C2-N3-C4	4.54	120.12	112.30
1	2A	2552	OMU	C4-N3-C2	-4.54	120.98	126.61
1	1A	1939	5MU	C5-C4-N3	4.53	119.26	115.32
1	1A	1939	5MU	N3-C2-N1	4.52	120.77	114.89
32	1a	527	G7M	C2-N3-C4	4.47	120.00	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1939	5MU	C5-C6-N1	-4.43	118.50	123.31
32	2a	966	M2G	N9-C4-N3	4.40	134.74	125.95
32	1a	966	M2G	C2-N3-C4	4.38	120.62	112.51
32	1a	1519	MA6	C5-C4-N3	-4.34	120.74	126.72
32	2a	1518	MA6	N1-C2-N3	-4.33	122.02	128.58
57	2y	54	5MU	N3-C2-N1	4.32	120.52	114.89
55	1x	55	PSU	C4-N3-C2	-4.30	120.44	126.37
32	2a	516	PSU	C4-N3-C2	-4.29	120.45	126.37
55	1x	54	5MU	C4-N3-C2	-4.29	121.71	127.34
55	1x	54	5MU	N3-C2-N1	4.29	120.48	114.89
32	1a	516	PSU	C4-N3-C2	-4.27	120.49	126.37
57	2y	54	5MU	C5-C4-N3	4.23	119.00	115.32
32	2a	516	PSU	O2-C2-N1	-4.22	118.43	122.79
57	1y	55	PSU	O2-C2-N1	-4.22	118.44	122.79
1	1A	1917	PSU	C4-N3-C2	-4.21	120.57	126.37
1	2A	1917	PSU	C4-N3-C2	-4.21	120.58	126.37
57	2y	54	5MU	C4-N3-C2	-4.12	121.94	127.34
32	1a	1518	MA6	C2-N1-C6	4.12	121.89	111.83
32	2a	1519	MA6	C4-C5-N7	-4.12	105.88	110.58
54	1w	54	5MU	O4-C4-C5	-4.11	120.21	124.92
1	2A	2503	2MA	N6-C6-N1	4.10	122.56	117.03
57	1y	54	5MU	C5-C4-N3	4.10	118.88	115.32
55	1x	54	5MU	C5-C4-N3	4.09	118.88	115.32
1	1A	1915	5MU	C5-C4-N3	4.09	118.88	115.32
54	2w	55	PSU	C4-N3-C2	-4.08	120.75	126.37
1	2A	1939	5MU	O4-C4-C5	-4.07	120.26	124.92
55	2x	54	5MU	C5-C4-N3	4.07	118.86	115.32
32	1a	1519	MA6	C2-N1-C6	4.06	121.75	111.83
1	1A	1911	PSU	C4-N3-C2	-4.04	120.81	126.37
55	2x	55	PSU	C4-N3-C2	-4.02	120.83	126.37
55	1x	54	5MU	O4-C4-C5	-3.97	120.38	124.92
54	2w	8	4SU	N3-C2-N1	3.96	120.05	114.89
32	1a	1519	MA6	C4-C5-N7	-3.96	106.06	110.58
1	1A	1915	5MU	O4-C4-C5	-3.95	120.40	124.92
54	1w	54	5MU	C5-C4-N3	3.94	118.75	115.32
32	1a	1518	MA6	C5-C4-N3	-3.94	121.29	126.72
57	1y	54	5MU	O4-C4-C5	-3.94	120.41	124.92
32	2a	1519	MA6	C2-N1-C6	3.93	121.43	111.83
55	1x	8	4SU	O2-C2-N1	3.93	127.91	122.80
55	2x	54	5MU	O4-C4-C5	-3.91	120.44	124.92
32	2a	1207	2MG	C6-C5-N7	3.91	137.41	130.29
32	1a	1519	MA6	C5-N7-C8	3.88	109.56	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1207	2MG	N9-C4-N3	3.88	133.72	125.95
57	2y	55	PSU	O2-C2-N1	-3.88	118.79	122.79
54	2w	55	PSU	O2-C2-N1	-3.86	118.80	122.79
32	2a	1519	MA6	C5-N7-C8	3.85	109.50	103.45
54	1w	55	PSU	C4-N3-C2	-3.84	121.08	126.37
57	2y	8	4SU	C5-C4-S4	-3.83	119.93	124.31
57	2y	55	PSU	C4-N3-C2	-3.81	121.12	126.37
32	1a	1518	MA6	C5-N7-C8	3.81	109.43	103.45
32	2a	1518	MA6	C2-N1-C6	3.79	121.09	111.83
57	1y	55	PSU	C4-N3-C2	-3.78	121.17	126.37
55	1x	8	4SU	S4-C4-N3	-3.77	116.25	120.20
1	2A	1911	PSU	C4-N3-C2	-3.77	121.18	126.37
55	1x	55	PSU	O2-C2-N1	-3.76	118.91	122.79
55	1x	32	5MC	C5-C6-N1	-3.75	119.24	123.31
55	2x	55	PSU	O2-C2-N1	-3.74	118.93	122.79
32	1a	967	5MC	C5-C6-N1	-3.74	119.26	123.31
32	2a	1207	2MG	N9-C4-N3	3.72	133.38	125.95
54	1w	55	PSU	O2-C2-N1	-3.71	118.96	122.79
1	1A	1917	PSU	O2-C2-N1	-3.70	118.98	122.79
55	2x	8	4SU	C5-C4-N3	3.68	118.17	114.75
54	2w	54	5MU	N3-C2-N1	3.67	119.66	114.89
54	2w	54	5MU	C5-C4-N3	3.66	118.51	115.32
32	2a	1518	MA6	C4-C5-N7	-3.66	106.40	110.58
55	1x	8	4SU	C5-C4-N3	3.64	118.14	114.75
32	1a	1207	2MG	C6-C5-N7	3.62	136.88	130.29
32	2a	1400	5MC	C5-C6-N1	-3.61	119.39	123.31
54	2w	54	5MU	O4-C4-C5	-3.59	120.81	124.92
32	1a	1518	MA6	N9-C8-N7	-3.59	108.85	113.94
57	2y	8	4SU	N3-C2-N1	3.57	119.54	114.89
1	2A	1917	PSU	O2-C2-N1	-3.56	119.12	122.79
32	2a	1518	MA6	C5-N7-C8	3.52	108.99	103.45
1	2A	1939	5MU	O2-C2-N1	-3.52	118.21	122.80
32	2a	1519	MA6	C2-N3-C4	3.52	120.43	111.83
54	2w	54	5MU	C4-N3-C2	-3.52	122.73	127.34
1	1A	1942	5MC	C5-C6-N1	-3.51	119.50	123.31
55	1x	76	8AN	N9-C8-N7	-3.47	109.02	113.94
32	1a	1518	MA6	C4-C5-N7	-3.46	106.63	110.58
55	2x	76	8AN	N9-C8-N7	-3.46	109.03	113.94
1	2A	1942	5MC	C5-C6-N1	-3.46	119.56	123.31
1	2A	1962	5MC	C5-C6-N1	-3.45	119.56	123.31
54	1w	8	4SU	N3-C2-N1	3.45	119.39	114.89
54	2w	76	L3X	N9-C8-N7	-3.45	109.04	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	54	5MU	C5-C6-N1	-3.42	119.60	123.31
57	2y	54	5MU	O4-C4-C5	-3.40	121.02	124.92
55	2x	76	8AN	O4'-C1'-N9	3.40	114.62	108.09
32	2a	966	M2G	C6-C5-N7	3.36	136.41	130.29
55	1x	76	8AN	C5-N7-C8	3.34	108.70	103.45
54	2w	76	L3X	C2-N3-C4	3.34	119.98	111.83
55	2x	32	5MC	C5-C6-N1	-3.33	119.69	123.31
32	1a	1519	MA6	N9-C8-N7	-3.32	109.22	113.94
32	1a	1519	MA6	C2-N3-C4	3.32	119.94	111.83
55	2x	76	8AN	C2-N3-C4	3.30	119.88	111.83
1	2A	2552	OMU	O2-C2-N1	-3.29	118.52	122.80
57	1y	54	5MU	C5-C6-N1	-3.28	119.75	123.31
1	2A	2605	PSU	O2-C2-N1	-3.28	119.41	122.79
32	2a	1518	MA6	C2-N3-C4	3.27	119.81	111.83
1	1A	2503	2MA	C4-N9-C8	3.26	109.16	105.74
54	2w	8	4SU	O2-C2-N1	-3.26	118.55	122.80
1	1A	2605	PSU	O2-C2-N1	-3.25	119.44	122.79
1	2A	1915	5MU	C5-C6-N1	-3.23	119.80	123.31
1	2A	1911	PSU	O2-C2-N1	-3.23	119.46	122.79
55	2x	76	8AN	C4'-O4'-C1'	-3.22	102.36	109.47
1	1A	1962	5MC	C5-C6-N1	-3.21	119.82	123.31
55	1x	76	8AN	C2-N3-C4	3.21	119.67	111.83
32	2a	1498	UR3	C5-C4-N3	3.21	119.26	115.04
54	1w	76	L3X	C5-C4-N3	-3.21	122.30	126.72
32	1a	1518	MA6	C2-N3-C4	3.20	119.64	111.83
32	2a	1404	5MC	C5-C6-N1	-3.19	119.85	123.31
32	1a	1407	5MC	C5-C6-N1	-3.18	119.86	123.31
55	1x	76	8AN	C5-C4-N9	3.17	109.26	105.81
55	1x	32	5MC	C5-C4-N3	-3.17	118.51	121.75
32	2a	1519	MA6	N9-C8-N7	-3.15	109.47	113.94
32	1a	1498	UR3	C5-C4-N3	3.10	119.12	115.04
1	2A	2552	OMU	C5-C4-N3	3.10	119.14	114.80
55	2x	54	5MU	C5-C6-N1	-3.10	119.95	123.31
32	2a	1407	5MC	C5-C6-N1	-3.09	119.96	123.31
32	1a	1400	5MC	C5-C6-N1	-3.08	119.96	123.31
32	1a	1404	5MC	C5-C4-N3	-3.08	118.60	121.75
32	1a	1207	2MG	C4-C5-N7	-3.08	105.79	110.67
32	1a	516	PSU	O2-C2-N1	-3.07	119.62	122.79
1	1A	2552	OMU	O4-C4-C5	-3.06	119.89	125.16
1	1A	1942	5MC	C5-C4-N3	-3.05	118.63	121.75
32	2a	1407	5MC	C5-C4-N3	-3.05	118.63	121.75
55	2x	76	8AN	C5-N7-C8	3.04	108.23	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	8	4SU	C1'-N1-C2	3.04	123.05	117.59
1	1A	1939	5MU	O4-C4-C5	-3.03	121.45	124.92
32	1a	1404	5MC	C5-C6-N1	-3.02	120.03	123.31
54	2w	76	L3X	C5-N7-C8	3.02	108.20	103.45
32	2a	1207	2MG	C4-C5-N7	-3.01	105.90	110.67
32	2a	967	5MC	C5-C6-N1	-3.01	120.05	123.31
1	2A	2503	2MA	C4-C5-N7	-3.01	107.15	110.58
32	2a	1207	2MG	N1-C2-N2	2.98	119.60	116.56
1	1A	2251	OMG	C6-C5-N7	2.98	135.71	130.29
1	2A	2503	2MA	C4-N9-C8	2.96	108.85	105.74
1	2A	2251	OMG	O6-C6-C5	-2.96	118.73	126.53
1	1A	2503	2MA	N6-C6-N1	2.95	121.01	117.03
1	1A	2552	OMU	C5-C4-N3	2.95	118.93	114.80
43	2l	92	0TD	OD2-CG-CB	2.95	119.52	113.15
32	1a	1400	5MC	C5-C4-N3	-2.94	118.74	121.75
54	1w	76	L3X	N9-C8-N7	-2.94	109.76	113.94
1	1A	2503	2MA	C2-N1-C6	2.93	122.61	118.10
1	1A	1911	PSU	O2-C2-N1	-2.93	119.77	122.79
1	1A	2503	2MA	C4-C5-N7	-2.92	107.24	110.58
32	2a	1518	MA6	C4-C5-C6	2.91	118.92	115.91
32	1a	966	M2G	C6-C5-N7	2.91	135.58	130.29
55	1x	76	8AN	C4'-O4'-C1'	-2.90	103.07	109.47
32	2a	1404	5MC	C5-C4-N3	-2.90	118.79	121.75
32	2a	1518	MA6	N9-C8-N7	-2.88	109.86	113.94
57	1y	8	4SU	N3-C2-N1	2.85	118.61	114.89
57	1y	8	4SU	C5-C4-S4	-2.85	121.05	124.31
1	1A	1962	5MC	C5-C4-N3	-2.85	118.84	121.75
54	1w	76	L3X	C2-N3-C4	2.85	118.78	111.83
1	2A	2605	PSU	C5-C6-N1	-2.81	118.24	122.14
32	2a	1518	MA6	N3-C4-N9	2.78	131.90	127.17
32	1a	1207	2MG	N1-C2-N2	2.78	119.40	116.56
1	2A	1962	5MC	C5-C4-N3	-2.74	118.94	121.75
32	1a	1407	5MC	C5-C4-N3	-2.74	118.95	121.75
1	1A	1920	OMC	O2-C2-N3	-2.72	118.03	122.33
43	1l	92	0TD	OD2-CG-CB	2.72	119.03	113.15
1	1A	2552	OMU	O2-C2-N1	-2.72	119.26	122.80
54	1w	8	4SU	C1'-N1-C2	2.71	122.47	117.59
55	1x	76	8AN	C4-C5-N7	-2.71	107.49	110.58
55	2x	32	5MC	O2-C2-N3	-2.70	118.07	122.33
55	2x	32	5MC	C5-C4-N3	-2.70	118.99	121.75
32	1a	967	5MC	C5-C4-N3	-2.69	119.00	121.75
32	2a	1207	2MG	N2-C2-N3	-2.68	117.10	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	966	M2G	C4-C5-N7	-2.68	106.43	110.67
1	2A	1942	5MC	C5-C4-N3	-2.67	119.02	121.75
54	2w	76	L3X	C5-C4-N9	2.66	108.70	105.81
32	1a	1518	MA6	N3-C4-N9	2.64	131.65	127.17
32	1a	1207	2MG	N2-C2-N3	-2.63	117.17	120.51
1	2A	2251	OMG	C6-C5-N7	2.62	135.06	130.29
57	2y	54	5MU	C5-C6-N1	-2.61	120.48	123.31
1	2A	2552	OMU	O4-C4-C5	-2.60	120.68	125.16
54	1w	54	5MU	C5-C6-N1	-2.59	120.50	123.31
32	2a	1407	5MC	O2-C2-N3	-2.58	118.26	122.33
55	2x	76	8AN	C5-C4-N9	2.57	108.61	105.81
55	2x	8	4SU	C6-C5-C4	-2.54	117.75	119.95
32	2a	1519	MA6	N3-C4-N9	2.54	131.48	127.17
1	1A	1915	5MU	C5-C6-N1	-2.53	120.57	123.31
32	2a	1400	5MC	C5-C4-N3	-2.51	119.18	121.75
32	1a	1519	MA6	C4-C5-C6	2.49	118.49	115.91
32	1a	966	M2G	C4-C5-N7	-2.49	106.73	110.67
54	2w	76	L3X	N3-C4-N9	2.47	131.38	127.17
32	1a	1519	MA6	N3-C4-N9	2.47	131.36	127.17
55	2x	76	8AN	N3-C4-N9	2.46	131.35	127.17
1	1A	2503	2MA	C5-N7-C8	2.44	107.28	103.45
32	2a	1519	MA6	C4-C5-C6	2.43	118.42	115.91
32	1a	1402	4OC	C6-C5-C4	2.41	119.91	117.00
55	1x	55	PSU	C5-C6-N1	-2.37	118.84	122.14
1	1A	2251	OMG	O6-C6-C5	-2.37	120.27	126.53
57	2y	8	4SU	C1'-N1-C2	2.37	121.85	117.59
54	1w	55	PSU	C6-C5-C4	-2.35	116.58	118.17
56	2z	1	FME	C-CA-N	2.35	114.04	109.50
1	2A	1917	PSU	C5-C6-N1	-2.34	118.89	122.14
1	1A	2503	2MA	N9-C8-N7	-2.33	110.63	113.94
32	2a	516	PSU	C5-C6-N1	-2.33	118.91	122.14
57	1y	54	5MU	O2-C2-N1	-2.32	119.78	122.80
32	1a	527	G7M	O6-C6-C5	-2.32	122.83	128.01
32	2a	1402	4OC	C6-C5-C4	2.31	119.78	117.00
32	1a	1404	5MC	O2-C2-N3	-2.30	118.71	122.33
32	2a	1404	5MC	O2-C2-N3	-2.29	118.72	122.33
1	2A	2503	2MA	C5-N7-C8	2.29	107.05	103.45
32	2a	967	5MC	C5-C4-N3	-2.28	119.42	121.75
54	1w	54	5MU	O2-C2-N1	-2.27	119.84	122.80
55	1x	8	4SU	C1'-N1-C2	2.27	121.67	117.59
54	2w	54	5MU	C5M-C5-C4	2.27	121.20	118.78
1	2A	2503	2MA	C2-N1-C6	2.24	121.55	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2y	54	5MU	C1'-N1-C2	2.24	121.62	117.59
1	1A	1962	5MC	O2-C2-N3	-2.24	118.80	122.33
1	2A	1920	OMC	O2-C2-N3	-2.24	118.80	122.33
54	2w	8	4SU	C1'-N1-C2	2.23	121.60	117.59
1	2A	2251	OMG	C5-C6-N1	2.23	118.93	113.25
54	2w	54	5MU	C5-C6-N1	-2.21	120.92	123.31
55	1x	76	8AN	N3-C4-N9	2.21	130.92	127.17
32	2a	1519	MA6	C5-C4-N9	2.19	108.20	105.81
32	1a	1518	MA6	C4-N9-C8	2.18	108.03	105.74
32	1a	527	G7M	C5-C6-N1	2.18	116.35	111.84
54	2w	76	L3X	C6-C5-C4	2.17	120.14	117.18
32	2a	516	PSU	O4'-C1'-C2'	2.17	108.15	105.15
1	1A	2552	OMU	C2'-C1'-N1	-2.16	110.14	114.24
1	1A	1917	PSU	C5-C6-N1	-2.16	119.15	122.14
32	2a	1498	UR3	C6-N1-C2	-2.15	120.05	121.80
1	1A	1942	5MC	CM5-C5-C6	-2.14	119.95	122.85
32	2a	967	5MC	C1'-N1-C6	-2.14	117.62	121.15
32	1a	1400	5MC	O2-C2-N3	-2.14	118.95	122.33
1	1A	1911	PSU	C5-C6-N1	-2.13	119.18	122.14
1	1A	2605	PSU	C5-C6-N1	-2.13	119.19	122.14
1	1A	1911	PSU	O4'-C1'-C2'	2.12	108.09	105.15
54	2w	76	L3X	C4-C5-N7	-2.12	108.16	110.58
1	2A	2605	PSU	O2-C2-N3	-2.11	118.11	121.86
32	2a	527	G7M	C5-C6-N1	2.11	116.21	111.84
55	2x	76	8AN	C4-C5-N7	-2.11	108.17	110.58
1	1A	2251	OMG	C4-C5-N7	-2.11	107.33	110.67
32	2a	966	M2G	O6-C6-C5	-2.10	120.98	126.53
57	2y	54	5MU	O2-C2-N3	-2.10	117.61	121.49
55	1x	76	8AN	O4'-C1'-C2'	-2.10	102.12	106.62
55	1x	76	8AN	C6-C5-C4	2.10	120.04	117.18
32	2a	1400	5MC	O2-C2-N3	-2.09	119.04	122.33
55	1x	8	4SU	O2-C2-N3	-2.09	117.64	121.49
32	2a	1498	UR3	C3U-N3-C4	2.09	120.76	117.87
32	1a	966	M2G	O6-C6-C5	-2.07	121.07	126.53
1	1A	1915	5MU	O2-C2-N1	-2.07	120.11	122.80
1	1A	1915	5MU	C5M-C5-C4	2.06	120.98	118.78
55	1x	32	5MC	O2-C2-N3	-2.05	119.10	122.33
54	1w	54	5MU	C5M-C5-C4	2.05	120.97	118.78
1	2A	1915	5MU	C5M-C5-C4	2.05	120.97	118.78
55	2x	54	5MU	O2-C2-N1	-2.04	120.14	122.80
32	1a	516	PSU	O4'-C1'-C2'	2.04	107.97	105.15
55	2x	55	PSU	C5-C6-N1	-2.03	119.32	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1402	4OC	CM4-N4-C4	-2.03	118.49	122.45
55	2x	8	4SU	O2-C2-N3	-2.03	117.75	121.49
1	2A	1915	5MU	O2-C2-N1	-2.02	120.17	122.80
32	1a	1518	MA6	C4-C5-C6	2.01	117.99	115.91
57	2y	54	5MU	C5M-C5-C4	2.01	120.93	118.78
1	1A	2503	2MA	C6-C5-N7	2.01	135.97	132.09
32	1a	1498	UR3	C6-N1-C2	-2.01	120.16	121.80

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N3-C2-N2-CM2
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1207	2MG	N3-C2-N2-CM2
54	2w	76	L3X	O4'-C4'-C5'-O5'
55	1x	76	8AN	C3'-C4'-C5'-O5'
57	2y	55	PSU	O4'-C4'-C5'-O5'
54	2w	76	L3X	C3'-C4'-C5'-O5'
55	2x	76	8AN	C3'-C4'-C5'-O5'
57	2y	8	4SU	O4'-C4'-C5'-O5'
57	2y	55	PSU	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
55	1x	76	8AN	O4'-C4'-C5'-O5'
55	2x	76	8AN	O4'-C4'-C5'-O5'
57	2y	54	5MU	O4'-C4'-C5'-O5'
56	1z	1	FME	N-CA-CB-CG
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
57	2y	8	4SU	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
57	2y	54	5MU	C3'-C4'-C5'-O5'
56	1z	1	FME	CB-CG-SD-CE
32	2a	527	G7M	O4'-C4'-C5'-O5'
56	1z	1	FME	C-CA-CB-CG
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
55	1x	76	8AN	C4'-C5'-O5'-P
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
43	2l	92	0TD	SB-CB-CG-OD1
57	1y	55	PSU	O4'-C1'-C5-C4
57	2y	55	PSU	O4'-C1'-C5-C4
32	1a	1519	MA6	C4'-C5'-O5'-P
55	2x	76	8AN	C4'-C5'-O5'-P
1	1A	2503	2MA	C4'-C5'-O5'-P
32	1a	527	G7M	C4'-C5'-O5'-P
43	2l	92	0TD	SB-CB-CG-OD2
57	1y	55	PSU	O4'-C1'-C5-C6
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
32	1a	967	5MC	C3'-C4'-C5'-O5'
1	1A	1920	OMC	C2'-C1'-N1-C2
55	2x	8	4SU	C2'-C1'-N1-C2
1	1A	2503	2MA	O4'-C4'-C5'-O5'
57	2y	54	5MU	C2'-C1'-N1-C2

There are no ring outliers.

36 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	516	PSU	1	0
1	2A	2251	OMG	1	0
54	2w	8	4SU	6	0
55	1x	8	4SU	2	0
54	2w	55	PSU	1	0
57	2y	8	4SU	2	0
1	2A	1917	PSU	1	0
54	1w	54	5MU	2	0
57	1y	8	4SU	2	0
32	1a	1402	4OC	2	0
32	1a	1519	MA6	2	0
32	2a	1402	4OC	2	0
32	2a	1519	MA6	1	0
43	2l	92	0TD	2	0
32	2a	967	5MC	1	0
32	2a	1498	UR3	1	0
43	1l	92	0TD	1	0
32	2a	1207	2MG	1	0
1	2A	2552	OMU	1	0
1	1A	2503	2MA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	1x	76	8AN	1	0
1	1A	1939	5MU	1	0
32	1a	1518	MA6	2	0
1	2A	1939	5MU	1	0
1	1A	1915	5MU	1	0
54	1w	76	L3X	1	0
32	2a	1404	5MC	1	0
54	2w	54	5MU	1	0
55	2x	54	5MU	2	0
56	2z	1	FME	1	0
54	1w	55	PSU	2	0
55	2x	76	8AN	2	0
32	2a	1518	MA6	5	0
1	1A	2552	OMU	1	0
32	1a	967	5MC	1	0
54	2w	76	L3X	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2669 ligands modelled in this entry, 2665 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
60	CLM	2w	103	54	20,20,20	0.84	0	23,27,27	0.85	0
62	SF4	1d	302	35	0,12,12	-	-	-		
62	SF4	2d	303	35	0,12,12	-	-	-		
60	CLM	1A	4087	-	20,20,20	0.97	1 (5%)	23,27,27	1.25	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	CLM	2w	103	54	-	2/20/22/22	0/1/1/1
62	SF4	1d	302	35	-	-	0/6/5/5
62	SF4	2d	303	35	-	-	0/6/5/5
60	CLM	1A	4087	-	-	4/20/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	1A	4087	CLM	C6-C5	-2.24	1.48	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	1A	4087	CLM	C6-C5-C3	2.96	117.02	111.72
60	1A	4087	CLM	O5-C5-C6	-2.90	104.90	111.20
60	1A	4087	CLM	C8-C9-N9	2.71	121.70	119.34

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	1A	4087	CLM	N2-C3-C4-O4
60	1A	4087	CLM	C5-C3-C4-O4
60	2w	103	CLM	C8-C9-N9-O9B
60	2w	103	CLM	C10-C9-N9-O9B
60	1A	4087	CLM	O2-C2-N2-C3
60	1A	4087	CLM	C1-C2-N2-C3

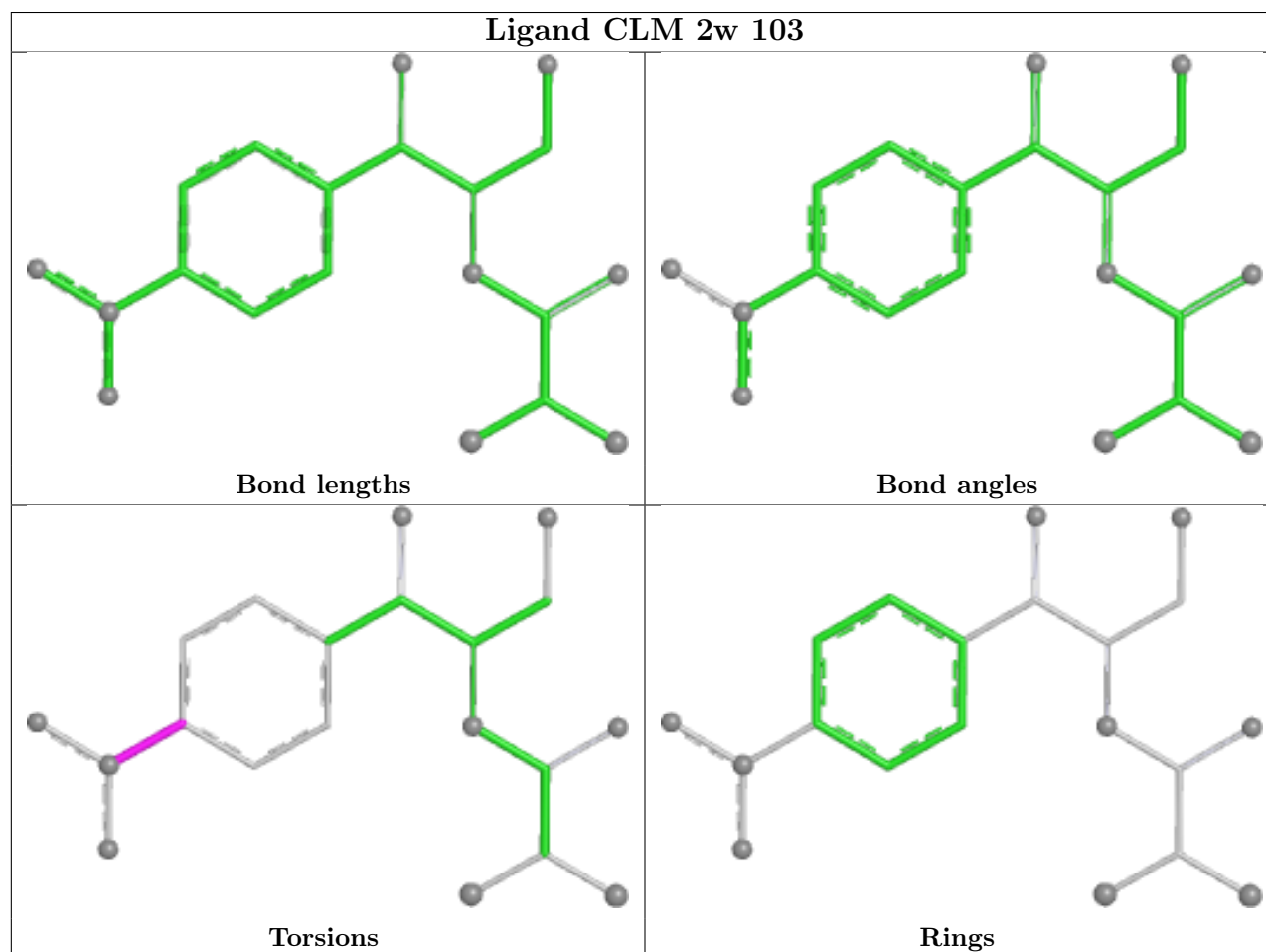
There are no ring outliers.

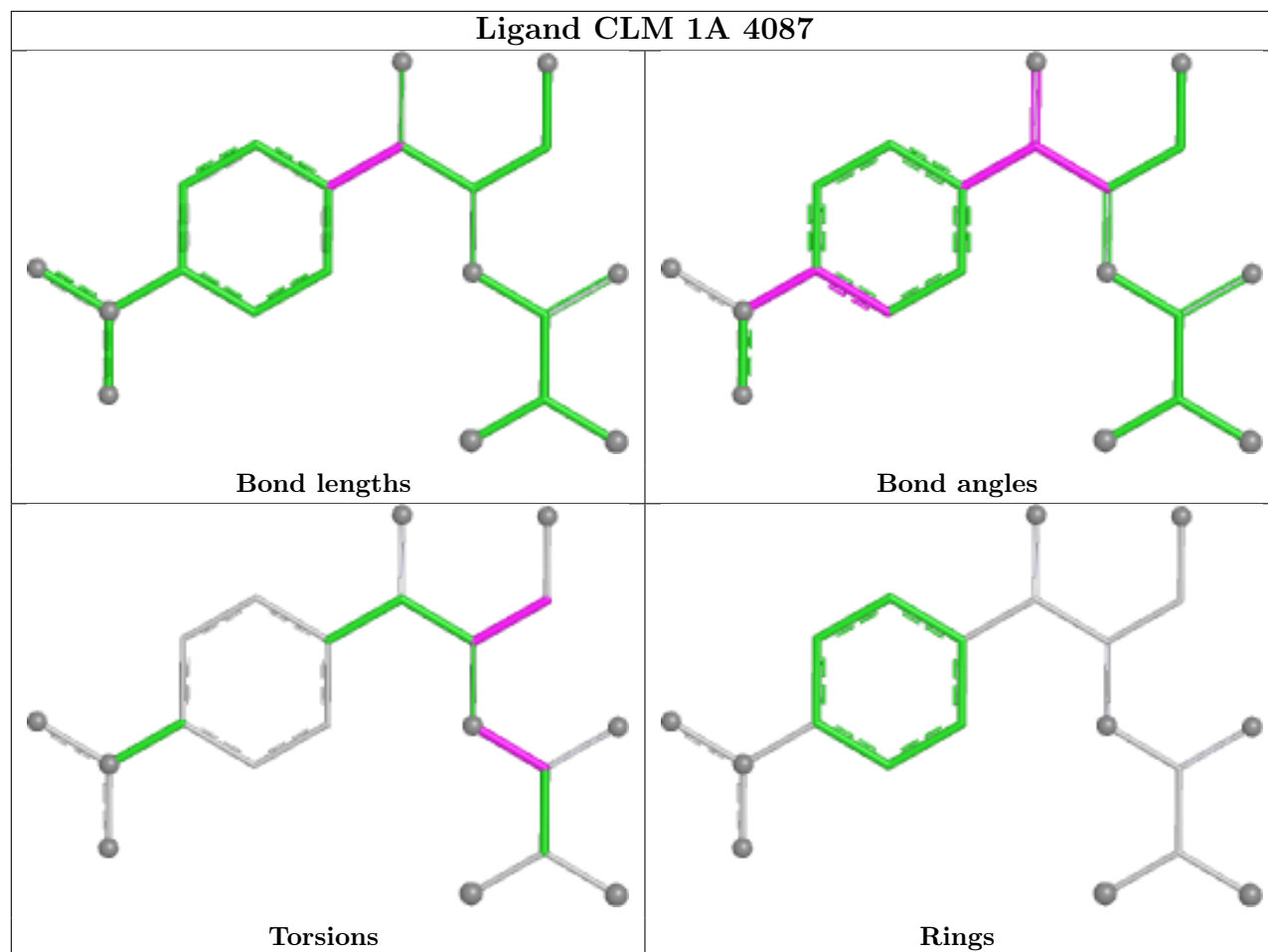
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	2w	103	CLM	1	0
62	1d	302	SF4	1	0
60	1A	4087	CLM	1	0

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

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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%)	-0.42	131 (4%)	37	38	28, 45, 105, 116	0
1	2A	2789/2915 (95%)	0.07	107 (3%)	44	45	42, 67, 102, 116	0
2	1B	120/121 (99%)	-0.39	0	100	100	38, 60, 73, 98	0
2	2B	120/121 (99%)	0.62	4 (3%)	49	50	70, 87, 94, 103	0
3	1D	275/276 (99%)	-0.04	2 (0%)	84	86	28, 46, 59, 88	0
3	2D	275/276 (99%)	0.49	8 (2%)	53	55	41, 59, 72, 88	0
4	1E	204/206 (99%)	0.02	1 (0%)	87	89	28, 49, 66, 82	0
4	2E	204/206 (99%)	0.73	12 (5%)	28	27	46, 69, 81, 90	0
5	1F	202/210 (96%)	0.09	3 (1%)	72	73	26, 51, 73, 94	0
5	2F	202/210 (96%)	0.68	5 (2%)	58	59	46, 77, 88, 94	0
6	1G	181/182 (99%)	0.74	12 (6%)	24	24	52, 69, 83, 96	0
6	2G	181/182 (99%)	1.31	26 (14%)	6	5	76, 88, 94, 99	0
7	1H	174/180 (96%)	0.38	3 (1%)	69	69	47, 61, 74, 83	0
7	2H	174/180 (96%)	1.58	53 (30%)	1	0	79, 92, 100, 102	0
8	1I	146/148 (98%)	0.84	6 (4%)	41	42	53, 81, 89, 92	0
8	2I	146/148 (98%)	1.00	13 (8%)	15	14	64, 82, 89, 94	0
9	1N	140/140 (100%)	0.10	2 (1%)	73	74	33, 45, 66, 81	0
9	2N	140/140 (100%)	1.05	14 (10%)	12	12	61, 76, 87, 96	0
10	1O	122/122 (100%)	0.23	3 (2%)	58	59	38, 49, 66, 71	0
10	2O	122/122 (100%)	0.62	0	100	100	58, 68, 79, 84	0
11	1P	149/150 (99%)	0.21	1 (0%)	84	86	29, 53, 74, 84	0
11	2P	149/150 (99%)	0.85	7 (4%)	36	36	51, 76, 91, 96	0
12	1Q	141/141 (100%)	0.24	1 (0%)	84	86	32, 50, 64, 85	0
12	2Q	141/141 (100%)	1.36	25 (17%)	4	3	63, 76, 86, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.04	0 100 100	32, 44, 58, 65	0
13	2R	118/118 (100%)	0.47	0 100 100	48, 63, 74, 80	0
14	1S	110/112 (98%)	0.34	2 (1%) 67 68	45, 59, 72, 75	0
14	2S	110/112 (98%)	1.38	19 (17%) 4 3	70, 82, 89, 94	0
15	1T	131/146 (89%)	0.44	4 (3%) 51 52	41, 54, 76, 84	0
15	2T	131/146 (89%)	0.93	9 (6%) 23 22	63, 71, 84, 91	0
16	1U	116/118 (98%)	-0.24	1 (0%) 81 83	30, 39, 55, 69	0
16	2U	116/118 (98%)	0.85	4 (3%) 48 49	55, 74, 86, 94	0
17	1V	101/101 (100%)	-0.18	1 (0%) 79 80	31, 48, 64, 78	0
17	2V	101/101 (100%)	0.77	3 (2%) 52 54	51, 82, 89, 92	0
18	1W	112/113 (99%)	-0.19	1 (0%) 81 83	31, 40, 58, 90	0
18	2W	112/113 (99%)	0.55	3 (2%) 56 57	50, 60, 75, 95	0
19	1X	95/96 (98%)	0.18	2 (2%) 63 64	35, 47, 72, 85	0
19	2X	95/96 (98%)	0.85	7 (7%) 20 19	52, 68, 80, 96	0
20	1Y	107/110 (97%)	0.65	7 (6%) 25 24	45, 59, 73, 88	0
20	2Y	107/110 (97%)	1.54	26 (24%) 2 1	66, 81, 89, 95	0
21	1Z	154/206 (74%)	0.91	16 (10%) 11 11	46, 70, 93, 99	0
21	2Z	160/206 (77%)	1.85	53 (33%) 1 0	79, 89, 99, 101	0
22	10	83/85 (97%)	0.40	5 (6%) 27 27	33, 46, 65, 78	0
22	20	83/85 (97%)	1.46	17 (20%) 2 2	56, 73, 85, 88	0
23	11	97/98 (98%)	0.36	3 (3%) 51 52	36, 54, 76, 87	0
23	21	97/98 (98%)	0.73	2 (2%) 63 64	46, 64, 81, 85	0
24	12	70/72 (97%)	0.42	2 (2%) 53 55	43, 58, 69, 78	0
24	22	70/72 (97%)	0.98	7 (10%) 12 12	66, 79, 86, 88	0
25	13	59/60 (98%)	0.07	2 (3%) 48 49	34, 43, 70, 89	0
25	23	59/60 (98%)	0.82	7 (11%) 9 8	66, 76, 86, 92	0
26	14	69/71 (97%)	0.93	9 (13%) 7 6	65, 83, 96, 99	0
26	24	69/71 (97%)	1.34	12 (17%) 4 3	87, 95, 101, 101	0
27	15	59/60 (98%)	-0.21	0 100 100	28, 42, 64, 69	0
27	25	59/60 (98%)	0.55	2 (3%) 48 49	46, 62, 80, 89	0
28	16	53/54 (98%)	0.31	2 (3%) 44 45	41, 51, 65, 70	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.85	5 (9%) 14 13	60, 71, 78, 85	0
29	17	48/49 (97%)	0.10	4 (8%) 17 17	29, 36, 70, 76	0
29	27	48/49 (97%)	0.53	6 (12%) 8 7	43, 50, 74, 81	0
30	18	64/65 (98%)	-0.15	0 100 100	34, 42, 50, 63	0
30	28	64/65 (98%)	0.83	2 (3%) 51 52	55, 65, 73, 80	0
31	19	37/37 (100%)	0.30	0 100 100	39, 48, 66, 69	0
31	29	37/37 (100%)	1.43	7 (18%) 3 2	72, 79, 89, 92	0
32	1a	1488/1521 (97%)	0.36	63 (4%) 40 41	44, 79, 103, 117	0
32	2a	1491/1521 (98%)	0.67	108 (7%) 21 20	57, 85, 105, 115	0
33	1b	231/256 (90%)	1.32	47 (20%) 3 2	75, 87, 97, 105	0
33	2b	231/256 (90%)	1.69	77 (33%) 1 0	81, 93, 98, 100	0
34	1c	206/239 (86%)	1.23	29 (14%) 6 5	75, 85, 94, 99	0
34	2c	206/239 (86%)	2.05	110 (53%) 0 0	85, 92, 98, 103	0
35	1d	208/209 (99%)	1.20	25 (12%) 9 8	67, 82, 90, 98	0
35	2d	208/209 (99%)	0.96	16 (7%) 19 18	68, 77, 85, 90	0
36	1e	148/162 (91%)	0.82	7 (4%) 36 36	55, 75, 84, 89	0
36	2e	148/162 (91%)	1.44	33 (22%) 2 2	72, 85, 92, 98	0
37	1f	100/101 (99%)	0.75	3 (3%) 52 54	65, 78, 85, 88	0
37	2f	100/101 (99%)	0.91	6 (6%) 27 27	71, 81, 88, 95	0
38	1g	155/156 (99%)	0.99	22 (14%) 6 5	73, 83, 94, 100	0
38	2g	155/156 (99%)	1.33	27 (17%) 4 3	79, 88, 97, 102	0
39	1h	137/138 (99%)	0.92	10 (7%) 21 20	64, 76, 82, 89	0
39	2h	137/138 (99%)	1.34	18 (13%) 7 6	78, 85, 90, 93	0
40	1i	127/128 (99%)	1.51	32 (25%) 1 1	69, 88, 93, 96	0
40	2i	127/128 (99%)	2.19	68 (53%) 0 0	78, 93, 98, 99	0
41	1j	97/105 (92%)	1.59	29 (29%) 1 1	73, 90, 96, 99	0
41	2j	96/105 (91%)	2.31	59 (61%) 0 0	86, 95, 100, 103	0
42	1k	114/129 (88%)	0.77	9 (7%) 18 18	50, 75, 88, 95	0
42	2k	114/129 (88%)	1.00	14 (12%) 8 7	65, 82, 91, 93	0
43	1l	121/132 (91%)	0.67	4 (3%) 49 50	55, 70, 79, 83	0
43	2l	121/132 (91%)	1.28	15 (12%) 8 7	69, 81, 88, 90	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	1.22	13 (10%) 11 11	69, 82, 90, 98	0
44	2m	122/126 (96%)	2.12	49 (40%) 0 0	83, 91, 97, 101	0
45	1n	60/61 (98%)	1.57	10 (16%) 4 3	74, 83, 89, 91	0
45	2n	60/61 (98%)	2.69	45 (75%) 0 0	88, 94, 98, 100	0
46	1o	88/89 (98%)	0.78	6 (6%) 23 22	56, 72, 82, 89	0
46	2o	88/89 (98%)	0.98	5 (5%) 29 29	69, 82, 89, 94	0
47	1p	82/88 (93%)	1.56	19 (23%) 2 1	68, 81, 89, 96	0
47	2p	82/88 (93%)	0.97	5 (6%) 27 26	67, 76, 84, 88	0
48	1q	99/105 (94%)	1.09	10 (10%) 12 11	63, 74, 85, 86	0
48	2q	99/105 (94%)	0.90	8 (8%) 18 17	71, 81, 89, 94	0
49	1r	68/88 (77%)	0.72	5 (7%) 20 19	66, 75, 86, 89	0
49	2r	68/88 (77%)	0.88	3 (4%) 39 39	75, 81, 89, 90	0
50	1s	83/93 (89%)	1.15	8 (9%) 13 13	74, 85, 92, 96	0
50	2s	83/93 (89%)	2.04	38 (45%) 0 0	87, 95, 100, 104	0
51	1t	96/106 (90%)	1.39	22 (22%) 2 2	68, 80, 89, 91	0
51	2t	96/106 (90%)	1.00	7 (7%) 21 20	65, 79, 89, 90	0
52	1u	23/27 (85%)	1.87	9 (39%) 1 0	74, 80, 83, 85	0
52	2u	23/27 (85%)	2.35	19 (82%) 0 0	84, 90, 94, 96	0
53	1v	13/24 (54%)	1.51	4 (30%) 1 0	58, 82, 104, 108	0
53	2v	13/24 (54%)	2.37	6 (46%) 0 0	81, 93, 107, 113	0
54	1w	69/74 (93%)	1.37	11 (15%) 5 4	62, 106, 112, 114	0
54	2w	68/74 (91%)	1.79	26 (38%) 1 0	78, 108, 113, 115	0
55	1x	72/77 (93%)	0.42	2 (2%) 55 56	43, 76, 93, 96	0
55	2x	72/77 (93%)	0.65	2 (2%) 55 56	62, 91, 99, 109	0
56	1z	2/3 (66%)	0.40	0 100 100	44, 44, 44, 46	0
56	2z	2/3 (66%)	1.13	0 100 100	64, 64, 64, 69	0
57	1y	70/74 (94%)	2.19	37 (52%) 0 0	68, 110, 113, 115	0
57	2y	70/74 (94%)	2.18	41 (58%) 0 0	80, 111, 115, 116	0
All	All	20889/21746 (96%)	0.56	1932 (9%) 14 14	26, 74, 99, 117	0

All (1932) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	12.3
44	2m	124	PRO	11.3
1	1A	2115	G	8.3
44	1m	123	ALA	8.0
44	2m	102	ARG	7.9
45	1n	2	ALA	7.7
1	1A	2145	C	6.6
38	2g	80	VAL	6.5
23	2l	2	SER	6.4
44	1m	122	LYS	6.4
21	1Z	146	ILE	6.1
44	1m	124	PRO	6.1
38	1g	80	VAL	6.0
44	2m	121	LYS	5.8
34	2c	8	ILE	5.8
44	2m	7	VAL	5.7
1	1A	2114	A	5.7
41	2j	65	LEU	5.6
41	2j	32	ALA	5.6
1	2A	2111	C	5.6
50	2s	2	PRO	5.6
7	1H	2	SER	5.6
45	2n	2	ALA	5.6
44	2m	122	LYS	5.5
45	2n	34	TYR	5.4
21	2Z	172	ALA	5.4
23	1l	2	SER	5.4
51	1t	10	LEU	5.4
1	1A	2117	A	5.2
1	1A	2119	A	5.2
21	2Z	171	ILE	5.2
43	2l	18	VAL	5.2
33	1b	237	ALA	5.2
1	1A	2121	G	5.1
34	2c	207	VAL	5.1
1	1A	2120	G	5.1
32	2a	1033	G	5.1
21	2Z	174	VAL	5.1
1	1A	2178	C	5.0
53	2v	13	A	5.0
45	2n	39	LEU	5.0
33	2b	237	ALA	5.0
1	2A	2145	C	4.9

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Mol	Chain	Res	Type	RSRZ
1	1A	2112	G	4.9
39	2h	53	VAL	4.9
52	1u	18	TYR	4.9
32	2a	1219	U	4.8
34	2c	158	GLY	4.8
1	1A	2179	C	4.8
15	1T	130	ALA	4.8
40	2i	36	TYR	4.8
7	2H	43	VAL	4.8
1	2A	2112	G	4.7
44	1m	121	LYS	4.7
1	2A	2104	G	4.7
1	1A	2174	C	4.7
40	2i	118	LYS	4.7
40	1i	19	LEU	4.7
1	1A	1081	U	4.7
40	2i	14	VAL	4.6
45	2n	38	GLY	4.6
34	2c	2	GLY	4.6
1	1A	2146	C	4.6
47	1p	82	GLN	4.6
1	1A	2111	C	4.6
33	2b	236	TYR	4.6
50	2s	71	LEU	4.6
41	2j	47	PHE	4.5
4	2E	204	ALA	4.5
45	2n	18	VAL	4.5
1	1A	1094	U	4.5
44	1m	2	ALA	4.5
21	2Z	125	LEU	4.5
1	2A	2115	G	4.4
32	2a	1034	G	4.4
1	2A	2137	C	4.4
21	2Z	144	LEU	4.4
21	2Z	150	LEU	4.4
1	2A	2114	A	4.4
36	2e	114	GLY	4.4
40	2i	119	ALA	4.4
1	2A	2138	C	4.4
21	1Z	141	VAL	4.4
15	1T	131	ALA	4.4
21	2Z	173	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
57	1y	75	C	4.4
1	1A	2110	G	4.4
1	2A	2134	A	4.4
22	10	3	HIS	4.4
3	2D	38	LYS	4.4
1	2A	2159	G	4.3
33	1b	188	ALA	4.3
48	1q	98	LEU	4.3
40	2i	117	HIS	4.3
1	2A	2135	A	4.3
1	1A	2116	G	4.3
45	2n	7	ILE	4.3
1	1A	2108	C	4.3
1	2A	2155	G	4.3
52	1u	24	ARG	4.3
57	2y	19	U	4.3
1	1A	2177	C	4.3
34	2c	189	ALA	4.3
53	2v	12	A	4.3
22	20	3	HIS	4.2
1	2A	2160	G	4.2
1	1A	2167	U	4.2
41	2j	63	PHE	4.2
1	2A	2146	C	4.2
32	1a	1038	C	4.2
1	1A	2113	U	4.2
1	1A	2130	U	4.2
40	2i	102	LEU	4.2
33	1b	7	VAL	4.2
38	1g	156	TRP	4.2
32	2a	1032	G	4.2
54	2w	71	G	4.2
45	2n	13	THR	4.1
45	2n	25	VAL	4.1
1	2A	2113	U	4.1
1	2A	2147	G	4.1
33	2b	38	GLY	4.1
38	1g	2	ALA	4.1
1	1A	2159	G	4.1
6	2G	139	LEU	4.1
49	2r	66	LEU	4.1
53	2v	14	A	4.1

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Mol	Chain	Res	Type	RSRZ
40	2i	11	LYS	4.1
1	1A	2122	U	4.0
1	1A	2147	G	4.0
38	2g	154	TYR	4.0
1	1A	1059	G	4.0
32	1a	1003	G	4.0
32	2a	1036	G	4.0
21	2Z	164	ALA	4.0
38	2g	83	ALA	4.0
40	2i	2	GLU	4.0
12	2Q	22	LYS	4.0
15	2T	131	ALA	4.0
15	2T	55	ASN	4.0
1	1A	2180	U	4.0
52	2u	2	GLY	3.9
1	2A	2117	A	3.9
34	2c	182	ILE	3.9
38	2g	156	TRP	3.9
57	1y	35	C	3.9
34	2c	128	PHE	3.9
1	1A	2135	A	3.9
54	1w	1	G	3.9
57	2y	18	G	3.9
1	1A	2109	U	3.9
33	2b	165	VAL	3.9
9	2N	45	ASN	3.9
51	1t	103	GLY	3.9
50	1s	13	ASP	3.9
33	1b	11	LEU	3.9
40	2i	19	LEU	3.9
1	2A	652(B)	A	3.9
1	2A	2158	A	3.9
1	2A	2174	C	3.9
12	2Q	15	GLY	3.9
40	2i	10	ARG	3.9
33	2b	7	VAL	3.9
41	2j	44	VAL	3.9
1	1A	2143	C	3.8
20	2Y	55	TYR	3.8
34	2c	186	PHE	3.8
44	2m	100	GLY	3.8
40	1i	18	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	1A	2160	G	3.8
7	2H	113	VAL	3.8
24	22	1	MET	3.8
22	20	5	LYS	3.8
34	2c	149	ALA	3.8
40	1i	106	ALA	3.8
47	1p	48	TRP	3.8
49	1r	20	ALA	3.8
41	1j	4	ILE	3.8
57	2y	34	C	3.8
32	1a	1001(A)	G	3.8
32	1a	1036	G	3.8
45	2n	33	VAL	3.8
57	2y	15	A	3.8
38	2g	84	ASN	3.8
33	2b	121	LEU	3.8
1	1A	2129	C	3.8
44	2m	117	VAL	3.7
7	2H	60	ARG	3.7
44	2m	6	GLY	3.7
1	1A	1057	A	3.7
6	2G	52	ILE	3.7
1	2A	2136	C	3.7
57	1y	36	C	3.7
7	2H	19	VAL	3.7
40	2i	126	SER	3.7
50	2s	4	SER	3.7
15	2T	130	ALA	3.7
33	2b	123	ALA	3.7
34	2c	41	GLY	3.7
20	2Y	90	LEU	3.7
34	2c	188	LEU	3.7
1	2A	2169	A	3.7
53	1v	13	A	3.7
43	1l	126	LYS	3.7
7	2H	44	VAL	3.7
33	2b	10	LEU	3.7
44	1m	27	LYS	3.7
47	1p	39	TYR	3.7
12	2Q	10	ARG	3.7
1	1A	1068	G	3.7
1	1A	2165	G	3.7

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Mol	Chain	Res	Type	RSRZ
38	2g	85	TYR	3.7
1	1A	1096	A	3.6
26	24	56	VAL	3.6
57	1y	34	C	3.6
12	2Q	104	PHE	3.6
21	2Z	146	ILE	3.6
40	2i	91	ASP	3.6
21	2Z	149	SER	3.6
21	2Z	76	LEU	3.6
34	1c	84	ILE	3.6
41	2j	74	ILE	3.6
1	1A	1060	U	3.6
1	2A	2133	G	3.6
1	2A	2802	G	3.6
57	2y	17	G	3.6
7	2H	2	SER	3.6
54	2w	15	A	3.6
12	2Q	1	MET	3.6
38	1g	82	GLY	3.6
40	2i	128	ARG	3.6
33	2b	200	ILE	3.6
1	1A	2136	C	3.6
1	2A	2179	C	3.6
32	2a	1030(B)	C	3.6
1	1A	2118	U	3.6
25	23	60	GLU	3.6
44	2m	53	VAL	3.6
1	1A	2169	A	3.6
20	2Y	22	GLY	3.6
38	2g	81	GLY	3.6
40	1i	56	LEU	3.6
41	2j	20	ALA	3.6
33	2b	122	PHE	3.6
7	2H	52	VAL	3.5
45	1n	3	ARG	3.5
32	2a	1220	G	3.5
41	2j	40	LEU	3.5
41	2j	75	ILE	3.5
48	2q	100	LYS	3.5
1	1A	2172	U	3.5
34	1c	70	VAL	3.5
21	2Z	157	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
34	2c	129	ALA	3.5
34	2c	5	ILE	3.5
1	1A	2141	G	3.5
1	1A	2166	G	3.5
1	2A	2148	G	3.5
29	27	46	VAL	3.5
33	2b	136	VAL	3.5
41	2j	34	VAL	3.5
1	1A	1078	U	3.5
1	1A	2150	U	3.5
19	1X	95	LEU	3.5
40	2i	96	LEU	3.5
7	1H	174	GLY	3.5
12	2Q	33	GLY	3.5
22	20	2	ALA	3.5
34	2c	168	ALA	3.5
45	2n	10	ALA	3.5
45	2n	55	GLY	3.5
51	2t	103	GLY	3.5
20	2Y	1	MET	3.5
21	1Z	1	MET	3.5
16	2U	8	VAL	3.5
57	2y	6	C	3.5
33	2b	138	LEU	3.5
33	1b	232	PRO	3.5
47	1p	41	PRO	3.5
51	2t	98	PRO	3.5
29	27	48	LYS	3.5
1	1A	2170	A	3.4
1	1A	2173	A	3.4
1	2A	2125	G	3.4
32	2a	1202	G	3.4
32	2a	1224	G	3.4
33	1b	230	VAL	3.4
50	1s	9	VAL	3.4
22	20	84	LEU	3.4
33	2b	187	LEU	3.4
40	2i	99	LEU	3.4
1	1A	2142	C	3.4
21	2Z	147	GLY	3.4
34	1c	2	GLY	3.4
41	2j	10	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	1A	2144	U	3.4
41	2j	59	SER	3.4
54	1w	73	U	3.4
20	2Y	89	PHE	3.4
38	1g	153	HIS	3.4
47	1p	16	HIS	3.4
1	1A	2181	G	3.4
1	2A	2120	G	3.4
1	1A	1064	C	3.4
1	1A	2175	C	3.4
1	2A	2167	U	3.4
40	2i	66	ARG	3.4
52	2u	14	TRP	3.4
47	2p	82	GLN	3.4
3	1D	276	LYS	3.4
21	2Z	141	VAL	3.4
6	2G	53	LEU	3.4
45	2n	11	LYS	3.4
7	2H	39	PRO	3.4
31	29	37	GLY	3.4
35	1d	167	GLY	3.4
1	1A	1058	G	3.4
1	2A	2110	G	3.4
45	2n	30	ALA	3.4
1	1A	1065	U	3.4
1	2A	2109	U	3.4
40	2i	120	ARG	3.4
1	1A	1100	C	3.4
7	2H	45	VAL	3.4
19	2X	95	LEU	3.4
21	1Z	170	THR	3.4
45	2n	22	THR	3.4
38	2g	82	GLY	3.4
29	17	47	ARG	3.4
44	2m	104	ARG	3.4
1	1A	1099	G	3.3
4	2E	51	PHE	3.3
32	1a	346	G	3.3
41	2j	54	PHE	3.3
46	2o	69	TYR	3.3
1	1A	2161	C	3.3
1	2A	2139	C	3.3

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Mol	Chain	Res	Type	RSRZ
32	1a	1007	C	3.3
3	2D	276	LYS	3.3
40	2i	108	VAL	3.3
50	2s	79	THR	3.3
50	2s	84	GLY	3.3
38	1g	85	TYR	3.3
47	1p	17	TYR	3.3
50	2s	52	TYR	3.3
22	20	12	ASN	3.3
23	11	98	LEU	3.3
33	1b	229	VAL	3.3
34	1c	75	VAL	3.3
33	2b	21	ARG	3.3
21	2Z	121	HIS	3.3
50	2s	14	HIS	3.3
1	1A	2171	A	3.3
32	1a	1531	A	3.3
43	2l	126	LYS	3.3
21	1Z	99	TYR	3.3
40	2i	92	TYR	3.3
1	1A	1082	U	3.3
32	1a	1000	U	3.3
39	2h	2	LEU	3.3
40	2i	21	PRO	3.3
36	2e	23	GLY	3.3
8	2I	146	ALA	3.3
50	2s	38	SER	3.3
51	1t	11	SER	3.3
43	2l	64	TYR	3.3
32	2a	1257	U	3.3
21	1Z	150	LEU	3.3
52	2u	24	ARG	3.3
1	2A	2116	G	3.3
34	2c	130	VAL	3.3
34	2c	138	VAL	3.3
41	2j	49	VAL	3.3
57	1y	18	G	3.3
1	1A	2164	C	3.3
1	2A	1536	C	3.3
1	2A	2128	C	3.3
39	2h	90	GLY	3.3
54	2w	72	C	3.3

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Mol	Chain	Res	Type	RSRZ
41	2j	50	ILE	3.3
33	2b	34	ALA	3.3
33	2b	161	ALA	3.3
44	2m	28	ALA	3.3
45	2n	36	PHE	3.2
32	1a	1257	U	3.2
46	2o	60	VAL	3.2
45	2n	4	LYS	3.2
34	2c	124	ILE	3.2
1	2A	2168	G	3.2
45	2n	61	TRP	3.2
19	2X	68	ARG	3.2
53	2v	24	A	3.2
6	2G	142	PRO	3.2
37	2f	45	LEU	3.2
41	2j	8	LEU	3.2
50	2s	80	TYR	3.2
1	2A	2130	U	3.2
21	2Z	96	VAL	3.2
39	1h	93	VAL	3.2
40	2i	17	VAL	3.2
44	2m	37	THR	3.2
36	2e	86	ALA	3.2
1	2A	2177	C	3.2
57	2y	35	C	3.2
57	2y	48	C	3.2
57	2y	75	C	3.2
32	2a	1002	G	3.2
21	1Z	149	SER	3.2
21	2Z	136	PHE	3.2
45	2n	37	PHE	3.2
32	1a	1035	A	3.2
32	2a	1016	A	3.2
41	2j	91	PRO	3.2
20	1Y	1	MET	3.2
40	2i	67	GLY	3.2
50	2s	9	VAL	3.2
45	2n	3	ARG	3.2
1	1A	2137	C	3.2
57	2y	36	C	3.2
57	1y	1	G	3.2
7	2H	7	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
34	2c	90	GLU	3.2
45	2n	53	LEU	3.2
42	1k	25	TYR	3.2
7	2H	11	VAL	3.2
7	2H	17	VAL	3.2
34	2c	159	GLY	3.2
42	2k	49	GLY	3.2
52	2u	16	GLY	3.2
1	2A	2108	C	3.1
32	1a	1008	C	3.1
32	2a	1018	C	3.1
32	2a	1039	C	3.1
32	2a	1149	C	3.1
33	2b	189	ASP	3.1
40	2i	105	ASP	3.1
34	1c	87	LEU	3.1
41	2j	88	LEU	3.1
6	2G	132	ASN	3.1
38	1g	84	ASN	3.1
1	2A	2154	G	3.1
32	1a	1009	G	3.1
21	2Z	170	THR	3.1
33	1b	127	ILE	3.1
34	2c	14	ILE	3.1
34	2c	191	THR	3.1
41	2j	87	THR	3.1
1	2A	2150	U	3.1
32	2a	1196	U	3.1
38	1g	79	ARG	3.1
33	1b	17	PHE	3.1
34	2c	43	LEU	3.1
34	2c	87	LEU	3.1
38	2g	16	LEU	3.1
32	2a	1030	C	3.1
1	1A	1056	G	3.1
1	1A	1093	G	3.1
1	2A	1533	G	3.1
1	2A	2318	G	3.1
21	2Z	71	VAL	3.1
32	1a	630	G	3.1
32	1a	1002	G	3.1
32	2a	1222	G	3.1

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Mol	Chain	Res	Type	RSRZ
44	2m	98	VAL	3.1
1	2A	899	A	3.1
1	2A	2170	A	3.1
11	2P	15	ARG	3.1
14	2S	20	ARG	3.1
33	1b	123	ALA	3.1
20	2Y	94	LYS	3.1
33	2b	22	LYS	3.1
10	1O	108	GLU	3.1
7	2H	61	HIS	3.1
12	2Q	2	LEU	3.1
34	2c	62	ASP	3.1
41	1j	88	LEU	3.1
1	1A	2185	C	3.1
1	2A	2129	C	3.1
11	2P	79	ARG	3.1
19	2X	94	GLY	3.1
32	2a	999	C	3.1
33	2b	214	ILE	3.1
34	2c	192	THR	3.1
1	2A	2149	G	3.1
40	2i	122	ALA	3.1
41	2j	41	PRO	3.1
20	2Y	107	ASP	3.1
40	2i	18	PHE	3.1
12	2Q	102	VAL	3.1
1	1A	34	C	3.1
14	2S	35	ILE	3.1
34	2c	99	VAL	3.1
32	1a	221	C	3.1
48	1q	7	THR	3.0
34	2c	200	ALA	3.0
1	1A	1087	G	3.0
32	2a	1124	G	3.0
33	2b	234	PRO	3.0
57	2y	1	G	3.0
35	1d	194	LEU	3.0
50	1s	71	LEU	3.0
40	1i	126	SER	3.0
6	1G	51	ARG	3.0
22	20	55	ARG	3.0
34	2c	190	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
36	2e	27	ARG	3.0
26	14	56	VAL	3.0
29	17	46	VAL	3.0
33	2b	80	ILE	3.0
34	2c	68	VAL	3.0
45	2n	42	ILE	3.0
50	2s	77	THR	3.0
32	2a	1043	C	3.0
20	2Y	5	MET	3.0
40	2i	114	TYR	3.0
32	1a	1005	A	3.0
32	2a	1001	A	3.0
9	2N	112	LEU	3.0
14	2S	110	LEU	3.0
34	2c	52	LEU	3.0
26	24	51	ASP	3.0
54	2w	18	G	3.0
9	2N	83	LYS	3.0
45	1n	4	LYS	3.0
36	2e	20	GLN	3.0
36	2e	109	ILE	3.0
41	2j	6	ILE	3.0
44	2m	101	GLN	3.0
44	2m	105	THR	3.0
1	2A	2175	C	3.0
26	14	63	TYR	3.0
34	1c	184	TYR	3.0
54	2w	2	C	3.0
54	2w	70	C	3.0
1	1A	1098	A	3.0
1	2A	2119	A	3.0
32	2a	1035	A	3.0
53	1v	12	A	3.0
55	2x	47	U	3.0
57	1y	15	A	3.0
36	2e	45	PHE	3.0
22	20	49	LYS	3.0
1	1A	2133	G	3.0
1	2A	2182	G	3.0
32	2a	1030(A)	G	3.0
41	2j	76	ASN	3.0
33	1b	227	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
40	2i	39	GLY	3.0
34	2c	157	ILE	3.0
34	2c	202	ILE	3.0
44	2m	103	THR	3.0
4	1E	204	ALA	3.0
29	27	45	ALA	3.0
40	2i	82	ALA	3.0
21	2Z	159	PRO	3.0
3	2D	262	ARG	3.0
46	1o	57	LEU	3.0
52	1u	6	ARG	3.0
1	1A	889	C	3.0
1	2A	2105	C	3.0
40	2i	101	PHE	3.0
50	2s	12	ASP	3.0
54	2w	73	U	3.0
57	1y	19	U	3.0
41	2j	93	GLY	3.0
51	1t	55	ILE	2.9
1	1A	2123	G	2.9
1	2A	2156	G	2.9
1	2A	2893	G	2.9
10	1O	1	MET	2.9
54	1w	4	G	2.9
41	1j	32	ALA	2.9
45	1n	5	ALA	2.9
21	2Z	95	PRO	2.9
35	1d	29	PRO	2.9
43	1l	64	TYR	2.9
1	2A	2188	C	2.9
32	2a	995	C	2.9
1	2A	1026	U	2.9
53	1v	14	A	2.9
43	1l	63	GLY	2.9
6	2G	31	VAL	2.9
7	2H	58	GLU	2.9
20	2Y	45	VAL	2.9
34	1c	76	VAL	2.9
32	1a	1023	G	2.9
32	2a	993	G	2.9
38	2g	5	ARG	2.9
41	1j	77	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
57	2y	57	G	2.9
33	1b	236	TYR	2.9
1	1A	1066	U	2.9
1	1A	1097	U	2.9
32	2a	980	C	2.9
32	2a	1020	U	2.9
57	1y	68	C	2.9
57	2y	56	C	2.9
18	1W	112	GLY	2.9
36	1e	85	GLY	2.9
52	2u	4	GLY	2.9
1	1A	899	A	2.9
32	2a	1044	A	2.9
33	1b	134	GLU	2.9
53	2v	23	A	2.9
57	1y	38	A	2.9
33	1b	93	VAL	2.9
29	17	48	LYS	2.9
34	1c	60	ALA	2.9
34	2c	24	ALA	2.9
50	2s	50	ALA	2.9
11	1P	105	LEU	2.9
34	2c	47	LEU	2.9
44	2m	96	LEU	2.9
50	1s	5	LEU	2.9
1	1A	2125	G	2.9
1	1A	2149	G	2.9
1	1A	2162	G	2.9
1	2A	652(U)	G	2.9
1	2A	2157	G	2.9
40	1i	125	TYR	2.9
36	2e	26	PHE	2.9
42	2k	13	GLN	2.9
34	1c	185	GLY	2.9
38	1g	81	GLY	2.9
40	2i	72	GLY	2.9
50	2s	46	GLY	2.9
1	1A	2128	C	2.9
1	1A	2138	C	2.9
32	1a	1037	C	2.9
33	2b	39	ILE	2.9
1	1A	1070	A	2.9

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Mol	Chain	Res	Type	RSRZ
7	2H	50	VAL	2.9
22	20	11	ARG	2.9
32	1a	1447	A	2.9
34	1c	207	VAL	2.9
45	2n	31	ARG	2.9
41	2j	55	LYS	2.9
51	1t	68	LYS	2.9
22	20	43	THR	2.9
36	2e	16	THR	2.9
41	1j	100	THR	2.9
45	1n	20	ALA	2.9
33	1b	24	TRP	2.9
21	2Z	88	PHE	2.9
26	14	49	PHE	2.9
26	24	67	TYR	2.9
38	1g	154	TYR	2.9
40	2i	37	PHE	2.9
57	1y	17	G	2.9
21	2Z	168	GLU	2.9
9	2N	77	GLY	2.9
36	2e	22	GLY	2.9
36	2e	85	GLY	2.9
44	1m	6	GLY	2.9
6	2G	20	ILE	2.8
20	2Y	44	ILE	2.8
20	2Y	75	ILE	2.8
38	2g	4	ARG	2.8
42	2k	117	ASN	2.8
40	2i	95	LYS	2.8
45	1n	7	ILE	2.8
32	2a	1040	U	2.8
50	2s	45	VAL	2.8
32	1a	1027	C	2.8
1	1A	2158	A	2.8
40	2i	103	THR	2.8
41	2j	42	THR	2.8
50	2s	59	PRO	2.8
52	2u	23	PRO	2.8
33	1b	221	LEU	2.8
34	2c	196	LEU	2.8
42	2k	103	LEU	2.8
21	1Z	148	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
22	20	69	PHE	2.8
33	2b	70	PHE	2.8
43	2l	16	GLU	2.8
21	2Z	99	TYR	2.8
34	2c	184	TYR	2.8
34	2c	171	GLY	2.8
36	2e	18	ARG	2.8
41	1j	46	ARG	2.8
52	2u	6	ARG	2.8
1	1A	2151	G	2.8
1	2A	2124	G	2.8
33	2b	201	ILE	2.8
54	2w	7	G	2.8
1	2A	2189	U	2.8
5	2F	114	VAL	2.8
21	2Z	165	VAL	2.8
33	2b	112	VAL	2.8
33	2b	230	VAL	2.8
45	1n	25	VAL	2.8
57	2y	33	U	2.8
29	27	24	THR	2.8
1	1A	2105	C	2.8
45	2n	40	CYS	2.8
32	1a	1001	A	2.8
32	1a	1030(D)	A	2.8
12	2Q	12	GLN	2.8
15	1T	125	ARG	2.8
19	2X	69	TYR	2.8
33	2b	99	GLY	2.8
6	1G	52	ILE	2.8
51	1t	9	ASN	2.8
21	2Z	68	PRO	2.8
36	2e	115	VAL	2.8
37	2f	6	VAL	2.8
32	2a	1117	G	2.8
34	2c	67	THR	2.8
34	2c	137	ALA	2.8
34	2c	178	LEU	2.8
36	2e	31	LEU	2.8
40	1i	15	ALA	2.8
47	1p	45	THR	2.8
1	1A	885	C	2.8

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Mol	Chain	Res	Type	RSRZ
32	2a	1027	C	2.8
32	2a	1531	A	2.8
57	1y	24	A	2.8
6	2G	88	ILE	2.8
51	1t	63	ILE	2.8
41	2j	37	PRO	2.8
29	17	45	ALA	2.8
33	2b	215	LEU	2.8
36	1e	21	ALA	2.8
41	1j	48	THR	2.8
32	2a	1126	U	2.8
45	2n	6	LEU	2.8
49	2r	20	ALA	2.8
1	2A	2100	G	2.8
1	2A	2121	G	2.8
32	2a	1017	G	2.8
41	2j	86	MET	2.8
6	1G	136	ARG	2.8
24	12	70	GLN	2.8
24	22	70	GLN	2.8
29	27	47	ARG	2.8
1	1A	1069	A	2.8
1	2A	896	A	2.8
1	2A	2103	C	2.8
1	2A	2803	C	2.8
32	1a	1039	C	2.8
32	1a	1158	C	2.8
33	1b	30	ARG	2.8
39	2h	30	ARG	2.8
57	1y	69	C	2.8
57	1y	74	C	2.8
57	2y	74	C	2.8
33	1b	113	HIS	2.8
47	1p	13	HIS	2.8
5	1F	207	GLY	2.7
31	29	21	GLY	2.7
40	2i	69	GLY	2.7
41	1j	47	PHE	2.8
7	2H	136	ILE	2.7
33	1b	214	ILE	2.7
33	2b	131	PRO	2.7
40	2i	86	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
24	22	60	LEU	2.7
40	2i	27	THR	2.7
41	2j	100	THR	2.7
50	2s	16	LEU	2.7
44	2m	5	ALA	2.7
45	2n	20	ALA	2.7
45	2n	59	ALA	2.7
1	1A	12	U	2.7
25	13	60	GLU	2.7
36	2e	25	ARG	2.7
1	2A	2805	G	2.7
1	2A	2126	A	2.7
54	1w	2	C	2.7
33	2b	17	PHE	2.7
35	1d	23	GLY	2.7
50	2s	10	PHE	2.7
48	1q	36	ILE	2.7
7	2H	168	PRO	2.7
34	2c	7	PRO	2.7
52	1u	23	PRO	2.7
14	2S	46	VAL	2.7
25	23	59	VAL	2.7
30	28	64	TYR	2.7
44	2m	21	TYR	2.7
45	2n	21	TYR	2.7
48	2q	95	TYR	2.7
8	1I	38	LEU	2.7
28	26	11	LEU	2.7
34	2c	42	LEU	2.7
41	2j	90	LEU	2.7
6	1G	50	ALA	2.7
12	2Q	121	ALA	2.7
34	2c	95	THR	2.7
36	1e	17	ALA	2.7
48	2q	82	MET	2.7
9	2N	74	ARG	2.7
40	2i	9	ARG	2.7
41	1j	45	ARG	2.7
46	1o	68	ARG	2.7
41	2j	13	HIS	2.7
1	2A	2127	G	2.7
1	2A	2166	G	2.7

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Mol	Chain	Res	Type	RSRZ
32	2a	1031	G	2.7
41	2j	36	GLY	2.7
1	2A	2140	C	2.7
1	2A	2176	A	2.7
16	2U	62	ILE	2.7
32	2a	1223	C	2.7
57	1y	27	A	2.7
34	1c	39	ILE	2.7
35	2d	5	ILE	2.7
44	2m	113	PRO	2.7
47	1p	46	PRO	2.7
6	1G	139	LEU	2.7
21	2Z	127	LYS	2.7
34	2c	151	VAL	2.7
34	2c	195	VAL	2.7
34	2c	198	VAL	2.7
35	1d	22	LYS	2.7
36	2e	51	VAL	2.7
33	1b	61	LEU	2.7
35	1d	157	LEU	2.7
39	1h	112	LEU	2.7
12	2Q	129	THR	2.7
14	2S	3	ARG	2.7
15	2T	108	ARG	2.7
21	2Z	152	ALA	2.7
34	2c	163	ALA	2.7
38	2g	128	ALA	2.7
41	2j	66	ARG	2.7
45	2n	29	ARG	2.7
47	1p	42	ARG	2.7
40	2i	110	GLU	2.7
32	1a	1025	U	2.7
6	2G	77	ILE	2.7
12	2Q	65	PHE	2.7
14	2S	29	PHE	2.7
7	2H	128	PRO	2.7
21	2Z	158	PRO	2.7
33	2b	42	ILE	2.7
38	2g	42	ILE	2.7
1	2A	2164	C	2.7
32	2a	1037	C	2.7
34	2c	45	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
37	2f	7	ASN	2.7
41	2j	78	ASN	2.7
45	2n	17	LYS	2.7
21	2Z	16	SER	2.7
34	2c	94	LEU	2.7
38	2g	32	ARG	2.7
43	2l	43	VAL	2.7
44	2m	90	LEU	2.7
45	2n	12	ARG	2.7
50	2s	15	LEU	2.7
50	2s	35	SER	2.7
28	16	4	GLU	2.7
33	2b	148	TYR	2.7
40	2i	4	TYR	2.7
44	2m	64	TRP	2.7
32	2a	1532	U	2.7
57	1y	32	U	2.7
50	2s	13	ASP	2.6
36	2e	99	GLY	2.6
9	2N	44	PRO	2.6
20	2Y	53	PRO	2.6
21	2Z	104	PHE	2.6
25	13	2	PRO	2.6
26	24	49	PHE	2.6
41	2j	77	PRO	2.6
52	2u	3	LYS	2.6
8	2I	82	ARG	2.6
7	2H	15	VAL	2.6
32	1a	1286	A	2.6
34	2c	12	LEU	2.6
34	2c	153	VAL	2.6
34	2c	173	VAL	2.6
38	2g	21	VAL	2.6
1	2A	2165	G	2.6
8	2I	122	GLU	2.6
33	1b	129	GLU	2.6
33	2b	86	GLU	2.6
35	1d	179	GLU	2.6
54	2w	1	G	2.6
6	2G	50	ALA	2.6
18	2W	93	ALA	2.6
35	2d	164	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
38	2g	40	ALA	2.6
40	1i	122	ALA	2.6
42	2k	25	TYR	2.6
47	1p	38	TYR	2.6
33	1b	97	TRP	2.6
1	2A	2122	U	2.6
20	1Y	107	ASP	2.6
26	24	65	ASP	2.6
32	1a	1532	U	2.6
26	24	29	PRO	2.6
34	2c	57	ILE	2.6
35	2d	206	PHE	2.6
52	2u	13	ILE	2.6
14	2S	17	ARG	2.6
45	2n	35	ARG	2.6
9	1N	138	LEU	2.6
9	2N	5	VAL	2.6
9	2N	140	VAL	2.6
42	2k	105	VAL	2.6
50	2s	41	VAL	2.6
1	1A	2134	A	2.6
1	1A	2163	C	2.6
6	1G	46	ALA	2.6
40	2i	84	ALA	2.6
44	2m	42	ALA	2.6
54	2w	61	C	2.6
1	2A	2131	G	2.6
35	2d	54	TYR	2.6
45	2n	49	HIS	2.6
42	2k	124	LYS	2.6
43	2l	47	LYS	2.6
7	2H	82	GLY	2.6
7	2H	21	PRO	2.6
33	2b	202	PRO	2.6
35	1d	51	PRO	2.6
52	2u	10	ARG	2.6
57	1y	33	U	2.6
21	1Z	136	PHE	2.6
33	2b	83	MET	2.6
47	1p	19	ILE	2.6
8	2I	64	GLU	2.6
32	2a	1286	A	2.6

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Mol	Chain	Res	Type	RSRZ
47	1p	69	THR	2.6
54	1w	15	A	2.6
14	2S	7	TYR	2.6
32	2a	1019	C	2.6
40	2i	125	TYR	2.6
54	1w	70	C	2.6
20	1Y	94	LYS	2.6
40	2i	112	LYS	2.6
1	1A	2131	G	2.6
1	2A	2123	G	2.6
32	1a	1024	G	2.6
32	2a	1001(A)	G	2.6
32	2a	1061	G	2.6
54	2w	3	G	2.6
57	2y	3	G	2.6
22	20	82	ARG	2.6
33	1b	18	GLY	2.6
33	1b	130	ARG	2.6
34	2c	205	GLY	2.6
35	1d	87	GLY	2.6
7	2H	41	MET	2.6
41	2j	53	PRO	2.6
33	1b	42	ILE	2.6
34	2c	152	ILE	2.6
32	1a	204	U	2.6
33	2b	163	PHE	2.6
38	1g	26	PHE	2.6
57	2y	12	U	2.6
6	2G	176	LEU	2.6
34	1c	195	VAL	2.6
34	2c	55	VAL	2.6
42	2k	14	VAL	2.6
31	29	20	HIS	2.6
33	1b	140	HIS	2.6
39	2h	3	THR	2.6
51	2t	97	ALA	2.6
39	2h	98	LYS	2.6
1	1A	1095	A	2.6
1	1A	2790	A	2.6
32	1a	344	A	2.6
32	2a	1447	A	2.6
42	1k	75	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	2A	2178	C	2.5
1	2A	2789	C	2.5
54	2w	56	C	2.5
57	2y	62	C	2.5
21	1Z	159	PRO	2.5
33	2b	48	MET	2.5
35	2d	183	GLY	2.5
36	2e	106	PRO	2.5
45	2n	14	PRO	2.5
1	2A	882	G	2.5
32	1a	348	G	2.5
41	1j	38	ILE	2.5
54	1w	3	G	2.5
21	1Z	2	GLU	2.5
6	2G	19	LEU	2.5
7	2H	103	LEU	2.5
15	1T	114	LEU	2.5
32	2a	1000	U	2.5
33	2b	145	LEU	2.5
35	1d	162	LEU	2.5
41	2j	71	LEU	2.5
8	1I	142	VAL	2.5
15	2T	30	VAL	2.5
41	1j	33	GLN	2.5
33	1b	19	HIS	2.5
34	1c	71	ALA	2.5
38	2g	2	ALA	2.5
51	1t	74	LYS	2.5
35	1d	89	THR	2.5
42	2k	31	THR	2.5
34	1c	79	ARG	2.5
52	2u	15	ARG	2.5
1	2A	229	A	2.5
21	2Z	9	TYR	2.5
22	20	26	TYR	2.5
9	2N	1	MET	2.5
4	2E	115	GLY	2.5
40	2i	98	PRO	2.5
32	1a	999	C	2.5
41	2j	52	GLY	2.5
50	1s	84	GLY	2.5
52	1u	19	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
15	2T	52	ILE	2.5
33	1b	223	ILE	2.5
44	2m	78	ILE	2.5
47	2p	48	TRP	2.5
1	1A	2168	G	2.5
1	2A	2181	G	2.5
57	2y	51	G	2.5
32	1a	202	U	2.5
57	1y	65	U	2.5
7	2H	37	VAL	2.5
7	2H	114	VAL	2.5
8	2I	81	VAL	2.5
20	2Y	49	VAL	2.5
34	1c	68	VAL	2.5
34	2c	135	LYS	2.5
40	2i	113	LYS	2.5
8	2I	55	ALA	2.5
19	2X	91	ALA	2.5
33	1b	186	ALA	2.5
35	2d	48	ALA	2.5
36	2e	17	ALA	2.5
38	1g	83	ALA	2.5
20	2Y	23	ARG	2.5
34	2c	172	ARG	2.5
44	1m	102	ARG	2.5
44	2m	88	ARG	2.5
44	2m	94	ARG	2.5
33	1b	131	PRO	2.5
39	1h	62	TYR	2.5
42	2k	50	TYR	2.5
43	2l	69	TYR	2.5
1	1A	1086	A	2.5
20	2Y	58	GLY	2.5
34	2c	25	GLY	2.5
33	2b	185	ILE	2.5
41	2j	83	GLU	2.5
45	2n	46	GLU	2.5
1	1A	2107	C	2.5
32	2a	1260	C	2.5
6	2G	152	LEU	2.5
22	10	84	LEU	2.5
22	20	45	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
26	24	59	PHE	2.5
33	1b	70	PHE	2.5
39	1h	2	LEU	2.5
40	2i	59	PHE	2.5
20	2Y	54	LYS	2.5
1	2A	2144	U	2.5
38	1g	9	VAL	2.5
39	2h	61	VAL	2.5
40	1i	53	VAL	2.5
1	1A	2207	G	2.5
32	1a	1026	G	2.5
32	2a	630	G	2.5
57	1y	67	G	2.5
33	2b	77	ALA	2.5
40	2i	20	ARG	2.5
42	2k	89	ALA	2.5
43	2l	56	ALA	2.5
44	2m	57	ARG	2.5
50	2s	75	ALA	2.5
34	2c	109	PRO	2.5
52	2u	11	GLY	2.5
7	2H	157	TYR	2.5
34	2c	23	TYR	2.5
36	2e	131	ILE	2.5
39	2h	8	ASP	2.5
2	2B	120	A	2.5
7	2H	64	LEU	2.5
33	1b	22	LYS	2.5
33	1b	133	LYS	2.5
34	2c	4	LYS	2.5
34	2c	32	LEU	2.5
44	2m	13	LYS	2.5
1	1A	2140	C	2.5
32	2a	1116	C	2.5
41	1j	62	HIS	2.5
7	2H	133	VAL	2.5
33	2b	15	VAL	2.5
37	1f	88	VAL	2.5
45	1n	33	VAL	2.5
14	2S	30	ARG	2.5
32	1a	65	U	2.5
38	1g	78	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
48	2q	38	ARG	2.5
51	1t	8	ARG	2.5
52	2u	7	ARG	2.5
7	2H	150	ALA	2.5
33	2b	29	ALA	2.5
40	2i	94	ALA	2.5
6	1G	145	THR	2.5
17	2V	73	SER	2.5
41	2j	48	THR	2.5
32	1a	64	G	2.5
32	1a	1031	G	2.5
32	1a	1034	G	2.5
32	2a	971	G	2.5
57	1y	39	G	2.5
6	2G	32	PRO	2.4
41	2j	39	PRO	2.4
24	22	66	GLU	2.4
33	1b	228	GLY	2.4
34	2c	9	GLY	2.4
34	2c	194	GLY	2.4
21	1Z	120	ILE	2.4
34	2c	84	ILE	2.4
34	2c	201	TYR	2.4
37	2f	59	TYR	2.4
40	2i	63	ILE	2.4
44	2m	4	ILE	2.4
44	2m	31	LYS	2.4
51	1t	14	LYS	2.4
52	2u	5	ASP	2.4
4	2E	5	LEU	2.4
14	2S	58	LEU	2.4
27	25	58	LEU	2.4
34	2c	33	LEU	2.4
40	2i	56	LEU	2.4
1	1A	1045	A	2.4
32	2a	1251	A	2.4
32	2a	1503	A	2.4
35	1d	49	ARG	2.4
7	2H	35	VAL	2.4
32	2a	979	C	2.4
47	2p	2	VAL	2.4
48	2q	9	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
49	1r	86	VAL	2.4
54	1w	72	C	2.4
1	1A	1026	U	2.4
44	1m	5	ALA	2.4
44	2m	72	ALA	2.4
9	2N	73	THR	2.4
6	2G	17	PRO	2.4
25	23	2	PRO	2.4
45	2n	54	PRO	2.4
1	1A	2104	G	2.4
1	2A	2833	G	2.4
20	2Y	46	LYS	2.4
32	1a	79	G	2.4
32	2a	953	G	2.4
41	1j	36	GLY	2.4
41	2j	14	LYS	2.4
50	2s	62	ILE	2.4
23	11	82	LEU	2.4
33	2b	31	TYR	2.4
40	2i	5	TYR	2.4
45	2n	44	LEU	2.4
51	2t	10	LEU	2.4
31	29	18	ARG	2.4
1	2A	2173	A	2.4
32	2a	965	A	2.4
32	2a	983	A	2.4
57	2y	21	A	2.4
8	2I	142	VAL	2.4
21	2Z	86	VAL	2.4
25	23	58	VAL	2.4
31	29	16	VAL	2.4
33	2b	93	VAL	2.4
35	1d	170	VAL	2.4
38	1g	17	VAL	2.4
50	1s	41	VAL	2.4
50	2s	11	VAL	2.4
1	2A	2143	C	2.4
40	2i	106	ALA	2.4
42	1k	89	ALA	2.4
45	2n	5	ALA	2.4
54	1w	69	C	2.4
54	2w	13	C	2.4

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Mol	Chain	Res	Type	RSRZ
1	1A	2132	U	2.4
32	1a	173	U	2.4
40	1i	7	THR	2.4
40	2i	7	THR	2.4
45	1n	13	THR	2.4
52	2u	17	THR	2.4
15	2T	67	SER	2.4
40	2i	97	LYS	2.4
43	2l	23	LYS	2.4
12	1Q	15	GLY	2.4
17	1V	101	GLY	2.4
36	2e	80	ILE	2.4
41	2j	96	ILE	2.4
8	2I	68	LEU	2.4
32	2a	1024	G	2.4
32	2a	1182	G	2.4
33	1b	187	LEU	2.4
33	2b	51	LEU	2.4
34	2c	28	GLN	2.4
34	2c	34	LEU	2.4
34	2c	170	GLN	2.4
35	1d	21	LEU	2.4
35	2d	176	LEU	2.4
36	1e	119	LEU	2.4
38	1g	124	LEU	2.4
40	1i	50	LEU	2.4
40	1i	99	LEU	2.4
50	2s	22	LEU	2.4
57	2y	7	G	2.4
7	1H	3	ARG	2.4
12	2Q	60	ARG	2.4
41	2j	9	ARG	2.4
6	1G	146	TYR	2.4
9	2N	75	TYR	2.4
34	1c	48	TYR	2.4
34	2c	48	TYR	2.4
44	2m	87	TYR	2.4
21	2Z	98	MET	2.4
21	2Z	105	VAL	2.4
34	2c	66	VAL	2.4
35	2d	198	VAL	2.4
40	1i	17	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
41	1j	86	MET	2.4
47	1p	2	VAL	2.4
48	1q	85	VAL	2.4
1	1A	1073	A	2.4
16	2U	44	ASN	2.4
32	2a	1236	A	2.4
57	2y	14	A	2.4
7	2H	145	ALA	2.4
28	26	42	TRP	2.4
33	1b	120	ALA	2.4
33	2b	88	ALA	2.4
34	2c	100	ALA	2.4
38	2g	65	ALA	2.4
34	2c	174	PRO	2.4
40	1i	2	GLU	2.4
1	1A	154(A)	C	2.4
1	2A	652(V)	C	2.4
1	2A	2183	C	2.4
40	2i	49	PRO	2.4
41	1j	91	PRO	2.4
50	2s	76	PRO	2.4
5	2F	207	GLY	2.4
7	2H	48	GLY	2.4
35	2d	2	GLY	2.4
38	2g	34	GLY	2.4
39	2h	130	GLY	2.4
46	1o	89	GLY	2.4
9	2N	61	ARG	2.4
24	12	69	ARG	2.4
26	14	51	ASP	2.4
28	16	28	ARG	2.4
29	27	23	ARG	2.4
33	2b	44	LEU	2.4
33	2b	118	LEU	2.4
33	2b	135	GLN	2.4
38	1g	4	ARG	2.4
38	2g	38	LEU	2.4
40	1i	102	LEU	2.4
41	2j	79	ARG	2.4
44	2m	66	LEU	2.4
52	2u	9	ARG	2.4
1	1A	2106	G	2.4

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Mol	Chain	Res	Type	RSRZ
26	24	32	TYR	2.4
32	2a	973	G	2.4
32	2a	1003	G	2.4
32	2a	1253	G	2.4
33	2b	152	PHE	2.4
41	2j	11	PHE	2.4
35	1d	112	VAL	2.4
35	1d	198	VAL	2.4
48	2q	23	VAL	2.4
39	2h	15	ASN	2.4
12	2Q	63	LYS	2.4
14	2S	19	LYS	2.4
40	2i	15	ALA	2.4
44	2m	33	ALA	2.4
6	1G	48	GLU	2.4
57	2y	46	A	2.4
7	2H	12	PRO	2.3
7	2H	55	PRO	2.3
34	2c	15	THR	2.3
52	1u	17	THR	2.3
54	2w	33	U	2.3
57	2y	59	U	2.3
32	2a	1242	C	2.3
41	2j	31	GLY	2.3
55	2x	1	C	2.3
6	2G	118	ARG	2.3
14	2S	13	ARG	2.3
20	1Y	50	ARG	2.3
34	2c	77	ILE	2.3
34	2c	79	ARG	2.3
19	2X	92	LEU	2.3
24	22	35	LEU	2.3
33	2b	149	LEU	2.3
41	1j	6	ILE	2.3
36	2e	133	TYR	2.3
21	1Z	139	VAL	2.3
34	2c	116	VAL	2.3
40	2i	65	VAL	2.3
45	2n	58	LYS	2.3
47	2p	12	LYS	2.3
1	1A	1089	G	2.3
1	1A	2148	G	2.3

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Mol	Chain	Res	Type	RSRZ
1	1A	2156	G	2.3
1	2A	2141	G	2.3
1	2A	2751	G	2.3
32	1a	1010	G	2.3
8	1I	146	ALA	2.3
34	1c	189	ALA	2.3
40	2i	43	ALA	2.3
51	1t	59	ALA	2.3
6	2G	2	PRO	2.3
21	2Z	167	PRO	2.3
33	2b	232	PRO	2.3
1	1A	1088	A	2.3
32	2a	978	A	2.3
32	2a	1110	A	2.3
32	2a	1256	A	2.3
34	2c	167	TRP	2.3
53	1v	24	A	2.3
7	2H	6	ARG	2.3
41	1j	35	SER	2.3
50	2s	68	GLY	2.3
51	1t	17	ARG	2.3
52	2u	22	ARG	2.3
32	1a	841	U	2.3
35	1d	201	GLN	2.3
36	1e	20	GLN	2.3
42	1k	13	GLN	2.3
54	2w	60	U	2.3
57	1y	64	U	2.3
4	2E	195	LEU	2.3
6	1G	152	LEU	2.3
14	1S	58	LEU	2.3
21	2Z	57	ILE	2.3
22	10	7	LEU	2.3
33	2b	11	LEU	2.3
36	2e	119	LEU	2.3
40	1i	96	LEU	2.3
41	2j	23	ILE	2.3
41	2j	85	LEU	2.3
1	2A	888	C	2.3
1	2A	2142	C	2.3
32	1a	1029	C	2.3
4	2E	96	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
35	1d	110	PHE	2.3
38	2g	26	PHE	2.3
41	2j	80	LYS	2.3
7	2H	79	VAL	2.3
40	1i	108	VAL	2.3
42	2k	75	TYR	2.3
44	2m	54	VAL	2.3
52	1u	21	TYR	2.3
8	1I	64	GLU	2.3
14	2S	55	ALA	2.3
34	2c	60	ALA	2.3
34	2c	133	ALA	2.3
38	2g	7	ALA	2.3
49	1r	24	ALA	2.3
1	1A	1176	G	2.3
1	2A	652(C)	G	2.3
7	2H	3	ARG	2.3
32	1a	1032	G	2.3
32	2a	1221	G	2.3
41	2j	67	THR	2.3
51	1t	86	ARG	2.3
54	2w	10	G	2.3
57	1y	53	G	2.3
32	2a	975	A	2.3
57	1y	37	A	2.3
57	1y	46	A	2.3
57	2y	23	A	2.3
33	2b	40	HIS	2.3
34	2c	6	HIS	2.3
25	23	26	LEU	2.3
33	1b	10	LEU	2.3
39	1h	111	ILE	2.3
39	2h	80	ILE	2.3
42	2k	48	ILE	2.3
43	2l	7	ILE	2.3
43	2l	93	LEU	2.3
51	1t	20	LEU	2.3
1	2A	2102	U	2.3
1	2A	2804	C	2.3
31	29	2	LYS	2.3
32	1a	1028	C	2.3
44	2m	65	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
48	1q	100	LYS	2.3
57	2y	13	C	2.3
7	2H	123	PHE	2.3
4	2E	73	GLU	2.3
8	2I	145	VAL	2.3
21	2Z	2	GLU	2.3
9	2N	78	TYR	2.3
22	20	66	VAL	2.3
34	1c	106	VAL	2.3
34	2c	29	TYR	2.3
35	2d	20	TYR	2.3
44	2m	17	VAL	2.3
50	2s	67	VAL	2.3
34	2c	3	ASN	2.3
34	2c	92	ALA	2.3
44	2m	106	ASN	2.3
34	1c	88	ARG	2.3
42	2k	126	ARG	2.3
52	1u	15	ARG	2.3
41	1j	87	THR	2.3
50	2s	39	THR	2.3
1	2A	1170	G	2.3
21	2Z	166	SER	2.3
32	2a	1042	G	2.3
33	1b	158	LEU	2.3
1	1A	1847	A	2.3
8	2I	109	ILE	2.3
39	2h	112	LEU	2.3
49	1r	76	LEU	2.3
50	2s	34	TRP	2.3
47	1p	43	LYS	2.3
32	2a	961	U	2.3
32	2a	992	U	2.3
1	1A	886	C	2.3
1	1A	2188	C	2.3
21	2Z	162	GLU	2.3
32	1a	345	C	2.3
32	1a	848	C	2.3
32	2a	972	C	2.3
11	2P	83	VAL	2.3
33	2b	229	VAL	2.3
36	2e	100	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
41	2j	94	VAL	2.3
25	23	29	ARG	2.3
40	2i	123	PRO	2.3
5	2F	115	ALA	2.2
7	2H	83	TYR	2.3
7	2H	96	ALA	2.2
18	2W	60	ASN	2.2
42	1k	96	ARG	2.3
33	2b	13	ALA	2.2
33	2b	207	ALA	2.2
34	2c	61	ALA	2.2
34	2c	65	ALA	2.2
44	2m	107	ALA	2.2
48	1q	95	TYR	2.3
51	1t	67	ALA	2.2
6	2G	161	THR	2.2
23	2l	79	GLY	2.2
33	1b	14	GLY	2.2
33	2b	140	HIS	2.2
38	1g	34	GLY	2.2
40	1i	39	GLY	2.2
46	2o	89	GLY	2.2
7	2H	72	ILE	2.2
7	2H	89	ILE	2.2
10	1O	112	MET	2.2
33	2b	132	LYS	2.2
34	2c	39	ILE	2.2
36	1e	10	MET	2.2
37	2f	14	LEU	2.2
40	1i	63	ILE	2.2
43	2l	54	LYS	2.2
45	2n	9	LYS	2.2
45	2n	15	LYS	2.2
48	1q	87	LYS	2.2
51	1t	24	LEU	2.2
51	2t	14	LYS	2.2
32	2a	974	A	2.2
33	2b	166	ASP	2.2
39	2h	4	ASP	2.2
41	2j	58	ASP	2.2
1	2A	2793	G	2.2
32	2a	1030(C)	G	2.2

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Mol	Chain	Res	Type	RSRZ
55	1x	46	G	2.2
1	1A	1083	U	2.2
1	1A	2189	U	2.2
32	2a	1150	U	2.2
57	1y	73	U	2.2
6	1G	137	GLU	2.2
33	2b	170	GLU	2.2
21	2Z	79	ARG	2.2
1	1A	1053	C	2.2
28	26	52	VAL	2.2
35	2d	73	ARG	2.2
36	2e	107	ARG	2.2
37	2f	56	PRO	2.2
38	2g	135	VAL	2.2
40	2i	111	ARG	2.2
43	2l	19	ARG	2.2
45	2n	56	VAL	2.2
50	1s	29	ARG	2.2
32	2a	1217	C	2.2
55	1x	1	C	2.2
57	1y	40	C	2.2
34	2c	187	ALA	2.2
35	2d	154	ASN	2.2
40	1i	43	ALA	2.2
42	1k	97	ALA	2.2
50	2s	24	ALA	2.2
14	2S	92	TYR	2.2
40	1i	62	TYR	2.2
46	1o	69	TYR	2.2
41	2j	92	THR	2.2
4	2E	29	GLY	2.2
11	2P	118	GLY	2.2
19	1X	94	GLY	2.2
26	14	54	GLY	2.2
34	2c	93	LYS	2.2
34	2c	91	LEU	2.2
35	1d	33	MET	2.2
46	2o	20	GLY	2.2
4	2E	63	LEU	2.2
17	2V	94	LEU	2.2
21	2Z	41	LEU	2.2
21	2Z	163	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
33	2b	127	ILE	2.2
3	2D	99	ASP	2.2
34	1c	62	ASP	2.2
33	2b	97	TRP	2.2
1	1A	1067	A	2.2
32	2a	1030(D)	A	2.2
34	1c	35	GLU	2.2
32	1a	223	U	2.2
32	2a	1278	U	2.2
57	2y	60	U	2.2
32	2a	1216	G	2.2
35	2d	132	ARG	2.2
57	1y	49	G	2.2
57	2y	49	G	2.2
20	1Y	60	PHE	2.2
8	2I	107	VAL	2.2
9	1N	9	VAL	2.2
21	1Z	95	PRO	2.2
33	1b	71	VAL	2.2
34	2c	73	PRO	2.2
34	2c	120	VAL	2.2
39	2h	79	VAL	2.2
1	1A	1076	C	2.2
1	1A	2103	C	2.2
36	2e	94	ALA	2.2
57	1y	13	C	2.2
57	1y	66	C	2.2
14	2S	83	LYS	2.2
26	24	63	TYR	2.2
33	2b	8	LYS	2.2
34	2c	27	LYS	2.2
40	1i	95	LYS	2.2
41	2j	56	HIS	2.2
44	1m	120	LYS	2.2
38	1g	89	MET	2.2
52	2u	8	THR	2.2
7	2H	166	GLY	2.2
21	1Z	157	LEU	2.2
41	1j	8	LEU	2.2
45	2n	47	LEU	2.2
28	26	54	ILE	2.2
48	1q	99	SER	2.2

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Mol	Chain	Res	Type	RSRZ
38	2g	33	ASP	2.2
8	2I	135	GLU	2.2
41	2j	64	GLU	2.2
7	2H	42	ARG	2.2
46	2o	88	ARG	2.2
1	1A	1054	A	2.2
1	1A	2176	A	2.2
1	2A	2118	U	2.2
32	1a	383	A	2.2
32	2a	946	A	2.2
32	2a	1180	A	2.2
57	2y	37	A	2.2
26	14	59	PHE	2.2
36	2e	96	PRO	2.2
34	2c	70	VAL	2.2
40	2i	109	VAL	2.2
1	1A	2127	G	2.2
4	2E	152	LYS	2.2
19	2X	33	LYS	2.2
20	2Y	34	LYS	2.2
26	24	2	LYS	2.2
32	1a	68	G	2.2
50	2s	32	LYS	2.2
52	2u	20	LYS	2.2
54	2w	5	G	2.2
57	1y	5	G	2.2
20	1Y	92	ASN	2.2
33	1b	13	ALA	2.2
33	1b	34	ALA	2.2
33	2b	186	ALA	2.2
34	2c	146	ALA	2.2
34	2c	180	ALA	2.2
3	2D	126	GLN	2.2
35	1d	181	MET	2.2
1	2A	2107	C	2.2
2	2B	88	C	2.2
3	2D	216	GLY	2.2
7	2H	67	LEU	2.2
12	2Q	19	GLY	2.2
26	14	45	GLY	2.2
32	1a	67	C	2.2
32	2a	1038	C	2.2

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Mol	Chain	Res	Type	RSRZ
32	2a	1059	C	2.2
32	2a	1060	C	2.2
34	2c	165	THR	2.2
35	2d	167	GLY	2.2
38	2g	99	LEU	2.2
40	1i	57	GLY	2.2
41	1j	40	LEU	2.2
44	2m	112	GLY	2.2
50	1s	15	LEU	2.2
54	2w	68	C	2.2
57	1y	25	C	2.2
57	2y	72	C	2.2
8	1l	51	ILE	2.2
16	2U	88	ILE	2.2
36	1e	109	ILE	2.2
41	1j	74	ILE	2.2
33	1b	9	GLU	2.2
25	23	55	ARG	2.2
34	2c	11	ARG	2.2
39	2h	18	ARG	2.2
39	1h	89	PRO	2.2
45	1n	61	TRP	2.2
1	2A	2180	U	2.2
3	1D	38	LYS	2.2
7	2H	85	LYS	2.2
32	2a	532	A	2.1
32	2a	997	U	2.2
44	2m	27	LYS	2.2
54	1w	23	A	2.1
57	2y	32	U	2.2
57	2y	73	U	2.2
22	10	2	ALA	2.1
34	2c	160	ALA	2.1
51	2t	9	ASN	2.1
1	2A	530	G	2.1
1	2A	883	G	2.1
1	2A	2101	G	2.1
6	2G	43	LEU	2.1
15	2T	69	GLY	2.1
20	2Y	93	GLY	2.1
22	20	10	THR	2.1
32	1a	78	G	2.1

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Mol	Chain	Res	Type	RSRZ
32	1a	181	G	2.1
32	1a	380	G	2.1
33	2b	168	THR	2.1
49	2r	79	LEU	2.1
51	1t	13	LEU	2.1
54	1w	71	G	2.1
54	2w	4	G	2.1
57	1y	22	G	2.1
57	2y	22	G	2.1
30	28	16	ILE	2.1
46	1o	3	ILE	2.1
47	2p	19	ILE	2.1
57	1y	48	C	2.1
57	1y	70	C	2.1
6	2G	54	GLU	2.1
7	2H	51	ARG	2.1
7	2H	170	ARG	2.1
24	22	51	ARG	2.1
35	1d	25	ARG	2.1
40	2i	107	ARG	2.1
40	2i	121	ARG	2.1
41	2j	46	ARG	2.1
47	1p	5	ARG	2.1
33	2b	43	ASP	2.1
47	1p	47	ASP	2.1
47	1p	68	ASP	2.1
48	2q	99	SER	2.1
7	2H	10	PRO	2.1
11	2P	76	LYS	2.1
43	1l	94	PRO	2.1
43	2l	94	PRO	2.1
44	2m	97	PRO	2.1
22	20	60	PHE	2.1
34	2c	10	PHE	2.1
40	1i	59	PHE	2.1
5	1F	89	VAL	2.1
33	2b	164	VAL	2.1
2	2B	1	U	2.1
12	2Q	103	MET	2.1
18	2W	111	HIS	2.1
34	1c	86	VAL	2.1
54	2w	11	U	2.1

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Mol	Chain	Res	Type	RSRZ
32	2a	1004	A	2.1
32	2a	1252	A	2.1
49	1r	73	ALA	2.1
54	2w	24	A	2.1
6	2G	34	LEU	2.1
12	2Q	24	GLY	2.1
14	2S	48	LEU	2.1
40	1i	67	GLY	2.1
47	1p	6	LEU	2.1
5	2F	82	ILE	2.1
21	2Z	124	ILE	2.1
37	1f	52	ILE	2.1
44	2m	22	ILE	2.1
1	1A	2152	G	2.1
1	2A	2321	G	2.1
6	2G	137	GLU	2.1
6	2G	146	TYR	2.1
7	2H	53	GLU	2.1
15	2T	115	ARG	2.1
21	2Z	94	GLU	2.1
21	2Z	103	ARG	2.1
41	1j	64	GLU	2.1
41	1j	79	ARG	2.1
41	2j	51	ARG	2.1
48	2q	96	GLU	2.1
51	2t	25	ARG	2.1
32	2a	1021	G	2.1
57	1y	4	G	2.1
57	2y	5	G	2.1
57	2y	39	G	2.1
32	2a	1118	C	2.1
32	2a	1119	C	2.1
57	1y	31	C	2.1
28	26	53	LYS	2.1
21	1Z	158	PRO	2.1
34	1c	73	PRO	2.1
35	1d	189	PRO	2.1
36	2e	49	PRO	2.1
39	1h	27	PRO	2.1
12	2Q	106	VAL	2.1
33	1b	15	VAL	2.1
41	1j	44	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	2A	2172	U	2.1
4	2E	28	ALA	2.1
12	2Q	114	ALA	2.1
32	1a	1040	U	2.1
1	1A	890	A	2.1
38	1g	16	LEU	2.1
39	1h	133	LEU	2.1
44	1m	56	LEU	2.1
53	2v	15	A	2.1
40	1i	103	THR	2.1
14	1S	13	ARG	2.1
34	2c	88	ARG	2.1
38	2g	3	ARG	2.1
21	2Z	53	ILE	2.1
33	1b	12	GLU	2.1
33	2b	208	ILE	2.1
38	2g	49	ILE	2.1
51	1t	100	ILE	2.1
26	24	25	TYR	2.1
34	2c	17	ASP	2.1
45	2n	60	SER	2.1
1	1A	1091	G	2.1
1	1A	2157	G	2.1
1	1A	2184	G	2.1
1	2A	2151	G	2.1
2	2B	118	G	2.1
32	1a	220	G	2.1
32	1a	1030(A)	G	2.1
32	2a	1058	G	2.1
32	2a	1356	G	2.1
1	1A	1080	C	2.1
32	1a	163	C	2.1
32	1a	1006	C	2.1
32	1a	1260	C	2.1
32	2a	1128	C	2.1
32	2a	1137	C	2.1
32	2a	1192	C	2.1
14	2S	34	HIS	2.1
35	1d	165	MET	2.1
44	2m	92	HIS	2.1
50	2s	57	HIS	2.1
5	1F	6	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
33	2b	28	PHE	2.1
34	1c	128	PHE	2.1
50	2s	58	VAL	2.1
12	2Q	28	ALA	2.1
21	2Z	21	ALA	2.1
20	2Y	92	ASN	2.1
6	1G	113	ARG	2.1
20	2Y	80	GLY	2.1
20	2Y	97	ARG	2.1
24	22	61	LEU	2.1
34	2c	204	LEU	2.1
39	2h	107	LEU	2.1
42	1k	42	TRP	2.1
40	1i	128	ARG	2.1
40	2i	104	ARG	2.1
51	1t	62	LEU	2.1
57	1y	59	U	2.1
52	1u	2	GLY	2.1
33	2b	47	THR	2.1
45	2n	8	GLU	2.1
1	1A	1077	A	2.1
1	2A	528	A	2.1
20	2Y	38	ILE	2.1
32	2a	1492	A	2.1
34	2c	26	LYS	2.1
43	2l	20	LYS	2.1
4	2E	151	TYR	2.1
6	2G	12	TYR	2.1
27	25	17	ASP	2.1
40	1i	91	ASP	2.1
6	2G	76	SER	2.1
7	2H	112	PRO	2.1
20	2Y	66	PRO	2.1
26	14	18	CYS	2.1
35	1d	37	PRO	2.1
39	2h	67	PRO	2.1
44	1m	97	PRO	2.1
36	2e	10	MET	2.1
1	1A	1092	C	2.1
1	2A	11	G	2.0
32	1a	1137	C	2.1
32	2a	970	C	2.1

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Mol	Chain	Res	Type	RSRZ
16	1U	117	GLN	2.0
32	2a	1026	G	2.0
32	2a	1109	C	2.1
32	2a	1184	G	2.0
54	2w	25	C	2.1
34	1c	107	GLN	2.0
54	2w	26	G	2.0
57	2y	26	G	2.0
57	2y	53	G	2.0
3	2D	15	PHE	2.0
6	2G	23	PHE	2.0
8	1I	127	VAL	2.0
9	2N	62	VAL	2.0
11	2P	91	PHE	2.0
21	2Z	139	VAL	2.0
36	2e	69	VAL	2.0
40	1i	41	VAL	2.0
42	1k	14	VAL	2.0
42	1k	84	VAL	2.0
44	1m	98	VAL	2.0
50	2s	51	VAL	2.0
14	2S	79	ALA	2.0
34	1c	113	ALA	2.0
34	2c	50	ALA	2.0
35	2d	32	ALA	2.0
41	2j	26	ALA	2.0
11	2P	6	LEU	2.0
34	2c	175	LEU	2.0
41	1j	65	LEU	2.0
44	2m	34	LEU	2.0
5	2F	131	GLY	2.0
20	1Y	91	GLU	2.0
21	2Z	169	GLU	2.0
40	1i	12	GLU	2.0
12	2Q	64	ILE	2.0
20	2Y	87	LYS	2.0
31	29	31	LYS	2.0
32	2a	1351	U	2.0
33	2b	67	THR	2.0
34	2c	18	TRP	2.0
34	2c	199	LYS	2.0
41	1j	42	THR	2.0

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Mol	Chain	Res	Type	RSRZ
44	2m	120	LYS	2.0
51	1t	29	LYS	2.0
54	2w	12	U	2.0
57	2y	65	U	2.0
41	1j	50	ILE	2.0
41	1j	98	ILE	2.0
1	1A	1103	A	2.0
32	2a	1225	A	2.0
33	2b	33	TYR	2.0
33	2b	199	TYR	2.0
35	2d	4	TYR	2.0
39	1h	4	ASP	2.0
40	1i	98	PRO	2.0
40	2i	62	TYR	2.0
14	2S	52	SER	2.0
33	2b	101	MET	2.0
40	2i	124	GLN	2.0
1	2A	2896	C	2.0
17	2V	22	VAL	2.0
21	2Z	89	PHE	2.0
22	20	30	VAL	2.0
32	1a	174	C	2.0
33	1b	136	VAL	2.0
33	2b	57	PHE	2.0
34	1c	99	VAL	2.0
36	2e	34	VAL	2.0
36	2e	41	VAL	2.0
37	1f	90	VAL	2.0
40	1i	101	PHE	2.0
41	1j	5	ARG	2.0
45	2n	16	PHE	2.0
57	2y	63	C	2.0
57	2y	69	C	2.0
1	1A	1063	G	2.0
32	1a	1021	G	2.0
32	2a	1079	G	2.0
3	2D	177	LEU	2.0
8	2I	38	LEU	2.0
12	2Q	117	ALA	2.0
35	1d	120	LEU	2.0
36	2e	111	GLU	2.0
38	1g	12	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
39	2h	10	LEU	2.0
40	2i	13	ALA	2.0
57	2y	4	G	2.0
7	2H	159	GLU	2.0
33	1b	44	LEU	2.0
40	2i	40	LEU	2.0
44	2m	19	LEU	2.0
46	1o	66	LEU	2.0
50	2s	20	LEU	2.0
22	10	5	LYS	2.0
34	1c	41	GLY	2.0
34	1c	98	ASN	2.0
50	2s	53	ASN	2.0
51	1t	75	ASN	2.0
12	2Q	127	ILE	2.0
20	2Y	61	ILE	2.0
26	24	22	ILE	2.0
33	2b	222	ILE	2.0
40	2i	74	ILE	2.0
1	1A	2102	U	2.0
32	2a	982	U	2.0
32	2a	1205	U	2.0
32	2a	1235	U	2.0
54	2w	59	U	2.0
1	1A	1046	A	2.0
7	2H	36	PRO	2.0
12	2Q	39	PRO	2.0
32	2a	1250	A	2.0
32	2a	1357	A	2.0
21	2Z	28	MET	2.0
21	2Z	87	ASP	2.0
38	1g	20	ASP	2.0
44	2m	16	ASP	2.0
48	1q	28	PRO	2.0
54	2w	23	A	2.0
12	2Q	74	TYR	2.0
26	14	32	TYR	2.0
39	1h	87	SER	2.0
41	2j	35	SER	2.0
48	1q	97	SER	2.0
51	1t	61	SER	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	5MU	2y	54	21/22	0.27	0.21	101,111,118,134	0
57	4SU	2y	8	20/21	0.32	0.19	105,113,122,131	0
57	5MU	1y	54	21/22	0.43	0.15	105,110,115,127	0
57	PSU	1y	55	20/21	0.44	0.16	104,112,117,130	0
54	5MU	2w	54	21/22	0.46	0.18	100,104,109,115	0
57	4SU	1y	8	20/21	0.46	0.14	105,110,118,129	0
54	4SU	2w	8	20/21	0.49	0.16	104,111,124,129	0
57	PSU	2y	55	20/21	0.50	0.17	107,112,118,123	0
54	PSU	2w	55	20/21	0.53	0.15	104,108,117,120	0
54	4SU	1w	8	20/21	0.56	0.14	102,109,124,127	0
54	PSU	1w	55	20/21	0.69	0.13	97,100,112,112	0
54	5MU	1w	54	21/22	0.76	0.13	78,95,98,101	0
1	5MU	2A	1915	21/22	0.77	0.15	80,89,91,95	0
32	2MG	2a	1207	24/25	0.83	0.14	91,96,103,113	0
55	4SU	2x	8	20/21	0.86	0.11	91,96,99,103	0
55	PSU	2x	55	20/21	0.87	0.11	86,92,99,102	0
55	5MU	2x	54	21/22	0.88	0.11	89,96,98,104	0
43	0TD	2l	92	10/11	0.88	0.14	78,82,86,87	0
32	2MG	1a	1207	24/25	0.89	0.11	81,85,89,95	0
1	PSU	2A	1917	20/21	0.89	0.10	74,83,87,88	0
32	PSU	2a	516	20/21	0.89	0.11	80,89,93,95	0
55	5MU	1x	54	21/22	0.89	0.12	74,81,89,91	0
43	0TD	1l	92	10/11	0.90	0.16	66,75,78,95	0
1	5MU	1A	1915	21/22	0.90	0.12	64,74,80,81	0
32	G7M	2a	527	24/25	0.90	0.14	75,82,88,93	0
32	PSU	1a	516	20/21	0.91	0.10	72,77,81,81	0
54	L3X	2w	76	26/27	0.91	0.14	63,71,76,83	0
32	5MC	2a	1404	21/22	0.91	0.12	60,71,76,79	0
56	FME	1z	1	10/11	0.91	0.18	50,57,73,78	0
55	5MC	2x	32	21/22	0.91	0.13	79,85,90,95	0
55	4SU	1x	8	20/21	0.92	0.10	64,71,75,80	0
32	4OC	2a	1402	22/23	0.92	0.13	68,76,80,81	0
32	M2G	2a	966	25/26	0.92	0.15	67,79,96,97	0
32	5MC	2a	967	21/22	0.92	0.12	75,80,88,98	0
1	PSU	2A	1911	20/21	0.92	0.09	72,75,80,80	0
55	PSU	1x	55	20/21	0.92	0.09	66,77,86,93	0
32	5MC	2a	1400	21/22	0.92	0.16	81,85,89,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	OMC	2A	1920	21/22	0.93	0.10	65,73,78,80	0
32	5MC	2a	1407	21/22	0.93	0.11	61,68,74,77	0
55	5MC	1x	32	21/22	0.93	0.14	62,68,72,78	0
32	UR3	2a	1498	21/22	0.93	0.13	63,69,77,78	0
32	MA6	2a	1519	24/25	0.93	0.14	63,77,83,84	0
32	5MC	1a	967	21/22	0.94	0.10	58,64,71,78	0
54	L3X	1w	76	26/27	0.94	0.09	42,52,59,67	0
32	MA6	2a	1518	24/25	0.94	0.12	64,79,83,84	0
55	8AN	2x	76	22/23	0.94	0.11	55,65,72,76	0
1	PSU	1A	1917	20/21	0.94	0.09	59,68,76,76	0
56	FME	2z	1	10/11	0.94	0.18	66,76,86,87	0
1	5MC	2A	1962	21/22	0.95	0.10	43,57,66,73	0
32	M2G	1a	966	25/26	0.95	0.11	58,63,72,80	0
1	5MC	1A	1942	21/22	0.95	0.09	42,47,52,61	0
32	G7M	1a	527	24/25	0.96	0.09	62,68,71,74	0
1	5MU	2A	1939	21/22	0.96	0.09	42,50,56,58	0
1	5MC	2A	1942	21/22	0.96	0.09	58,69,73,79	0
1	PSU	1A	1911	20/21	0.96	0.08	51,59,64,65	0
1	PSU	2A	2605	20/21	0.96	0.08	40,49,59,59	0
32	5MC	1a	1400	21/22	0.96	0.12	56,65,67,70	0
55	8AN	1x	76	22/23	0.96	0.09	35,46,52,62	0
32	5MC	1a	1407	21/22	0.96	0.10	44,52,56,59	0
1	2MA	2A	2503	23/24	0.97	0.09	43,48,51,53	0
1	OMU	2A	2552	21/22	0.97	0.09	47,55,61,64	0
32	MA6	1a	1519	24/25	0.97	0.10	45,55,58,61	0
32	4OC	1a	1402	22/23	0.97	0.11	47,56,61,67	0
1	OMC	1A	1920	21/22	0.97	0.07	45,54,59,63	0
1	OMG	2A	2251	24/25	0.97	0.09	47,52,58,64	0
32	UR3	1a	1498	21/22	0.98	0.09	46,52,57,61	0
32	MA6	1a	1518	24/25	0.98	0.08	46,52,55,58	0
1	OMG	1A	2251	24/25	0.98	0.07	26,33,37,41	0
1	2MA	1A	2503	23/24	0.98	0.06	24,31,33,35	0
1	OMU	1A	2552	21/22	0.98	0.07	30,37,40,41	0
1	PSU	1A	2605	20/21	0.98	0.06	33,37,45,46	0
1	5MU	1A	1939	21/22	0.98	0.08	31,36,41,43	0
32	5MC	1a	1404	21/22	0.98	0.08	46,52,55,58	0
1	5MC	1A	1962	21/22	0.98	0.07	40,43,48,56	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

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
58	MG	1A	4051	1/1	0.22	0.28	78,78,78,78	0
58	MG	1x	101	1/1	0.42	0.37	98,98,98,98	0
58	MG	2a	1722	1/1	0.46	0.31	85,85,85,85	0
58	MG	2A	3281	1/1	0.50	0.31	89,89,89,89	0
58	MG	1a	1727	1/1	0.51	0.53	90,90,90,90	0
58	MG	1A	3524	1/1	0.55	0.30	72,72,72,72	0
58	MG	1a	1708	1/1	0.55	0.24	98,98,98,98	0
58	MG	2a	1822	1/1	0.55	0.41	98,98,98,98	0
58	MG	2a	1606	1/1	0.58	0.35	86,86,86,86	0
58	MG	2A	3588	1/1	0.60	0.22	81,81,81,81	0
58	MG	2A	3201	1/1	0.61	0.27	86,86,86,86	0
58	MG	18	106	1/1	0.61	0.23	76,76,76,76	0
58	MG	1A	3705	1/1	0.61	0.26	86,86,86,86	0
58	MG	2B	210	1/1	0.62	0.24	92,92,92,92	0
58	MG	2a	1795	1/1	0.63	0.22	93,93,93,93	0
58	MG	2w	102	1/1	0.64	0.36	92,92,92,92	0
58	MG	1B	229	1/1	0.65	0.16	93,93,93,93	0
58	MG	1a	1747	1/1	0.65	0.29	80,80,80,80	0
58	MG	1w	108	1/1	0.65	0.14	87,87,87,87	0
58	MG	2a	1608	1/1	0.65	0.45	89,89,89,89	0
58	MG	2x	108	1/1	0.65	0.23	79,79,79,79	0
58	MG	1B	228	1/1	0.66	0.17	87,87,87,87	0
58	MG	1w	106	1/1	0.66	0.24	97,97,97,97	0
58	MG	2a	1802	1/1	0.66	0.28	76,76,76,76	0
58	MG	2a	1782	1/1	0.67	0.17	97,97,97,97	0
58	MG	1a	1652	1/1	0.67	0.30	83,83,83,83	0
58	MG	1x	109	1/1	0.67	0.29	84,84,84,84	0
58	MG	2A	3097	1/1	0.67	0.18	75,75,75,75	0
58	MG	2A	3787	1/1	0.67	0.24	79,79,79,79	0
58	MG	2a	1780	1/1	0.67	0.27	73,73,73,73	0
58	MG	1A	3254	1/1	0.68	0.19	75,75,75,75	0
58	MG	2A	3599	1/1	0.68	0.27	73,73,73,73	0
58	MG	2a	1806	1/1	0.68	0.36	87,87,87,87	0
58	MG	2A	3678	1/1	0.68	0.20	62,62,62,62	0
58	MG	1a	1808	1/1	0.68	0.38	85,85,85,85	0
58	MG	1A	3691	1/1	0.68	0.23	56,56,56,56	0
58	MG	2a	1634	1/1	0.69	0.25	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1B	234	1/1	0.69	0.21	80,80,80,80	0
58	MG	2A	3346	1/1	0.69	0.17	80,80,80,80	0
58	MG	2A	3546	1/1	0.69	0.23	91,91,91,91	0
58	MG	2A	3780	1/1	0.69	0.17	80,80,80,80	0
58	MG	1A	3773	1/1	0.70	0.35	95,95,95,95	0
58	MG	2a	1697	1/1	0.70	0.40	86,86,86,86	0
58	MG	2v	101	1/1	0.70	0.56	85,85,85,85	0
58	MG	2a	1706	1/1	0.70	0.28	89,89,89,89	0
58	MG	2A	3654	1/1	0.70	0.14	79,79,79,79	0
58	MG	2A	3067	1/1	0.71	0.23	75,75,75,75	0
58	MG	2a	1785	1/1	0.71	0.24	80,80,80,80	0
58	MG	2A	3310	1/1	0.71	0.27	85,85,85,85	0
58	MG	2a	1800	1/1	0.71	0.27	80,80,80,80	0
58	MG	1a	1771	1/1	0.71	0.49	97,97,97,97	0
58	MG	2A	3702	1/1	0.71	0.23	86,86,86,86	0
58	MG	2A	3543	1/1	0.71	0.26	83,83,83,83	0
58	MG	2A	3118	1/1	0.71	0.24	89,89,89,89	0
58	MG	2a	1726	1/1	0.71	0.29	88,88,88,88	0
58	MG	1w	105	1/1	0.71	0.18	84,84,84,84	0
58	MG	2a	1779	1/1	0.72	0.23	95,95,95,95	0
58	MG	2A	3566	1/1	0.72	0.26	82,82,82,82	0
58	MG	2Q	203	1/1	0.72	0.24	72,72,72,72	0
58	MG	1A	3420	1/1	0.72	0.29	76,76,76,76	0
58	MG	1A	3247	1/1	0.72	0.52	80,80,80,80	0
58	MG	2a	1633	1/1	0.72	0.40	86,86,86,86	0
58	MG	1A	3531	1/1	0.72	0.33	71,71,71,71	0
58	MG	1A	3828	1/1	0.72	0.27	69,69,69,69	0
58	MG	2a	1813	1/1	0.72	0.32	95,95,95,95	0
58	MG	2A	3405	1/1	0.72	0.38	85,85,85,85	0
58	MG	1A	3583	1/1	0.72	0.17	60,60,60,60	0
58	MG	1B	220	1/1	0.72	0.18	65,65,65,65	0
58	MG	2a	1778	1/1	0.72	0.35	76,76,76,76	0
58	MG	1A	3792	1/1	0.73	0.25	59,59,59,59	0
58	MG	2A	3284	1/1	0.73	0.27	66,66,66,66	0
58	MG	2A	3295	1/1	0.73	0.25	83,83,83,83	0
58	MG	2a	1635	1/1	0.73	0.27	76,76,76,76	0
58	MG	1w	101	1/1	0.73	0.17	97,97,97,97	0
58	MG	1w	104	1/1	0.73	0.18	81,81,81,81	0
58	MG	2A	3351	1/1	0.73	0.27	77,77,77,77	0
58	MG	1A	3753	1/1	0.73	0.14	27,27,27,27	0
58	MG	1A	3352	1/1	0.73	0.36	80,80,80,80	0
58	MG	2A	3184	1/1	0.73	0.25	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1661	1/1	0.73	0.18	88,88,88,88	0
58	MG	1A	3821	1/1	0.74	0.18	68,68,68,68	0
58	MG	1A	4060	1/1	0.74	0.24	49,49,49,49	0
58	MG	1A	3478	1/1	0.74	0.31	81,81,81,81	0
58	MG	2A	3147	1/1	0.74	0.13	90,90,90,90	0
58	MG	1a	1666	1/1	0.74	0.19	86,86,86,86	0
58	MG	2a	1670	1/1	0.74	0.19	84,84,84,84	0
58	MG	2A	3533	1/1	0.75	0.25	68,68,68,68	0
58	MG	1A	3261	1/1	0.75	0.22	77,77,77,77	0
58	MG	2a	1759	1/1	0.75	0.19	85,85,85,85	0
58	MG	2A	3189	1/1	0.75	0.32	76,76,76,76	0
58	MG	2B	216	1/1	0.75	0.21	83,83,83,83	0
58	MG	2E	307	1/1	0.75	0.23	75,75,75,75	0
58	MG	2A	3336	1/1	0.75	0.28	76,76,76,76	0
58	MG	2Z	301	1/1	0.75	0.15	97,97,97,97	0
58	MG	1a	1777	1/1	0.75	0.41	82,82,82,82	0
58	MG	2A	3037	1/1	0.75	0.22	74,74,74,74	0
58	MG	2a	1801	1/1	0.75	0.24	76,76,76,76	0
58	MG	2A	3604	1/1	0.75	0.19	80,80,80,80	0
58	MG	2A	3652	1/1	0.75	0.16	75,75,75,75	0
58	MG	2A	3051	1/1	0.75	0.38	90,90,90,90	0
58	MG	2A	3416	1/1	0.75	0.44	90,90,90,90	0
58	MG	2a	1685	1/1	0.75	0.21	84,84,84,84	0
58	MG	2A	3442	1/1	0.75	0.33	86,86,86,86	0
58	MG	2A	3743	1/1	0.75	0.25	61,61,61,61	0
58	MG	2B	211	1/1	0.76	0.27	86,86,86,86	0
58	MG	2A	3562	1/1	0.76	0.25	71,71,71,71	0
58	MG	2A	3342	1/1	0.76	0.15	73,73,73,73	0
58	MG	1A	4057	1/1	0.76	0.28	80,80,80,80	0
58	MG	1A	4058	1/1	0.76	0.25	69,69,69,69	0
58	MG	2A	3390	1/1	0.76	0.43	73,73,73,73	0
58	MG	1a	1664	1/1	0.76	0.19	80,80,80,80	0
58	MG	1A	3429	1/1	0.76	0.21	77,77,77,77	0
58	MG	2A	3098	1/1	0.76	0.24	88,88,88,88	0
58	MG	2A	3693	1/1	0.76	0.24	64,64,64,64	0
58	MG	2a	1646	1/1	0.76	0.24	84,84,84,84	0
58	MG	2a	1805	1/1	0.76	0.21	88,88,88,88	0
58	MG	2a	1658	1/1	0.76	0.25	79,79,79,79	0
58	MG	2A	3478	1/1	0.76	0.23	69,69,69,69	0
58	MG	2A	3109	1/1	0.76	0.21	71,71,71,71	0
58	MG	2A	3538	1/1	0.76	0.22	81,81,81,81	0
58	MG	1A	3783	1/1	0.76	0.14	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1717	1/1	0.76	0.37	88,88,88,88	0
58	MG	1x	108	1/1	0.77	0.24	90,90,90,90	0
58	MG	2A	3191	1/1	0.77	0.27	78,78,78,78	0
58	MG	1A	4059	1/1	0.77	0.16	57,57,57,57	0
58	MG	2A	3236	1/1	0.77	0.20	89,89,89,89	0
58	MG	2A	3274	1/1	0.77	0.21	80,80,80,80	0
58	MG	2A	3005	1/1	0.77	0.28	75,75,75,75	0
58	MG	2A	3023	1/1	0.77	0.19	84,84,84,84	0
58	MG	2a	1711	1/1	0.77	0.42	91,91,91,91	0
58	MG	1A	3809	1/1	0.77	0.17	61,61,61,61	0
58	MG	1A	3469	1/1	0.77	0.16	72,72,72,72	0
58	MG	2A	3058	1/1	0.77	0.17	80,80,80,80	0
58	MG	1A	3060	1/1	0.77	0.25	73,73,73,73	0
58	MG	1w	102	1/1	0.77	0.24	93,93,93,93	0
58	MG	1a	1697	1/1	0.77	0.55	80,80,80,80	0
58	MG	2A	3381	1/1	0.77	0.29	68,68,68,68	0
58	MG	2B	204	1/1	0.77	0.27	83,83,83,83	0
58	MG	2A	3382	1/1	0.77	0.20	87,87,87,87	0
58	MG	2A	3102	1/1	0.77	0.29	86,86,86,86	0
58	MG	1A	3489	1/1	0.77	0.36	77,77,77,77	0
58	MG	1A	3791	1/1	0.77	0.20	67,67,67,67	0
58	MG	2A	3427	1/1	0.77	0.15	71,71,71,71	0
58	MG	2A	3132	1/1	0.77	0.21	69,69,69,69	0
58	MG	20	103	1/1	0.77	0.23	76,76,76,76	0
58	MG	1O	206	1/1	0.77	0.22	74,74,74,74	0
58	MG	2A	3164	1/1	0.77	0.14	88,88,88,88	0
58	MG	2A	3166	1/1	0.77	0.22	87,87,87,87	0
58	MG	1A	3231	1/1	0.77	0.22	76,76,76,76	0
58	MG	1s	101	1/1	0.78	0.20	86,86,86,86	0
58	MG	1A	3217	1/1	0.78	0.19	84,84,84,84	0
58	MG	1a	1620	1/1	0.78	0.25	67,67,67,67	0
58	MG	2A	3586	1/1	0.78	0.20	82,82,82,82	0
58	MG	2A	3239	1/1	0.78	0.19	65,65,65,65	0
58	MG	2A	3265	1/1	0.78	0.25	84,84,84,84	0
58	MG	2T	202	1/1	0.78	0.32	81,81,81,81	0
58	MG	1a	1640	1/1	0.78	0.30	76,76,76,76	0
58	MG	1A	3836	1/1	0.78	0.13	78,78,78,78	0
58	MG	2a	1605	1/1	0.78	0.36	86,86,86,86	0
58	MG	1A	3582	1/1	0.78	0.17	79,79,79,79	0
58	MG	1F	308	1/1	0.78	0.21	67,67,67,67	0
58	MG	2a	1615	1/1	0.78	0.29	79,79,79,79	0
58	MG	2A	3681	1/1	0.78	0.25	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3307	1/1	0.78	0.27	78,78,78,78	0
58	MG	1A	3431	1/1	0.78	0.18	65,65,65,65	0
58	MG	2A	3729	1/1	0.78	0.17	72,72,72,72	0
58	MG	2A	3734	1/1	0.78	0.25	87,87,87,87	0
58	MG	2A	3327	1/1	0.78	0.26	77,77,77,77	0
58	MG	2A	3330	1/1	0.78	0.43	77,77,77,77	0
58	MG	2x	101	1/1	0.78	0.27	79,79,79,79	0
58	MG	1a	1680	1/1	0.78	0.24	93,93,93,93	0
58	MG	1a	1605	1/1	0.79	0.12	78,78,78,78	0
58	MG	2A	3499	1/1	0.79	0.17	82,82,82,82	0
58	MG	2A	3738	1/1	0.79	0.30	81,81,81,81	0
58	MG	1A	3867	1/1	0.79	0.13	34,34,34,34	0
58	MG	2a	1705	1/1	0.79	0.34	90,90,90,90	0
58	MG	2A	3064	1/1	0.79	0.22	87,87,87,87	0
58	MG	2a	1707	1/1	0.79	0.27	86,86,86,86	0
58	MG	1A	3939	1/1	0.79	0.16	91,91,91,91	0
58	MG	2A	3792	1/1	0.79	0.19	63,63,63,63	0
58	MG	2A	3068	1/1	0.79	0.14	62,62,62,62	0
58	MG	2A	3089	1/1	0.79	0.23	72,72,72,72	0
58	MG	2a	1764	1/1	0.79	0.10	97,97,97,97	0
58	MG	1A	3364	1/1	0.79	0.17	68,68,68,68	0
58	MG	1A	3535	1/1	0.79	0.29	76,76,76,76	0
58	MG	2A	3358	1/1	0.79	0.21	71,71,71,71	0
58	MG	2G	201	1/1	0.79	0.29	81,81,81,81	0
58	MG	2A	3589	1/1	0.79	0.13	72,72,72,72	0
58	MG	2A	3264	1/1	0.79	0.20	77,77,77,77	0
58	MG	1D	3610	1/1	0.79	0.26	80,80,80,80	0
58	MG	20	102	1/1	0.79	0.21	72,72,72,72	0
58	MG	2A	3641	1/1	0.79	0.17	64,64,64,64	0
58	MG	2A	3642	1/1	0.79	0.21	80,80,80,80	0
58	MG	1A	3208	1/1	0.79	0.16	81,81,81,81	0
58	MG	1a	1677	1/1	0.79	0.20	77,77,77,77	0
58	MG	2a	1820	1/1	0.79	0.37	80,80,80,80	0
58	MG	2A	3672	1/1	0.79	0.21	52,52,52,52	0
58	MG	2A	3413	1/1	0.79	0.46	78,78,78,78	0
58	MG	1A	3349	1/1	0.79	0.21	68,68,68,68	0
58	MG	2A	3286	1/1	0.79	0.28	83,83,83,83	0
58	MG	2x	105	1/1	0.79	0.25	80,80,80,80	0
58	MG	2x	107	1/1	0.79	0.18	80,80,80,80	0
58	MG	1A	3232	1/1	0.79	0.19	65,65,65,65	0
58	MG	2a	1691	1/1	0.80	0.51	83,83,83,83	0
58	MG	2A	3767	1/1	0.80	0.14	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3591	1/1	0.80	0.13	69,69,69,69	0
58	MG	1a	1675	1/1	0.80	0.18	67,67,67,67	0
58	MG	1A	3851	1/1	0.80	0.27	56,56,56,56	0
58	MG	1A	3668	1/1	0.80	0.18	80,80,80,80	0
58	MG	2B	208	1/1	0.80	0.17	93,93,93,93	0
58	MG	1A	3826	1/1	0.80	0.14	73,73,73,73	0
58	MG	2a	1733	1/1	0.80	0.14	95,95,95,95	0
58	MG	2a	1736	1/1	0.80	0.30	83,83,83,83	0
58	MG	2a	1742	1/1	0.80	0.29	103,103,103,103	0
58	MG	2A	3252	1/1	0.80	0.21	89,89,89,89	0
58	MG	2a	1760	1/1	0.80	0.31	90,90,90,90	0
58	MG	1A	3988	1/1	0.80	0.18	78,78,78,78	0
58	MG	2a	1771	1/1	0.80	0.26	80,80,80,80	0
58	MG	2A	3595	1/1	0.80	0.24	58,58,58,58	0
58	MG	1a	1639	1/1	0.80	0.20	79,79,79,79	0
58	MG	1a	1719	1/1	0.80	0.33	72,72,72,72	0
58	MG	2A	3609	1/1	0.80	0.19	74,74,74,74	0
58	MG	1x	103	1/1	0.80	0.34	87,87,87,87	0
58	MG	2A	3408	1/1	0.80	0.18	83,83,83,83	0
58	MG	1A	4017	1/1	0.80	0.14	89,89,89,89	0
58	MG	1A	3073	1/1	0.80	0.24	67,67,67,67	0
58	MG	1A	3830	1/1	0.80	0.16	70,70,70,70	0
58	MG	2A	3428	1/1	0.80	0.15	48,48,48,48	0
58	MG	2A	3303	1/1	0.80	0.18	86,86,86,86	0
58	MG	2a	1631	1/1	0.80	0.57	74,74,74,74	0
58	MG	2a	1818	1/1	0.80	0.36	83,83,83,83	0
58	MG	2A	3459	1/1	0.80	0.21	81,81,81,81	0
58	MG	1a	1663	1/1	0.80	0.33	86,86,86,86	0
58	MG	2q	202	1/1	0.80	0.16	92,92,92,92	0
58	MG	2A	3717	1/1	0.80	0.15	69,69,69,69	0
58	MG	2A	3498	1/1	0.80	0.24	84,84,84,84	0
58	MG	1a	1791	1/1	0.80	0.18	65,65,65,65	0
58	MG	2a	1666	1/1	0.80	0.46	87,87,87,87	0
58	MG	2A	3322	1/1	0.80	0.23	84,84,84,84	0
58	MG	1E	312	1/1	0.80	0.17	66,66,66,66	0
58	MG	2A	3262	1/1	0.81	0.30	89,89,89,89	0
58	MG	2A	3553	1/1	0.81	0.26	52,52,52,52	0
58	MG	1a	1695	1/1	0.81	0.31	63,63,63,63	0
58	MG	1a	1696	1/1	0.81	0.37	69,69,69,69	0
58	MG	2A	3581	1/1	0.81	0.20	79,79,79,79	0
58	MG	1A	3608	1/1	0.81	0.21	64,64,64,64	0
58	MG	2A	3034	1/1	0.81	0.25	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1a	1707	1/1	0.81	0.31	72,72,72,72	0
58	MG	2A	3592	1/1	0.81	0.23	69,69,69,69	0
58	MG	2A	3040	1/1	0.81	0.21	73,73,73,73	0
58	MG	1A	4000	1/1	0.81	0.15	94,94,94,94	0
58	MG	1A	3499	1/1	0.81	0.23	73,73,73,73	0
58	MG	12	101	1/1	0.81	0.23	66,66,66,66	0
58	MG	2a	1690	1/1	0.81	0.15	95,95,95,95	0
58	MG	2A	3065	1/1	0.81	0.35	78,78,78,78	0
58	MG	2a	1696	1/1	0.81	0.18	85,85,85,85	0
58	MG	2A	3312	1/1	0.81	0.47	82,82,82,82	0
58	MG	2A	3319	1/1	0.81	0.27	70,70,70,70	0
58	MG	1A	4018	1/1	0.81	0.17	72,72,72,72	0
58	MG	2A	3660	1/1	0.81	0.27	73,73,73,73	0
58	MG	1A	4037	1/1	0.81	0.15	55,55,55,55	0
58	MG	2A	3072	1/1	0.81	0.19	70,70,70,70	0
58	MG	1a	1748	1/1	0.81	0.19	81,81,81,81	0
58	MG	2A	3682	1/1	0.81	0.19	75,75,75,75	0
58	MG	2A	3688	1/1	0.81	0.25	74,74,74,74	0
58	MG	1A	4045	1/1	0.81	0.15	76,76,76,76	0
58	MG	2a	1758	1/1	0.81	0.28	93,93,93,93	0
58	MG	2A	3696	1/1	0.81	0.13	87,87,87,87	0
58	MG	1a	1775	1/1	0.81	0.23	78,78,78,78	0
58	MG	2a	1761	1/1	0.81	0.23	86,86,86,86	0
58	MG	2A	3716	1/1	0.81	0.15	90,90,90,90	0
58	MG	2A	3099	1/1	0.81	0.23	77,77,77,77	0
58	MG	1a	1622	1/1	0.81	0.34	83,83,83,83	0
58	MG	2A	3363	1/1	0.81	0.27	68,68,68,68	0
58	MG	1a	1623	1/1	0.81	0.34	84,84,84,84	0
58	MG	1a	1799	1/1	0.81	0.16	89,89,89,89	0
58	MG	1a	1636	1/1	0.81	0.17	86,86,86,86	0
58	MG	2A	3769	1/1	0.81	0.16	49,49,49,49	0
58	MG	1A	3521	1/1	0.81	0.14	81,81,81,81	0
58	MG	1A	3333	1/1	0.81	0.32	71,71,71,71	0
58	MG	1A	3246	1/1	0.81	0.17	73,73,73,73	0
58	MG	2A	3178	1/1	0.81	0.20	76,76,76,76	0
58	MG	1A	3832	1/1	0.81	0.25	72,72,72,72	0
58	MG	1A	3269	1/1	0.81	0.20	60,60,60,60	0
58	MG	2A	3190	1/1	0.81	0.41	85,85,85,85	0
58	MG	2A	3444	1/1	0.81	0.19	75,75,75,75	0
58	MG	1A	3354	1/1	0.81	0.14	63,63,63,63	0
58	MG	2f	202	1/1	0.81	0.14	89,89,89,89	0
58	MG	2j	201	1/1	0.81	0.23	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2F	305	1/1	0.81	0.21	66,66,66,66	0
58	MG	2A	3194	1/1	0.81	0.21	89,89,89,89	0
58	MG	1A	3299	1/1	0.81	0.15	65,65,65,65	0
58	MG	2A	3234	1/1	0.81	0.39	73,73,73,73	0
58	MG	1A	3933	1/1	0.81	0.14	39,39,39,39	0
58	MG	1A	3365	1/1	0.81	0.25	60,60,60,60	0
58	MG	1A	3963	1/1	0.81	0.15	89,89,89,89	0
58	MG	1A	3456	1/1	0.82	0.18	69,69,69,69	0
58	MG	1a	1728	1/1	0.82	0.14	76,76,76,76	0
58	MG	1B	230	1/1	0.82	0.14	81,81,81,81	0
58	MG	1A	3615	1/1	0.82	0.10	31,31,31,31	0
58	MG	2A	3749	1/1	0.82	0.31	76,76,76,76	0
58	MG	1A	3859	1/1	0.82	0.25	56,56,56,56	0
58	MG	1A	3863	1/1	0.82	0.17	69,69,69,69	0
58	MG	1A	3822	1/1	0.82	0.14	53,53,53,53	0
58	MG	2a	1708	1/1	0.82	0.24	82,82,82,82	0
58	MG	2a	1709	1/1	0.82	0.34	90,90,90,90	0
58	MG	2A	3579	1/1	0.82	0.23	71,71,71,71	0
58	MG	2a	1712	1/1	0.82	0.21	84,84,84,84	0
58	MG	2A	3345	1/1	0.82	0.19	86,86,86,86	0
58	MG	2A	3585	1/1	0.82	0.15	73,73,73,73	0
58	MG	1A	3891	1/1	0.82	0.15	62,62,62,62	0
58	MG	2A	3063	1/1	0.82	0.22	66,66,66,66	0
58	MG	2A	3209	1/1	0.82	0.44	74,74,74,74	0
58	MG	2a	1756	1/1	0.82	0.14	85,85,85,85	0
58	MG	2B	212	1/1	0.82	0.15	86,86,86,86	0
58	MG	1U	203	1/1	0.82	0.22	64,64,64,64	0
58	MG	2E	302	1/1	0.82	0.18	71,71,71,71	0
58	MG	2A	3373	1/1	0.82	0.47	86,86,86,86	0
58	MG	1a	1804	1/1	0.82	0.09	91,91,91,91	0
58	MG	1A	3906	1/1	0.82	0.20	83,83,83,83	0
58	MG	2A	3251	1/1	0.82	0.19	77,77,77,77	0
58	MG	1A	3622	1/1	0.82	0.28	68,68,68,68	0
58	MG	1a	1602	1/1	0.82	0.20	79,79,79,79	0
58	MG	2A	3087	1/1	0.82	0.28	76,76,76,76	0
58	MG	2a	1784	1/1	0.82	0.46	81,81,81,81	0
58	MG	1a	1691	1/1	0.82	0.29	78,78,78,78	0
58	MG	26	101	1/1	0.82	0.35	76,76,76,76	0
58	MG	27	102	1/1	0.82	0.15	68,68,68,68	0
58	MG	2a	1601	1/1	0.82	0.39	87,87,87,87	0
58	MG	1a	1603	1/1	0.82	0.10	67,67,67,67	0
58	MG	2A	3661	1/1	0.82	0.21	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3632	1/1	0.82	0.14	64,64,64,64	0
58	MG	2a	1614	1/1	0.82	0.17	73,73,73,73	0
58	MG	2a	1816	1/1	0.82	0.25	87,87,87,87	0
58	MG	1a	1607	1/1	0.82	0.28	80,80,80,80	0
58	MG	2a	1621	1/1	0.82	0.31	81,81,81,81	0
58	MG	1w	107	1/1	0.82	0.22	78,78,78,78	0
58	MG	2A	3451	1/1	0.82	0.18	66,66,66,66	0
58	MG	1A	3518	1/1	0.82	0.10	82,82,82,82	0
58	MG	2l	201	1/1	0.82	0.13	84,84,84,84	0
58	MG	1A	3205	1/1	0.82	0.21	70,70,70,70	0
58	MG	2a	1644	1/1	0.82	0.28	76,76,76,76	0
58	MG	1A	3995	1/1	0.82	0.28	45,45,45,45	0
58	MG	2a	1650	1/1	0.82	0.19	95,95,95,95	0
58	MG	1a	1633	1/1	0.82	0.19	88,88,88,88	0
58	MG	2A	3510	1/1	0.82	0.23	74,74,74,74	0
58	MG	2A	3532	1/1	0.82	0.13	51,51,51,51	0
58	MG	2A	3393	1/1	0.83	0.35	84,84,84,84	0
58	MG	1a	1704	1/1	0.83	0.30	72,72,72,72	0
58	MG	2A	3266	1/1	0.83	0.25	83,83,83,83	0
58	MG	2E	306	1/1	0.83	0.14	51,51,51,51	0
58	MG	1b	302	1/1	0.83	0.11	93,93,93,93	0
58	MG	1a	1660	1/1	0.83	0.09	83,83,83,83	0
58	MG	2a	1717	1/1	0.83	0.15	85,85,85,85	0
58	MG	2A	3648	1/1	0.83	0.14	67,67,67,67	0
58	MG	1A	3263	1/1	0.83	0.24	77,77,77,77	0
58	MG	2R	202	1/1	0.83	0.20	75,75,75,75	0
58	MG	1a	1710	1/1	0.83	0.24	70,70,70,70	0
58	MG	1A	3507	1/1	0.83	0.26	78,78,78,78	0
58	MG	2A	3296	1/1	0.83	0.16	72,72,72,72	0
58	MG	2A	3188	1/1	0.83	0.22	69,69,69,69	0
58	MG	1A	4052	1/1	0.83	0.23	83,83,83,83	0
58	MG	1A	3402	1/1	0.83	0.40	72,72,72,72	0
58	MG	1a	1670	1/1	0.83	0.31	75,75,75,75	0
58	MG	2A	3685	1/1	0.83	0.29	79,79,79,79	0
58	MG	1A	3099	1/1	0.83	0.13	68,68,68,68	0
58	MG	1H	201	1/1	0.83	0.20	76,76,76,76	0
58	MG	2A	3517	1/1	0.83	0.25	74,74,74,74	0
58	MG	2A	3207	1/1	0.83	0.18	74,74,74,74	0
58	MG	2A	3329	1/1	0.83	0.34	66,66,66,66	0
58	MG	2a	1623	1/1	0.83	0.34	83,83,83,83	0
58	MG	2a	1624	1/1	0.83	0.39	83,83,83,83	0
58	MG	2a	1625	1/1	0.83	0.25	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1628	1/1	0.83	0.29	93,93,93,93	0
58	MG	1A	3893	1/1	0.83	0.18	67,67,67,67	0
58	MG	2A	3540	1/1	0.83	0.24	80,80,80,80	0
58	MG	2A	3732	1/1	0.83	0.19	78,78,78,78	0
58	MG	2A	3216	1/1	0.83	0.25	74,74,74,74	0
58	MG	2A	3233	1/1	0.83	0.29	84,84,84,84	0
58	MG	2a	1645	1/1	0.83	0.15	80,80,80,80	0
58	MG	2A	3091	1/1	0.83	0.12	63,63,63,63	0
58	MG	2a	1647	1/1	0.83	0.22	93,93,93,93	0
58	MG	1a	1687	1/1	0.83	0.19	76,76,76,76	0
58	MG	1A	3843	1/1	0.83	0.13	53,53,53,53	0
58	MG	2A	3243	1/1	0.83	0.36	83,83,83,83	0
58	MG	2A	3359	1/1	0.83	0.33	57,57,57,57	0
58	MG	2a	1682	1/1	0.83	0.21	84,84,84,84	0
58	MG	2r	101	1/1	0.83	0.18	89,89,89,89	0
58	MG	1A	3907	1/1	0.83	0.16	81,81,81,81	0
58	MG	2w	101	1/1	0.83	0.14	98,98,98,98	0
58	MG	2A	3006	1/1	0.83	0.32	73,73,73,73	0
58	MG	2A	3379	1/1	0.83	0.30	70,70,70,70	0
58	MG	2x	104	1/1	0.83	0.11	85,85,85,85	0
58	MG	2A	3255	1/1	0.83	0.18	85,85,85,85	0
58	MG	1A	3693	1/1	0.83	0.14	65,65,65,65	0
58	MG	1A	4041	1/1	0.83	0.13	59,59,59,59	0
58	MG	1a	1669	1/1	0.84	0.23	77,77,77,77	0
58	MG	2A	3722	1/1	0.84	0.11	83,83,83,83	0
58	MG	2A	3501	1/1	0.84	0.17	80,80,80,80	0
58	MG	2A	3299	1/1	0.84	0.26	68,68,68,68	0
58	MG	1a	1751	1/1	0.84	0.27	81,81,81,81	0
58	MG	2a	1684	1/1	0.84	0.30	75,75,75,75	0
58	MG	2A	3183	1/1	0.84	0.20	77,77,77,77	0
58	MG	2a	1688	1/1	0.84	0.18	75,75,75,75	0
58	MG	2A	3309	1/1	0.84	0.16	70,70,70,70	0
58	MG	2A	3016	1/1	0.84	0.20	87,87,87,87	0
58	MG	2a	1692	1/1	0.84	0.25	67,67,67,67	0
58	MG	1a	1752	1/1	0.84	0.26	89,89,89,89	0
58	MG	2A	3768	1/1	0.84	0.17	76,76,76,76	0
58	MG	2a	1701	1/1	0.84	0.22	81,81,81,81	0
58	MG	1a	1757	1/1	0.84	0.35	79,79,79,79	0
58	MG	2A	3779	1/1	0.84	0.14	86,86,86,86	0
58	MG	1A	3819	1/1	0.84	0.12	58,58,58,58	0
58	MG	1A	3520	1/1	0.84	0.18	91,91,91,91	0
58	MG	2A	3559	1/1	0.84	0.19	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3192	1/1	0.84	0.20	65,65,65,65	0
58	MG	2B	207	1/1	0.84	0.27	77,77,77,77	0
58	MG	2A	3564	1/1	0.84	0.16	65,65,65,65	0
58	MG	1a	1676	1/1	0.84	0.32	85,85,85,85	0
58	MG	2A	3572	1/1	0.84	0.19	82,82,82,82	0
58	MG	1A	3646	1/1	0.84	0.15	71,71,71,71	0
58	MG	2B	214	1/1	0.84	0.22	81,81,81,81	0
58	MG	2B	215	1/1	0.84	0.27	79,79,79,79	0
58	MG	2a	1744	1/1	0.84	0.21	86,86,86,86	0
58	MG	2a	1748	1/1	0.84	0.19	94,94,94,94	0
58	MG	2a	1752	1/1	0.84	0.14	83,83,83,83	0
58	MG	2A	3338	1/1	0.84	0.22	67,67,67,67	0
58	MG	2B	217	1/1	0.84	0.30	80,80,80,80	0
58	MG	1A	3661	1/1	0.84	0.18	67,67,67,67	0
58	MG	1a	1684	1/1	0.84	0.26	63,63,63,63	0
58	MG	1A	3468	1/1	0.84	0.14	74,74,74,74	0
58	MG	1A	3984	1/1	0.84	0.14	68,68,68,68	0
58	MG	2A	3357	1/1	0.84	0.22	54,54,54,54	0
58	MG	2A	3593	1/1	0.84	0.16	66,66,66,66	0
58	MG	1n	101	1/1	0.84	0.31	77,77,77,77	0
58	MG	1A	3355	1/1	0.84	0.25	69,69,69,69	0
58	MG	1A	3472	1/1	0.84	0.29	78,78,78,78	0
58	MG	1B	232	1/1	0.84	0.15	79,79,79,79	0
58	MG	2A	3637	1/1	0.84	0.22	67,67,67,67	0
58	MG	2a	1792	1/1	0.84	0.25	72,72,72,72	0
58	MG	2A	3639	1/1	0.84	0.17	74,74,74,74	0
58	MG	2A	3244	1/1	0.84	0.22	79,79,79,79	0
58	MG	2A	3245	1/1	0.84	0.36	75,75,75,75	0
58	MG	1A	3377	1/1	0.84	0.24	68,68,68,68	0
58	MG	2a	1804	1/1	0.84	0.32	75,75,75,75	0
58	MG	2A	3651	1/1	0.84	0.22	80,80,80,80	0
58	MG	1A	3057	1/1	0.84	0.22	60,60,60,60	0
58	MG	2a	1613	1/1	0.84	0.23	79,79,79,79	0
58	MG	1A	3762	1/1	0.84	0.11	41,41,41,41	0
58	MG	2A	3261	1/1	0.84	0.26	73,73,73,73	0
58	MG	1A	3408	1/1	0.84	0.23	59,59,59,59	0
58	MG	1A	3502	1/1	0.84	0.32	70,70,70,70	0
58	MG	1A	3461	1/1	0.84	0.25	81,81,81,81	0
58	MG	1x	102	1/1	0.84	0.15	67,67,67,67	0
58	MG	2a	1626	1/1	0.84	0.13	98,98,98,98	0
58	MG	2A	3268	1/1	0.84	0.20	70,70,70,70	0
58	MG	2A	3683	1/1	0.84	0.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1T	202	1/1	0.84	0.17	67,67,67,67	0
58	MG	2A	3141	1/1	0.84	0.23	78,78,78,78	0
58	MG	2A	3282	1/1	0.84	0.23	75,75,75,75	0
58	MG	2a	1641	1/1	0.84	0.31	81,81,81,81	0
58	MG	1A	3512	1/1	0.84	0.23	65,65,65,65	0
58	MG	2A	3698	1/1	0.84	0.17	66,66,66,66	0
58	MG	2A	3156	1/1	0.84	0.11	74,74,74,74	0
58	MG	1A	3462	1/1	0.84	0.17	65,65,65,65	0
58	MG	2E	305	1/1	0.85	0.23	68,68,68,68	0
58	MG	12	102	1/1	0.85	0.17	56,56,56,56	0
58	MG	1a	1766	1/1	0.85	0.13	81,81,81,81	0
58	MG	1A	4080	1/1	0.85	0.15	49,49,49,49	0
58	MG	1a	1601	1/1	0.85	0.34	71,71,71,71	0
58	MG	2A	3052	1/1	0.85	0.12	65,65,65,65	0
58	MG	1A	3340	1/1	0.85	0.16	63,63,63,63	0
58	MG	2A	3480	1/1	0.85	0.11	67,67,67,67	0
58	MG	2A	3492	1/1	0.85	0.12	61,61,61,61	0
58	MG	20	101	1/1	0.85	0.31	81,81,81,81	0
58	MG	2A	3061	1/1	0.85	0.21	70,70,70,70	0
58	MG	2A	3315	1/1	0.85	0.29	80,80,80,80	0
58	MG	1A	3884	1/1	0.85	0.15	74,74,74,74	0
58	MG	2A	3684	1/1	0.85	0.17	73,73,73,73	0
58	MG	1A	4015	1/1	0.85	0.13	72,72,72,72	0
58	MG	2a	1602	1/1	0.85	0.29	81,81,81,81	0
58	MG	1a	1606	1/1	0.85	0.16	65,65,65,65	0
58	MG	2A	3690	1/1	0.85	0.17	65,65,65,65	0
58	MG	1a	1681	1/1	0.85	0.14	81,81,81,81	0
58	MG	1A	3730	1/1	0.85	0.19	55,55,55,55	0
58	MG	2A	3332	1/1	0.85	0.24	74,74,74,74	0
58	MG	2A	3700	1/1	0.85	0.24	73,73,73,73	0
58	MG	2a	1619	1/1	0.85	0.16	80,80,80,80	0
58	MG	2a	1620	1/1	0.85	0.24	82,82,82,82	0
58	MG	1e	202	1/1	0.85	0.19	81,81,81,81	0
58	MG	1a	1610	1/1	0.85	0.12	82,82,82,82	0
58	MG	1A	3793	1/1	0.85	0.10	50,50,50,50	0
58	MG	1A	3905	1/1	0.85	0.13	44,44,44,44	0
58	MG	2A	3093	1/1	0.85	0.23	82,82,82,82	0
58	MG	1D	3608	1/1	0.85	0.21	59,59,59,59	0
58	MG	2A	3355	1/1	0.85	0.26	66,66,66,66	0
58	MG	1a	1628	1/1	0.85	0.33	68,68,68,68	0
58	MG	1a	1703	1/1	0.85	0.33	77,77,77,77	0
58	MG	2A	3573	1/1	0.85	0.20	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3797	1/1	0.85	0.24	77,77,77,77	0
58	MG	1A	3799	1/1	0.85	0.12	64,64,64,64	0
58	MG	2A	3367	1/1	0.85	0.48	79,79,79,79	0
58	MG	1A	3837	1/1	0.85	0.14	78,78,78,78	0
58	MG	2a	1815	1/1	0.85	0.19	85,85,85,85	0
58	MG	1A	3558	1/1	0.85	0.32	65,65,65,65	0
58	MG	1a	1649	1/1	0.85	0.13	73,73,73,73	0
58	MG	2a	1657	1/1	0.85	0.10	88,88,88,88	0
58	MG	2a	1821	1/1	0.85	0.19	76,76,76,76	0
58	MG	2A	3267	1/1	0.85	0.36	89,89,89,89	0
58	MG	2a	1662	1/1	0.85	0.33	70,70,70,70	0
58	MG	2B	203	1/1	0.85	0.15	77,77,77,77	0
58	MG	1a	1651	1/1	0.85	0.26	71,71,71,71	0
58	MG	1A	3572	1/1	0.85	0.21	81,81,81,81	0
58	MG	1A	3981	1/1	0.85	0.10	84,84,84,84	0
58	MG	1A	3528	1/1	0.85	0.13	69,69,69,69	0
58	MG	2A	3606	1/1	0.85	0.16	65,65,65,65	0
58	MG	1a	1662	1/1	0.85	0.17	78,78,78,78	0
58	MG	2A	3415	1/1	0.85	0.17	72,72,72,72	0
58	MG	1W	203	1/1	0.85	0.15	55,55,55,55	0
58	MG	2A	3418	1/1	0.85	0.11	78,78,78,78	0
58	MG	1A	3289	1/1	0.85	0.19	67,67,67,67	0
58	MG	2A	3645	1/1	0.85	0.28	79,79,79,79	0
58	MG	2A	3218	1/1	0.86	0.14	57,57,57,57	0
58	MG	2A	3411	1/1	0.86	0.09	63,63,63,63	0
58	MG	2a	1648	1/1	0.86	0.38	81,81,81,81	0
58	MG	2A	3695	1/1	0.86	0.29	73,73,73,73	0
58	MG	2a	1654	1/1	0.86	0.23	81,81,81,81	0
58	MG	2a	1656	1/1	0.86	0.19	76,76,76,76	0
58	MG	2A	3230	1/1	0.86	0.47	84,84,84,84	0
58	MG	1A	3455	1/1	0.86	0.29	74,74,74,74	0
58	MG	2a	1660	1/1	0.86	0.17	86,86,86,86	0
58	MG	1A	3686	1/1	0.86	0.20	65,65,65,65	0
58	MG	1A	3688	1/1	0.86	0.16	41,41,41,41	0
58	MG	2A	3423	1/1	0.86	0.18	69,69,69,69	0
58	MG	2a	1675	1/1	0.86	0.29	81,81,81,81	0
58	MG	2a	1676	1/1	0.86	0.25	75,75,75,75	0
58	MG	1A	4039	1/1	0.86	0.16	72,72,72,72	0
58	MG	1A	3260	1/1	0.86	0.18	66,66,66,66	0
58	MG	1A	3270	1/1	0.86	0.13	51,51,51,51	0
58	MG	1A	3375	1/1	0.86	0.38	64,64,64,64	0
58	MG	2A	3249	1/1	0.86	0.19	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3454	1/1	0.86	0.24	71,71,71,71	0
58	MG	1A	3467	1/1	0.86	0.30	79,79,79,79	0
58	MG	1A	3343	1/1	0.86	0.35	57,57,57,57	0
58	MG	2A	3763	1/1	0.86	0.24	70,70,70,70	0
58	MG	1A	3393	1/1	0.86	0.50	49,49,49,49	0
58	MG	2a	1703	1/1	0.86	0.14	74,74,74,74	0
58	MG	1a	1632	1/1	0.86	0.42	68,68,68,68	0
58	MG	2A	3496	1/1	0.86	0.18	59,59,59,59	0
58	MG	2A	3059	1/1	0.86	0.29	80,80,80,80	0
58	MG	1a	1733	1/1	0.86	0.18	71,71,71,71	0
58	MG	1a	1740	1/1	0.86	0.20	71,71,71,71	0
58	MG	1A	3180	1/1	0.86	0.27	58,58,58,58	0
58	MG	2A	3801	1/1	0.86	0.18	79,79,79,79	0
58	MG	1A	3878	1/1	0.86	0.17	35,35,35,35	0
58	MG	2a	1718	1/1	0.86	0.18	80,80,80,80	0
58	MG	1A	3775	1/1	0.86	0.12	64,64,64,64	0
58	MG	1B	212	1/1	0.86	0.14	73,73,73,73	0
58	MG	2A	3277	1/1	0.86	0.36	65,65,65,65	0
58	MG	1a	1644	1/1	0.86	0.18	79,79,79,79	0
58	MG	2A	3073	1/1	0.86	0.17	62,62,62,62	0
58	MG	2A	3084	1/1	0.86	0.20	67,67,67,67	0
58	MG	1A	3189	1/1	0.86	0.30	50,50,50,50	0
58	MG	1A	3785	1/1	0.86	0.21	59,59,59,59	0
58	MG	2A	3560	1/1	0.86	0.18	51,51,51,51	0
58	MG	1A	3483	1/1	0.86	0.13	69,69,69,69	0
58	MG	1A	3410	1/1	0.86	0.62	93,93,93,93	0
58	MG	1a	1779	1/1	0.86	0.14	71,71,71,71	0
58	MG	1a	1781	1/1	0.86	0.19	85,85,85,85	0
58	MG	2a	1762	1/1	0.86	0.26	74,74,74,74	0
58	MG	1A	3497	1/1	0.86	0.23	77,77,77,77	0
58	MG	1a	1795	1/1	0.86	0.23	64,64,64,64	0
58	MG	2a	1775	1/1	0.86	0.27	83,83,83,83	0
58	MG	1A	3908	1/1	0.86	0.21	62,62,62,62	0
58	MG	2A	3111	1/1	0.86	0.25	75,75,75,75	0
58	MG	1A	3796	1/1	0.86	0.14	78,78,78,78	0
58	MG	2a	1781	1/1	0.86	0.24	82,82,82,82	0
58	MG	2A	3122	1/1	0.86	0.10	62,62,62,62	0
58	MG	1A	3305	1/1	0.86	0.28	56,56,56,56	0
58	MG	1a	1809	1/1	0.86	0.19	58,58,58,58	0
58	MG	2a	1791	1/1	0.86	0.25	69,69,69,69	0
58	MG	2A	3145	1/1	0.86	0.20	70,70,70,70	0
58	MG	1A	3312	1/1	0.86	0.18	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3965	1/1	0.86	0.10	75,75,75,75	0
58	MG	2A	3159	1/1	0.86	0.26	70,70,70,70	0
58	MG	2A	3341	1/1	0.86	0.22	79,79,79,79	0
58	MG	1m	3001	1/1	0.86	0.10	75,75,75,75	0
58	MG	2A	3613	1/1	0.86	0.13	57,57,57,57	0
58	MG	1A	3973	1/1	0.86	0.11	89,89,89,89	0
58	MG	1n	102	1/1	0.86	0.25	74,74,74,74	0
58	MG	1a	1674	1/1	0.86	0.22	69,69,69,69	0
58	MG	1A	3626	1/1	0.86	0.14	83,83,83,83	0
58	MG	1Q	208	1/1	0.86	0.20	59,59,59,59	0
58	MG	2a	1617	1/1	0.86	0.18	82,82,82,82	0
58	MG	1A	3815	1/1	0.86	0.21	64,64,64,64	0
58	MG	1A	3985	1/1	0.86	0.13	75,75,75,75	0
58	MG	1A	3361	1/1	0.86	0.11	79,79,79,79	0
58	MG	2g	201	1/1	0.86	0.25	89,89,89,89	0
58	MG	1a	1683	1/1	0.86	0.36	70,70,70,70	0
58	MG	1A	3436	1/1	0.86	0.38	60,60,60,60	0
58	MG	2l	202	1/1	0.86	0.11	88,88,88,88	0
58	MG	1A	3449	1/1	0.86	0.32	78,78,78,78	0
58	MG	2A	3662	1/1	0.86	0.13	64,64,64,64	0
58	MG	2A	3380	1/1	0.86	0.29	66,66,66,66	0
58	MG	2A	3203	1/1	0.86	0.14	68,68,68,68	0
58	MG	2A	3206	1/1	0.86	0.20	79,79,79,79	0
58	MG	1a	1689	1/1	0.86	0.16	74,74,74,74	0
58	MG	1A	4011	1/1	0.86	0.15	68,68,68,68	0
58	MG	2A	3394	1/1	0.86	0.35	69,69,69,69	0
58	MG	1A	3664	1/1	0.86	0.16	73,73,73,73	0
58	MG	2A	3406	1/1	0.86	0.28	76,76,76,76	0
58	MG	2T	201	1/1	0.87	0.17	72,72,72,72	0
58	MG	2A	3232	1/1	0.87	0.37	84,84,84,84	0
58	MG	1G	204	1/1	0.87	0.17	84,84,84,84	0
58	MG	1x	104	1/1	0.87	0.21	84,84,84,84	0
58	MG	2A	3509	1/1	0.87	0.12	59,59,59,59	0
58	MG	1x	106	1/1	0.87	0.29	73,73,73,73	0
58	MG	23	102	1/1	0.87	0.21	75,75,75,75	0
58	MG	2A	3513	1/1	0.87	0.10	84,84,84,84	0
58	MG	1A	3968	1/1	0.87	0.13	85,85,85,85	0
58	MG	28	102	1/1	0.87	0.27	71,71,71,71	0
58	MG	2A	3521	1/1	0.87	0.26	75,75,75,75	0
58	MG	2A	3522	1/1	0.87	0.20	67,67,67,67	0
58	MG	2A	3526	1/1	0.87	0.16	67,67,67,67	0
58	MG	1A	3148	1/1	0.87	0.24	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1607	1/1	0.87	0.27	77,77,77,77	0
58	MG	1Q	205	1/1	0.87	0.20	76,76,76,76	0
58	MG	2a	1612	1/1	0.87	0.22	74,74,74,74	0
58	MG	1A	3811	1/1	0.87	0.25	61,61,61,61	0
58	MG	2A	3248	1/1	0.87	0.17	83,83,83,83	0
58	MG	2A	3008	1/1	0.87	0.16	70,70,70,70	0
58	MG	1S	203	1/1	0.87	0.14	66,66,66,66	0
58	MG	1a	1693	1/1	0.87	0.10	80,80,80,80	0
58	MG	2A	3254	1/1	0.87	0.38	82,82,82,82	0
58	MG	2A	3030	1/1	0.87	0.24	69,69,69,69	0
58	MG	1A	3298	1/1	0.87	0.29	60,60,60,60	0
58	MG	1A	3024	1/1	0.87	0.26	75,75,75,75	0
58	MG	1A	3187	1/1	0.87	0.12	58,58,58,58	0
58	MG	10	108	1/1	0.87	0.09	54,54,54,54	0
58	MG	1A	3448	1/1	0.87	0.23	49,49,49,49	0
58	MG	2A	3577	1/1	0.87	0.20	84,84,84,84	0
58	MG	1A	3824	1/1	0.87	0.33	71,71,71,71	0
58	MG	1A	3356	1/1	0.87	0.19	67,67,67,67	0
58	MG	1A	3310	1/1	0.87	0.33	67,67,67,67	0
58	MG	2a	1638	1/1	0.87	0.30	76,76,76,76	0
58	MG	1A	3044	1/1	0.87	0.13	50,50,50,50	0
58	MG	1A	3317	1/1	0.87	0.10	47,47,47,47	0
58	MG	1a	1721	1/1	0.87	0.12	72,72,72,72	0
58	MG	2A	3066	1/1	0.87	0.43	73,73,73,73	0
58	MG	1a	1604	1/1	0.87	0.22	71,71,71,71	0
58	MG	2A	3594	1/1	0.87	0.23	79,79,79,79	0
58	MG	1A	4023	1/1	0.87	0.10	96,96,96,96	0
58	MG	1a	1731	1/1	0.87	0.20	81,81,81,81	0
58	MG	1A	4036	1/1	0.87	0.12	57,57,57,57	0
58	MG	2A	3302	1/1	0.87	0.25	79,79,79,79	0
58	MG	2A	3078	1/1	0.87	0.14	67,67,67,67	0
58	MG	2A	3304	1/1	0.87	0.13	62,62,62,62	0
58	MG	2A	3621	1/1	0.87	0.19	71,71,71,71	0
58	MG	2A	3623	1/1	0.87	0.11	78,78,78,78	0
58	MG	2A	3636	1/1	0.87	0.16	71,71,71,71	0
58	MG	2a	1671	1/1	0.87	0.26	78,78,78,78	0
58	MG	2A	3081	1/1	0.87	0.23	69,69,69,69	0
58	MG	1A	3322	1/1	0.87	0.10	59,59,59,59	0
58	MG	2a	1679	1/1	0.87	0.33	78,78,78,78	0
58	MG	1A	3703	1/1	0.87	0.13	44,44,44,44	0
58	MG	1A	3332	1/1	0.87	0.10	65,65,65,65	0
58	MG	2A	3643	1/1	0.87	0.10	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3314	1/1	0.87	0.21	79,79,79,79	0
58	MG	1A	3728	1/1	0.87	0.15	75,75,75,75	0
58	MG	2A	3316	1/1	0.87	0.23	81,81,81,81	0
58	MG	2A	3092	1/1	0.87	0.14	59,59,59,59	0
58	MG	1A	3532	1/1	0.87	0.20	46,46,46,46	0
58	MG	2A	3323	1/1	0.87	0.10	79,79,79,79	0
58	MG	2A	3324	1/1	0.87	0.41	77,77,77,77	0
58	MG	2A	3095	1/1	0.87	0.15	63,63,63,63	0
58	MG	1A	3744	1/1	0.87	0.13	30,30,30,30	0
58	MG	2A	3674	1/1	0.87	0.18	76,76,76,76	0
58	MG	1a	1630	1/1	0.87	0.24	75,75,75,75	0
58	MG	1A	3392	1/1	0.87	0.18	65,65,65,65	0
58	MG	1a	1773	1/1	0.87	0.15	63,63,63,63	0
58	MG	1A	3541	1/1	0.87	0.28	72,72,72,72	0
58	MG	1A	3556	1/1	0.87	0.13	75,75,75,75	0
58	MG	2A	3115	1/1	0.87	0.20	79,79,79,79	0
58	MG	2A	3686	1/1	0.87	0.17	71,71,71,71	0
58	MG	1A	3886	1/1	0.87	0.20	65,65,65,65	0
58	MG	1A	4077	1/1	0.87	0.17	75,75,75,75	0
58	MG	2A	3349	1/1	0.87	0.11	66,66,66,66	0
58	MG	2a	1734	1/1	0.87	0.14	79,79,79,79	0
58	MG	2A	3128	1/1	0.87	0.18	75,75,75,75	0
58	MG	2a	1738	1/1	0.87	0.17	75,75,75,75	0
58	MG	2A	3354	1/1	0.87	0.27	66,66,66,66	0
58	MG	1A	3267	1/1	0.87	0.33	69,69,69,69	0
58	MG	1a	1794	1/1	0.87	0.23	68,68,68,68	0
58	MG	2a	1751	1/1	0.87	0.15	88,88,88,88	0
58	MG	2A	3701	1/1	0.87	0.26	82,82,82,82	0
58	MG	1a	1645	1/1	0.87	0.20	77,77,77,77	0
58	MG	2A	3707	1/1	0.87	0.16	73,73,73,73	0
58	MG	2A	3708	1/1	0.87	0.26	81,81,81,81	0
58	MG	1B	207	1/1	0.87	0.17	75,75,75,75	0
58	MG	2A	3362	1/1	0.87	0.30	49,49,49,49	0
58	MG	2A	3148	1/1	0.87	0.27	79,79,79,79	0
58	MG	2A	3153	1/1	0.87	0.16	72,72,72,72	0
58	MG	2A	3730	1/1	0.87	0.15	74,74,74,74	0
58	MG	1a	1801	1/1	0.87	0.14	57,57,57,57	0
58	MG	2A	3378	1/1	0.87	0.46	75,75,75,75	0
58	MG	2A	3158	1/1	0.87	0.28	83,83,83,83	0
58	MG	1A	3570	1/1	0.87	0.21	54,54,54,54	0
58	MG	2A	3745	1/1	0.87	0.12	71,71,71,71	0
58	MG	2A	3746	1/1	0.87	0.21	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3160	1/1	0.87	0.12	57,57,57,57	0
58	MG	1a	1806	1/1	0.87	0.28	73,73,73,73	0
58	MG	1A	3904	1/1	0.87	0.29	70,70,70,70	0
58	MG	1a	1658	1/1	0.87	0.25	76,76,76,76	0
58	MG	1B	224	1/1	0.87	0.14	74,74,74,74	0
58	MG	2A	3400	1/1	0.87	0.18	77,77,77,77	0
58	MG	2A	3402	1/1	0.87	0.10	71,71,71,71	0
58	MG	2A	3784	1/1	0.87	0.14	90,90,90,90	0
58	MG	1A	3396	1/1	0.87	0.24	73,73,73,73	0
58	MG	1A	3191	1/1	0.87	0.17	66,66,66,66	0
58	MG	1A	3479	1/1	0.87	0.14	61,61,61,61	0
58	MG	2a	1812	1/1	0.87	0.07	87,87,87,87	0
58	MG	1A	3128	1/1	0.87	0.14	61,61,61,61	0
58	MG	1a	1665	1/1	0.87	0.12	69,69,69,69	0
58	MG	2B	205	1/1	0.87	0.20	79,79,79,79	0
58	MG	1A	3484	1/1	0.87	0.27	65,65,65,65	0
58	MG	2A	3193	1/1	0.87	0.30	79,79,79,79	0
58	MG	1B	235	1/1	0.87	0.14	79,79,79,79	0
58	MG	2A	3199	1/1	0.87	0.14	76,76,76,76	0
58	MG	1A	3345	1/1	0.87	0.15	69,69,69,69	0
58	MG	1a	1671	1/1	0.87	0.16	77,77,77,77	0
58	MG	1A	3960	1/1	0.87	0.21	73,73,73,73	0
58	MG	1E	302	1/1	0.87	0.27	64,64,64,64	0
58	MG	1A	3496	1/1	0.87	0.26	77,77,77,77	0
58	MG	1w	109	1/1	0.87	0.15	80,80,80,80	0
58	MG	2A	3217	1/1	0.87	0.20	71,71,71,71	0
58	MG	2A	3472	1/1	0.87	0.16	76,76,76,76	0
58	MG	1A	3806	1/1	0.87	0.17	54,54,54,54	0
58	MG	2F	303	1/1	0.87	0.17	83,83,83,83	0
58	MG	2F	304	1/1	0.87	0.23	78,78,78,78	0
58	MG	2A	3219	1/1	0.87	0.31	73,73,73,73	0
58	MG	2A	3491	1/1	0.87	0.16	77,77,77,77	0
58	MG	2A	3222	1/1	0.87	0.17	70,70,70,70	0
58	MG	1F	311	1/1	0.87	0.16	63,63,63,63	0
58	MG	2A	3126	1/1	0.88	0.17	59,59,59,59	0
58	MG	1A	3629	1/1	0.88	0.13	46,46,46,46	0
58	MG	1e	203	1/1	0.88	0.30	74,74,74,74	0
58	MG	2A	3136	1/1	0.88	0.21	69,69,69,69	0
58	MG	1A	3860	1/1	0.88	0.27	46,46,46,46	0
58	MG	2a	1609	1/1	0.88	0.31	80,80,80,80	0
58	MG	2A	3144	1/1	0.88	0.14	53,53,53,53	0
58	MG	1A	3360	1/1	0.88	0.25	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	10	107	1/1	0.88	0.19	63,63,63,63	0
58	MG	1A	3866	1/1	0.88	0.12	53,53,53,53	0
58	MG	2A	3150	1/1	0.88	0.23	69,69,69,69	0
58	MG	2A	3603	1/1	0.88	0.26	76,76,76,76	0
58	MG	1A	3480	1/1	0.88	0.30	57,57,57,57	0
58	MG	2A	3335	1/1	0.88	0.14	74,74,74,74	0
58	MG	2A	3155	1/1	0.88	0.27	77,77,77,77	0
58	MG	2A	3611	1/1	0.88	0.12	62,62,62,62	0
58	MG	2A	3612	1/1	0.88	0.16	75,75,75,75	0
58	MG	1A	3048	1/1	0.88	0.16	54,54,54,54	0
58	MG	2A	3339	1/1	0.88	0.14	73,73,73,73	0
58	MG	2a	1629	1/1	0.88	0.23	65,65,65,65	0
58	MG	2a	1630	1/1	0.88	0.31	66,66,66,66	0
58	MG	1w	103	1/1	0.88	0.09	71,71,71,71	0
58	MG	2A	3624	1/1	0.88	0.11	62,62,62,62	0
58	MG	2A	3628	1/1	0.88	0.17	74,74,74,74	0
58	MG	1A	3157	1/1	0.88	0.17	38,38,38,38	0
58	MG	1A	3248	1/1	0.88	0.23	46,46,46,46	0
58	MG	1A	3888	1/1	0.88	0.21	49,49,49,49	0
58	MG	1A	4053	1/1	0.88	0.11	28,28,28,28	0
58	MG	2A	3168	1/1	0.88	0.12	77,77,77,77	0
58	MG	2A	3173	1/1	0.88	0.16	65,65,65,65	0
58	MG	2A	3174	1/1	0.88	0.15	71,71,71,71	0
58	MG	1A	3545	1/1	0.88	0.10	77,77,77,77	0
58	MG	1A	3549	1/1	0.88	0.19	64,64,64,64	0
58	MG	1a	1702	1/1	0.88	0.37	71,71,71,71	0
58	MG	2A	3185	1/1	0.88	0.33	75,75,75,75	0
58	MG	2A	3655	1/1	0.88	0.13	81,81,81,81	0
58	MG	2A	3658	1/1	0.88	0.12	68,68,68,68	0
58	MG	1A	3900	1/1	0.88	0.11	31,31,31,31	0
58	MG	1A	3902	1/1	0.88	0.19	49,49,49,49	0
58	MG	2A	3370	1/1	0.88	0.24	79,79,79,79	0
58	MG	2A	3665	1/1	0.88	0.11	70,70,70,70	0
58	MG	2A	3371	1/1	0.88	0.31	59,59,59,59	0
58	MG	1A	4070	1/1	0.88	0.14	72,72,72,72	0
58	MG	1A	4071	1/1	0.88	0.09	29,29,29,29	0
58	MG	1x	107	1/1	0.88	0.22	71,71,71,71	0
58	MG	2a	1681	1/1	0.88	0.11	80,80,80,80	0
58	MG	1A	4075	1/1	0.88	0.13	91,91,91,91	0
58	MG	1a	1712	1/1	0.88	0.19	74,74,74,74	0
58	MG	2A	3003	1/1	0.88	0.33	65,65,65,65	0
58	MG	2a	1686	1/1	0.88	0.11	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3384	1/1	0.88	0.14	58,58,58,58	0
58	MG	2A	3386	1/1	0.88	0.21	60,60,60,60	0
58	MG	2A	3388	1/1	0.88	0.19	67,67,67,67	0
58	MG	2A	3389	1/1	0.88	0.37	71,71,71,71	0
58	MG	2a	1693	1/1	0.88	0.17	80,80,80,80	0
58	MG	1A	3275	1/1	0.88	0.16	64,64,64,64	0
58	MG	2A	3391	1/1	0.88	0.35	69,69,69,69	0
58	MG	1a	1624	1/1	0.88	0.16	63,63,63,63	0
58	MG	1a	1625	1/1	0.88	0.24	67,67,67,67	0
58	MG	2a	1704	1/1	0.88	0.20	84,84,84,84	0
58	MG	1a	1723	1/1	0.88	0.35	66,66,66,66	0
58	MG	1a	1725	1/1	0.88	0.17	77,77,77,77	0
58	MG	2A	3212	1/1	0.88	0.11	65,65,65,65	0
58	MG	1A	3810	1/1	0.88	0.13	56,56,56,56	0
58	MG	1A	3557	1/1	0.88	0.32	73,73,73,73	0
58	MG	2A	3712	1/1	0.88	0.20	78,78,78,78	0
58	MG	1A	3812	1/1	0.88	0.26	58,58,58,58	0
58	MG	1A	3698	1/1	0.88	0.16	59,59,59,59	0
58	MG	2A	3046	1/1	0.88	0.21	75,75,75,75	0
58	MG	2A	3727	1/1	0.88	0.14	78,78,78,78	0
58	MG	1a	1735	1/1	0.88	0.13	71,71,71,71	0
58	MG	2a	1729	1/1	0.88	0.21	90,90,90,90	0
58	MG	1A	3922	1/1	0.88	0.14	78,78,78,78	0
58	MG	2A	3054	1/1	0.88	0.17	76,76,76,76	0
58	MG	2A	3056	1/1	0.88	0.43	75,75,75,75	0
58	MG	1A	3816	1/1	0.88	0.10	58,58,58,58	0
58	MG	2A	3429	1/1	0.88	0.27	66,66,66,66	0
58	MG	2A	3430	1/1	0.88	0.10	89,89,89,89	0
58	MG	2a	1747	1/1	0.88	0.23	83,83,83,83	0
58	MG	1A	3818	1/1	0.88	0.11	48,48,48,48	0
58	MG	1A	3164	1/1	0.88	0.15	71,71,71,71	0
58	MG	2A	3756	1/1	0.88	0.09	92,92,92,92	0
58	MG	1A	3820	1/1	0.88	0.18	79,79,79,79	0
58	MG	1A	3381	1/1	0.88	0.19	63,63,63,63	0
58	MG	1a	1762	1/1	0.88	0.23	71,71,71,71	0
58	MG	1a	1765	1/1	0.88	0.20	84,84,84,84	0
58	MG	1A	3716	1/1	0.88	0.16	68,68,68,68	0
58	MG	1A	3971	1/1	0.88	0.14	81,81,81,81	0
58	MG	1a	1772	1/1	0.88	0.24	74,74,74,74	0
58	MG	2A	3786	1/1	0.88	0.19	56,56,56,56	0
58	MG	2a	1773	1/1	0.88	0.19	77,77,77,77	0
58	MG	1a	1656	1/1	0.88	0.27	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3293	1/1	0.88	0.21	56,56,56,56	0
58	MG	1A	3259	1/1	0.88	0.21	62,62,62,62	0
58	MG	1A	3101	1/1	0.88	0.23	85,85,85,85	0
58	MG	1A	3516	1/1	0.88	0.30	73,73,73,73	0
58	MG	2A	3508	1/1	0.88	0.21	73,73,73,73	0
58	MG	2B	206	1/1	0.88	0.33	73,73,73,73	0
58	MG	1a	1785	1/1	0.88	0.23	75,75,75,75	0
58	MG	2a	1789	1/1	0.88	0.19	76,76,76,76	0
58	MG	1a	1787	1/1	0.88	0.18	67,67,67,67	0
58	MG	1F	309	1/1	0.88	0.27	48,48,48,48	0
58	MG	2A	3516	1/1	0.88	0.21	66,66,66,66	0
58	MG	2A	3273	1/1	0.88	0.09	81,81,81,81	0
58	MG	1a	1793	1/1	0.88	0.17	83,83,83,83	0
58	MG	2A	3094	1/1	0.88	0.14	86,86,86,86	0
58	MG	2A	3525	1/1	0.88	0.26	70,70,70,70	0
58	MG	2A	3279	1/1	0.88	0.26	74,74,74,74	0
58	MG	2E	301	1/1	0.88	0.26	77,77,77,77	0
58	MG	2A	3530	1/1	0.88	0.17	75,75,75,75	0
58	MG	1A	3760	1/1	0.88	0.10	43,43,43,43	0
58	MG	1A	3990	1/1	0.88	0.15	59,59,59,59	0
58	MG	1A	3300	1/1	0.88	0.25	44,44,44,44	0
58	MG	2E	308	1/1	0.88	0.14	55,55,55,55	0
58	MG	2A	3539	1/1	0.88	0.14	63,63,63,63	0
58	MG	1a	1668	1/1	0.88	0.19	73,73,73,73	0
58	MG	2A	3288	1/1	0.88	0.21	72,72,72,72	0
58	MG	2d	301	1/1	0.88	0.28	69,69,69,69	0
58	MG	2A	3291	1/1	0.88	0.38	82,82,82,82	0
58	MG	1A	3122	1/1	0.88	0.13	58,58,58,58	0
58	MG	2A	3106	1/1	0.88	0.18	78,78,78,78	0
58	MG	1a	1805	1/1	0.88	0.18	79,79,79,79	0
58	MG	2A	3561	1/1	0.88	0.17	69,69,69,69	0
58	MG	2q	201	1/1	0.88	0.10	81,81,81,81	0
58	MG	2A	3110	1/1	0.88	0.46	83,83,83,83	0
58	MG	1A	3842	1/1	0.88	0.25	44,44,44,44	0
58	MG	2A	3112	1/1	0.88	0.43	84,84,84,84	0
58	MG	2A	3570	1/1	0.88	0.27	79,79,79,79	0
58	MG	1A	3026	1/1	0.88	0.18	64,64,64,64	0
58	MG	25	102	1/1	0.88	0.16	63,63,63,63	0
58	MG	1A	3264	1/1	0.88	0.11	63,63,63,63	0
58	MG	2A	3575	1/1	0.88	0.14	66,66,66,66	0
58	MG	2A	3120	1/1	0.88	0.30	73,73,73,73	0
58	MG	1T	201	1/1	0.88	0.25	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3823	1/1	0.89	0.12	45,45,45,45	0
58	MG	1A	3527	1/1	0.89	0.23	59,59,59,59	0
58	MG	1a	1672	1/1	0.89	0.13	80,80,80,80	0
58	MG	1O	205	1/1	0.89	0.23	82,82,82,82	0
58	MG	2A	3670	1/1	0.89	0.12	85,85,85,85	0
58	MG	1A	3143	1/1	0.89	0.13	54,54,54,54	0
58	MG	1A	3695	1/1	0.89	0.09	87,87,87,87	0
58	MG	2a	1637	1/1	0.89	0.44	76,76,76,76	0
58	MG	2A	3677	1/1	0.89	0.31	56,56,56,56	0
58	MG	2a	1640	1/1	0.89	0.16	74,74,74,74	0
58	MG	1a	1810	1/1	0.89	0.24	80,80,80,80	0
58	MG	2A	3420	1/1	0.89	0.12	60,60,60,60	0
58	MG	1a	1814	1/1	0.89	0.10	64,64,64,64	0
58	MG	1A	3342	1/1	0.89	0.14	68,68,68,68	0
58	MG	2A	3100	1/1	0.89	0.08	38,38,38,38	0
58	MG	1A	4003	1/1	0.89	0.08	27,27,27,27	0
58	MG	1A	3387	1/1	0.89	0.12	67,67,67,67	0
58	MG	2A	3687	1/1	0.89	0.28	68,68,68,68	0
58	MG	2A	3435	1/1	0.89	0.21	61,61,61,61	0
58	MG	2A	3689	1/1	0.89	0.17	80,80,80,80	0
58	MG	2A	3439	1/1	0.89	0.18	68,68,68,68	0
58	MG	2A	3440	1/1	0.89	0.16	77,77,77,77	0
58	MG	1f	202	1/1	0.89	0.20	80,80,80,80	0
58	MG	1A	3224	1/1	0.89	0.13	55,55,55,55	0
58	MG	1A	3715	1/1	0.89	0.14	72,72,72,72	0
58	MG	1A	3255	1/1	0.89	0.16	73,73,73,73	0
58	MG	2A	3114	1/1	0.89	0.19	60,60,60,60	0
58	MG	2A	3465	1/1	0.89	0.10	53,53,53,53	0
58	MG	2a	1677	1/1	0.89	0.17	76,76,76,76	0
58	MG	1X	105	1/1	0.89	0.13	60,60,60,60	0
58	MG	1Y	201	1/1	0.89	0.20	71,71,71,71	0
58	MG	1A	3721	1/1	0.89	0.09	51,51,51,51	0
58	MG	2A	3485	1/1	0.89	0.16	43,43,43,43	0
58	MG	2A	3489	1/1	0.89	0.11	85,85,85,85	0
58	MG	2A	3121	1/1	0.89	0.18	68,68,68,68	0
58	MG	1A	4029	1/1	0.89	0.15	69,69,69,69	0
58	MG	2A	3493	1/1	0.89	0.14	63,63,63,63	0
58	MG	2A	3289	1/1	0.89	0.24	75,75,75,75	0
58	MG	1A	4033	1/1	0.89	0.14	79,79,79,79	0
58	MG	2A	3293	1/1	0.89	0.15	77,77,77,77	0
58	MG	2A	3500	1/1	0.89	0.09	37,37,37,37	0
58	MG	2A	3294	1/1	0.89	0.14	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3846	1/1	0.89	0.20	71,71,71,71	0
58	MG	17	105	1/1	0.89	0.20	64,64,64,64	0
58	MG	2A	3298	1/1	0.89	0.30	69,69,69,69	0
58	MG	1A	3542	1/1	0.89	0.12	62,62,62,62	0
58	MG	2A	3140	1/1	0.89	0.23	81,81,81,81	0
58	MG	1A	3120	1/1	0.89	0.34	56,56,56,56	0
58	MG	1A	3737	1/1	0.89	0.09	44,44,44,44	0
58	MG	2A	3306	1/1	0.89	0.20	69,69,69,69	0
58	MG	1A	3546	1/1	0.89	0.30	70,70,70,70	0
58	MG	2A	3146	1/1	0.89	0.33	66,66,66,66	0
58	MG	1A	3315	1/1	0.89	0.32	68,68,68,68	0
58	MG	1A	3759	1/1	0.89	0.13	44,44,44,44	0
58	MG	1a	1716	1/1	0.89	0.42	80,80,80,80	0
58	MG	1A	3088	1/1	0.89	0.22	61,61,61,61	0
58	MG	2a	1728	1/1	0.89	0.12	92,92,92,92	0
58	MG	1A	4054	1/1	0.89	0.10	64,64,64,64	0
58	MG	2a	1732	1/1	0.89	0.17	90,90,90,90	0
58	MG	1A	3321	1/1	0.89	0.37	43,43,43,43	0
58	MG	1a	1613	1/1	0.89	0.18	79,79,79,79	0
58	MG	2a	1735	1/1	0.89	0.17	83,83,83,83	0
58	MG	1A	3412	1/1	0.89	0.25	65,65,65,65	0
58	MG	2A	3550	1/1	0.89	0.10	60,60,60,60	0
58	MG	1A	3418	1/1	0.89	0.21	62,62,62,62	0
58	MG	1A	3243	1/1	0.89	0.10	55,55,55,55	0
58	MG	1A	3580	1/1	0.89	0.09	50,50,50,50	0
58	MG	2A	3010	1/1	0.89	0.15	73,73,73,73	0
58	MG	1A	3423	1/1	0.89	0.23	64,64,64,64	0
58	MG	2A	3018	1/1	0.89	0.12	66,66,66,66	0
58	MG	2a	1753	1/1	0.89	0.10	88,88,88,88	0
58	MG	2a	1754	1/1	0.89	0.17	75,75,75,75	0
58	MG	2A	3020	1/1	0.89	0.15	76,76,76,76	0
58	MG	1A	3494	1/1	0.89	0.27	56,56,56,56	0
58	MG	2A	3024	1/1	0.89	0.22	72,72,72,72	0
58	MG	2B	218	1/1	0.89	0.31	78,78,78,78	0
58	MG	2D	301	1/1	0.89	0.13	58,58,58,58	0
58	MG	2D	305	1/1	0.89	0.28	70,70,70,70	0
58	MG	2A	3340	1/1	0.89	0.22	66,66,66,66	0
58	MG	2a	1768	1/1	0.89	0.24	76,76,76,76	0
58	MG	2A	3028	1/1	0.89	0.28	64,64,64,64	0
58	MG	2A	3029	1/1	0.89	0.19	87,87,87,87	0
58	MG	1A	3587	1/1	0.89	0.14	60,60,60,60	0
58	MG	2A	3031	1/1	0.89	0.10	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3348	1/1	0.89	0.18	72,72,72,72	0
58	MG	1A	4079	1/1	0.89	0.12	31,31,31,31	0
58	MG	1A	3326	1/1	0.89	0.28	65,65,65,65	0
58	MG	1A	4083	1/1	0.89	0.26	82,82,82,82	0
58	MG	2A	3042	1/1	0.89	0.17	71,71,71,71	0
58	MG	2A	3356	1/1	0.89	0.27	59,59,59,59	0
58	MG	2a	1788	1/1	0.89	0.26	75,75,75,75	0
58	MG	2A	3043	1/1	0.89	0.33	69,69,69,69	0
58	MG	2a	1790	1/1	0.89	0.22	73,73,73,73	0
58	MG	2A	3200	1/1	0.89	0.18	70,70,70,70	0
58	MG	1B	203	1/1	0.89	0.12	52,52,52,52	0
58	MG	2A	3601	1/1	0.89	0.17	68,68,68,68	0
58	MG	1A	3430	1/1	0.89	0.21	75,75,75,75	0
58	MG	1a	1642	1/1	0.89	0.33	82,82,82,82	0
58	MG	1A	3327	1/1	0.89	0.16	65,65,65,65	0
58	MG	2A	3208	1/1	0.89	0.15	80,80,80,80	0
58	MG	1A	3433	1/1	0.89	0.17	73,73,73,73	0
58	MG	1A	3330	1/1	0.89	0.31	61,61,61,61	0
58	MG	2a	1808	1/1	0.89	0.25	73,73,73,73	0
58	MG	2a	1810	1/1	0.89	0.27	76,76,76,76	0
58	MG	2A	3375	1/1	0.89	0.35	70,70,70,70	0
58	MG	1A	3443	1/1	0.89	0.24	50,50,50,50	0
58	MG	2A	3622	1/1	0.89	0.19	81,81,81,81	0
58	MG	1A	3514	1/1	0.89	0.14	67,67,67,67	0
58	MG	2a	1603	1/1	0.89	0.31	76,76,76,76	0
58	MG	2a	1604	1/1	0.89	0.26	72,72,72,72	0
58	MG	1A	3942	1/1	0.89	0.09	62,62,62,62	0
58	MG	2A	3626	1/1	0.89	0.10	42,42,42,42	0
58	MG	1A	3950	1/1	0.89	0.09	31,31,31,31	0
58	MG	2A	3635	1/1	0.89	0.11	59,59,59,59	0
58	MG	1A	3089	1/1	0.89	0.19	52,52,52,52	0
58	MG	2a	1611	1/1	0.89	0.34	74,74,74,74	0
58	MG	2A	3224	1/1	0.89	0.15	66,66,66,66	0
58	MG	1A	3371	1/1	0.89	0.18	58,58,58,58	0
58	MG	1A	3519	1/1	0.89	0.09	80,80,80,80	0
58	MG	1A	3666	1/1	0.89	0.08	45,45,45,45	0
58	MG	1A	3450	1/1	0.89	0.21	72,72,72,72	0
58	MG	1A	3452	1/1	0.89	0.27	78,78,78,78	0
58	MG	1A	3138	1/1	0.89	0.18	63,63,63,63	0
58	MG	2A	3241	1/1	0.89	0.22	77,77,77,77	0
58	MG	2A	3397	1/1	0.89	0.14	70,70,70,70	0
58	MG	2x	102	1/1	0.89	0.22	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3983	1/1	0.89	0.13	61,61,61,61	0
58	MG	1a	1796	1/1	0.89	0.21	77,77,77,77	0
58	MG	1A	3690	1/1	0.89	0.16	47,47,47,47	0
58	MG	2a	1627	1/1	0.89	0.12	89,89,89,89	0
59	K	2A	3403	1/1	0.89	0.12	84,84,84,84	0
58	MG	1A	4043	1/1	0.90	0.16	41,41,41,41	0
58	MG	1A	4044	1/1	0.90	0.10	33,33,33,33	0
58	MG	2A	3032	1/1	0.90	0.27	69,69,69,69	0
58	MG	1A	3885	1/1	0.90	0.13	63,63,63,63	0
58	MG	2A	3647	1/1	0.90	0.10	55,55,55,55	0
58	MG	2A	3385	1/1	0.90	0.26	61,61,61,61	0
58	MG	1A	3409	1/1	0.90	0.14	65,65,65,65	0
58	MG	1A	3466	1/1	0.90	0.14	60,60,60,60	0
58	MG	1A	3182	1/1	0.90	0.12	58,58,58,58	0
58	MG	1A	3411	1/1	0.90	0.16	68,68,68,68	0
58	MG	1A	3895	1/1	0.90	0.38	72,72,72,72	0
58	MG	1a	1612	1/1	0.90	0.12	78,78,78,78	0
58	MG	1A	3006	1/1	0.90	0.18	69,69,69,69	0
58	MG	2A	3395	1/1	0.90	0.31	73,73,73,73	0
58	MG	2A	3053	1/1	0.90	0.20	88,88,88,88	0
58	MG	2a	1636	1/1	0.90	0.31	70,70,70,70	0
58	MG	2A	3666	1/1	0.90	0.18	72,72,72,72	0
58	MG	1a	1619	1/1	0.90	0.10	74,74,74,74	0
58	MG	2A	3231	1/1	0.90	0.20	69,69,69,69	0
58	MG	2A	3055	1/1	0.90	0.15	70,70,70,70	0
58	MG	2a	1642	1/1	0.90	0.18	75,75,75,75	0
58	MG	1A	3901	1/1	0.90	0.14	37,37,37,37	0
58	MG	1A	3649	1/1	0.90	0.14	39,39,39,39	0
58	MG	1A	3903	1/1	0.90	0.24	50,50,50,50	0
58	MG	1A	3798	1/1	0.90	0.14	41,41,41,41	0
58	MG	2A	3062	1/1	0.90	0.15	60,60,60,60	0
58	MG	1A	3530	1/1	0.90	0.21	57,57,57,57	0
58	MG	1a	1767	1/1	0.90	0.22	81,81,81,81	0
58	MG	2a	1655	1/1	0.90	0.15	91,91,91,91	0
58	MG	1a	1627	1/1	0.90	0.28	64,64,64,64	0
58	MG	1A	3257	1/1	0.90	0.07	44,44,44,44	0
58	MG	1A	3258	1/1	0.90	0.13	41,41,41,41	0
58	MG	1a	1774	1/1	0.90	0.20	66,66,66,66	0
58	MG	1a	1631	1/1	0.90	0.15	80,80,80,80	0
58	MG	1A	3533	1/1	0.90	0.21	44,44,44,44	0
58	MG	2a	1668	1/1	0.90	0.35	67,67,67,67	0
58	MG	2A	3694	1/1	0.90	0.19	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3673	1/1	0.90	0.08	28,28,28,28	0
58	MG	2a	1672	1/1	0.90	0.15	77,77,77,77	0
58	MG	2A	3256	1/1	0.90	0.37	80,80,80,80	0
58	MG	1a	1635	1/1	0.90	0.31	84,84,84,84	0
58	MG	2A	3082	1/1	0.90	0.17	61,61,61,61	0
58	MG	2A	3083	1/1	0.90	0.18	64,64,64,64	0
58	MG	2a	1680	1/1	0.90	0.23	65,65,65,65	0
58	MG	1a	1783	1/1	0.90	0.16	74,74,74,74	0
58	MG	2A	3704	1/1	0.90	0.18	86,86,86,86	0
58	MG	2A	3452	1/1	0.90	0.10	46,46,46,46	0
58	MG	1B	201	1/1	0.90	0.20	73,73,73,73	0
58	MG	2A	3709	1/1	0.90	0.07	83,83,83,83	0
58	MG	1A	3684	1/1	0.90	0.09	33,33,33,33	0
58	MG	2a	1689	1/1	0.90	0.27	85,85,85,85	0
58	MG	1a	1788	1/1	0.90	0.23	67,67,67,67	0
58	MG	2A	3272	1/1	0.90	0.33	82,82,82,82	0
58	MG	2A	3718	1/1	0.90	0.08	52,52,52,52	0
58	MG	1A	3534	1/1	0.90	0.20	60,60,60,60	0
58	MG	2A	3723	1/1	0.90	0.19	61,61,61,61	0
58	MG	2A	3725	1/1	0.90	0.21	65,65,65,65	0
58	MG	1A	3004	1/1	0.90	0.09	33,33,33,33	0
58	MG	2a	1702	1/1	0.90	0.30	76,76,76,76	0
58	MG	1B	216	1/1	0.90	0.09	61,61,61,61	0
58	MG	1A	3366	1/1	0.90	0.09	55,55,55,55	0
58	MG	2A	3731	1/1	0.90	0.29	69,69,69,69	0
58	MG	1B	221	1/1	0.90	0.12	74,74,74,74	0
58	MG	1a	1798	1/1	0.90	0.26	60,60,60,60	0
58	MG	1a	1650	1/1	0.90	0.09	67,67,67,67	0
58	MG	2A	3739	1/1	0.90	0.09	89,89,89,89	0
58	MG	2a	1710	1/1	0.90	0.15	78,78,78,78	0
58	MG	2A	3494	1/1	0.90	0.17	50,50,50,50	0
58	MG	1A	3956	1/1	0.90	0.13	70,70,70,70	0
58	MG	2a	1713	1/1	0.90	0.15	70,70,70,70	0
58	MG	2a	1714	1/1	0.90	0.29	82,82,82,82	0
58	MG	2a	1715	1/1	0.90	0.24	72,72,72,72	0
58	MG	1a	1802	1/1	0.90	0.14	78,78,78,78	0
58	MG	1A	3335	1/1	0.90	0.22	67,67,67,67	0
58	MG	2A	3752	1/1	0.90	0.12	52,52,52,52	0
58	MG	2a	1725	1/1	0.90	0.18	80,80,80,80	0
58	MG	2A	3290	1/1	0.90	0.11	61,61,61,61	0
58	MG	2A	3107	1/1	0.90	0.35	72,72,72,72	0
58	MG	2A	3507	1/1	0.90	0.17	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3962	1/1	0.90	0.09	79,79,79,79	0
58	MG	1A	3107	1/1	0.90	0.40	43,43,43,43	0
58	MG	2A	3773	1/1	0.90	0.20	72,72,72,72	0
58	MG	2A	3776	1/1	0.90	0.22	85,85,85,85	0
58	MG	2A	3778	1/1	0.90	0.12	75,75,75,75	0
58	MG	1a	1659	1/1	0.90	0.32	78,78,78,78	0
58	MG	1A	3237	1/1	0.90	0.32	60,60,60,60	0
58	MG	1A	3696	1/1	0.90	0.20	59,59,59,59	0
58	MG	1a	1811	1/1	0.90	0.09	70,70,70,70	0
58	MG	1a	1812	1/1	0.90	0.13	68,68,68,68	0
58	MG	2a	1750	1/1	0.90	0.17	62,62,62,62	0
58	MG	2A	3790	1/1	0.90	0.10	55,55,55,55	0
58	MG	1A	3969	1/1	0.90	0.14	69,69,69,69	0
58	MG	2A	3799	1/1	0.90	0.12	74,74,74,74	0
58	MG	2A	3800	1/1	0.90	0.17	86,86,86,86	0
58	MG	1A	3493	1/1	0.90	0.12	60,60,60,60	0
58	MG	1A	3262	1/1	0.90	0.21	77,77,77,77	0
58	MG	2A	3123	1/1	0.90	0.07	81,81,81,81	0
58	MG	1A	3442	1/1	0.90	0.21	53,53,53,53	0
58	MG	1E	309	1/1	0.90	0.12	60,60,60,60	0
58	MG	1A	3195	1/1	0.90	0.39	77,77,77,77	0
58	MG	1A	3346	1/1	0.90	0.19	60,60,60,60	0
58	MG	2B	209	1/1	0.90	0.21	81,81,81,81	0
58	MG	2A	3137	1/1	0.90	0.34	67,67,67,67	0
58	MG	1A	3245	1/1	0.90	0.19	60,60,60,60	0
58	MG	2A	3317	1/1	0.90	0.15	76,76,76,76	0
58	MG	2A	3547	1/1	0.90	0.22	52,52,52,52	0
58	MG	1A	3574	1/1	0.90	0.19	63,63,63,63	0
58	MG	1A	3579	1/1	0.90	0.12	47,47,47,47	0
58	MG	2A	3558	1/1	0.90	0.20	65,65,65,65	0
58	MG	1A	3993	1/1	0.90	0.14	43,43,43,43	0
58	MG	1N	202	1/1	0.90	0.09	53,53,53,53	0
58	MG	2D	304	1/1	0.90	0.42	53,53,53,53	0
58	MG	1A	3841	1/1	0.90	0.13	65,65,65,65	0
58	MG	1A	3998	1/1	0.90	0.11	70,70,70,70	0
58	MG	1P	205	1/1	0.90	0.23	53,53,53,53	0
58	MG	1A	3505	1/1	0.90	0.31	57,57,57,57	0
58	MG	1A	3168	1/1	0.90	0.23	70,70,70,70	0
58	MG	1A	3398	1/1	0.90	0.34	47,47,47,47	0
58	MG	2A	3157	1/1	0.90	0.21	62,62,62,62	0
58	MG	1A	3847	1/1	0.90	0.10	55,55,55,55	0
58	MG	1A	3848	1/1	0.90	0.09	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2a	1803	1/1	0.90	0.12	72,72,72,72	0
58	MG	1A	3584	1/1	0.90	0.14	53,53,53,53	0
58	MG	2A	3162	1/1	0.90	0.15	74,74,74,74	0
58	MG	1a	1692	1/1	0.90	0.43	74,74,74,74	0
58	MG	1U	204	1/1	0.90	0.24	45,45,45,45	0
58	MG	2A	3347	1/1	0.90	0.13	77,77,77,77	0
58	MG	1A	3090	1/1	0.90	0.18	62,62,62,62	0
58	MG	2A	3171	1/1	0.90	0.25	70,70,70,70	0
58	MG	1A	4028	1/1	0.90	0.18	78,78,78,78	0
58	MG	2A	3352	1/1	0.90	0.35	60,60,60,60	0
58	MG	1A	3407	1/1	0.90	0.42	72,72,72,72	0
58	MG	1y	101	1/1	0.90	0.15	70,70,70,70	0
58	MG	25	101	1/1	0.90	0.28	65,65,65,65	0
58	MG	1a	1700	1/1	0.90	0.30	62,62,62,62	0
58	MG	1Z	302	1/1	0.90	0.17	75,75,75,75	0
58	MG	1A	3771	1/1	0.90	0.09	54,54,54,54	0
58	MG	28	101	1/1	0.90	0.12	65,65,65,65	0
58	MG	1A	3592	1/1	0.90	0.10	37,37,37,37	0
58	MG	2A	3361	1/1	0.90	0.35	75,75,75,75	0
58	MG	11	102	1/1	0.90	0.14	54,54,54,54	0
58	MG	11	104	1/1	0.90	0.10	78,78,78,78	0
58	MG	2A	3365	1/1	0.90	0.34	66,66,66,66	0
58	MG	1A	3460	1/1	0.90	0.13	59,59,59,59	0
58	MG	2t	201	1/1	0.90	0.23	62,62,62,62	0
58	MG	2A	3368	1/1	0.90	0.33	71,71,71,71	0
58	MG	1A	4038	1/1	0.90	0.08	48,48,48,48	0
58	MG	13	104	1/1	0.90	0.13	58,58,58,58	0
58	MG	2A	3625	1/1	0.90	0.12	58,58,58,58	0
58	MG	1A	3781	1/1	0.90	0.12	52,52,52,52	0
58	MG	2A	3374	1/1	0.90	0.22	71,71,71,71	0
58	MG	2A	3026	1/1	0.90	0.21	65,65,65,65	0
58	MG	2A	3377	1/1	0.90	0.28	77,77,77,77	0
58	MG	18	103	1/1	0.90	0.14	59,59,59,59	0
58	MG	1A	3216	1/1	0.90	0.18	44,44,44,44	0
58	MG	1A	3948	1/1	0.91	0.08	40,40,40,40	0
58	MG	2A	3587	1/1	0.91	0.15	77,77,77,77	0
58	MG	1A	3039	1/1	0.91	0.23	65,65,65,65	0
58	MG	1B	233	1/1	0.91	0.16	60,60,60,60	0
58	MG	1A	3955	1/1	0.91	0.12	51,51,51,51	0
58	MG	2A	3143	1/1	0.91	0.26	49,49,49,49	0
58	MG	1l	202	1/1	0.91	0.08	76,76,76,76	0
58	MG	1A	3307	1/1	0.91	0.27	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3337	1/1	0.91	0.15	73,73,73,73	0
58	MG	2A	3600	1/1	0.91	0.13	88,88,88,88	0
58	MG	1A	3814	1/1	0.91	0.16	64,64,64,64	0
58	MG	1A	3401	1/1	0.91	0.12	46,46,46,46	0
58	MG	1A	3100	1/1	0.91	0.12	64,64,64,64	0
58	MG	1A	3817	1/1	0.91	0.17	49,49,49,49	0
58	MG	2A	3608	1/1	0.91	0.23	70,70,70,70	0
58	MG	1A	3671	1/1	0.91	0.12	40,40,40,40	0
58	MG	2A	3343	1/1	0.91	0.12	83,83,83,83	0
58	MG	2a	1618	1/1	0.91	0.21	91,91,91,91	0
58	MG	1A	3404	1/1	0.91	0.12	60,60,60,60	0
58	MG	1A	3682	1/1	0.91	0.14	63,63,63,63	0
58	MG	1F	310	1/1	0.91	0.22	65,65,65,65	0
58	MG	1A	3020	1/1	0.91	0.23	64,64,64,64	0
58	MG	1a	1679	1/1	0.91	0.08	84,84,84,84	0
58	MG	1A	3152	1/1	0.91	0.17	56,56,56,56	0
58	MG	1A	3029	1/1	0.91	0.10	46,46,46,46	0
58	MG	2A	3353	1/1	0.91	0.23	53,53,53,53	0
58	MG	2A	3163	1/1	0.91	0.09	75,75,75,75	0
58	MG	1A	3471	1/1	0.91	0.22	59,59,59,59	0
58	MG	1N	205	1/1	0.91	0.17	60,60,60,60	0
58	MG	1O	204	1/1	0.91	0.10	68,68,68,68	0
58	MG	2a	1632	1/1	0.91	0.17	87,87,87,87	0
58	MG	2A	3638	1/1	0.91	0.14	70,70,70,70	0
58	MG	1A	3249	1/1	0.91	0.12	78,78,78,78	0
58	MG	1A	3477	1/1	0.91	0.19	47,47,47,47	0
58	MG	2A	3360	1/1	0.91	0.42	70,70,70,70	0
58	MG	1A	3989	1/1	0.91	0.09	55,55,55,55	0
58	MG	2A	3177	1/1	0.91	0.31	64,64,64,64	0
58	MG	1Q	201	1/1	0.91	0.33	49,49,49,49	0
58	MG	2A	3179	1/1	0.91	0.12	70,70,70,70	0
58	MG	2A	3182	1/1	0.91	0.32	78,78,78,78	0
58	MG	1A	3251	1/1	0.91	0.13	71,71,71,71	0
58	MG	2A	3653	1/1	0.91	0.23	78,78,78,78	0
58	MG	1Q	206	1/1	0.91	0.09	69,69,69,69	0
58	MG	1A	3992	1/1	0.91	0.11	62,62,62,62	0
58	MG	1a	1698	1/1	0.91	0.40	70,70,70,70	0
58	MG	1a	1699	1/1	0.91	0.27	60,60,60,60	0
58	MG	2A	3007	1/1	0.91	0.12	59,59,59,59	0
58	MG	1R	207	1/1	0.91	0.21	50,50,50,50	0
58	MG	1A	3111	1/1	0.91	0.16	47,47,47,47	0
58	MG	1A	3834	1/1	0.91	0.09	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3555	1/1	0.91	0.25	48,48,48,48	0
58	MG	1a	1705	1/1	0.91	0.57	89,89,89,89	0
58	MG	1a	1706	1/1	0.91	0.20	66,66,66,66	0
58	MG	2A	3383	1/1	0.91	0.27	66,66,66,66	0
58	MG	1A	3999	1/1	0.91	0.07	83,83,83,83	0
58	MG	1A	3414	1/1	0.91	0.34	72,72,72,72	0
58	MG	1a	1709	1/1	0.91	0.36	72,72,72,72	0
58	MG	2A	3387	1/1	0.91	0.29	77,77,77,77	0
58	MG	2a	1673	1/1	0.91	0.15	73,73,73,73	0
58	MG	2a	1674	1/1	0.91	0.28	63,63,63,63	0
58	MG	1A	3482	1/1	0.91	0.09	61,61,61,61	0
58	MG	1A	3707	1/1	0.91	0.16	66,66,66,66	0
58	MG	1a	1713	1/1	0.91	0.13	67,67,67,67	0
58	MG	2A	3210	1/1	0.91	0.37	68,68,68,68	0
58	MG	1a	1714	1/1	0.91	0.30	75,75,75,75	0
58	MG	2A	3215	1/1	0.91	0.16	68,68,68,68	0
58	MG	1A	4012	1/1	0.91	0.15	51,51,51,51	0
58	MG	2A	3035	1/1	0.91	0.11	71,71,71,71	0
58	MG	2A	3399	1/1	0.91	0.17	69,69,69,69	0
58	MG	1A	3417	1/1	0.91	0.14	67,67,67,67	0
58	MG	1A	4016	1/1	0.91	0.10	78,78,78,78	0
58	MG	1A	3845	1/1	0.91	0.10	73,73,73,73	0
58	MG	2A	3223	1/1	0.91	0.16	75,75,75,75	0
58	MG	1A	3560	1/1	0.91	0.11	63,63,63,63	0
58	MG	2A	3226	1/1	0.91	0.32	68,68,68,68	0
58	MG	2A	3703	1/1	0.91	0.16	74,74,74,74	0
58	MG	2A	3412	1/1	0.91	0.16	69,69,69,69	0
58	MG	2A	3228	1/1	0.91	0.16	74,74,74,74	0
58	MG	2A	3229	1/1	0.91	0.20	70,70,70,70	0
58	MG	1a	1724	1/1	0.91	0.32	61,61,61,61	0
58	MG	2A	3710	1/1	0.91	0.22	69,69,69,69	0
58	MG	1A	3286	1/1	0.91	0.35	57,57,57,57	0
58	MG	2A	3714	1/1	0.91	0.26	80,80,80,80	0
58	MG	1A	4024	1/1	0.91	0.15	68,68,68,68	0
58	MG	1A	3093	1/1	0.91	0.20	60,60,60,60	0
58	MG	1A	3422	1/1	0.91	0.10	68,68,68,68	0
58	MG	2A	3235	1/1	0.91	0.12	77,77,77,77	0
58	MG	1A	3855	1/1	0.91	0.20	40,40,40,40	0
58	MG	1A	3733	1/1	0.91	0.14	55,55,55,55	0
58	MG	1A	3576	1/1	0.91	0.11	65,65,65,65	0
58	MG	1a	1741	1/1	0.91	0.10	74,74,74,74	0
58	MG	1A	3577	1/1	0.91	0.25	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3865	1/1	0.91	0.10	50,50,50,50	0
58	MG	1a	1749	1/1	0.91	0.16	70,70,70,70	0
58	MG	2A	3445	1/1	0.91	0.17	49,49,49,49	0
58	MG	1A	3179	1/1	0.91	0.27	46,46,46,46	0
58	MG	2a	1724	1/1	0.91	0.14	77,77,77,77	0
58	MG	2A	3250	1/1	0.91	0.15	69,69,69,69	0
58	MG	2A	3740	1/1	0.91	0.19	61,61,61,61	0
58	MG	2A	3742	1/1	0.91	0.08	66,66,66,66	0
58	MG	1A	4042	1/1	0.91	0.15	42,42,42,42	0
58	MG	2a	1731	1/1	0.91	0.15	64,64,64,64	0
58	MG	2A	3455	1/1	0.91	0.17	67,67,67,67	0
58	MG	1A	3758	1/1	0.91	0.07	72,72,72,72	0
58	MG	2A	3460	1/1	0.91	0.10	38,38,38,38	0
58	MG	1A	3873	1/1	0.91	0.06	48,48,48,48	0
58	MG	1A	3368	1/1	0.91	0.17	62,62,62,62	0
58	MG	2A	3757	1/1	0.91	0.20	69,69,69,69	0
58	MG	2a	1740	1/1	0.91	0.17	72,72,72,72	0
58	MG	2A	3758	1/1	0.91	0.12	55,55,55,55	0
58	MG	2A	3475	1/1	0.91	0.14	57,57,57,57	0
58	MG	2A	3764	1/1	0.91	0.18	60,60,60,60	0
58	MG	2A	3071	1/1	0.91	0.14	64,64,64,64	0
58	MG	1A	3295	1/1	0.91	0.25	77,77,77,77	0
58	MG	2A	3482	1/1	0.91	0.14	67,67,67,67	0
58	MG	1A	3372	1/1	0.91	0.16	55,55,55,55	0
58	MG	2A	3263	1/1	0.91	0.09	76,76,76,76	0
58	MG	2A	3777	1/1	0.91	0.31	91,91,91,91	0
58	MG	2a	1755	1/1	0.91	0.08	87,87,87,87	0
58	MG	1A	3769	1/1	0.91	0.10	54,54,54,54	0
58	MG	2a	1757	1/1	0.91	0.07	92,92,92,92	0
58	MG	1A	3373	1/1	0.91	0.11	56,56,56,56	0
58	MG	1A	4055	1/1	0.91	0.27	67,67,67,67	0
58	MG	2A	3782	1/1	0.91	0.14	80,80,80,80	0
58	MG	1A	3772	1/1	0.91	0.08	30,30,30,30	0
58	MG	1A	3435	1/1	0.91	0.10	61,61,61,61	0
58	MG	2a	1763	1/1	0.91	0.20	73,73,73,73	0
58	MG	2A	3269	1/1	0.91	0.31	74,74,74,74	0
58	MG	2a	1765	1/1	0.91	0.20	82,82,82,82	0
58	MG	2A	3270	1/1	0.91	0.09	68,68,68,68	0
58	MG	1A	3506	1/1	0.91	0.14	66,66,66,66	0
58	MG	2a	1772	1/1	0.91	0.14	81,81,81,81	0
58	MG	1A	3897	1/1	0.91	0.26	40,40,40,40	0
58	MG	1a	1780	1/1	0.91	0.13	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	4067	1/1	0.91	0.09	52,52,52,52	0
58	MG	2B	201	1/1	0.91	0.18	79,79,79,79	0
58	MG	2A	3278	1/1	0.91	0.23	75,75,75,75	0
58	MG	1A	3296	1/1	0.91	0.19	67,67,67,67	0
58	MG	1A	3599	1/1	0.91	0.08	18,18,18,18	0
58	MG	1a	1786	1/1	0.91	0.18	79,79,79,79	0
58	MG	1A	3606	1/1	0.91	0.13	50,50,50,50	0
58	MG	2a	1786	1/1	0.91	0.32	71,71,71,71	0
58	MG	2A	3285	1/1	0.91	0.08	68,68,68,68	0
58	MG	1A	3376	1/1	0.91	0.30	67,67,67,67	0
58	MG	2A	3523	1/1	0.91	0.17	63,63,63,63	0
58	MG	2A	3287	1/1	0.91	0.14	63,63,63,63	0
58	MG	1a	1789	1/1	0.91	0.12	85,85,85,85	0
58	MG	1A	4078	1/1	0.91	0.10	54,54,54,54	0
58	MG	2a	1798	1/1	0.91	0.28	72,72,72,72	0
58	MG	2a	1799	1/1	0.91	0.12	83,83,83,83	0
58	MG	2A	3531	1/1	0.91	0.11	43,43,43,43	0
58	MG	2A	3101	1/1	0.91	0.27	72,72,72,72	0
58	MG	1A	3336	1/1	0.91	0.14	59,59,59,59	0
58	MG	1A	3446	1/1	0.91	0.28	47,47,47,47	0
58	MG	1A	3094	1/1	0.91	0.17	64,64,64,64	0
58	MG	2A	3108	1/1	0.91	0.18	62,62,62,62	0
58	MG	1A	3341	1/1	0.91	0.16	64,64,64,64	0
58	MG	2a	1807	1/1	0.91	0.26	61,61,61,61	0
58	MG	1a	1641	1/1	0.91	0.19	69,69,69,69	0
58	MG	1A	3630	1/1	0.91	0.11	38,38,38,38	0
58	MG	2a	1811	1/1	0.91	0.14	76,76,76,76	0
58	MG	1A	3915	1/1	0.91	0.12	40,40,40,40	0
58	MG	1B	209	1/1	0.91	0.12	56,56,56,56	0
58	MG	1A	3390	1/1	0.91	0.29	49,49,49,49	0
58	MG	2A	3117	1/1	0.91	0.21	59,59,59,59	0
58	MG	2F	301	1/1	0.91	0.20	51,51,51,51	0
58	MG	1A	3095	1/1	0.91	0.22	51,51,51,51	0
58	MG	2A	3308	1/1	0.91	0.09	63,63,63,63	0
58	MG	2A	3119	1/1	0.91	0.42	76,76,76,76	0
58	MG	1B	219	1/1	0.91	0.11	59,59,59,59	0
58	MG	2N	201	1/1	0.91	0.13	73,73,73,73	0
58	MG	2O	201	1/1	0.91	0.13	67,67,67,67	0
58	MG	1A	3934	1/1	0.91	0.09	71,71,71,71	0
58	MG	2A	3567	1/1	0.91	0.17	57,57,57,57	0
58	MG	2A	3568	1/1	0.91	0.12	61,61,61,61	0
58	MG	2A	3313	1/1	0.91	0.18	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2U	201	1/1	0.91	0.21	70,70,70,70	0
58	MG	2W	201	1/1	0.91	0.22	79,79,79,79	0
58	MG	2Y	201	1/1	0.91	0.19	63,63,63,63	0
58	MG	2A	3571	1/1	0.91	0.25	68,68,68,68	0
58	MG	1A	3935	1/1	0.91	0.10	55,55,55,55	0
58	MG	1A	3936	1/1	0.91	0.09	61,61,61,61	0
58	MG	2A	3125	1/1	0.91	0.14	76,76,76,76	0
58	MG	2I	101	1/1	0.91	0.23	80,80,80,80	0
58	MG	1B	225	1/1	0.91	0.31	68,68,68,68	0
58	MG	1A	3647	1/1	0.91	0.09	46,46,46,46	0
58	MG	1A	3130	1/1	0.91	0.08	68,68,68,68	0
58	MG	2A	3583	1/1	0.91	0.12	73,73,73,73	0
58	MG	2A	3134	1/1	0.91	0.10	78,78,78,78	0
58	MG	1A	3374	1/1	0.92	0.13	63,63,63,63	0
58	MG	1A	3434	1/1	0.92	0.26	56,56,56,56	0
58	MG	1A	3288	1/1	0.92	0.33	73,73,73,73	0
58	MG	1B	223	1/1	0.92	0.10	67,67,67,67	0
58	MG	1A	3017	1/1	0.92	0.17	60,60,60,60	0
58	MG	1A	3290	1/1	0.92	0.17	61,61,61,61	0
58	MG	2a	1610	1/1	0.92	0.23	72,72,72,72	0
58	MG	2A	3619	1/1	0.92	0.14	67,67,67,67	0
58	MG	2A	3620	1/1	0.92	0.17	70,70,70,70	0
58	MG	1A	3944	1/1	0.92	0.10	68,68,68,68	0
58	MG	1A	3292	1/1	0.92	0.08	48,48,48,48	0
58	MG	1A	3949	1/1	0.92	0.17	54,54,54,54	0
58	MG	1B	231	1/1	0.92	0.07	82,82,82,82	0
58	MG	2A	3172	1/1	0.92	0.22	72,72,72,72	0
58	MG	1a	1667	1/1	0.92	0.11	65,65,65,65	0
58	MG	2A	3627	1/1	0.92	0.17	75,75,75,75	0
58	MG	1A	3805	1/1	0.92	0.16	39,39,39,39	0
58	MG	1A	3953	1/1	0.92	0.18	61,61,61,61	0
58	MG	1A	3633	1/1	0.92	0.18	62,62,62,62	0
58	MG	1A	3635	1/1	0.92	0.08	51,51,51,51	0
58	MG	1D	3604	1/1	0.92	0.13	54,54,54,54	0
58	MG	1A	3957	1/1	0.92	0.12	64,64,64,64	0
58	MG	1A	3384	1/1	0.92	0.10	71,71,71,71	0
58	MG	1A	3447	1/1	0.92	0.11	60,60,60,60	0
58	MG	2A	3187	1/1	0.92	0.33	73,73,73,73	0
58	MG	1A	3385	1/1	0.92	0.17	52,52,52,52	0
58	MG	2A	3372	1/1	0.92	0.28	77,77,77,77	0
58	MG	1A	3964	1/1	0.92	0.12	56,56,56,56	0
58	MG	2A	3650	1/1	0.92	0.15	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3338	1/1	0.92	0.24	62,62,62,62	0
58	MG	1A	3114	1/1	0.92	0.29	53,53,53,53	0
58	MG	1A	3529	1/1	0.92	0.29	61,61,61,61	0
58	MG	1x	111	1/1	0.92	0.27	66,66,66,66	0
58	MG	1A	3294	1/1	0.92	0.29	75,75,75,75	0
58	MG	2A	3198	1/1	0.92	0.11	66,66,66,66	0
58	MG	2A	3001	1/1	0.92	0.33	70,70,70,70	0
58	MG	2A	3002	1/1	0.92	0.46	70,70,70,70	0
58	MG	1a	1685	1/1	0.92	0.17	66,66,66,66	0
58	MG	2A	3202	1/1	0.92	0.21	76,76,76,76	0
58	MG	1G	202	1/1	0.92	0.36	75,75,75,75	0
58	MG	2A	3668	1/1	0.92	0.14	62,62,62,62	0
58	MG	2a	1649	1/1	0.92	0.20	81,81,81,81	0
58	MG	2A	3669	1/1	0.92	0.12	63,63,63,63	0
58	MG	2a	1651	1/1	0.92	0.33	80,80,80,80	0
58	MG	2a	1652	1/1	0.92	0.26	84,84,84,84	0
58	MG	1a	1688	1/1	0.92	0.32	74,74,74,74	0
58	MG	1A	3203	1/1	0.92	0.08	32,32,32,32	0
58	MG	1A	3980	1/1	0.92	0.12	40,40,40,40	0
58	MG	1A	3672	1/1	0.92	0.16	37,37,37,37	0
58	MG	1N	204	1/1	0.92	0.17	52,52,52,52	0
58	MG	2A	3680	1/1	0.92	0.08	72,72,72,72	0
58	MG	2A	3211	1/1	0.92	0.31	69,69,69,69	0
58	MG	2a	1664	1/1	0.92	0.21	75,75,75,75	0
58	MG	1A	3394	1/1	0.92	0.12	65,65,65,65	0
58	MG	2A	3214	1/1	0.92	0.31	52,52,52,52	0
58	MG	1O	202	1/1	0.92	0.19	56,56,56,56	0
58	MG	1A	3674	1/1	0.92	0.10	39,39,39,39	0
58	MG	2A	3398	1/1	0.92	0.36	52,52,52,52	0
58	MG	1A	3680	1/1	0.92	0.11	36,36,36,36	0
58	MG	1A	3681	1/1	0.92	0.13	38,38,38,38	0
58	MG	1A	3459	1/1	0.92	0.17	58,58,58,58	0
58	MG	1A	3116	1/1	0.92	0.27	39,39,39,39	0
58	MG	1A	3061	1/1	0.92	0.14	58,58,58,58	0
58	MG	2a	1678	1/1	0.92	0.10	70,70,70,70	0
58	MG	1A	3537	1/1	0.92	0.10	37,37,37,37	0
58	MG	1A	3539	1/1	0.92	0.24	59,59,59,59	0
58	MG	2A	3227	1/1	0.92	0.31	62,62,62,62	0
58	MG	1A	3540	1/1	0.92	0.30	69,69,69,69	0
58	MG	2a	1683	1/1	0.92	0.17	67,67,67,67	0
58	MG	1A	3692	1/1	0.92	0.07	69,69,69,69	0
58	MG	1A	3213	1/1	0.92	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3417	1/1	0.92	0.24	63,63,63,63	0
58	MG	1A	3214	1/1	0.92	0.12	59,59,59,59	0
58	MG	1A	3304	1/1	0.92	0.32	45,45,45,45	0
58	MG	2A	3705	1/1	0.92	0.12	70,70,70,70	0
58	MG	2A	3421	1/1	0.92	0.18	73,73,73,73	0
58	MG	1A	3405	1/1	0.92	0.13	59,59,59,59	0
58	MG	2A	3426	1/1	0.92	0.12	67,67,67,67	0
58	MG	1A	3700	1/1	0.92	0.11	67,67,67,67	0
58	MG	1W	205	1/1	0.92	0.20	50,50,50,50	0
58	MG	2a	1698	1/1	0.92	0.07	90,90,90,90	0
58	MG	1a	1715	1/1	0.92	0.17	69,69,69,69	0
58	MG	2A	3237	1/1	0.92	0.09	80,80,80,80	0
58	MG	2A	3238	1/1	0.92	0.12	60,60,60,60	0
58	MG	2A	3438	1/1	0.92	0.12	61,61,61,61	0
58	MG	2A	3721	1/1	0.92	0.11	72,72,72,72	0
58	MG	1A	3353	1/1	0.92	0.11	69,69,69,69	0
58	MG	1A	3047	1/1	0.92	0.05	27,27,27,27	0
58	MG	2A	3724	1/1	0.92	0.44	69,69,69,69	0
58	MG	1Y	203	1/1	0.92	0.20	58,58,58,58	0
58	MG	2A	3443	1/1	0.92	0.09	53,53,53,53	0
58	MG	1A	3171	1/1	0.92	0.12	57,57,57,57	0
58	MG	1a	1722	1/1	0.92	0.11	51,51,51,51	0
58	MG	10	103	1/1	0.92	0.12	57,57,57,57	0
58	MG	10	105	1/1	0.92	0.18	69,69,69,69	0
58	MG	1A	4020	1/1	0.92	0.16	70,70,70,70	0
58	MG	2A	3736	1/1	0.92	0.12	82,82,82,82	0
58	MG	1A	3850	1/1	0.92	0.09	44,44,44,44	0
58	MG	1A	3711	1/1	0.92	0.09	51,51,51,51	0
58	MG	1a	1730	1/1	0.92	0.29	69,69,69,69	0
58	MG	2A	3741	1/1	0.92	0.13	78,78,78,78	0
58	MG	2A	3463	1/1	0.92	0.12	56,56,56,56	0
58	MG	1A	3854	1/1	0.92	0.05	46,46,46,46	0
58	MG	2A	3468	1/1	0.92	0.14	58,58,58,58	0
58	MG	1a	1732	1/1	0.92	0.24	63,63,63,63	0
58	MG	2A	3259	1/1	0.92	0.19	66,66,66,66	0
58	MG	1A	3086	1/1	0.92	0.29	55,55,55,55	0
58	MG	1A	3040	1/1	0.92	0.10	45,45,45,45	0
58	MG	1A	3717	1/1	0.92	0.10	67,67,67,67	0
58	MG	15	101	1/1	0.92	0.28	44,44,44,44	0
58	MG	2A	3076	1/1	0.92	0.15	62,62,62,62	0
58	MG	1a	1742	1/1	0.92	0.17	70,70,70,70	0
58	MG	15	105	1/1	0.92	0.45	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	15	106	1/1	0.92	0.18	41,41,41,41	0
58	MG	15	108	1/1	0.92	0.12	63,63,63,63	0
58	MG	1a	1750	1/1	0.92	0.14	65,65,65,65	0
58	MG	2A	3086	1/1	0.92	0.14	71,71,71,71	0
58	MG	1A	3720	1/1	0.92	0.08	63,63,63,63	0
58	MG	2A	3088	1/1	0.92	0.17	74,74,74,74	0
58	MG	1A	3313	1/1	0.92	0.25	74,74,74,74	0
58	MG	1a	1754	1/1	0.92	0.18	64,64,64,64	0
58	MG	18	105	1/1	0.92	0.12	55,55,55,55	0
58	MG	2A	3783	1/1	0.92	0.08	40,40,40,40	0
58	MG	1A	3562	1/1	0.92	0.15	37,37,37,37	0
58	MG	1A	4040	1/1	0.92	0.07	55,55,55,55	0
58	MG	2A	3283	1/1	0.92	0.23	63,63,63,63	0
58	MG	1A	3568	1/1	0.92	0.42	51,51,51,51	0
58	MG	1A	3870	1/1	0.92	0.10	39,39,39,39	0
58	MG	2A	3797	1/1	0.92	0.16	73,73,73,73	0
58	MG	2A	3798	1/1	0.92	0.09	74,74,74,74	0
58	MG	2A	3519	1/1	0.92	0.09	50,50,50,50	0
58	MG	1A	3871	1/1	0.92	0.13	53,53,53,53	0
58	MG	1A	3413	1/1	0.92	0.20	53,53,53,53	0
58	MG	1A	3875	1/1	0.92	0.09	37,37,37,37	0
58	MG	1A	3877	1/1	0.92	0.08	38,38,38,38	0
58	MG	1A	3481	1/1	0.92	0.18	58,58,58,58	0
58	MG	2A	3529	1/1	0.92	0.15	72,72,72,72	0
58	MG	1A	3879	1/1	0.92	0.15	77,77,77,77	0
58	MG	2A	3292	1/1	0.92	0.12	64,64,64,64	0
58	MG	1A	3740	1/1	0.92	0.14	60,60,60,60	0
58	MG	1a	1614	1/1	0.92	0.25	75,75,75,75	0
58	MG	1a	1616	1/1	0.92	0.22	68,68,68,68	0
58	MG	1A	3362	1/1	0.92	0.14	58,58,58,58	0
58	MG	1A	3750	1/1	0.92	0.13	50,50,50,50	0
58	MG	1A	3363	1/1	0.92	0.12	55,55,55,55	0
58	MG	2A	3544	1/1	0.92	0.20	64,64,64,64	0
58	MG	1A	3890	1/1	0.92	0.23	64,64,64,64	0
58	MG	1A	3041	1/1	0.92	0.26	44,44,44,44	0
58	MG	2A	3548	1/1	0.92	0.17	71,71,71,71	0
58	MG	1A	4064	1/1	0.92	0.08	50,50,50,50	0
58	MG	1a	1790	1/1	0.92	0.20	77,77,77,77	0
58	MG	2a	1797	1/1	0.92	0.20	76,76,76,76	0
58	MG	2A	3555	1/1	0.92	0.10	58,58,58,58	0
58	MG	1A	3486	1/1	0.92	0.15	55,55,55,55	0
58	MG	1A	3419	1/1	0.92	0.18	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3234	1/1	0.92	0.09	67,67,67,67	0
58	MG	1A	3183	1/1	0.92	0.10	79,79,79,79	0
58	MG	1A	3495	1/1	0.92	0.14	78,78,78,78	0
58	MG	2A	3563	1/1	0.92	0.10	51,51,51,51	0
58	MG	1a	1797	1/1	0.92	0.21	62,62,62,62	0
58	MG	2F	302	1/1	0.92	0.14	68,68,68,68	0
58	MG	1A	3184	1/1	0.92	0.09	50,50,50,50	0
58	MG	1A	3425	1/1	0.92	0.11	45,45,45,45	0
58	MG	2A	3131	1/1	0.92	0.12	68,68,68,68	0
58	MG	1A	3427	1/1	0.92	0.15	55,55,55,55	0
58	MG	1a	1637	1/1	0.92	0.25	82,82,82,82	0
58	MG	2A	3321	1/1	0.92	0.18	58,58,58,58	0
58	MG	2A	3135	1/1	0.92	0.20	54,54,54,54	0
58	MG	2R	201	1/1	0.92	0.12	58,58,58,58	0
58	MG	2A	3574	1/1	0.92	0.16	53,53,53,53	0
58	MG	1a	1803	1/1	0.92	0.13	69,69,69,69	0
58	MG	1A	3780	1/1	0.92	0.11	26,26,26,26	0
58	MG	2A	3325	1/1	0.92	0.18	68,68,68,68	0
58	MG	1A	4084	1/1	0.92	0.11	63,63,63,63	0
58	MG	2f	201	1/1	0.92	0.14	62,62,62,62	0
58	MG	1A	3185	1/1	0.92	0.12	55,55,55,55	0
58	MG	2A	3142	1/1	0.92	0.37	68,68,68,68	0
58	MG	1a	1807	1/1	0.92	0.18	74,74,74,74	0
58	MG	2A	3334	1/1	0.92	0.20	86,86,86,86	0
58	MG	1B	202	1/1	0.92	0.29	64,64,64,64	0
58	MG	1A	3782	1/1	0.92	0.07	49,49,49,49	0
58	MG	23	101	1/1	0.92	0.12	72,72,72,72	0
58	MG	1A	3604	1/1	0.92	0.09	44,44,44,44	0
58	MG	1a	1647	1/1	0.92	0.29	74,74,74,74	0
58	MG	1B	208	1/1	0.92	0.19	55,55,55,55	0
58	MG	25	104	1/1	0.92	0.14	63,63,63,63	0
58	MG	1A	3784	1/1	0.92	0.07	60,60,60,60	0
58	MG	2A	3152	1/1	0.92	0.18	61,61,61,61	0
58	MG	1A	3059	1/1	0.92	0.11	40,40,40,40	0
58	MG	2x	103	1/1	0.92	0.25	86,86,86,86	0
58	MG	1d	301	1/1	0.92	0.43	74,74,74,74	0
58	MG	28	103	1/1	0.92	0.10	84,84,84,84	0
58	MG	2A	3344	1/1	0.92	0.07	66,66,66,66	0
58	MG	1A	3144	1/1	0.92	0.12	51,51,51,51	0
59	K	1A	3559	1/1	0.92	0.12	81,81,81,81	0
58	MG	2A	3605	1/1	0.92	0.14	71,71,71,71	0
58	MG	1A	3924	1/1	0.93	0.11	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3927	1/1	0.93	0.15	68,68,68,68	0
58	MG	1A	3930	1/1	0.93	0.10	66,66,66,66	0
58	MG	2A	3419	1/1	0.93	0.12	76,76,76,76	0
58	MG	2A	3242	1/1	0.93	0.11	71,71,71,71	0
58	MG	1a	1746	1/1	0.93	0.23	51,51,51,51	0
58	MG	1A	3328	1/1	0.93	0.25	70,70,70,70	0
58	MG	1A	3813	1/1	0.93	0.27	71,71,71,71	0
58	MG	2A	3246	1/1	0.93	0.18	61,61,61,61	0
58	MG	2a	1639	1/1	0.93	0.28	74,74,74,74	0
58	MG	2A	3247	1/1	0.93	0.16	74,74,74,74	0
58	MG	1A	3488	1/1	0.93	0.10	56,56,56,56	0
58	MG	1A	4081	1/1	0.93	0.22	50,50,50,50	0
58	MG	1A	3285	1/1	0.93	0.14	58,58,58,58	0
58	MG	2A	3074	1/1	0.93	0.19	52,52,52,52	0
58	MG	1A	3062	1/1	0.93	0.29	61,61,61,61	0
58	MG	1a	1753	1/1	0.93	0.25	54,54,54,54	0
58	MG	2A	3080	1/1	0.93	0.18	67,67,67,67	0
58	MG	1A	4085	1/1	0.93	0.11	63,63,63,63	0
58	MG	1a	1755	1/1	0.93	0.26	75,75,75,75	0
58	MG	1A	3287	1/1	0.93	0.18	56,56,56,56	0
58	MG	1a	1760	1/1	0.93	0.14	61,61,61,61	0
58	MG	1A	3151	1/1	0.93	0.11	45,45,45,45	0
58	MG	1a	1763	1/1	0.93	0.22	62,62,62,62	0
58	MG	1a	1764	1/1	0.93	0.19	75,75,75,75	0
58	MG	2A	3457	1/1	0.93	0.09	58,58,58,58	0
58	MG	1A	3946	1/1	0.93	0.09	60,60,60,60	0
58	MG	1a	1617	1/1	0.93	0.12	74,74,74,74	0
58	MG	1B	206	1/1	0.93	0.14	55,55,55,55	0
58	MG	1A	3194	1/1	0.93	0.35	44,44,44,44	0
58	MG	1A	3337	1/1	0.93	0.35	60,60,60,60	0
58	MG	2a	1667	1/1	0.93	0.10	56,56,56,56	0
58	MG	1A	3437	1/1	0.93	0.33	62,62,62,62	0
58	MG	2a	1669	1/1	0.93	0.31	83,83,83,83	0
58	MG	2A	3096	1/1	0.93	0.10	68,68,68,68	0
58	MG	1B	210	1/1	0.93	0.11	56,56,56,56	0
58	MG	1B	211	1/1	0.93	0.13	58,58,58,58	0
58	MG	1A	3438	1/1	0.93	0.17	69,69,69,69	0
58	MG	1B	214	1/1	0.93	0.09	54,54,54,54	0
58	MG	2A	3280	1/1	0.93	0.16	60,60,60,60	0
58	MG	1a	1629	1/1	0.93	0.12	71,71,71,71	0
58	MG	1A	3578	1/1	0.93	0.26	48,48,48,48	0
58	MG	1B	218	1/1	0.93	0.14	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3071	1/1	0.93	0.30	36,36,36,36	0
58	MG	1A	3708	1/1	0.93	0.16	77,77,77,77	0
58	MG	1A	3198	1/1	0.93	0.09	55,55,55,55	0
58	MG	1A	3581	1/1	0.93	0.29	58,58,58,58	0
58	MG	1A	3202	1/1	0.93	0.07	53,53,53,53	0
58	MG	1A	3510	1/1	0.93	0.55	54,54,54,54	0
58	MG	2A	3503	1/1	0.93	0.34	68,68,68,68	0
58	MG	2A	3505	1/1	0.93	0.14	67,67,67,67	0
58	MG	2a	1687	1/1	0.93	0.18	57,57,57,57	0
58	MG	1A	3051	1/1	0.93	0.11	55,55,55,55	0
58	MG	1A	3253	1/1	0.93	0.12	40,40,40,40	0
58	MG	1A	3726	1/1	0.93	0.09	45,45,45,45	0
58	MG	1a	1643	1/1	0.93	0.19	65,65,65,65	0
58	MG	1A	3515	1/1	0.93	0.10	69,69,69,69	0
58	MG	1A	3972	1/1	0.93	0.15	69,69,69,69	0
58	MG	2a	1695	1/1	0.93	0.18	63,63,63,63	0
58	MG	2A	3747	1/1	0.93	0.09	59,59,59,59	0
58	MG	1A	3397	1/1	0.93	0.08	72,72,72,72	0
58	MG	2A	3297	1/1	0.93	0.18	70,70,70,70	0
58	MG	2a	1699	1/1	0.93	0.09	74,74,74,74	0
58	MG	2A	3755	1/1	0.93	0.08	61,61,61,61	0
58	MG	1a	1648	1/1	0.93	0.24	71,71,71,71	0
58	MG	1A	3976	1/1	0.93	0.09	41,41,41,41	0
58	MG	2A	3301	1/1	0.93	0.08	76,76,76,76	0
58	MG	2A	3524	1/1	0.93	0.14	70,70,70,70	0
58	MG	2A	3124	1/1	0.93	0.25	73,73,73,73	0
58	MG	1A	3079	1/1	0.93	0.12	62,62,62,62	0
58	MG	2A	3528	1/1	0.93	0.08	65,65,65,65	0
58	MG	1D	3601	1/1	0.93	0.23	54,54,54,54	0
58	MG	2A	3770	1/1	0.93	0.10	61,61,61,61	0
58	MG	2A	3771	1/1	0.93	0.07	53,53,53,53	0
58	MG	1A	3083	1/1	0.93	0.16	47,47,47,47	0
58	MG	2A	3129	1/1	0.93	0.12	62,62,62,62	0
58	MG	1a	1653	1/1	0.93	0.09	66,66,66,66	0
58	MG	1A	3739	1/1	0.93	0.12	56,56,56,56	0
58	MG	2a	1716	1/1	0.93	0.22	76,76,76,76	0
58	MG	2A	3535	1/1	0.93	0.18	54,54,54,54	0
58	MG	1a	1657	1/1	0.93	0.14	62,62,62,62	0
58	MG	2a	1720	1/1	0.93	0.15	77,77,77,77	0
58	MG	1A	3453	1/1	0.93	0.11	58,58,58,58	0
58	MG	1A	3741	1/1	0.93	0.12	25,25,25,25	0
58	MG	1E	308	1/1	0.93	0.24	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3607	1/1	0.93	0.09	59,59,59,59	0
58	MG	1E	310	1/1	0.93	0.09	29,29,29,29	0
58	MG	1A	3853	1/1	0.93	0.11	43,43,43,43	0
58	MG	1A	3746	1/1	0.93	0.07	35,35,35,35	0
58	MG	2A	3793	1/1	0.93	0.15	47,47,47,47	0
58	MG	2A	3320	1/1	0.93	0.10	79,79,79,79	0
58	MG	2A	3551	1/1	0.93	0.13	75,75,75,75	0
58	MG	1A	3748	1/1	0.93	0.07	34,34,34,34	0
58	MG	1A	3098	1/1	0.93	0.19	51,51,51,51	0
58	MG	2a	1737	1/1	0.93	0.10	77,77,77,77	0
58	MG	1A	3994	1/1	0.93	0.07	18,18,18,18	0
58	MG	2a	1739	1/1	0.93	0.14	61,61,61,61	0
58	MG	1A	3614	1/1	0.93	0.08	41,41,41,41	0
58	MG	1l	201	1/1	0.93	0.07	76,76,76,76	0
58	MG	1G	203	1/1	0.93	0.08	59,59,59,59	0
58	MG	2a	1746	1/1	0.93	0.17	85,85,85,85	0
58	MG	2A	3328	1/1	0.93	0.14	68,68,68,68	0
58	MG	1A	3861	1/1	0.93	0.30	43,43,43,43	0
58	MG	2a	1749	1/1	0.93	0.09	96,96,96,96	0
58	MG	1A	3754	1/1	0.93	0.10	65,65,65,65	0
58	MG	2A	3331	1/1	0.93	0.33	71,71,71,71	0
58	MG	1A	3864	1/1	0.93	0.09	36,36,36,36	0
58	MG	1a	1673	1/1	0.93	0.30	75,75,75,75	0
58	MG	1A	3172	1/1	0.93	0.13	52,52,52,52	0
58	MG	1A	4005	1/1	0.93	0.10	44,44,44,44	0
58	MG	2B	213	1/1	0.93	0.26	74,74,74,74	0
58	MG	1A	4006	1/1	0.93	0.07	34,34,34,34	0
58	MG	1A	3525	1/1	0.93	0.22	55,55,55,55	0
58	MG	1A	3018	1/1	0.93	0.12	45,45,45,45	0
58	MG	1A	4014	1/1	0.93	0.08	59,59,59,59	0
58	MG	2A	3576	1/1	0.93	0.10	69,69,69,69	0
58	MG	1A	3406	1/1	0.93	0.11	47,47,47,47	0
58	MG	1A	3765	1/1	0.93	0.09	32,32,32,32	0
58	MG	2A	3580	1/1	0.93	0.13	75,75,75,75	0
58	MG	1A	3087	1/1	0.93	0.22	47,47,47,47	0
58	MG	2A	3582	1/1	0.93	0.14	68,68,68,68	0
58	MG	2a	1769	1/1	0.93	0.34	66,66,66,66	0
58	MG	2a	1770	1/1	0.93	0.22	65,65,65,65	0
58	MG	2A	3170	1/1	0.93	0.13	53,53,53,53	0
58	MG	1A	3874	1/1	0.93	0.11	31,31,31,31	0
58	MG	1a	1686	1/1	0.93	0.13	69,69,69,69	0
58	MG	2a	1774	1/1	0.93	0.20	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3306	1/1	0.93	0.32	68,68,68,68	0
58	MG	2a	1777	1/1	0.93	0.22	68,68,68,68	0
58	MG	1R	206	1/1	0.93	0.11	40,40,40,40	0
58	MG	1A	3465	1/1	0.93	0.14	61,61,61,61	0
58	MG	1S	201	1/1	0.93	0.15	55,55,55,55	0
58	MG	1S	202	1/1	0.93	0.12	61,61,61,61	0
58	MG	1A	3131	1/1	0.93	0.25	52,52,52,52	0
58	MG	1a	1694	1/1	0.93	0.24	70,70,70,70	0
58	MG	1A	3639	1/1	0.93	0.13	62,62,62,62	0
58	MG	1A	3881	1/1	0.93	0.12	47,47,47,47	0
58	MG	2a	1787	1/1	0.93	0.17	73,73,73,73	0
58	MG	1A	3883	1/1	0.93	0.09	35,35,35,35	0
58	MG	1A	3359	1/1	0.93	0.11	65,65,65,65	0
58	MG	1U	207	1/1	0.93	0.34	44,44,44,44	0
58	MG	1W	202	1/1	0.93	0.21	58,58,58,58	0
58	MG	1a	1701	1/1	0.93	0.36	63,63,63,63	0
58	MG	2a	1793	1/1	0.93	0.17	70,70,70,70	0
58	MG	1A	3058	1/1	0.93	0.29	66,66,66,66	0
58	MG	2a	1796	1/1	0.93	0.20	89,89,89,89	0
58	MG	1A	3311	1/1	0.93	0.09	66,66,66,66	0
58	MG	2A	3610	1/1	0.93	0.09	70,70,70,70	0
58	MG	1A	3103	1/1	0.93	0.24	49,49,49,49	0
58	MG	1A	3233	1/1	0.93	0.23	53,53,53,53	0
58	MG	1A	3106	1/1	0.93	0.34	50,50,50,50	0
58	MG	1A	3145	1/1	0.93	0.27	38,38,38,38	0
58	MG	10	101	1/1	0.93	0.26	57,57,57,57	0
58	MG	2A	3025	1/1	0.93	0.12	70,70,70,70	0
58	MG	1A	3318	1/1	0.93	0.09	52,52,52,52	0
58	MG	2A	3204	1/1	0.93	0.15	58,58,58,58	0
58	MG	2A	3205	1/1	0.93	0.24	61,61,61,61	0
58	MG	25	103	1/1	0.93	0.31	61,61,61,61	0
58	MG	2a	1809	1/1	0.93	0.22	80,80,80,80	0
58	MG	2A	3376	1/1	0.93	0.33	69,69,69,69	0
58	MG	1A	3239	1/1	0.93	0.09	43,43,43,43	0
58	MG	1a	1711	1/1	0.93	0.07	59,59,59,59	0
58	MG	10	106	1/1	0.93	0.09	59,59,59,59	0
58	MG	2a	1814	1/1	0.93	0.11	75,75,75,75	0
58	MG	1A	3273	1/1	0.93	0.08	54,54,54,54	0
58	MG	1A	3547	1/1	0.93	0.28	51,51,51,51	0
58	MG	2a	1817	1/1	0.93	0.15	91,91,91,91	0
58	MG	1A	3678	1/1	0.93	0.09	43,43,43,43	0
58	MG	1A	3679	1/1	0.93	0.08	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3036	1/1	0.93	0.12	41,41,41,41	0
58	MG	1A	3800	1/1	0.93	0.33	37,37,37,37	0
58	MG	2A	3038	1/1	0.93	0.12	57,57,57,57	0
58	MG	1a	1718	1/1	0.93	0.40	80,80,80,80	0
58	MG	2A	3644	1/1	0.93	0.12	54,54,54,54	0
58	MG	2A	3041	1/1	0.93	0.13	64,64,64,64	0
58	MG	1A	3325	1/1	0.93	0.21	61,61,61,61	0
58	MG	2A	3221	1/1	0.93	0.29	61,61,61,61	0
58	MG	1A	3553	1/1	0.93	0.52	56,56,56,56	0
58	MG	2A	3045	1/1	0.93	0.13	63,63,63,63	0
58	MG	1A	3807	1/1	0.93	0.10	50,50,50,50	0
58	MG	2A	3225	1/1	0.93	0.17	58,58,58,58	0
58	MG	2A	3047	1/1	0.93	0.12	68,68,68,68	0
58	MG	15	103	1/1	0.93	0.29	47,47,47,47	0
58	MG	1A	3554	1/1	0.93	0.27	48,48,48,48	0
58	MG	1A	3914	1/1	0.93	0.15	65,65,65,65	0
58	MG	1A	3274	1/1	0.93	0.18	57,57,57,57	0
58	MG	16	101	1/1	0.93	0.30	57,57,57,57	0
58	MG	16	102	1/1	0.93	0.11	64,64,64,64	0
58	MG	2A	3057	1/1	0.93	0.22	78,78,78,78	0
58	MG	16	103	1/1	0.93	0.27	64,64,64,64	0
58	MG	2x	106	1/1	0.93	0.11	81,81,81,81	0
58	MG	1A	4065	1/1	0.93	0.10	63,63,63,63	0
58	MG	1A	3916	1/1	0.93	0.08	54,54,54,54	0
58	MG	1A	3241	1/1	0.93	0.24	46,46,46,46	0
58	MG	2A	3673	1/1	0.93	0.08	75,75,75,75	0
60	CLM	2w	103	20/20	0.93	0.12	51,55,72,76	0
61	ZN	2n	501	1/1	0.93	0.08	117,117,117,117	0
58	MG	1A	3166	1/1	0.94	0.08	38,38,38,38	0
58	MG	2a	1643	1/1	0.94	0.08	80,80,80,80	0
58	MG	1A	3833	1/1	0.94	0.21	55,55,55,55	0
58	MG	1A	3256	1/1	0.94	0.30	37,37,37,37	0
58	MG	1A	3712	1/1	0.94	0.08	58,58,58,58	0
58	MG	1A	3395	1/1	0.94	0.12	67,67,67,67	0
58	MG	2A	3275	1/1	0.94	0.17	74,74,74,74	0
58	MG	2A	3697	1/1	0.94	0.10	71,71,71,71	0
58	MG	2A	3276	1/1	0.94	0.08	67,67,67,67	0
58	MG	2A	3104	1/1	0.94	0.12	62,62,62,62	0
58	MG	1A	3840	1/1	0.94	0.12	42,42,42,42	0
58	MG	2A	3471	1/1	0.94	0.16	56,56,56,56	0
58	MG	1A	3009	1/1	0.94	0.08	35,35,35,35	0
58	MG	1A	3064	1/1	0.94	0.10	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3476	1/1	0.94	0.11	66,66,66,66	0
58	MG	1A	3718	1/1	0.94	0.09	61,61,61,61	0
58	MG	1A	3068	1/1	0.94	0.13	35,35,35,35	0
58	MG	1E	303	1/1	0.94	0.15	52,52,52,52	0
58	MG	1A	3593	1/1	0.94	0.16	73,73,73,73	0
58	MG	2A	3487	1/1	0.94	0.08	42,42,42,42	0
58	MG	2A	3488	1/1	0.94	0.10	72,72,72,72	0
58	MG	2A	3715	1/1	0.94	0.09	74,74,74,74	0
58	MG	1A	3986	1/1	0.94	0.12	55,55,55,55	0
58	MG	1A	3987	1/1	0.94	0.08	64,64,64,64	0
58	MG	1A	3722	1/1	0.94	0.09	60,60,60,60	0
58	MG	2A	3719	1/1	0.94	0.12	59,59,59,59	0
58	MG	1E	313	1/1	0.94	0.29	46,46,46,46	0
58	MG	1F	307	1/1	0.94	0.09	60,60,60,60	0
58	MG	1A	3724	1/1	0.94	0.09	26,26,26,26	0
58	MG	2A	3497	1/1	0.94	0.10	54,54,54,54	0
58	MG	1A	3596	1/1	0.94	0.13	59,59,59,59	0
58	MG	1A	3991	1/1	0.94	0.07	52,52,52,52	0
58	MG	2A	3728	1/1	0.94	0.16	61,61,61,61	0
58	MG	1A	3597	1/1	0.94	0.08	35,35,35,35	0
58	MG	1A	3135	1/1	0.94	0.17	53,53,53,53	0
58	MG	1A	3731	1/1	0.94	0.12	46,46,46,46	0
58	MG	1A	3136	1/1	0.94	0.28	37,37,37,37	0
58	MG	2A	3733	1/1	0.94	0.08	72,72,72,72	0
58	MG	1A	3223	1/1	0.94	0.30	63,63,63,63	0
58	MG	1a	1813	1/1	0.94	0.09	69,69,69,69	0
58	MG	1I	201	1/1	0.94	0.08	73,73,73,73	0
58	MG	2A	3300	1/1	0.94	0.17	64,64,64,64	0
58	MG	1N	201	1/1	0.94	0.29	50,50,50,50	0
58	MG	1A	3523	1/1	0.94	0.14	61,61,61,61	0
58	MG	1N	203	1/1	0.94	0.09	41,41,41,41	0
58	MG	2A	3518	1/1	0.94	0.16	75,75,75,75	0
58	MG	1A	3181	1/1	0.94	0.19	56,56,56,56	0
58	MG	2A	3520	1/1	0.94	0.13	72,72,72,72	0
58	MG	1A	4001	1/1	0.94	0.10	62,62,62,62	0
58	MG	2A	3748	1/1	0.94	0.09	55,55,55,55	0
58	MG	1k	201	1/1	0.94	0.19	56,56,56,56	0
58	MG	2A	3750	1/1	0.94	0.10	58,58,58,58	0
58	MG	1A	3611	1/1	0.94	0.05	38,38,38,38	0
58	MG	1A	3228	1/1	0.94	0.19	40,40,40,40	0
58	MG	1A	3112	1/1	0.94	0.18	47,47,47,47	0
58	MG	1A	4008	1/1	0.94	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3616	1/1	0.94	0.13	70,70,70,70	0
58	MG	1p	101	1/1	0.94	0.09	77,77,77,77	0
58	MG	1a	1678	1/1	0.94	0.24	65,65,65,65	0
58	MG	1A	3749	1/1	0.94	0.12	35,35,35,35	0
58	MG	1A	4013	1/1	0.94	0.07	51,51,51,51	0
58	MG	1A	3463	1/1	0.94	0.21	46,46,46,46	0
58	MG	2A	3534	1/1	0.94	0.16	62,62,62,62	0
58	MG	1A	3625	1/1	0.94	0.12	54,54,54,54	0
58	MG	2A	3537	1/1	0.94	0.12	48,48,48,48	0
58	MG	2A	3775	1/1	0.94	0.16	86,86,86,86	0
58	MG	1R	201	1/1	0.94	0.11	53,53,53,53	0
58	MG	1R	203	1/1	0.94	0.23	64,64,64,64	0
58	MG	1A	3052	1/1	0.94	0.07	59,59,59,59	0
58	MG	1A	3627	1/1	0.94	0.10	24,24,24,24	0
58	MG	1A	3357	1/1	0.94	0.12	69,69,69,69	0
58	MG	1A	3314	1/1	0.94	0.25	61,61,61,61	0
58	MG	1a	1690	1/1	0.94	0.42	64,64,64,64	0
58	MG	1A	3115	1/1	0.94	0.28	50,50,50,50	0
58	MG	1A	3316	1/1	0.94	0.34	82,82,82,82	0
58	MG	2a	1727	1/1	0.94	0.08	84,84,84,84	0
58	MG	1x	105	1/1	0.94	0.19	71,71,71,71	0
58	MG	2A	3167	1/1	0.94	0.25	65,65,65,65	0
58	MG	2a	1730	1/1	0.94	0.15	79,79,79,79	0
58	MG	1A	4025	1/1	0.94	0.09	82,82,82,82	0
58	MG	1A	3766	1/1	0.94	0.06	78,78,78,78	0
58	MG	2A	3794	1/1	0.94	0.07	74,74,74,74	0
58	MG	2A	3796	1/1	0.94	0.11	59,59,59,59	0
58	MG	1A	3882	1/1	0.94	0.10	51,51,51,51	0
58	MG	1U	205	1/1	0.94	0.24	44,44,44,44	0
58	MG	1x	110	1/1	0.94	0.10	69,69,69,69	0
58	MG	1A	3470	1/1	0.94	0.12	67,67,67,67	0
58	MG	2A	3175	1/1	0.94	0.12	61,61,61,61	0
58	MG	1U	210	1/1	0.94	0.09	64,64,64,64	0
58	MG	2A	3565	1/1	0.94	0.10	64,64,64,64	0
58	MG	1V	206	1/1	0.94	0.11	55,55,55,55	0
58	MG	1A	3636	1/1	0.94	0.14	53,53,53,53	0
58	MG	1A	3053	1/1	0.94	0.18	62,62,62,62	0
58	MG	2A	3004	1/1	0.94	0.39	63,63,63,63	0
58	MG	1A	3642	1/1	0.94	0.07	38,38,38,38	0
58	MG	1W	207	1/1	0.94	0.16	32,32,32,32	0
58	MG	1A	3774	1/1	0.94	0.17	59,59,59,59	0
58	MG	1A	3645	1/1	0.94	0.07	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3119	1/1	0.94	0.10	47,47,47,47	0
58	MG	1A	3538	1/1	0.94	0.20	57,57,57,57	0
58	MG	1Z	303	1/1	0.94	0.29	74,74,74,74	0
58	MG	2A	3019	1/1	0.94	0.07	46,46,46,46	0
58	MG	1A	3476	1/1	0.94	0.26	56,56,56,56	0
58	MG	2A	3022	1/1	0.94	0.24	58,58,58,58	0
58	MG	1A	3653	1/1	0.94	0.08	41,41,41,41	0
58	MG	1A	3188	1/1	0.94	0.25	47,47,47,47	0
58	MG	2D	302	1/1	0.94	0.15	59,59,59,59	0
58	MG	2A	3584	1/1	0.94	0.07	46,46,46,46	0
58	MG	1A	4046	1/1	0.94	0.07	43,43,43,43	0
58	MG	1A	4048	1/1	0.94	0.08	47,47,47,47	0
58	MG	1A	4049	1/1	0.94	0.16	57,57,57,57	0
58	MG	1A	3662	1/1	0.94	0.08	60,60,60,60	0
58	MG	1A	3786	1/1	0.94	0.06	25,25,25,25	0
58	MG	1A	3790	1/1	0.94	0.36	33,33,33,33	0
58	MG	1A	3279	1/1	0.94	0.14	40,40,40,40	0
58	MG	1A	3324	1/1	0.94	0.10	59,59,59,59	0
58	MG	2A	3369	1/1	0.94	0.11	65,65,65,65	0
58	MG	2A	3597	1/1	0.94	0.13	74,74,74,74	0
58	MG	2A	3598	1/1	0.94	0.12	82,82,82,82	0
58	MG	1A	3367	1/1	0.94	0.12	68,68,68,68	0
58	MG	2F	307	1/1	0.94	0.20	57,57,57,57	0
58	MG	1A	3794	1/1	0.94	0.12	59,59,59,59	0
58	MG	1A	3025	1/1	0.94	0.18	42,42,42,42	0
58	MG	1A	3910	1/1	0.94	0.18	53,53,53,53	0
58	MG	2Q	202	1/1	0.94	0.22	68,68,68,68	0
58	MG	2a	1783	1/1	0.94	0.12	77,77,77,77	0
58	MG	1A	4063	1/1	0.94	0.08	36,36,36,36	0
58	MG	2A	3213	1/1	0.94	0.09	91,91,91,91	0
58	MG	1a	1726	1/1	0.94	0.14	52,52,52,52	0
58	MG	1A	3913	1/1	0.94	0.07	75,75,75,75	0
58	MG	1A	3369	1/1	0.94	0.29	58,58,58,58	0
58	MG	2A	3044	1/1	0.94	0.16	76,76,76,76	0
58	MG	1A	3121	1/1	0.94	0.17	51,51,51,51	0
58	MG	17	103	1/1	0.94	0.19	40,40,40,40	0
58	MG	1A	3153	1/1	0.94	0.06	32,32,32,32	0
58	MG	2A	3617	1/1	0.94	0.07	69,69,69,69	0
58	MG	2A	3618	1/1	0.94	0.09	53,53,53,53	0
58	MG	1A	3920	1/1	0.94	0.08	64,64,64,64	0
58	MG	1A	3675	1/1	0.94	0.08	78,78,78,78	0
58	MG	1A	3923	1/1	0.94	0.09	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3801	1/1	0.94	0.07	58,58,58,58	0
58	MG	1A	3155	1/1	0.94	0.15	51,51,51,51	0
58	MG	1a	1744	1/1	0.94	0.15	63,63,63,63	0
58	MG	1A	3329	1/1	0.94	0.30	64,64,64,64	0
58	MG	1A	3932	1/1	0.94	0.14	34,34,34,34	0
58	MG	1A	3197	1/1	0.94	0.14	43,43,43,43	0
58	MG	2A	3392	1/1	0.94	0.37	70,70,70,70	0
58	MG	2A	3629	1/1	0.94	0.16	75,75,75,75	0
58	MG	1A	3490	1/1	0.94	0.27	62,62,62,62	0
58	MG	1A	3331	1/1	0.94	0.12	51,51,51,51	0
58	MG	1A	3156	1/1	0.94	0.35	46,46,46,46	0
58	MG	2A	3396	1/1	0.94	0.09	70,70,70,70	0
58	MG	1A	3380	1/1	0.94	0.09	47,47,47,47	0
58	MG	1A	3941	1/1	0.94	0.10	60,60,60,60	0
58	MG	1A	3566	1/1	0.94	0.15	50,50,50,50	0
58	MG	1A	3943	1/1	0.94	0.08	61,61,61,61	0
58	MG	2A	3401	1/1	0.94	0.39	66,66,66,66	0
58	MG	1a	1756	1/1	0.94	0.06	75,75,75,75	0
58	MG	1A	3567	1/1	0.94	0.16	39,39,39,39	0
58	MG	1a	1758	1/1	0.94	0.14	75,75,75,75	0
58	MG	2A	3407	1/1	0.94	0.30	75,75,75,75	0
58	MG	1a	1759	1/1	0.94	0.09	69,69,69,69	0
58	MG	2A	3410	1/1	0.94	0.17	55,55,55,55	0
58	MG	2a	1823	1/1	0.94	0.24	73,73,73,73	0
58	MG	1a	1618	1/1	0.94	0.08	58,58,58,58	0
58	MG	2d	302	1/1	0.94	0.10	67,67,67,67	0
58	MG	2e	201	1/1	0.94	0.09	83,83,83,83	0
58	MG	1A	3291	1/1	0.94	0.20	37,37,37,37	0
58	MG	2A	3077	1/1	0.94	0.10	40,40,40,40	0
58	MG	1A	3947	1/1	0.94	0.07	43,43,43,43	0
58	MG	2A	3079	1/1	0.94	0.17	62,62,62,62	0
58	MG	1A	3200	1/1	0.94	0.10	43,43,43,43	0
58	MG	1A	3201	1/1	0.94	0.19	38,38,38,38	0
58	MG	1A	3501	1/1	0.94	0.09	56,56,56,56	0
58	MG	1A	3952	1/1	0.94	0.09	55,55,55,55	0
58	MG	1a	1626	1/1	0.94	0.17	79,79,79,79	0
58	MG	2A	3085	1/1	0.94	0.08	61,61,61,61	0
58	MG	1A	3439	1/1	0.94	0.17	59,59,59,59	0
58	MG	1A	3697	1/1	0.94	0.06	26,26,26,26	0
58	MG	2A	3257	1/1	0.94	0.28	82,82,82,82	0
58	MG	2A	3258	1/1	0.94	0.19	64,64,64,64	0
58	MG	1A	3504	1/1	0.94	0.10	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3260	1/1	0.94	0.15	69,69,69,69	0
58	MG	1A	3082	1/1	0.94	0.29	53,53,53,53	0
58	MG	1A	3701	1/1	0.94	0.23	56,56,56,56	0
58	MG	1A	3961	1/1	0.94	0.10	76,76,76,76	0
58	MG	1A	3127	1/1	0.94	0.34	41,41,41,41	0
58	MG	1A	3339	1/1	0.94	0.07	64,64,64,64	0
58	MG	1A	3706	1/1	0.94	0.11	56,56,56,56	0
58	MG	1a	1784	1/1	0.94	0.17	69,69,69,69	0
58	MG	2A	3450	1/1	0.94	0.12	70,70,70,70	0
58	MG	1A	3509	1/1	0.94	0.25	40,40,40,40	0
58	MG	1B	204	1/1	0.95	0.25	70,70,70,70	0
58	MG	2A	3070	1/1	0.95	0.12	68,68,68,68	0
58	MG	1A	3543	1/1	0.95	0.28	63,63,63,63	0
58	MG	1A	3544	1/1	0.95	0.10	47,47,47,47	0
58	MG	2A	3659	1/1	0.95	0.11	51,51,51,51	0
58	MG	1A	3945	1/1	0.95	0.11	59,59,59,59	0
58	MG	2A	3422	1/1	0.95	0.15	74,74,74,74	0
58	MG	1A	3141	1/1	0.95	0.08	25,25,25,25	0
58	MG	2A	3663	1/1	0.95	0.05	78,78,78,78	0
58	MG	2A	3664	1/1	0.95	0.16	47,47,47,47	0
58	MG	2A	3075	1/1	0.95	0.19	54,54,54,54	0
58	MG	1A	3276	1/1	0.95	0.12	48,48,48,48	0
58	MG	1A	3142	1/1	0.95	0.08	58,58,58,58	0
58	MG	2A	3253	1/1	0.95	0.14	70,70,70,70	0
58	MG	1A	3548	1/1	0.95	0.18	43,43,43,43	0
58	MG	2A	3431	1/1	0.95	0.14	49,49,49,49	0
58	MG	2A	3433	1/1	0.95	0.09	32,32,32,32	0
58	MG	1a	1615	1/1	0.95	0.07	81,81,81,81	0
58	MG	2A	3675	1/1	0.95	0.08	46,46,46,46	0
58	MG	1A	3280	1/1	0.95	0.34	43,43,43,43	0
58	MG	1B	215	1/1	0.95	0.11	61,61,61,61	0
58	MG	1A	3552	1/1	0.95	0.18	43,43,43,43	0
58	MG	2A	3441	1/1	0.95	0.20	60,60,60,60	0
58	MG	1A	3281	1/1	0.95	0.39	42,42,42,42	0
58	MG	1a	1770	1/1	0.95	0.39	78,78,78,78	0
58	MG	1A	3230	1/1	0.95	0.16	59,59,59,59	0
58	MG	1A	3075	1/1	0.95	0.06	36,36,36,36	0
58	MG	2A	3447	1/1	0.95	0.08	48,48,48,48	0
58	MG	2a	1653	1/1	0.95	0.06	73,73,73,73	0
58	MG	2A	3448	1/1	0.95	0.07	52,52,52,52	0
58	MG	2A	3449	1/1	0.95	0.08	50,50,50,50	0
58	MG	1A	3474	1/1	0.95	0.08	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1B	222	1/1	0.95	0.18	60,60,60,60	0
58	MG	1A	3019	1/1	0.95	0.24	57,57,57,57	0
58	MG	2A	3090	1/1	0.95	0.28	56,56,56,56	0
58	MG	1A	3016	1/1	0.95	0.23	53,53,53,53	0
58	MG	1a	1778	1/1	0.95	0.16	84,84,84,84	0
58	MG	1A	3186	1/1	0.95	0.18	54,54,54,54	0
58	MG	1A	3694	1/1	0.95	0.10	58,58,58,58	0
58	MG	2A	3699	1/1	0.95	0.13	53,53,53,53	0
58	MG	2A	3461	1/1	0.95	0.09	59,59,59,59	0
58	MG	2A	3271	1/1	0.95	0.20	73,73,73,73	0
58	MG	2A	3464	1/1	0.95	0.08	64,64,64,64	0
58	MG	1A	3561	1/1	0.95	0.20	43,43,43,43	0
58	MG	2A	3466	1/1	0.95	0.11	51,51,51,51	0
58	MG	1A	3235	1/1	0.95	0.29	37,37,37,37	0
58	MG	1A	3564	1/1	0.95	0.09	58,58,58,58	0
58	MG	1A	3829	1/1	0.95	0.12	60,60,60,60	0
58	MG	2A	3473	1/1	0.95	0.12	54,54,54,54	0
58	MG	2A	3474	1/1	0.95	0.12	42,42,42,42	0
58	MG	2A	3711	1/1	0.95	0.06	50,50,50,50	0
58	MG	1A	3236	1/1	0.95	0.20	39,39,39,39	0
58	MG	1A	3030	1/1	0.95	0.34	36,36,36,36	0
58	MG	1A	3344	1/1	0.95	0.21	49,49,49,49	0
58	MG	2A	3479	1/1	0.95	0.08	71,71,71,71	0
58	MG	1B	236	1/1	0.95	0.08	51,51,51,51	0
58	MG	2A	3481	1/1	0.95	0.07	48,48,48,48	0
58	MG	1a	1638	1/1	0.95	0.09	56,56,56,56	0
58	MG	2A	3720	1/1	0.95	0.09	70,70,70,70	0
58	MG	2A	3105	1/1	0.95	0.11	52,52,52,52	0
58	MG	1B	237	1/1	0.95	0.12	46,46,46,46	0
58	MG	1A	3150	1/1	0.95	0.38	50,50,50,50	0
58	MG	1D	3602	1/1	0.95	0.09	49,49,49,49	0
58	MG	2A	3490	1/1	0.95	0.10	56,56,56,56	0
58	MG	1A	3978	1/1	0.95	0.09	27,27,27,27	0
58	MG	2a	1694	1/1	0.95	0.12	65,65,65,65	0
58	MG	1D	3606	1/1	0.95	0.20	45,45,45,45	0
58	MG	1A	3835	1/1	0.95	0.17	47,47,47,47	0
58	MG	1A	3571	1/1	0.95	0.24	46,46,46,46	0
58	MG	1a	1646	1/1	0.95	0.15	66,66,66,66	0
58	MG	1A	3049	1/1	0.95	0.19	34,34,34,34	0
58	MG	1A	3348	1/1	0.95	0.15	43,43,43,43	0
58	MG	1A	3123	1/1	0.95	0.18	45,45,45,45	0
58	MG	1A	3415	1/1	0.95	0.27	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3416	1/1	0.95	0.07	53,53,53,53	0
58	MG	2A	3502	1/1	0.95	0.17	55,55,55,55	0
58	MG	1A	3491	1/1	0.95	0.20	34,34,34,34	0
58	MG	1A	3192	1/1	0.95	0.23	40,40,40,40	0
58	MG	1a	1655	1/1	0.95	0.09	69,69,69,69	0
58	MG	1E	314	1/1	0.95	0.19	61,61,61,61	0
58	MG	2A	3744	1/1	0.95	0.07	58,58,58,58	0
58	MG	1F	301	1/1	0.95	0.25	50,50,50,50	0
58	MG	1F	304	1/1	0.95	0.11	50,50,50,50	0
58	MG	1F	305	1/1	0.95	0.14	39,39,39,39	0
58	MG	2A	3515	1/1	0.95	0.10	65,65,65,65	0
58	MG	1A	3193	1/1	0.95	0.34	42,42,42,42	0
58	MG	2A	3130	1/1	0.95	0.17	65,65,65,65	0
58	MG	1A	3124	1/1	0.95	0.30	40,40,40,40	0
58	MG	2A	3754	1/1	0.95	0.09	44,44,44,44	0
58	MG	1A	3125	1/1	0.95	0.26	31,31,31,31	0
58	MG	1A	3301	1/1	0.95	0.32	57,57,57,57	0
58	MG	2a	1723	1/1	0.95	0.06	79,79,79,79	0
58	MG	1A	3852	1/1	0.95	0.19	47,47,47,47	0
58	MG	1A	3498	1/1	0.95	0.08	73,73,73,73	0
58	MG	2A	3759	1/1	0.95	0.15	60,60,60,60	0
58	MG	1A	3302	1/1	0.95	0.22	59,59,59,59	0
58	MG	2A	3311	1/1	0.95	0.23	60,60,60,60	0
58	MG	1A	3725	1/1	0.95	0.10	41,41,41,41	0
58	MG	1A	3424	1/1	0.95	0.27	51,51,51,51	0
58	MG	1A	3727	1/1	0.95	0.05	24,24,24,24	0
58	MG	1A	3358	1/1	0.95	0.15	52,52,52,52	0
58	MG	1A	3729	1/1	0.95	0.07	64,64,64,64	0
58	MG	2A	3772	1/1	0.95	0.10	60,60,60,60	0
58	MG	1A	3594	1/1	0.95	0.09	41,41,41,41	0
58	MG	1A	3196	1/1	0.95	0.09	56,56,56,56	0
58	MG	1A	3732	1/1	0.95	0.11	44,44,44,44	0
58	MG	1t	201	1/1	0.95	0.19	63,63,63,63	0
58	MG	1A	3126	1/1	0.95	0.25	52,52,52,52	0
58	MG	2A	3151	1/1	0.95	0.16	58,58,58,58	0
58	MG	1A	3598	1/1	0.95	0.08	42,42,42,42	0
58	MG	2a	1743	1/1	0.95	0.16	78,78,78,78	0
58	MG	1A	3738	1/1	0.95	0.09	61,61,61,61	0
58	MG	2a	1745	1/1	0.95	0.11	76,76,76,76	0
58	MG	1A	3032	1/1	0.95	0.18	33,33,33,33	0
58	MG	2A	3542	1/1	0.95	0.07	48,48,48,48	0
58	MG	1A	3602	1/1	0.95	0.12	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3163	1/1	0.95	0.30	67,67,67,67	0
58	MG	1Q	202	1/1	0.95	0.26	47,47,47,47	0
58	MG	1A	3432	1/1	0.95	0.07	56,56,56,56	0
58	MG	1A	3308	1/1	0.95	0.08	42,42,42,42	0
58	MG	2A	3333	1/1	0.95	0.27	76,76,76,76	0
58	MG	1A	3747	1/1	0.95	0.10	52,52,52,52	0
58	MG	1A	3511	1/1	0.95	0.45	53,53,53,53	0
58	MG	2A	3554	1/1	0.95	0.17	53,53,53,53	0
58	MG	1R	202	1/1	0.95	0.15	63,63,63,63	0
58	MG	2A	3165	1/1	0.95	0.11	76,76,76,76	0
58	MG	1A	3309	1/1	0.95	0.21	59,59,59,59	0
58	MG	1A	3613	1/1	0.95	0.06	27,27,27,27	0
58	MG	1A	3513	1/1	0.95	0.28	45,45,45,45	0
58	MG	2A	3169	1/1	0.95	0.13	41,41,41,41	0
58	MG	1A	4030	1/1	0.95	0.05	47,47,47,47	0
58	MG	1A	3021	1/1	0.95	0.10	34,34,34,34	0
58	MG	1A	4035	1/1	0.95	0.09	53,53,53,53	0
58	MG	2a	1766	1/1	0.95	0.07	74,74,74,74	0
58	MG	2a	1767	1/1	0.95	0.16	69,69,69,69	0
58	MG	1A	3755	1/1	0.95	0.08	27,27,27,27	0
58	MG	1A	3165	1/1	0.95	0.16	40,40,40,40	0
58	MG	1A	3620	1/1	0.95	0.10	57,57,57,57	0
58	MG	1A	3621	1/1	0.95	0.14	46,46,46,46	0
58	MG	1A	3066	1/1	0.95	0.11	38,38,38,38	0
58	MG	2A	3350	1/1	0.95	0.18	48,48,48,48	0
58	MG	1A	3623	1/1	0.95	0.10	27,27,27,27	0
58	MG	2A	3181	1/1	0.95	0.18	76,76,76,76	0
58	MG	1A	3896	1/1	0.95	0.14	40,40,40,40	0
58	MG	1V	202	1/1	0.95	0.27	48,48,48,48	0
58	MG	1A	3002	1/1	0.95	0.07	53,53,53,53	0
58	MG	1A	3767	1/1	0.95	0.08	45,45,45,45	0
58	MG	1A	3206	1/1	0.95	0.14	44,44,44,44	0
58	MG	1A	3207	1/1	0.95	0.09	63,63,63,63	0
58	MG	2A	3012	1/1	0.95	0.07	47,47,47,47	0
58	MG	2A	3013	1/1	0.95	0.09	58,58,58,58	0
58	MG	1A	3170	1/1	0.95	0.16	59,59,59,59	0
58	MG	1X	104	1/1	0.95	0.13	53,53,53,53	0
58	MG	1A	3444	1/1	0.95	0.19	49,49,49,49	0
58	MG	2A	3364	1/1	0.95	0.17	59,59,59,59	0
58	MG	1A	3445	1/1	0.95	0.27	46,46,46,46	0
58	MG	2A	3366	1/1	0.95	0.37	70,70,70,70	0
58	MG	2A	3590	1/1	0.95	0.08	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3591	1/1	0.95	0.13	71,71,71,71	0
58	MG	2A	3195	1/1	0.95	0.22	64,64,64,64	0
58	MG	2A	3196	1/1	0.95	0.12	68,68,68,68	0
58	MG	1A	3210	1/1	0.95	0.16	57,57,57,57	0
58	MG	1Z	301	1/1	0.95	0.21	62,62,62,62	0
58	MG	2A	3596	1/1	0.95	0.11	57,57,57,57	0
58	MG	1A	3779	1/1	0.95	0.12	32,32,32,32	0
58	MG	2Q	201	1/1	0.95	0.09	61,61,61,61	0
58	MG	1A	3526	1/1	0.95	0.31	47,47,47,47	0
58	MG	1A	3212	1/1	0.95	0.07	44,44,44,44	0
58	MG	1A	3912	1/1	0.95	0.11	68,68,68,68	0
58	MG	1A	3638	1/1	0.95	0.08	44,44,44,44	0
58	MG	1A	3319	1/1	0.95	0.29	68,68,68,68	0
58	MG	1A	3641	1/1	0.95	0.13	43,43,43,43	0
58	MG	2T	203	1/1	0.95	0.20	60,60,60,60	0
58	MG	1A	4061	1/1	0.95	0.11	58,58,58,58	0
58	MG	2A	3033	1/1	0.95	0.10	53,53,53,53	0
58	MG	2A	3607	1/1	0.95	0.20	67,67,67,67	0
58	MG	1a	1720	1/1	0.95	0.16	53,53,53,53	0
58	MG	1A	3320	1/1	0.95	0.07	48,48,48,48	0
58	MG	1l	103	1/1	0.95	0.10	48,48,48,48	0
58	MG	1A	3917	1/1	0.95	0.12	44,44,44,44	0
58	MG	1A	3644	1/1	0.95	0.07	30,30,30,30	0
58	MG	1A	3132	1/1	0.95	0.06	45,45,45,45	0
58	MG	2A	3614	1/1	0.95	0.09	88,88,88,88	0
58	MG	2A	3615	1/1	0.95	0.09	45,45,45,45	0
58	MG	2A	3616	1/1	0.95	0.10	76,76,76,76	0
58	MG	13	103	1/1	0.95	0.31	64,64,64,64	0
58	MG	1A	4068	1/1	0.95	0.11	18,18,18,18	0
58	MG	1A	3378	1/1	0.95	0.11	55,55,55,55	0
58	MG	1A	3266	1/1	0.95	0.11	63,63,63,63	0
58	MG	1A	4072	1/1	0.95	0.09	72,72,72,72	0
58	MG	1A	3454	1/1	0.95	0.21	53,53,53,53	0
58	MG	15	107	1/1	0.95	0.11	54,54,54,54	0
58	MG	2A	3048	1/1	0.95	0.25	63,63,63,63	0
58	MG	2A	3049	1/1	0.95	0.26	62,62,62,62	0
58	MG	2A	3050	1/1	0.95	0.07	37,37,37,37	0
58	MG	1a	1734	1/1	0.95	0.14	56,56,56,56	0
58	MG	1A	3929	1/1	0.95	0.06	66,66,66,66	0
58	MG	1a	1736	1/1	0.95	0.08	60,60,60,60	0
58	MG	2A	3633	1/1	0.95	0.11	44,44,44,44	0
58	MG	1A	3650	1/1	0.95	0.08	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3323	1/1	0.95	0.23	48,48,48,48	0
58	MG	1A	3382	1/1	0.95	0.16	55,55,55,55	0
58	MG	1a	1743	1/1	0.95	0.11	64,64,64,64	0
58	MG	1A	3091	1/1	0.95	0.15	63,63,63,63	0
58	MG	1A	3268	1/1	0.95	0.36	61,61,61,61	0
58	MG	2A	3060	1/1	0.95	0.16	58,58,58,58	0
58	MG	1A	3215	1/1	0.95	0.28	51,51,51,51	0
58	MG	2a	1616	1/1	0.95	0.10	89,89,89,89	0
58	MG	1A	3938	1/1	0.95	0.13	61,61,61,61	0
58	MG	1A	4086	1/1	0.95	0.12	66,66,66,66	0
58	MG	19	101	1/1	0.95	0.24	58,58,58,58	0
58	MG	1A	3177	1/1	0.95	0.10	26,26,26,26	0
58	MG	2A	3414	1/1	0.95	0.10	62,62,62,62	0
58	MG	2a	1622	1/1	0.95	0.30	76,76,76,76	0
60	CLM	1A	4087	20/20	0.95	0.09	29,38,62,63	0
58	MG	1A	3055	1/1	0.95	0.26	56,56,56,56	0
61	ZN	24	501	1/1	0.95	0.14	140,140,140,140	0
58	MG	1A	3010	1/1	0.95	0.07	39,39,39,39	0
58	MG	1A	3652	1/1	0.96	0.09	37,37,37,37	0
58	MG	1A	3102	1/1	0.96	0.05	42,42,42,42	0
58	MG	1A	3656	1/1	0.96	0.06	29,29,29,29	0
58	MG	1A	3657	1/1	0.96	0.11	24,24,24,24	0
58	MG	2A	3039	1/1	0.96	0.15	42,42,42,42	0
58	MG	1a	1608	1/1	0.96	0.07	71,71,71,71	0
58	MG	2A	3536	1/1	0.96	0.08	45,45,45,45	0
58	MG	1a	1609	1/1	0.96	0.17	62,62,62,62	0
58	MG	1A	3763	1/1	0.96	0.09	59,59,59,59	0
58	MG	1A	3868	1/1	0.96	0.08	29,29,29,29	0
58	MG	1A	3219	1/1	0.96	0.08	51,51,51,51	0
58	MG	2A	3541	1/1	0.96	0.10	46,46,46,46	0
58	MG	1A	3220	1/1	0.96	0.07	54,54,54,54	0
58	MG	1A	3569	1/1	0.96	0.07	44,44,44,44	0
58	MG	2A	3737	1/1	0.96	0.09	82,82,82,82	0
58	MG	1A	3347	1/1	0.96	0.39	44,44,44,44	0
58	MG	1D	3605	1/1	0.96	0.18	41,41,41,41	0
58	MG	1A	3038	1/1	0.96	0.38	39,39,39,39	0
58	MG	1A	3154	1/1	0.96	0.20	48,48,48,48	0
58	MG	2A	3549	1/1	0.96	0.09	42,42,42,42	0
58	MG	1A	3350	1/1	0.96	0.36	40,40,40,40	0
58	MG	1a	1621	1/1	0.96	0.06	50,50,50,50	0
58	MG	1D	3611	1/1	0.96	0.16	45,45,45,45	0
58	MG	1A	3575	1/1	0.96	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3451	1/1	0.96	0.10	55,55,55,55	0
58	MG	2A	3556	1/1	0.96	0.12	63,63,63,63	0
58	MG	1a	1761	1/1	0.96	0.11	68,68,68,68	0
58	MG	1A	4004	1/1	0.96	0.06	37,37,37,37	0
58	MG	2A	3751	1/1	0.96	0.13	49,49,49,49	0
58	MG	1A	3776	1/1	0.96	0.10	59,59,59,59	0
58	MG	2A	3753	1/1	0.96	0.14	52,52,52,52	0
58	MG	1A	3351	1/1	0.96	0.11	49,49,49,49	0
58	MG	1A	3225	1/1	0.96	0.10	43,43,43,43	0
58	MG	1A	4009	1/1	0.96	0.07	49,49,49,49	0
58	MG	1A	4010	1/1	0.96	0.10	45,45,45,45	0
58	MG	1a	1769	1/1	0.96	0.11	80,80,80,80	0
58	MG	2A	3220	1/1	0.96	0.14	59,59,59,59	0
58	MG	2A	3760	1/1	0.96	0.07	60,60,60,60	0
58	MG	1A	3403	1/1	0.96	0.10	61,61,61,61	0
58	MG	1F	303	1/1	0.96	0.07	45,45,45,45	0
58	MG	2A	3765	1/1	0.96	0.07	69,69,69,69	0
58	MG	2A	3569	1/1	0.96	0.08	68,68,68,68	0
58	MG	1A	3226	1/1	0.96	0.12	56,56,56,56	0
58	MG	1A	3887	1/1	0.96	0.10	59,59,59,59	0
58	MG	1A	3227	1/1	0.96	0.13	48,48,48,48	0
58	MG	1A	3889	1/1	0.96	0.30	36,36,36,36	0
58	MG	1a	1776	1/1	0.96	0.07	78,78,78,78	0
58	MG	1A	3190	1/1	0.96	0.30	48,48,48,48	0
58	MG	1A	3104	1/1	0.96	0.11	36,36,36,36	0
58	MG	1A	3012	1/1	0.96	0.07	37,37,37,37	0
58	MG	2A	3578	1/1	0.96	0.20	73,73,73,73	0
58	MG	1G	201	1/1	0.96	0.14	51,51,51,51	0
58	MG	1A	3894	1/1	0.96	0.09	53,53,53,53	0
58	MG	1A	4021	1/1	0.96	0.05	65,65,65,65	0
58	MG	1A	3787	1/1	0.96	0.05	25,25,25,25	0
58	MG	1A	3129	1/1	0.96	0.10	47,47,47,47	0
58	MG	1A	3689	1/1	0.96	0.09	47,47,47,47	0
58	MG	2A	3785	1/1	0.96	0.07	66,66,66,66	0
58	MG	1A	4026	1/1	0.96	0.11	59,59,59,59	0
58	MG	1A	3588	1/1	0.96	0.12	33,33,33,33	0
58	MG	2A	3788	1/1	0.96	0.18	63,63,63,63	0
58	MG	1A	3590	1/1	0.96	0.07	29,29,29,29	0
58	MG	2A	3240	1/1	0.96	0.07	73,73,73,73	0
58	MG	1A	3522	1/1	0.96	0.11	61,61,61,61	0
58	MG	2a	1721	1/1	0.96	0.19	81,81,81,81	0
58	MG	1A	3158	1/1	0.96	0.11	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3795	1/1	0.96	0.09	53,53,53,53	0
58	MG	1a	1792	1/1	0.96	0.10	58,58,58,58	0
58	MG	1O	201	1/1	0.96	0.11	65,65,65,65	0
58	MG	1A	3464	1/1	0.96	0.21	42,42,42,42	0
58	MG	1A	3015	1/1	0.96	0.16	46,46,46,46	0
58	MG	1A	3108	1/1	0.96	0.32	39,39,39,39	0
58	MG	1A	3277	1/1	0.96	0.19	33,33,33,33	0
58	MG	1P	201	1/1	0.96	0.39	40,40,40,40	0
58	MG	1A	3109	1/1	0.96	0.05	46,46,46,46	0
58	MG	2A	3409	1/1	0.96	0.21	56,56,56,56	0
58	MG	1a	1800	1/1	0.96	0.09	66,66,66,66	0
58	MG	1A	3802	1/1	0.96	0.07	49,49,49,49	0
58	MG	2A	3602	1/1	0.96	0.09	60,60,60,60	0
58	MG	1A	3699	1/1	0.96	0.10	43,43,43,43	0
58	MG	1A	3133	1/1	0.96	0.10	49,49,49,49	0
58	MG	1A	3067	1/1	0.96	0.13	58,58,58,58	0
58	MG	1A	3808	1/1	0.96	0.05	42,42,42,42	0
58	MG	1A	3603	1/1	0.96	0.11	39,39,39,39	0
58	MG	2a	1741	1/1	0.96	0.17	76,76,76,76	0
58	MG	1A	3283	1/1	0.96	0.13	51,51,51,51	0
58	MG	1A	3918	1/1	0.96	0.05	47,47,47,47	0
58	MG	2A	3103	1/1	0.96	0.07	59,59,59,59	0
58	MG	1A	3919	1/1	0.96	0.09	52,52,52,52	0
58	MG	1A	3240	1/1	0.96	0.39	39,39,39,39	0
58	MG	1A	3921	1/1	0.96	0.06	18,18,18,18	0
58	MG	1A	3473	1/1	0.96	0.09	55,55,55,55	0
58	MG	2A	3424	1/1	0.96	0.14	64,64,64,64	0
58	MG	1A	3054	1/1	0.96	0.07	41,41,41,41	0
58	MG	1A	3709	1/1	0.96	0.06	54,54,54,54	0
58	MG	1A	3926	1/1	0.96	0.08	37,37,37,37	0
58	MG	1A	3710	1/1	0.96	0.08	57,57,57,57	0
58	MG	2E	303	1/1	0.96	0.10	68,68,68,68	0
58	MG	2E	304	1/1	0.96	0.19	57,57,57,57	0
58	MG	1e	201	1/1	0.96	0.41	73,73,73,73	0
58	MG	1A	3610	1/1	0.96	0.08	59,59,59,59	0
58	MG	2A	3432	1/1	0.96	0.12	56,56,56,56	0
58	MG	1A	3242	1/1	0.96	0.10	55,55,55,55	0
58	MG	1U	206	1/1	0.96	0.21	42,42,42,42	0
58	MG	2A	3437	1/1	0.96	0.08	69,69,69,69	0
58	MG	1A	3536	1/1	0.96	0.39	55,55,55,55	0
58	MG	1A	3027	1/1	0.96	0.13	79,79,79,79	0
58	MG	1A	3244	1/1	0.96	0.26	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2F	306	1/1	0.96	0.17	65,65,65,65	0
58	MG	1V	203	1/1	0.96	0.25	45,45,45,45	0
58	MG	2F	308	1/1	0.96	0.27	64,64,64,64	0
58	MG	2A	3630	1/1	0.96	0.07	72,72,72,72	0
58	MG	2A	3631	1/1	0.96	0.10	58,58,58,58	0
58	MG	1A	3139	1/1	0.96	0.13	50,50,50,50	0
58	MG	2A	3634	1/1	0.96	0.07	44,44,44,44	0
58	MG	1A	3619	1/1	0.96	0.13	72,72,72,72	0
58	MG	1A	3204	1/1	0.96	0.09	44,44,44,44	0
58	MG	1A	3426	1/1	0.96	0.09	57,57,57,57	0
58	MG	2A	3446	1/1	0.96	0.07	69,69,69,69	0
58	MG	1W	206	1/1	0.96	0.18	53,53,53,53	0
58	MG	2A	3127	1/1	0.96	0.13	60,60,60,60	0
58	MG	1A	3174	1/1	0.96	0.15	39,39,39,39	0
58	MG	2T	204	1/1	0.96	0.10	74,74,74,74	0
58	MG	1X	101	1/1	0.96	0.33	50,50,50,50	0
58	MG	2V	201	1/1	0.96	0.07	70,70,70,70	0
58	MG	1X	102	1/1	0.96	0.15	48,48,48,48	0
58	MG	1A	3092	1/1	0.96	0.05	32,32,32,32	0
58	MG	2A	3453	1/1	0.96	0.09	66,66,66,66	0
58	MG	1A	4073	1/1	0.96	0.07	63,63,63,63	0
58	MG	2A	3133	1/1	0.96	0.25	57,57,57,57	0
58	MG	2A	3456	1/1	0.96	0.22	64,64,64,64	0
58	MG	1A	3042	1/1	0.96	0.27	39,39,39,39	0
58	MG	2A	3458	1/1	0.96	0.07	52,52,52,52	0
58	MG	1A	3485	1/1	0.96	0.15	47,47,47,47	0
58	MG	1A	3831	1/1	0.96	0.12	56,56,56,56	0
58	MG	2A	3656	1/1	0.96	0.11	73,73,73,73	0
58	MG	2A	3657	1/1	0.96	0.07	70,70,70,70	0
58	MG	1A	3022	1/1	0.96	0.07	47,47,47,47	0
58	MG	2A	3462	1/1	0.96	0.07	50,50,50,50	0
58	MG	27	101	1/1	0.96	0.15	48,48,48,48	0
58	MG	2A	3138	1/1	0.96	0.12	48,48,48,48	0
58	MG	2A	3139	1/1	0.96	0.10	54,54,54,54	0
58	MG	1A	3628	1/1	0.96	0.08	42,42,42,42	0
58	MG	1A	3487	1/1	0.96	0.08	58,58,58,58	0
58	MG	10	102	1/1	0.96	0.11	56,56,56,56	0
58	MG	1A	3379	1/1	0.96	0.21	42,42,42,42	0
58	MG	1A	3631	1/1	0.96	0.05	41,41,41,41	0
58	MG	1A	3951	1/1	0.96	0.08	66,66,66,66	0
58	MG	1A	3252	1/1	0.96	0.20	53,53,53,53	0
58	MG	1A	3839	1/1	0.96	0.08	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	11	101	1/1	0.96	0.45	45,45,45,45	0
58	MG	2A	3149	1/1	0.96	0.07	62,62,62,62	0
58	MG	2A	3305	1/1	0.96	0.07	68,68,68,68	0
58	MG	1A	3551	1/1	0.96	0.16	42,42,42,42	0
58	MG	2A	3676	1/1	0.96	0.08	65,65,65,65	0
58	MG	1A	3023	1/1	0.96	0.08	25,25,25,25	0
58	MG	1x	112	1/1	0.96	0.11	67,67,67,67	0
58	MG	1A	3081	1/1	0.96	0.26	44,44,44,44	0
58	MG	1A	3959	1/1	0.96	0.18	72,72,72,72	0
58	MG	1A	3492	1/1	0.96	0.23	38,38,38,38	0
58	MG	13	102	1/1	0.96	0.12	51,51,51,51	0
58	MG	1A	3844	1/1	0.96	0.06	48,48,48,48	0
58	MG	1A	3005	1/1	0.96	0.07	55,55,55,55	0
58	MG	1A	3742	1/1	0.96	0.12	53,53,53,53	0
58	MG	2A	3161	1/1	0.96	0.08	64,64,64,64	0
58	MG	1A	3149	1/1	0.96	0.22	33,33,33,33	0
58	MG	2A	3318	1/1	0.96	0.09	63,63,63,63	0
58	MG	15	104	1/1	0.96	0.20	39,39,39,39	0
58	MG	1A	3386	1/1	0.96	0.10	53,53,53,53	0
58	MG	2A	3011	1/1	0.96	0.08	64,64,64,64	0
58	MG	1B	213	1/1	0.96	0.05	71,71,71,71	0
58	MG	1A	3643	1/1	0.96	0.08	31,31,31,31	0
58	MG	2A	3014	1/1	0.96	0.07	45,45,45,45	0
58	MG	1A	3035	1/1	0.96	0.05	55,55,55,55	0
58	MG	2A	3017	1/1	0.96	0.26	58,58,58,58	0
58	MG	1A	3970	1/1	0.96	0.07	55,55,55,55	0
58	MG	1A	3440	1/1	0.96	0.22	45,45,45,45	0
58	MG	1A	3441	1/1	0.96	0.25	60,60,60,60	0
58	MG	2A	3021	1/1	0.96	0.09	39,39,39,39	0
58	MG	17	101	1/1	0.96	0.12	41,41,41,41	0
58	MG	2A	3176	1/1	0.96	0.07	52,52,52,52	0
58	MG	1A	3751	1/1	0.96	0.10	38,38,38,38	0
58	MG	1A	3975	1/1	0.96	0.08	30,30,30,30	0
58	MG	18	101	1/1	0.96	0.21	52,52,52,52	0
58	MG	2A	3180	1/1	0.96	0.07	66,66,66,66	0
58	MG	1a	1729	1/1	0.96	0.12	66,66,66,66	0
58	MG	1A	3084	1/1	0.96	0.16	37,37,37,37	0
58	MG	1A	3857	1/1	0.96	0.27	43,43,43,43	0
58	MG	1A	3858	1/1	0.96	0.25	46,46,46,46	0
58	MG	1A	3563	1/1	0.96	0.14	43,43,43,43	0
58	MG	2A	3186	1/1	0.96	0.07	65,65,65,65	0
58	MG	1A	3391	1/1	0.96	0.13	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
61	ZN	14	501	1/1	0.96	0.12	115,115,115,115	0
58	MG	1A	3756	1/1	0.96	0.06	33,33,33,33	0
58	MG	1A	3862	1/1	0.96	0.12	39,39,39,39	0
58	MG	2A	3514	1/1	0.97	0.10	60,60,60,60	0
58	MG	1A	3400	1/1	0.97	0.24	42,42,42,42	0
58	MG	18	102	1/1	0.97	0.07	50,50,50,50	0
58	MG	2A	3113	1/1	0.97	0.15	56,56,56,56	0
58	MG	1A	3687	1/1	0.97	0.09	39,39,39,39	0
58	MG	1A	3173	1/1	0.97	0.36	46,46,46,46	0
58	MG	2a	1700	1/1	0.97	0.08	73,73,73,73	0
58	MG	1A	3768	1/1	0.97	0.07	40,40,40,40	0
58	MG	1A	3238	1/1	0.97	0.14	43,43,43,43	0
58	MG	1A	3940	1/1	0.97	0.09	68,68,68,68	0
58	MG	2D	303	1/1	0.97	0.10	42,42,42,42	0
58	MG	1A	3105	1/1	0.97	0.07	34,34,34,34	0
58	MG	2A	3667	1/1	0.97	0.22	50,50,50,50	0
58	MG	1A	3175	1/1	0.97	0.05	44,44,44,44	0
58	MG	1A	3612	1/1	0.97	0.05	39,39,39,39	0
58	MG	1A	3550	1/1	0.97	0.16	41,41,41,41	0
58	MG	2A	3671	1/1	0.97	0.08	67,67,67,67	0
58	MG	1A	3278	1/1	0.97	0.14	46,46,46,46	0
58	MG	1A	3856	1/1	0.97	0.10	42,42,42,42	0
58	MG	1A	4047	1/1	0.97	0.07	59,59,59,59	0
58	MG	1A	3146	1/1	0.97	0.26	41,41,41,41	0
58	MG	1A	3777	1/1	0.97	0.10	33,33,33,33	0
58	MG	1A	4050	1/1	0.97	0.09	33,33,33,33	0
58	MG	1A	3500	1/1	0.97	0.14	49,49,49,49	0
58	MG	2A	3679	1/1	0.97	0.08	69,69,69,69	0
58	MG	2a	1719	1/1	0.97	0.12	73,73,73,73	0
58	MG	1A	3617	1/1	0.97	0.12	39,39,39,39	0
58	MG	1A	3007	1/1	0.97	0.04	39,39,39,39	0
58	MG	1A	3077	1/1	0.97	0.16	46,46,46,46	0
58	MG	1A	3503	1/1	0.97	0.19	34,34,34,34	0
58	MG	1A	3282	1/1	0.97	0.20	55,55,55,55	0
58	MG	1A	3702	1/1	0.97	0.15	55,55,55,55	0
58	MG	1a	1738	1/1	0.97	0.19	43,43,43,43	0
58	MG	1a	1739	1/1	0.97	0.09	49,49,49,49	0
58	MG	1A	3209	1/1	0.97	0.10	44,44,44,44	0
58	MG	1A	3958	1/1	0.97	0.12	61,61,61,61	0
58	MG	2A	3545	1/1	0.97	0.05	54,54,54,54	0
58	MG	2A	3691	1/1	0.97	0.07	53,53,53,53	0
58	MG	2A	3692	1/1	0.97	0.15	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1O	203	1/1	0.97	0.08	56,56,56,56	0
58	MG	1A	3284	1/1	0.97	0.09	56,56,56,56	0
58	MG	1A	4062	1/1	0.97	0.04	44,44,44,44	0
58	MG	1a	1745	1/1	0.97	0.05	54,54,54,54	0
58	MG	1A	3457	1/1	0.97	0.12	53,53,53,53	0
58	MG	1A	3458	1/1	0.97	0.10	55,55,55,55	0
58	MG	2W	202	1/1	0.97	0.07	63,63,63,63	0
58	MG	2X	101	1/1	0.97	0.11	60,60,60,60	0
58	MG	2A	3552	1/1	0.97	0.07	46,46,46,46	0
58	MG	1P	202	1/1	0.97	0.36	46,46,46,46	0
58	MG	1P	204	1/1	0.97	0.28	41,41,41,41	0
58	MG	1A	3078	1/1	0.97	0.07	31,31,31,31	0
58	MG	1A	3211	1/1	0.97	0.25	42,42,42,42	0
58	MG	2A	3557	1/1	0.97	0.07	51,51,51,51	0
58	MG	1A	3034	1/1	0.97	0.17	42,42,42,42	0
58	MG	1Q	204	1/1	0.97	0.07	46,46,46,46	0
58	MG	1A	3795	1/1	0.97	0.04	66,66,66,66	0
58	MG	2A	3154	1/1	0.97	0.09	71,71,71,71	0
58	MG	2A	3027	1/1	0.97	0.05	45,45,45,45	0
58	MG	1a	1634	1/1	0.97	0.09	40,40,40,40	0
58	MG	1A	3876	1/1	0.97	0.09	31,31,31,31	0
58	MG	2A	3713	1/1	0.97	0.11	56,56,56,56	0
58	MG	1Q	207	1/1	0.97	0.10	54,54,54,54	0
58	MG	1A	3110	1/1	0.97	0.16	41,41,41,41	0
58	MG	1A	3370	1/1	0.97	0.20	47,47,47,47	0
58	MG	1A	3065	1/1	0.97	0.10	36,36,36,36	0
58	MG	1A	4076	1/1	0.97	0.12	58,58,58,58	0
58	MG	1R	204	1/1	0.97	0.24	49,49,49,49	0
58	MG	1A	3880	1/1	0.97	0.04	41,41,41,41	0
58	MG	1A	3634	1/1	0.97	0.06	50,50,50,50	0
58	MG	2A	3425	1/1	0.97	0.12	65,65,65,65	0
58	MG	1A	3974	1/1	0.97	0.10	52,52,52,52	0
58	MG	1A	3250	1/1	0.97	0.14	55,55,55,55	0
58	MG	1A	3043	1/1	0.97	0.06	46,46,46,46	0
58	MG	1a	1768	1/1	0.97	0.09	69,69,69,69	0
58	MG	1A	3977	1/1	0.97	0.10	43,43,43,43	0
58	MG	1A	3719	1/1	0.97	0.08	54,54,54,54	0
58	MG	1U	202	1/1	0.97	0.23	47,47,47,47	0
58	MG	1A	3803	1/1	0.97	0.04	34,34,34,34	0
58	MG	1A	3804	1/1	0.97	0.06	38,38,38,38	0
58	MG	1A	3637	1/1	0.97	0.11	67,67,67,67	0
58	MG	1A	3113	1/1	0.97	0.06	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	2A	3735	1/1	0.97	0.09	71,71,71,71	0
58	MG	2a	1776	1/1	0.97	0.10	69,69,69,69	0
58	MG	1A	3573	1/1	0.97	0.15	49,49,49,49	0
58	MG	1U	208	1/1	0.97	0.21	42,42,42,42	0
58	MG	1A	3421	1/1	0.97	0.07	62,62,62,62	0
58	MG	1V	201	1/1	0.97	0.20	38,38,38,38	0
58	MG	1B	205	1/1	0.97	0.05	53,53,53,53	0
58	MG	1A	3096	1/1	0.97	0.05	45,45,45,45	0
58	MG	1a	1782	1/1	0.97	0.07	85,85,85,85	0
58	MG	1V	205	1/1	0.97	0.27	59,59,59,59	0
58	MG	1A	3218	1/1	0.97	0.09	45,45,45,45	0
58	MG	1A	3050	1/1	0.97	0.20	38,38,38,38	0
58	MG	1A	3028	1/1	0.97	0.34	42,42,42,42	0
58	MG	1A	3297	1/1	0.97	0.11	44,44,44,44	0
58	MG	1A	3159	1/1	0.97	0.19	44,44,44,44	0
58	MG	1A	3475	1/1	0.97	0.12	47,47,47,47	0
58	MG	1A	3428	1/1	0.97	0.09	56,56,56,56	0
58	MG	1A	3160	1/1	0.97	0.15	38,38,38,38	0
58	MG	1A	3996	1/1	0.97	0.11	31,31,31,31	0
58	MG	2a	1794	1/1	0.97	0.18	75,75,75,75	0
58	MG	1A	3735	1/1	0.97	0.07	46,46,46,46	0
58	MG	1B	217	1/1	0.97	0.10	51,51,51,51	0
58	MG	1Y	202	1/1	0.97	0.20	60,60,60,60	0
58	MG	2A	3197	1/1	0.97	0.15	63,63,63,63	0
58	MG	2A	3069	1/1	0.97	0.07	35,35,35,35	0
58	MG	1A	3162	1/1	0.97	0.37	35,35,35,35	0
58	MG	1A	3586	1/1	0.97	0.08	40,40,40,40	0
58	MG	1A	3137	1/1	0.97	0.33	41,41,41,41	0
58	MG	2A	3761	1/1	0.97	0.08	48,48,48,48	0
58	MG	1A	4002	1/1	0.97	0.08	40,40,40,40	0
58	MG	1A	3118	1/1	0.97	0.16	46,46,46,46	0
58	MG	1A	3589	1/1	0.97	0.06	45,45,45,45	0
58	MG	2A	3467	1/1	0.97	0.09	48,48,48,48	0
58	MG	1A	3909	1/1	0.97	0.08	69,69,69,69	0
58	MG	2A	3470	1/1	0.97	0.08	44,44,44,44	0
58	MG	10	104	1/1	0.97	0.08	52,52,52,52	0
58	MG	1a	1682	1/1	0.97	0.18	64,64,64,64	0
58	MG	1A	3663	1/1	0.97	0.07	32,32,32,32	0
58	MG	1B	227	1/1	0.97	0.05	47,47,47,47	0
58	MG	1A	3303	1/1	0.97	0.09	42,42,42,42	0
58	MG	1A	3827	1/1	0.97	0.05	63,63,63,63	0
58	MG	2A	3477	1/1	0.97	0.07	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3085	1/1	0.97	0.25	42,42,42,42	0
58	MG	1A	3389	1/1	0.97	0.21	44,44,44,44	0
58	MG	2a	1659	1/1	0.97	0.09	58,58,58,58	0
58	MG	1A	3669	1/1	0.97	0.05	41,41,41,41	0
58	MG	2a	1661	1/1	0.97	0.06	68,68,68,68	0
58	MG	1A	3229	1/1	0.97	0.32	46,46,46,46	0
58	MG	2a	1663	1/1	0.97	0.05	68,68,68,68	0
58	MG	1A	3140	1/1	0.97	0.12	46,46,46,46	0
58	MG	2a	1665	1/1	0.97	0.10	61,61,61,61	0
58	MG	2A	3484	1/1	0.97	0.10	53,53,53,53	0
58	MG	1A	3595	1/1	0.97	0.19	57,57,57,57	0
58	MG	2A	3486	1/1	0.97	0.09	62,62,62,62	0
58	MG	1b	301	1/1	0.97	0.05	90,90,90,90	0
58	MG	13	101	1/1	0.97	0.16	40,40,40,40	0
58	MG	1A	3752	1/1	0.97	0.08	40,40,40,40	0
58	MG	2A	3791	1/1	0.97	0.13	57,57,57,57	0
58	MG	1A	3265	1/1	0.97	0.19	46,46,46,46	0
58	MG	1A	3069	1/1	0.97	0.06	25,25,25,25	0
58	MG	1A	4019	1/1	0.97	0.07	62,62,62,62	0
58	MG	1f	201	1/1	0.97	0.15	61,61,61,61	0
58	MG	15	102	1/1	0.97	0.32	38,38,38,38	0
58	MG	1A	3676	1/1	0.97	0.11	34,34,34,34	0
58	MG	1A	3838	1/1	0.97	0.07	29,29,29,29	0
58	MG	1A	4022	1/1	0.97	0.05	60,60,60,60	0
58	MG	1A	3925	1/1	0.97	0.05	42,42,42,42	0
58	MG	1A	3169	1/1	0.97	0.09	43,43,43,43	0
58	MG	2A	3646	1/1	0.97	0.07	44,44,44,44	0
58	MG	2B	202	1/1	0.97	0.12	74,74,74,74	0
58	MG	1A	3199	1/1	0.97	0.15	29,29,29,29	0
58	MG	1A	3928	1/1	0.97	0.06	44,44,44,44	0
58	MG	1A	3045	1/1	0.97	0.08	50,50,50,50	0
58	MG	1E	305	1/1	0.97	0.10	34,34,34,34	0
58	MG	1A	3046	1/1	0.97	0.15	38,38,38,38	0
58	MG	17	102	1/1	0.97	0.11	42,42,42,42	0
58	MG	1A	3074	1/1	0.97	0.04	39,39,39,39	0
58	MG	17	104	1/1	0.97	0.17	45,45,45,45	0
58	MG	1A	3605	1/1	0.97	0.08	38,38,38,38	0
58	MG	1F	302	1/1	0.98	0.22	42,42,42,42	0
58	MG	1A	3167	1/1	0.98	0.21	39,39,39,39	0
58	MG	1A	3954	1/1	0.98	0.09	33,33,33,33	0
58	MG	2A	3116	1/1	0.98	0.06	48,48,48,48	0
58	MG	1A	3654	1/1	0.98	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1F	306	1/1	0.98	0.12	36,36,36,36	0
58	MG	1A	3655	1/1	0.98	0.10	33,33,33,33	0
58	MG	1A	3508	1/1	0.98	0.25	37,37,37,37	0
58	MG	1A	3849	1/1	0.98	0.07	51,51,51,51	0
58	MG	1A	3388	1/1	0.98	0.11	47,47,47,47	0
58	MG	2A	3469	1/1	0.98	0.09	39,39,39,39	0
58	MG	1A	3659	1/1	0.98	0.05	32,32,32,32	0
58	MG	1A	3660	1/1	0.98	0.03	34,34,34,34	0
58	MG	1A	3014	1/1	0.98	0.06	33,33,33,33	0
58	MG	1A	3624	1/1	0.98	0.12	20,20,20,20	0
58	MG	1A	3221	1/1	0.98	0.05	59,59,59,59	0
58	MG	1A	3911	1/1	0.98	0.07	51,51,51,51	0
58	MG	1A	3966	1/1	0.98	0.06	76,76,76,76	0
58	MG	1A	3967	1/1	0.98	0.04	58,58,58,58	0
58	MG	1A	3565	1/1	0.98	0.21	43,43,43,43	0
58	MG	1A	3757	1/1	0.98	0.06	42,42,42,42	0
58	MG	1a	1654	1/1	0.98	0.14	52,52,52,52	0
58	MG	1A	3222	1/1	0.98	0.15	40,40,40,40	0
58	MG	1a	1737	1/1	0.98	0.06	35,35,35,35	0
58	MG	2A	3483	1/1	0.98	0.06	47,47,47,47	0
58	MG	1A	3080	1/1	0.98	0.12	48,48,48,48	0
58	MG	1A	4034	1/1	0.98	0.06	61,61,61,61	0
58	MG	1A	3031	1/1	0.98	0.30	42,42,42,42	0
58	MG	1A	3761	1/1	0.98	0.04	27,27,27,27	0
58	MG	1A	3670	1/1	0.98	0.04	30,30,30,30	0
58	MG	1A	3713	1/1	0.98	0.05	29,29,29,29	0
58	MG	1A	3764	1/1	0.98	0.09	70,70,70,70	0
58	MG	1A	3070	1/1	0.98	0.10	36,36,36,36	0
58	MG	1A	3117	1/1	0.98	0.17	42,42,42,42	0
58	MG	1P	203	1/1	0.98	0.18	33,33,33,33	0
58	MG	1A	3979	1/1	0.98	0.08	31,31,31,31	0
58	MG	2A	3495	1/1	0.98	0.04	47,47,47,47	0
58	MG	2A	3404	1/1	0.98	0.11	25,25,25,25	0
58	MG	1A	3517	1/1	0.98	0.09	58,58,58,58	0
58	MG	1A	3601	1/1	0.98	0.17	40,40,40,40	0
58	MG	2A	3789	1/1	0.98	0.06	40,40,40,40	0
58	MG	1A	3982	1/1	0.98	0.04	59,59,59,59	0
58	MG	1Q	203	1/1	0.98	0.11	37,37,37,37	0
58	MG	1A	3003	1/1	0.98	0.06	33,33,33,33	0
58	MG	1A	3770	1/1	0.98	0.03	49,49,49,49	0
58	MG	1A	3063	1/1	0.98	0.14	45,45,45,45	0
58	MG	1A	3677	1/1	0.98	0.09	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3033	1/1	0.98	0.32	37,37,37,37	0
58	MG	2A	3326	1/1	0.98	0.04	48,48,48,48	0
58	MG	1A	3399	1/1	0.98	0.06	44,44,44,44	0
58	MG	1A	3931	1/1	0.98	0.06	52,52,52,52	0
58	MG	2A	3511	1/1	0.98	0.08	39,39,39,39	0
58	MG	2A	3512	1/1	0.98	0.05	57,57,57,57	0
58	MG	18	104	1/1	0.98	0.11	53,53,53,53	0
58	MG	1A	3825	1/1	0.98	0.10	41,41,41,41	0
58	MG	1A	3011	1/1	0.98	0.05	54,54,54,54	0
58	MG	1R	205	1/1	0.98	0.29	54,54,54,54	0
58	MG	1A	3178	1/1	0.98	0.07	45,45,45,45	0
58	MG	1A	4056	1/1	0.98	0.05	42,42,42,42	0
58	MG	1A	3640	1/1	0.98	0.10	51,51,51,51	0
58	MG	2a	1819	1/1	0.98	0.20	60,60,60,60	0
58	MG	1A	3683	1/1	0.98	0.08	36,36,36,36	0
58	MG	1A	3161	1/1	0.98	0.15	40,40,40,40	0
58	MG	1A	3685	1/1	0.98	0.06	18,18,18,18	0
58	MG	1D	3603	1/1	0.98	0.12	30,30,30,30	0
58	MG	1A	3997	1/1	0.98	0.05	40,40,40,40	0
58	MG	1A	3334	1/1	0.98	0.24	62,62,62,62	0
58	MG	1A	3271	1/1	0.98	0.16	49,49,49,49	0
58	MG	2A	3527	1/1	0.98	0.11	54,54,54,54	0
58	MG	1a	1611	1/1	0.98	0.09	39,39,39,39	0
58	MG	1D	3607	1/1	0.98	0.06	52,52,52,52	0
58	MG	1A	3272	1/1	0.98	0.14	41,41,41,41	0
58	MG	1D	3609	1/1	0.98	0.16	33,33,33,33	0
58	MG	1A	3147	1/1	0.98	0.04	39,39,39,39	0
58	MG	1U	209	1/1	0.98	0.28	41,41,41,41	0
58	MG	2A	3009	1/1	0.98	0.04	45,45,45,45	0
58	MG	1A	4066	1/1	0.98	0.04	49,49,49,49	0
58	MG	2A	3726	1/1	0.98	0.11	56,56,56,56	0
58	MG	1E	301	1/1	0.98	0.42	41,41,41,41	0
58	MG	1A	3134	1/1	0.98	0.10	48,48,48,48	0
58	MG	1A	3076	1/1	0.98	0.18	58,58,58,58	0
58	MG	1E	304	1/1	0.98	0.14	41,41,41,41	0
58	MG	2A	3015	1/1	0.98	0.08	58,58,58,58	0
58	MG	1A	3789	1/1	0.98	0.04	32,32,32,32	0
58	MG	1E	306	1/1	0.98	0.20	42,42,42,42	0
58	MG	1E	307	1/1	0.98	0.15	44,44,44,44	0
58	MG	1W	204	1/1	0.98	0.22	50,50,50,50	0
58	MG	1A	3648	1/1	0.98	0.09	41,41,41,41	0
58	MG	1A	3585	1/1	0.98	0.08	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3001	1/1	0.98	0.15	43,43,43,43	0
58	MG	1E	311	1/1	0.98	0.09	32,32,32,32	0
58	MG	1A	4074	1/1	0.98	0.04	39,39,39,39	0
58	MG	1X	103	1/1	0.98	0.09	54,54,54,54	0
58	MG	1A	3651	1/1	0.98	0.08	28,28,28,28	0
61	ZN	1n	103	1/1	0.98	0.04	87,87,87,87	0
61	ZN	2Y	202	1/1	0.98	0.05	97,97,97,97	0
58	MG	1A	3037	1/1	0.98	0.19	46,46,46,46	0
61	ZN	29	501	1/1	0.98	0.04	83,83,83,83	0
58	MG	1A	3745	1/1	0.98	0.05	52,52,52,52	0
62	SF4	1d	302	8/8	0.98	0.05	72,80,88,90	0
62	SF4	2d	303	8/8	0.98	0.05	74,78,87,89	0
58	MG	1A	3618	1/1	0.99	0.03	29,29,29,29	0
58	MG	1A	3723	1/1	0.99	0.04	68,68,68,68	0
58	MG	1U	201	1/1	0.99	0.15	35,35,35,35	0
58	MG	2A	3640	1/1	0.99	0.04	53,53,53,53	0
58	MG	1A	3743	1/1	0.99	0.09	54,54,54,54	0
58	MG	1B	226	1/1	0.99	0.04	53,53,53,53	0
58	MG	1A	3892	1/1	0.99	0.08	45,45,45,45	0
58	MG	2A	3774	1/1	0.99	0.03	38,38,38,38	0
58	MG	1A	3013	1/1	0.99	0.18	35,35,35,35	0
58	MG	1A	3665	1/1	0.99	0.07	25,25,25,25	0
58	MG	1A	3872	1/1	0.99	0.05	53,53,53,53	0
58	MG	1A	3609	1/1	0.99	0.07	30,30,30,30	0
58	MG	1A	3788	1/1	0.99	0.05	49,49,49,49	0
58	MG	2A	3649	1/1	0.99	0.08	44,44,44,44	0
58	MG	2A	3781	1/1	0.99	0.05	66,66,66,66	0
58	MG	1E	315	1/1	0.99	0.06	46,46,46,46	0
58	MG	1A	3898	1/1	0.99	0.06	36,36,36,36	0
58	MG	1A	3899	1/1	0.99	0.02	31,31,31,31	0
58	MG	1A	4031	1/1	0.99	0.02	33,33,33,33	0
58	MG	1V	204	1/1	0.99	0.22	39,39,39,39	0
58	MG	1A	4032	1/1	0.99	0.05	55,55,55,55	0
58	MG	1A	3667	1/1	0.99	0.08	35,35,35,35	0
58	MG	1W	201	1/1	0.99	0.11	48,48,48,48	0
58	MG	1A	3600	1/1	0.99	0.11	41,41,41,41	0
58	MG	1A	3383	1/1	0.99	0.22	35,35,35,35	0
58	MG	1A	3036	1/1	0.99	0.05	25,25,25,25	0
58	MG	1A	4007	1/1	0.99	0.02	41,41,41,41	0
58	MG	1A	3714	1/1	0.99	0.05	26,26,26,26	0
58	MG	2A	3504	1/1	0.99	0.11	59,59,59,59	0
58	MG	2A	3706	1/1	0.99	0.04	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
58	MG	1A	3008	1/1	0.99	0.08	31,31,31,31	0
58	MG	2A	3506	1/1	0.99	0.06	52,52,52,52	0
58	MG	1A	3658	1/1	0.99	0.04	30,30,30,30	0
58	MG	1A	3734	1/1	0.99	0.04	46,46,46,46	0
58	MG	1A	3097	1/1	0.99	0.11	25,25,25,25	0
58	MG	2A	3434	1/1	0.99	0.06	75,75,75,75	0
58	MG	1A	3736	1/1	0.99	0.04	29,29,29,29	0
58	MG	2A	3436	1/1	0.99	0.11	54,54,54,54	0
61	ZN	1Y	204	1/1	0.99	0.03	69,69,69,69	0
58	MG	1A	3176	1/1	0.99	0.16	38,38,38,38	0
61	ZN	15	109	1/1	0.99	0.02	56,56,56,56	0
61	ZN	16	104	1/1	0.99	0.03	50,50,50,50	0
61	ZN	19	102	1/1	0.99	0.20	104,104,104,104	0
58	MG	1X	106	1/1	0.99	0.07	34,34,34,34	0
58	MG	2A	3632	1/1	0.99	0.06	42,42,42,42	0
58	MG	1A	3072	1/1	0.99	0.06	18,18,18,18	0
61	ZN	25	105	1/1	0.99	0.03	84,84,84,84	0
61	ZN	26	102	1/1	0.99	0.04	74,74,74,74	0
58	MG	2A	3762	1/1	0.99	0.05	52,52,52,52	0
58	MG	1A	3937	1/1	0.99	0.04	55,55,55,55	0
58	MG	1A	3704	1/1	0.99	0.07	24,24,24,24	0
58	MG	1A	3056	1/1	0.99	0.04	41,41,41,41	0
58	MG	1A	4027	1/1	1.00	0.01	52,52,52,52	0
58	MG	1A	3869	1/1	1.00	0.08	38,38,38,38	0
58	MG	1A	3778	1/1	1.00	0.05	24,24,24,24	0
58	MG	2A	3766	1/1	1.00	0.07	57,57,57,57	0
58	MG	1A	4069	1/1	1.00	0.08	38,38,38,38	0
58	MG	1A	4082	1/1	1.00	0.04	48,48,48,48	0

6.5 Other polymers

There are no such residues in this entry.