Full wwPDB X-ray Structure Validation Report (i)

Mar 18, 2026 – 12:22 AM UTC

PDB ID	:	7U2I / pdb_00007u2i
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with mRNA, aminoacylated A-site Gly-NH-tRNAgly, aminoacylated P-site fMet-NH-tRNAmet, deacylated E-site tRNAgly, and chloramphenicol at 2.55A resolution
Authors	:	Syroegin, E.A.; Aleksandrova, E.V.; Polikanov, Y.S.
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 (i) 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:

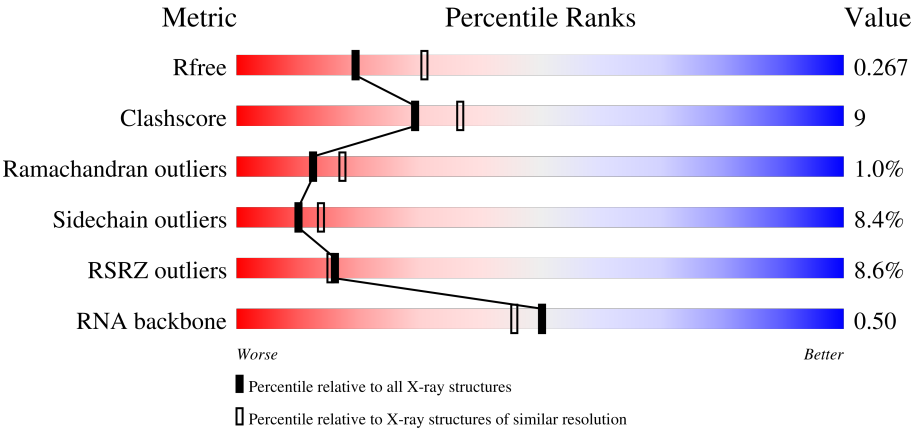
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 <=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% 67% 25% 6%
1	2A	2915	4% 60% 29% 7%
2	1B	121	79% 19%
2	2B	121	55% 32% 12%

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Mol	Chain	Length	Quality of chain
3	1D	276	83% 15%
3	2D	276	3% 78% 20%
4	1E	206	84% 13%
4	2E	206	2% 77% 18%
5	1F	210	72% 20%
5	2F	210	68% 25%
6	1G	182	7% 69% 26%
6	2G	182	18% 53% 41% 5%
7	1H	180	2% 69% 25%
7	2H	180	22% 68% 25%
8	1I	148	4% 64% 27% 7%
8	2I	148	19% 61% 34%
9	1N	140	83% 14%
9	2N	140	7% 75% 21%
10	1O	122	81% 18%
10	2O	122	75% 24%
11	1P	150	74% 21% 5%
11	2P	150	5% 73% 22%
12	1Q	141	80% 18%
12	2Q	141	8% 73% 26%
13	1R	118	83% 14%
13	2R	118	2% 71% 26%
14	1S	112	79% 18%
14	2S	112	28% 50% 43% 5%
15	1T	146	3% 70% 17% 10%

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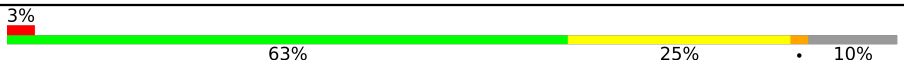
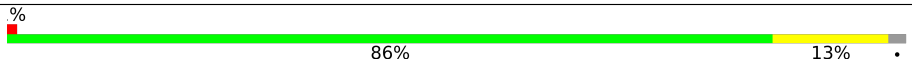
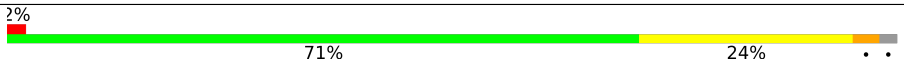
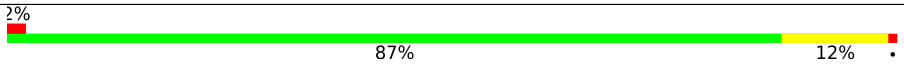
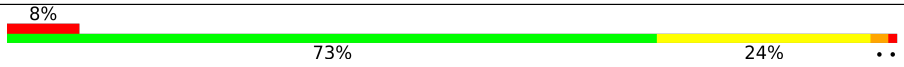
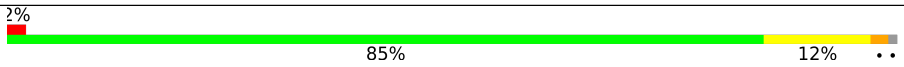
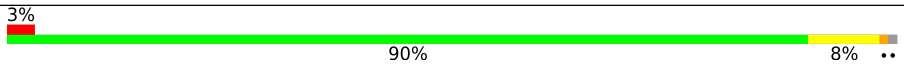
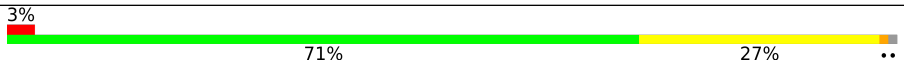
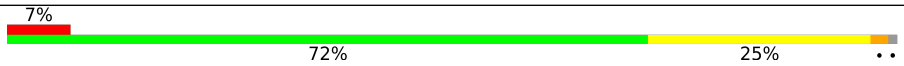
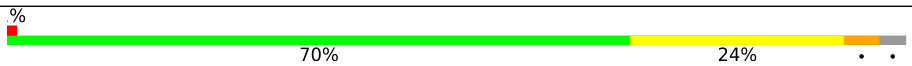
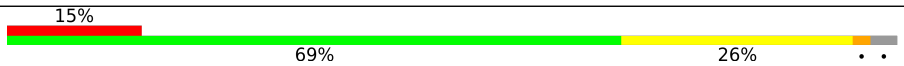
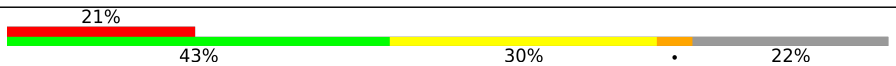
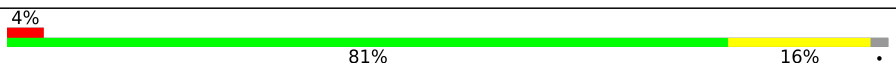
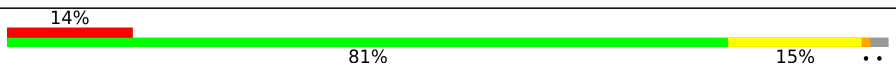
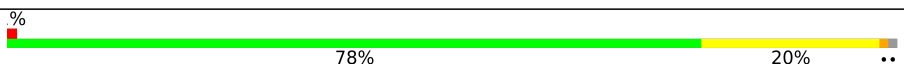
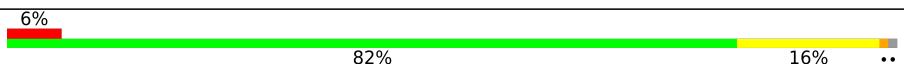
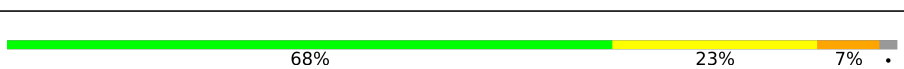
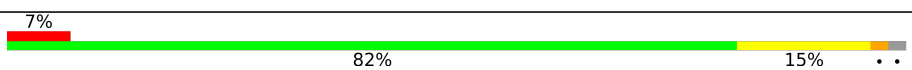
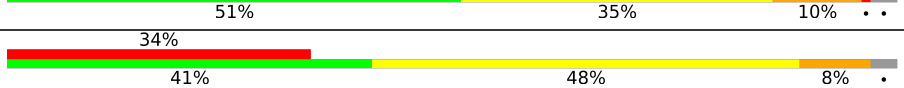
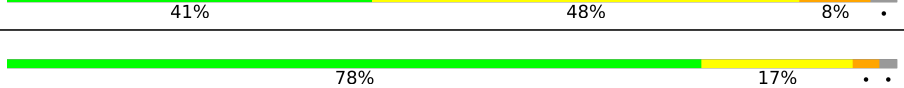
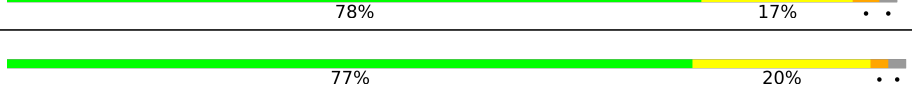
Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	
27	25	60	

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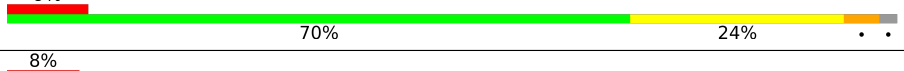
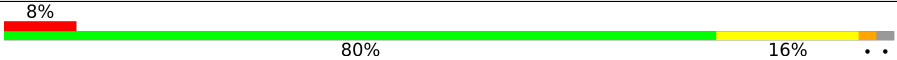
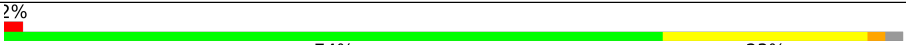
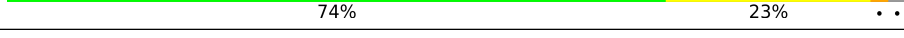
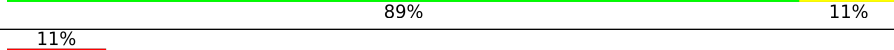
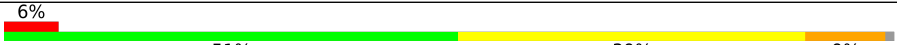
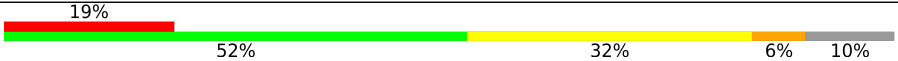
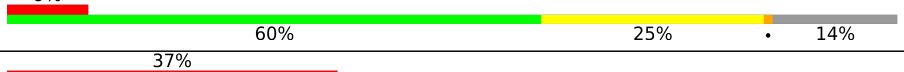
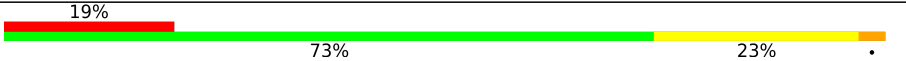
Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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Mol	Chain	Length	Quality of chain
40	2i	128	60% 55% 37% 7%
41	1j	105	31% 56% 30% 6% 8%
41	2j	105	50% 47% 37% 8% 9%
42	1k	129	5% 67% 17% 12%
42	2k	129	12% 62% 23% 12%
43	1l	132	5% 79% 14% 8%
43	2l	132	21% 64% 26% 8%
44	1m	126	10% 60% 31% 6%
44	2m	126	26% 52% 41%
45	1n	61	11% 74% 23%
45	2n	61	61% 54% 39% 5%
46	1o	89	7% 67% 27%
46	2o	89	9% 65% 30%
47	1p	88	18% 57% 35% 7%
47	2p	88	8% 59% 31% 7%
48	1q	105	15% 74% 18% 6%
48	2q	105	7% 70% 23% 6%
49	1r	88	% 57% 18% 23%
49	2r	88	7% 48% 28% 23%
50	1s	93	12% 61% 24% 11%
50	2s	93	58% 42% 40% 8% 11%
51	1t	106	16% 62% 24% 5% 9%
51	2t	106	6% 67% 20% 9%
52	1u	27	15% 52% 33% 15%
52	2u	27	41% 44% 41% 15%

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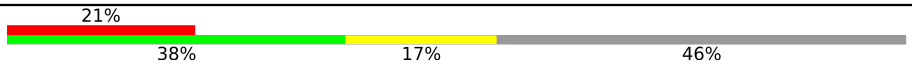
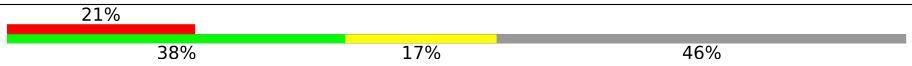
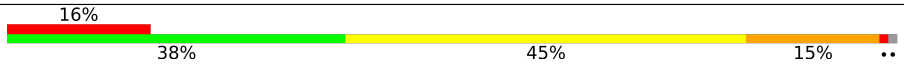
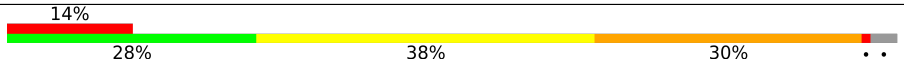
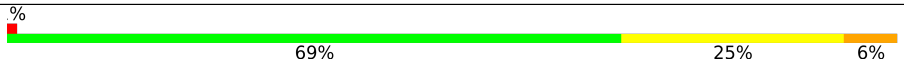
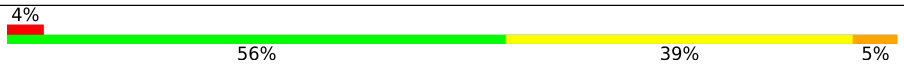
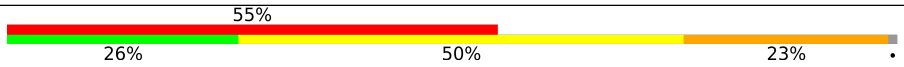
Mol	Chain	Length	Quality of chain
53	1v	24	
53	2v	24	
54	1w	74	
54	2w	74	
55	1x	77	
55	2x	77	
56	1y	74	
56	2y	74	

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
54	4SU	2w	8	-	-	X	-
57	MG	1U	210	-	-	-	X
57	MG	1a	1636	-	-	-	X
57	MG	1a	1722	-	-	-	X
57	MG	2A	3218	-	-	-	X
57	MG	2A	3325	-	-	-	X
57	MG	2A	3424	-	-	-	X
57	MG	2v	103	-	-	-	X

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 300046 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 Aminoacyl-tRNA fMet-NH-tRNAmet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1656	740	299	538	77	2			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1656	740	299	538	77	2			

- Molecule 56 is a RNA chain called E-site Deacylated tRNAgly.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
56	1y	73	Total	C	N	O	P	S	0	0	0
			1552	693	273	512	73	1			
56	2y	73	Total	C	N	O	P	S	0	0	0
			1552	693	273	512	73	1			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1095	Total	Mg	0	0
			1095	1095		
57	1B	36	Total	Mg	0	0
			36	36		
57	1D	13	Total	Mg	0	0
			13	13		
57	1E	12	Total	Mg	0	0
			12	12		
57	1F	15	Total	Mg	0	0
			15	15		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1G	4	Total Mg 4 4	0	0
57	1I	1	Total Mg 1 1	0	0
57	1N	5	Total Mg 5 5	0	0
57	1O	5	Total Mg 5 5	0	0
57	1P	5	Total Mg 5 5	0	0
57	1Q	7	Total Mg 7 7	0	0
57	1R	7	Total Mg 7 7	0	0
57	1S	3	Total Mg 3 3	0	0
57	1T	3	Total Mg 3 3	0	0
57	1U	10	Total Mg 10 10	0	0
57	1V	7	Total Mg 7 7	0	0
57	1W	7	Total Mg 7 7	0	0
57	1X	7	Total Mg 7 7	0	0
57	1Y	3	Total Mg 3 3	0	0
57	1Z	3	Total Mg 3 3	0	0
57	10	9	Total Mg 9 9	0	0
57	11	3	Total Mg 3 3	0	0
57	12	2	Total Mg 2 2	0	0
57	13	5	Total Mg 5 5	0	0
57	15	6	Total Mg 6 6	0	0
57	16	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	17	5	Total Mg 5 5	0	0
57	18	6	Total Mg 6 6	0	0
57	19	1	Total Mg 1 1	0	0
57	1a	226	Total Mg 226 226	0	0
57	1b	2	Total Mg 2 2	0	0
57	1e	2	Total Mg 2 2	0	0
57	1f	2	Total Mg 2 2	0	0
57	1h	1	Total Mg 1 1	0	0
57	1l	2	Total Mg 2 2	0	0
57	1m	1	Total Mg 1 1	0	0
57	1n	2	Total Mg 2 2	0	0
57	1s	1	Total Mg 1 1	0	0
57	1t	1	Total Mg 1 1	0	0
57	1v	1	Total Mg 1 1	0	0
57	1w	7	Total Mg 7 7	0	0
57	1x	12	Total Mg 12 12	0	0
57	2A	861	Total Mg 861 861	0	0
57	2B	20	Total Mg 20 20	0	0
57	2D	5	Total Mg 5 5	0	0
57	2E	8	Total Mg 8 8	0	0
57	2F	7	Total Mg 7 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2G	1	Total Mg 1 1	0	0
57	2N	1	Total Mg 1 1	0	0
57	2O	1	Total Mg 1 1	0	0
57	2P	2	Total Mg 2 2	0	0
57	2Q	3	Total Mg 3 3	0	0
57	2R	2	Total Mg 2 2	0	0
57	2T	4	Total Mg 4 4	0	0
57	2U	2	Total Mg 2 2	0	0
57	2V	3	Total Mg 3 3	0	0
57	2W	2	Total Mg 2 2	0	0
57	2X	1	Total Mg 1 1	0	0
57	2Y	1	Total Mg 1 1	0	0
57	2Z	1	Total Mg 1 1	0	0
57	20	2	Total Mg 2 2	0	0
57	21	1	Total Mg 1 1	0	0
57	23	4	Total Mg 4 4	0	0
57	25	5	Total Mg 5 5	0	0
57	26	1	Total Mg 1 1	0	0
57	27	3	Total Mg 3 3	0	0
57	28	2	Total Mg 2 2	0	0
57	2a	225	Total Mg 225 225	0	0

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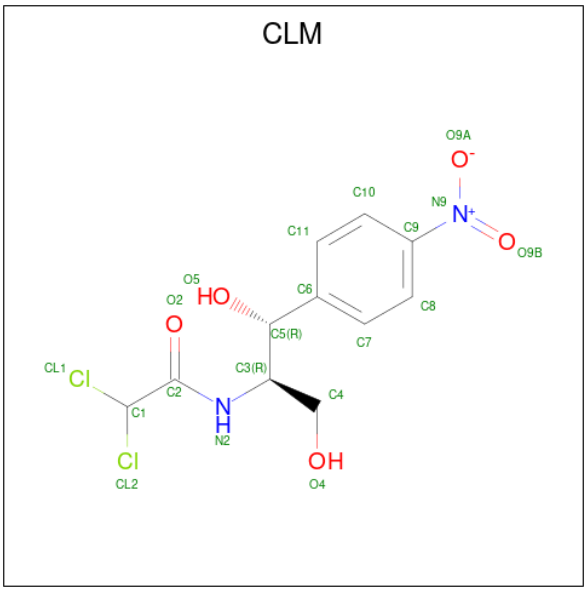
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2d	2	Total Mg 2 2	0	0
57	2e	1	Total Mg 1 1	0	0
57	2f	2	Total Mg 2 2	0	0
57	2i	1	Total Mg 1 1	0	0
57	2j	1	Total Mg 1 1	0	0
57	2k	1	Total Mg 1 1	0	0
57	2l	3	Total Mg 3 3	0	0
57	2q	2	Total Mg 2 2	0	0
57	2r	1	Total Mg 1 1	0	0
57	2t	1	Total Mg 1 1	0	0
57	2v	4	Total Mg 4 4	0	0
57	2w	4	Total Mg 4 4	0	0
57	2x	4	Total Mg 4 4	0	0
57	2y	1	Total Mg 1 1	0	0

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 59 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
59	1A	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		
59	2A	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1Y	1	Total	Zn	0	0
			1	1		
60	14	1	Total	Zn	0	0
			1	1		
60	15	1	Total	Zn	0	0
			1	1		
60	16	1	Total	Zn	0	0
			1	1		
60	19	1	Total	Zn	0	0
			1	1		
60	1n	1	Total	Zn	0	0
			1	1		
60	2Y	1	Total	Zn	0	0
			1	1		
60	24	1	Total	Zn	0	0
			1	1		
60	25	1	Total	Zn	0	0
			1	1		
60	26	1	Total	Zn	0	0
			1	1		

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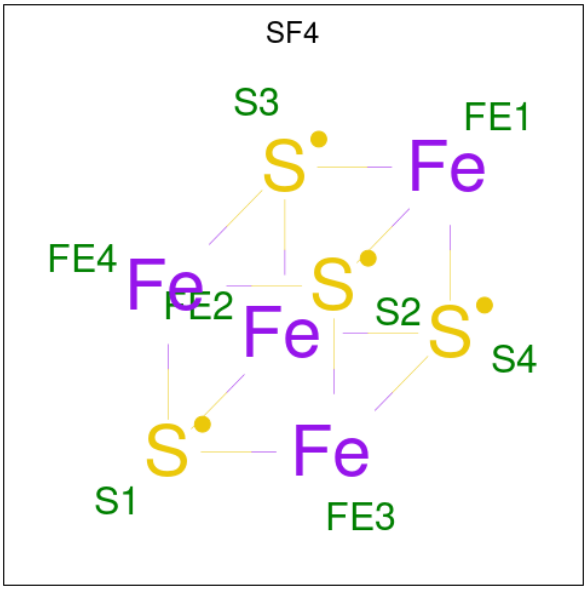
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

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



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

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1A	2086	Total O 2086 2086	0	0
62	1B	65	Total O 65 65	0	0
62	1D	28	Total O 28 28	0	0
62	1E	28	Total O 28 28	0	0
62	1F	17	Total O 17 17	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1G	7	Total O 7 7	0	0
62	1H	2	Total O 2 2	0	0
62	1N	5	Total O 5 5	0	0
62	1O	6	Total O 6 6	0	0
62	1P	21	Total O 21 21	0	0
62	1Q	7	Total O 7 7	0	0
62	1R	7	Total O 7 7	0	0
62	1S	3	Total O 3 3	0	0
62	1T	9	Total O 9 9	0	0
62	1U	13	Total O 13 13	0	0
62	1V	9	Total O 9 9	0	0
62	1W	5	Total O 5 5	0	0
62	1X	6	Total O 6 6	0	0
62	1Y	3	Total O 3 3	0	0
62	1Z	1	Total O 1 1	0	0
62	10	12	Total O 12 12	0	0
62	11	10	Total O 10 10	0	0
62	12	3	Total O 3 3	0	0
62	13	6	Total O 6 6	0	0
62	14	1	Total O 1 1	0	0
62	15	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	16	5	Total O 5 5	0	0
62	17	9	Total O 9 9	0	0
62	18	10	Total O 10 10	0	0
62	1a	331	Total O 331 331	0	0
62	1b	1	Total O 1 1	0	0
62	1d	1	Total O 1 1	0	0
62	1e	1	Total O 1 1	0	0
62	1l	3	Total O 3 3	0	0
62	1m	2	Total O 2 2	0	0
62	1q	3	Total O 3 3	0	0
62	1u	1	Total O 1 1	0	0
62	1v	6	Total O 6 6	0	0
62	1w	9	Total O 9 9	0	0
62	1x	11	Total O 11 11	0	0
62	1y	1	Total O 1 1	0	0
62	2A	1147	Total O 1147 1147	0	0
62	2B	21	Total O 21 21	0	0
62	2D	18	Total O 18 18	0	0
62	2E	14	Total O 14 14	0	0
62	2F	12	Total O 12 12	0	0
62	2I	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2N	2	Total O 2 2	0	0
62	2O	2	Total O 2 2	0	0
62	2P	10	Total O 10 10	0	0
62	2Q	1	Total O 1 1	0	0
62	2R	5	Total O 5 5	0	0
62	2T	3	Total O 3 3	0	0
62	2U	3	Total O 3 3	0	0
62	2W	4	Total O 4 4	0	0
62	2X	5	Total O 5 5	0	0
62	2Z	2	Total O 2 2	0	0
62	20	1	Total O 1 1	0	0
62	21	8	Total O 8 8	0	0
62	23	2	Total O 2 2	0	0
62	25	3	Total O 3 3	0	0
62	27	5	Total O 5 5	0	0
62	28	3	Total O 3 3	0	0
62	29	1	Total O 1 1	0	0
62	2a	205	Total O 205 205	0	0
62	2c	1	Total O 1 1	0	0
62	2i	1	Total O 1 1	0	0
62	2j	3	Total O 3 3	0	0

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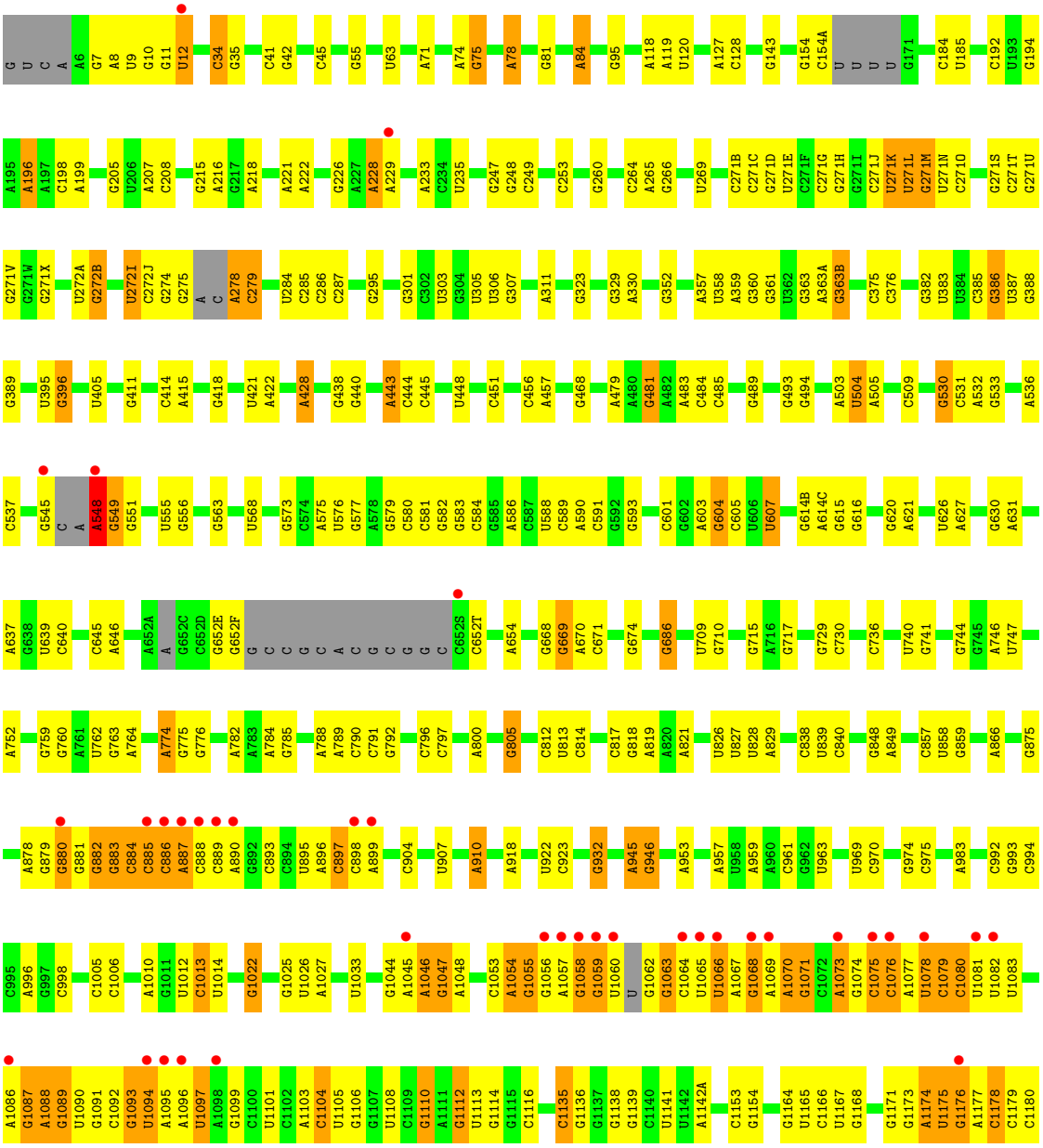
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	2l	4	Total O 4 4	0	0
62	2r	1	Total O 1 1	0	0
62	2t	2	Total O 2 2	0	0
62	2v	2	Total O 2 2	0	0
62	2w	1	Total O 1 1	0	0
62	2x	7	Total O 7 7	0	0

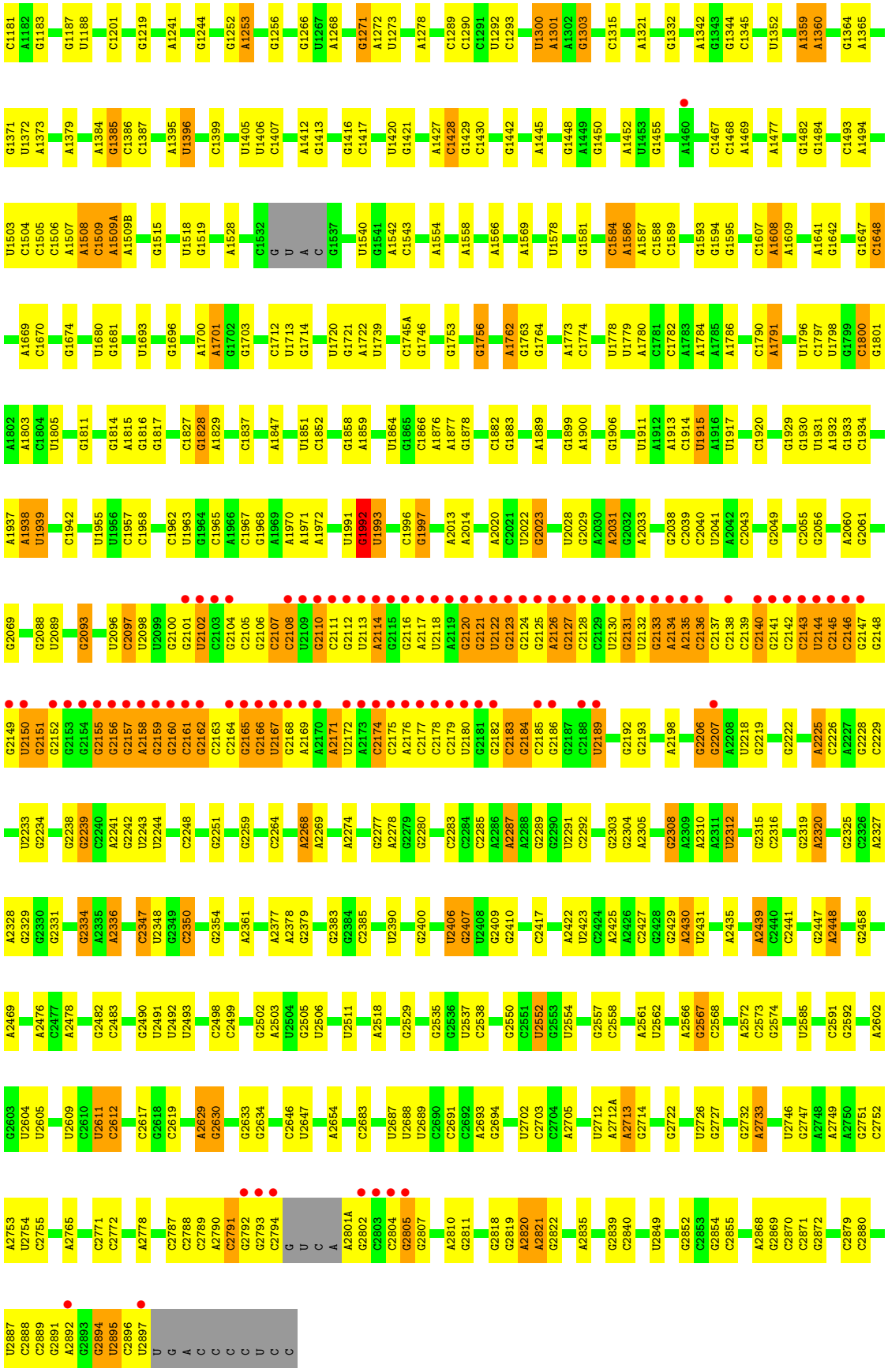
3 Residue-property plots (i)

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

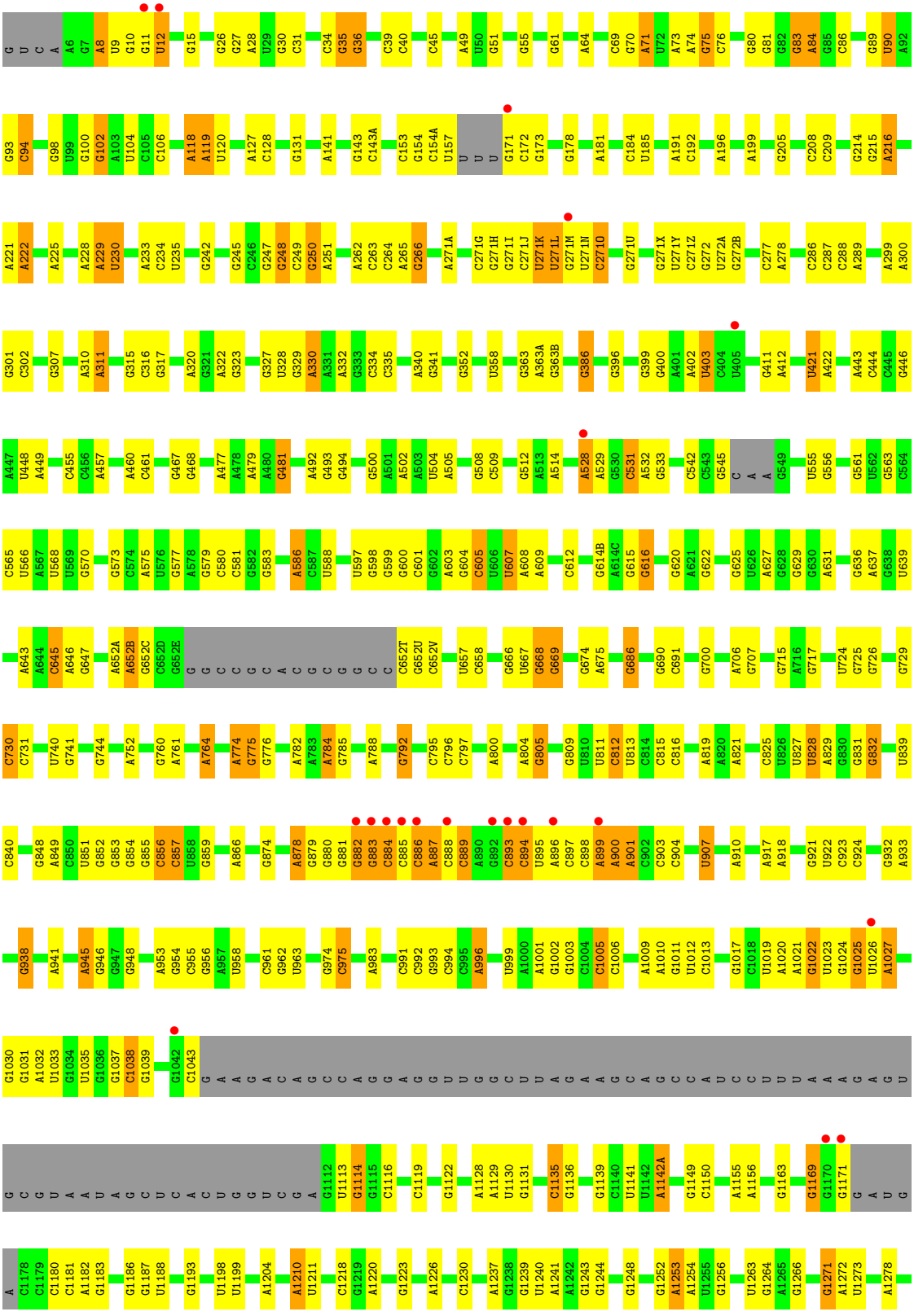
Chain 1A:

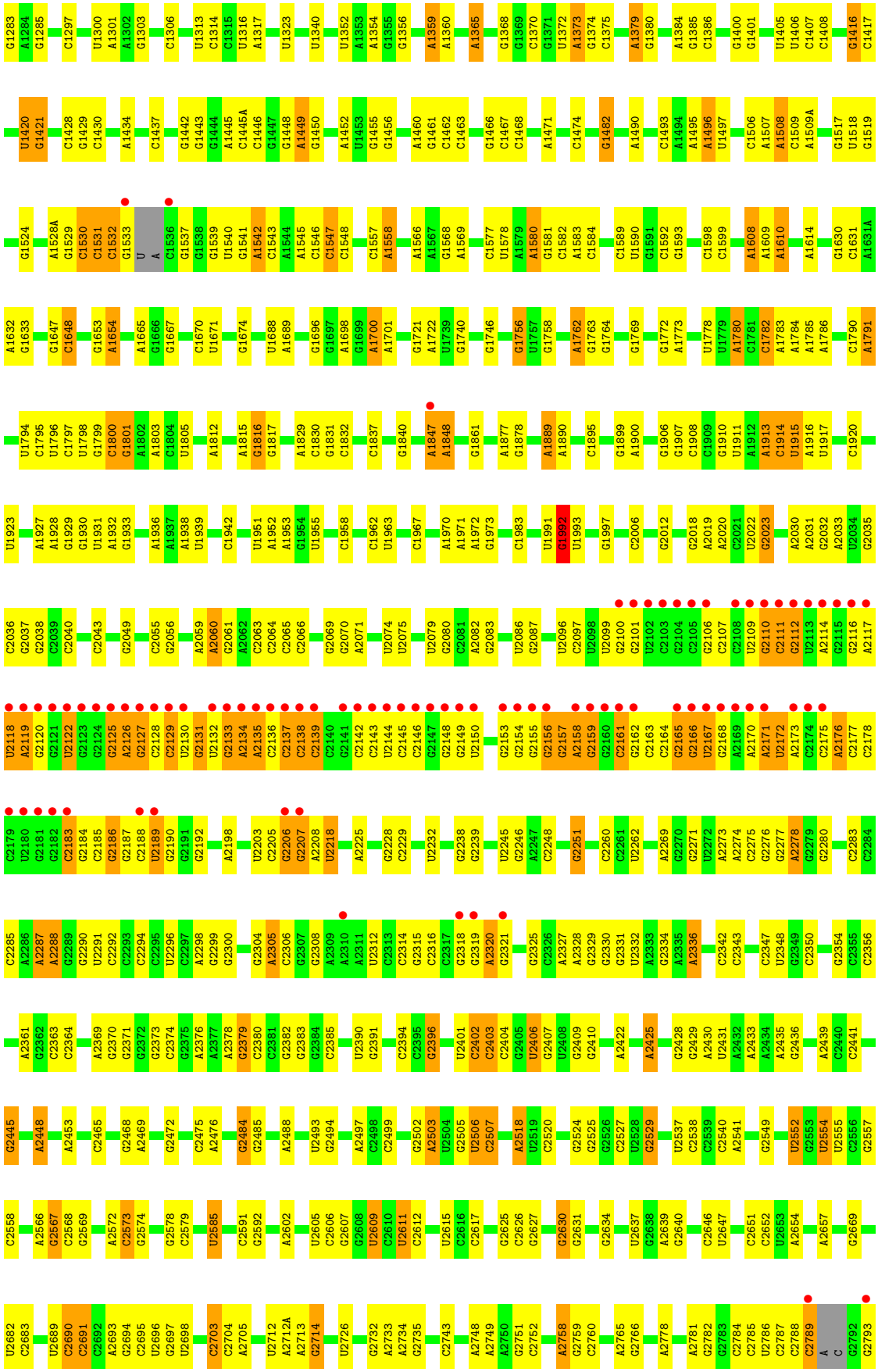




• Molecule 1: 23S Ribosomal RNA

Chain 2A:

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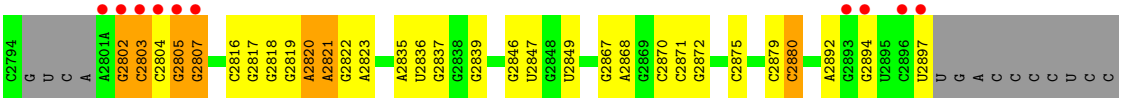
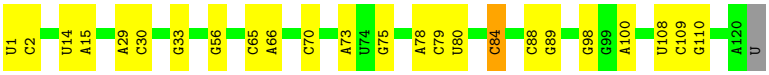
U1420 G1421 C1428 C1429 C1430 A1434 C1437 G1442 G1443 G1444 A1445 C1445A C1446 G1447 G1448 A1449 G1450 A1452 U1453 G1455 G1456 A1460 G1461 C1462 C1463 G1466 C1467 C1468 A1471 C1474 G1482 A1490 C1493 A1494 A1495 A1496 U1497 C1506 A1507 A1508 C1509 A1509A G1517 U1518 G1519
G1524 A1528A G1529 C1530 C1531 C1532 G1533 U A C1536 G1537 G1538 G1539 U1540 G1541 A1542 C1543 A1544 A1545 C1546 C1547 C1548 C1557 A1558 A1566 A1567 G1568 A1569 C1577 U1578 A1579 A1580 G1581 C1582 A1583 C1584 C1589 U1590 G1591 C1592 G1593 C1598 C1599 A1608 A1609 A1610 A1614 G1630 C1631 A1631A
A1632 G1633 G1647 C1648 G1653 A1654 A1665 G1666 G1667 C1670 U1671 G1674 U1688 A1689 G1696 G1697 A1698 G1699 A1700 A1701 G1721 A1722 U1739 G1740 G1746 G1756 U1757 G1758 A1762 G1763 G1764 G1769 G1772 A1773 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 C1790 A1791
U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 C1804 U1805 A1812 A1815 G1816 G1817 A1829 C1830 G1831 C1832 C1837 G1840 A1847 A1848 G1861 A1877 G1878 A1889 A1890 C1895 G1899 A1900 G1906 G1907 C1908 C1909 G1910 U1911 A1912 A1913 C1914 U1915 A1916 U1917 C1920
U1923 A1927 A1928 G1929 G1930 U1931 A1932 G1933 A1936 A1937 A1938 U1939 C1942 U1951 A1952 A1953 C1954 U1955 C1958 C1962 U1963 C1967 A1970 A1971 A1972 G1973 C1983 U1991 G1992 U1993 G1997 C2006 G2012 G2018 A2019 A2020 C2021 U2022 G2023 A2030 A2031 G2032 A2033 U2034 G2035
C2036 G2037 G2038 C2039 C2040 C2043 G2049 C2055 G2056 A2059 A2060 G2061 A2062 C2063 C2064 C2065 C2066 G2069 G2070 A2071 U2074 U2075 U2079 G2080 C2081 A2082 G2083 U2086 G2087 U2096 C2097 U2098 U2099 G2100 G2101 U2102 C2103 G2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117
U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 C2141 C2142 C2143 U2144 C2145 C2146 C2147 G2148 G2149 U2150 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178
C2179 U2180 G2181 G2182 C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 G2191 G2192 A2198 U2203 C2205 G2206 G2207 A2208 U2218 A2225 G2228 C2229 U2232 G2238 G2239 U2245 G2246 A2247 C2248 G2251 C2260 C2261 U2262 A2269 G2270 G2271 U2272 A2273 A2274 C2275 G2276 G2277 A2278 G2279 G2280 C2283 C2284
C2285 A2286 A2287 A2288 G2289 G2290 U2291 C2292 C2293 C2294 C2295 U2296 C2297 A2298 G2299 G2300 G2304 A2305 C2306 C2307 G2308 A2309 A2310 A2311 U2312 C2313 C2314 G2315 C2316 C2317 G2318 G2319 A2320 G2321 G2325 C2326 A2327 A2328 G2329 G2330 G2331 U2332 A2333 G2334 A2335 A2336 C2342 C2343 C2347 U2348 G2349 C2350 G2354 C2355 C2356
A2361 G2362 C2363 C2364 A2369 G2370 G2371 G2372 G2373 C2374 G2375 A2376 A2377 A2378 G2379 C2380 C2381 G2382 G2383 G2384 C2385 U2390 G2391 C2394 C2395 G2396 U2401 C2402 C2403 C2404 G2405 U2406 G2407 U2408 G2409 G2410 A2422 A2425 G2428 G2429 A2430 U2431 A2432 A2433 A2434 A2435 G2436 A2439 C2440 C2441
G2445 A2448 A2453 C2465 G2468 A2469 G2472 C2475 A2476 G2484 G2485 A2488 U2493 G2494 A2497 C2498 C2499 G2502 A2503 U2504 G2505 U2506 C2507 A2518 U2519 C2520 G2524 G2525 G2526 C2527 U2528 G2529 U2537 C2538 C2539 C2540 A2541 G2549 U2552 G2553 U2554 U2555 C2556 G2557
C2558 A2566 G2567 C2568 G2569 A2572 C2573 G2574 G2578 C2579 U2585 C2591 G2592 A2602 U2605 C2606 G2607 G2608 U2609 C2610 U2611 C2612 U2615 C2616 C2617 G2625 C2626 G2627 G2630 G2631 G2634 U2637 G2638 A2639 G2640 C2646 U2647 C2651 C2652 U2653 A2654 A2657 G2669
U2682 C2683 U2689 C2690 C2691 C2692 A2693 G2694 C2695 U2696 G2697 U2698 C2703 C2704 A2705 U2712 A2712A A2713 G2714 U2726 G2732 A2733 A2734 G2735 C2743 A2748 A2749 A2750 G2751 C2752 A2758 G2759 C2760 A2765 G2766 A2778 A2781 G2782 G2783 C2784 C2785 U2786 C2787 C2788 C2789 A C G2792 G2793



• Molecule 2: 5S Ribosomal RNA

Chain 1B:

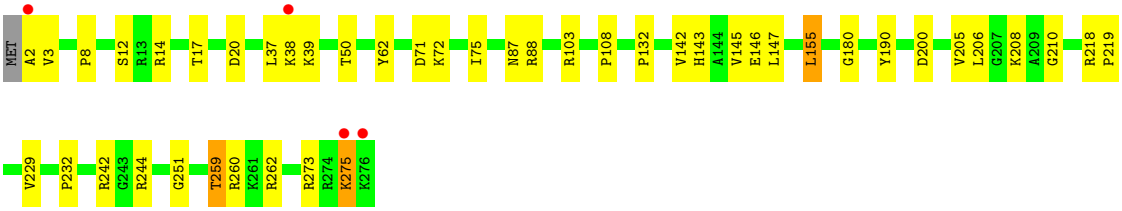


• Molecule 2: 5S Ribosomal RNA

Chain 2B:

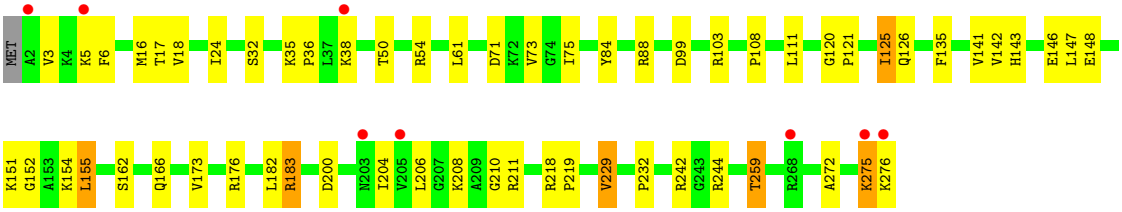
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



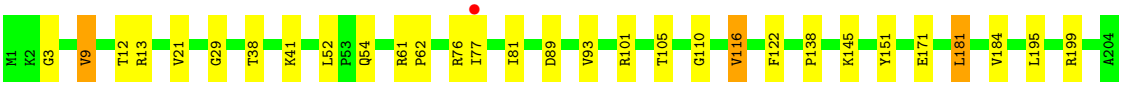
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



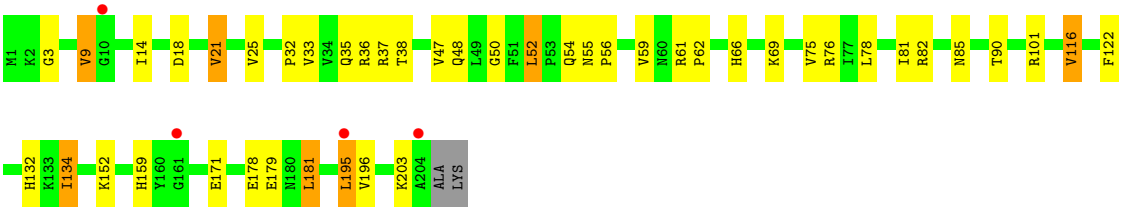
• Molecule 4: 50S ribosomal protein L3

Chain 1E:



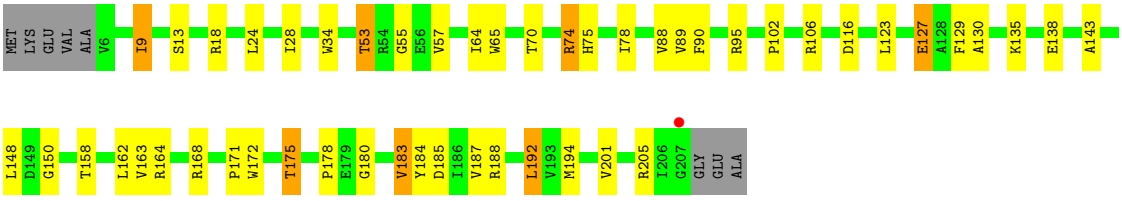
• Molecule 4: 50S ribosomal protein L3

Chain 2E:



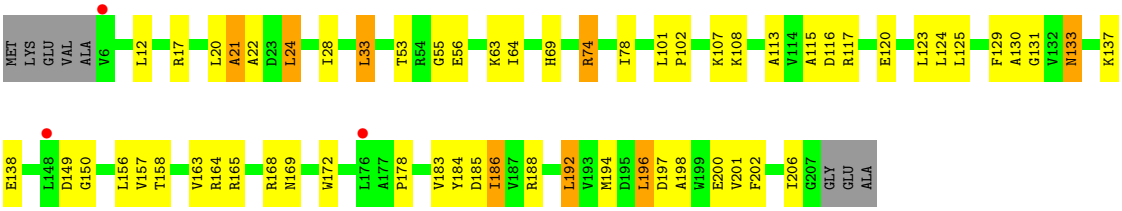
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



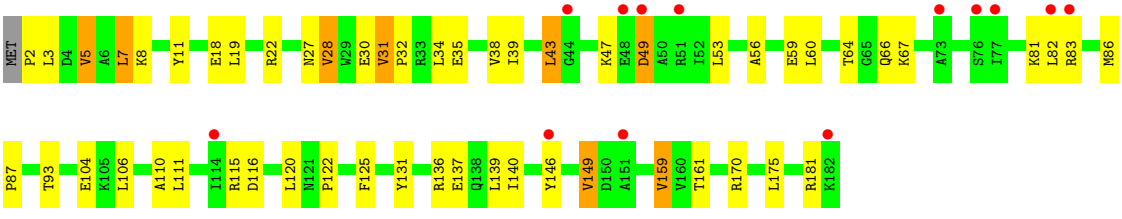
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



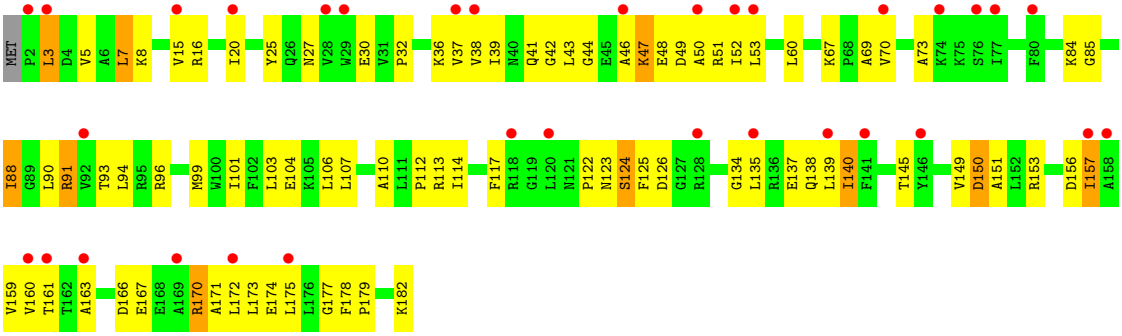
• Molecule 6: 50S ribosomal protein L5

Chain 1G:

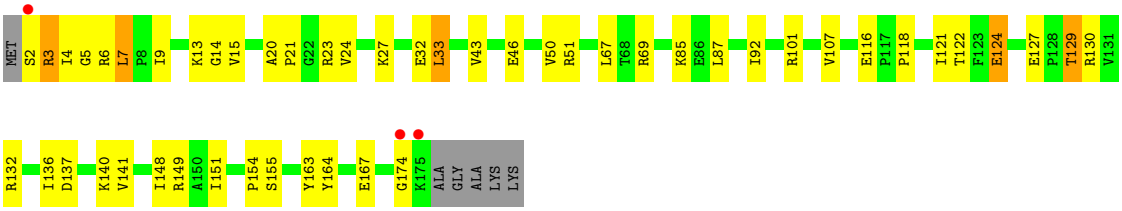


• Molecule 6: 50S ribosomal protein L5

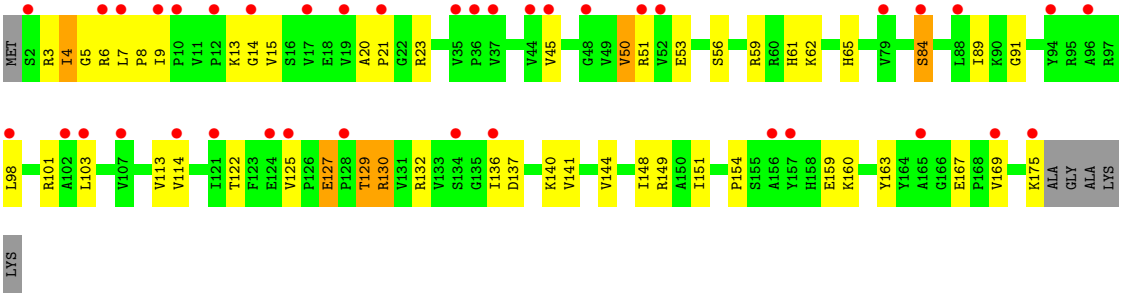
Chain 2G:



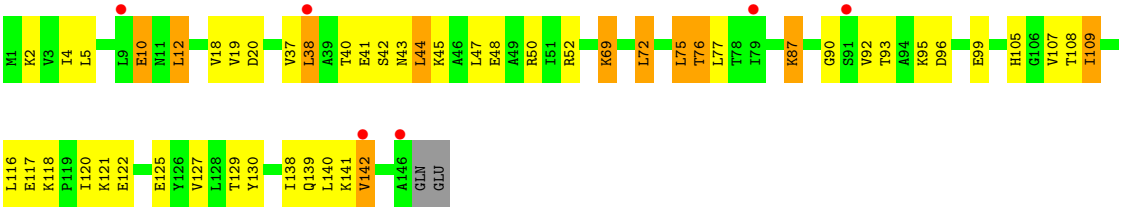
• Molecule 7: 50S ribosomal protein L6



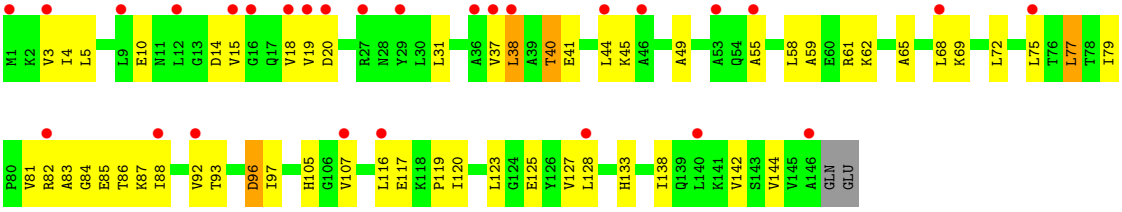
• Molecule 7: 50S ribosomal protein L6



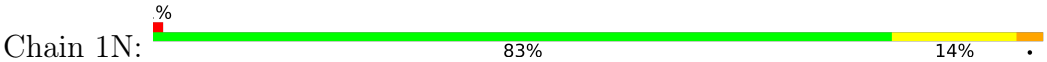
• Molecule 8: 50S ribosomal protein L9



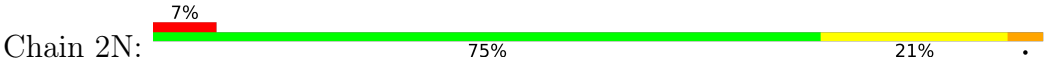
• Molecule 8: 50S ribosomal protein L9

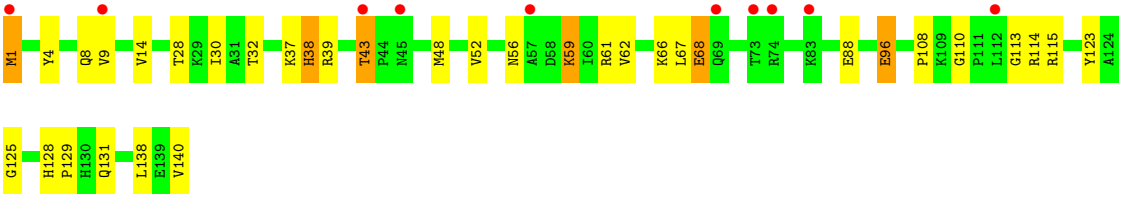


• Molecule 9: 50S ribosomal protein L13

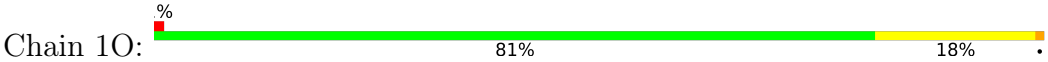


• Molecule 9: 50S ribosomal protein L13

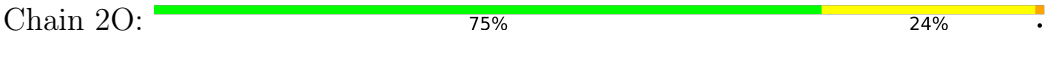




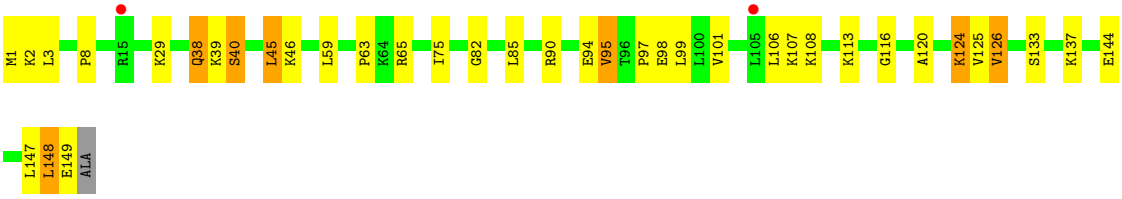
• Molecule 10: 50S ribosomal protein L14



• Molecule 10: 50S ribosomal protein L14

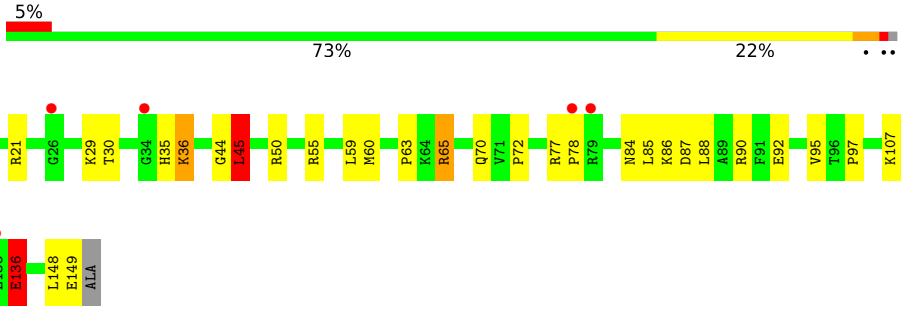


• Molecule 11: 50S ribosomal protein L15



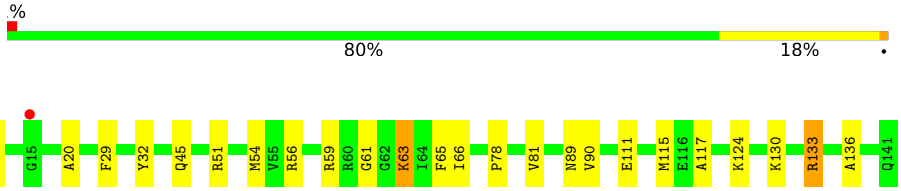
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



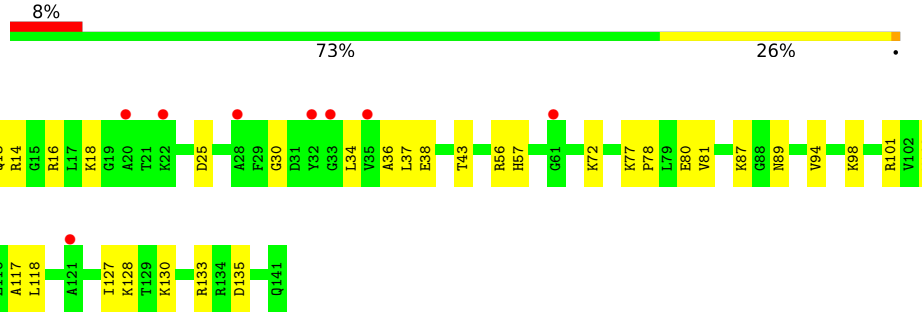
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



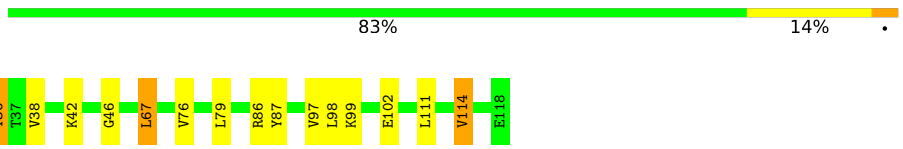
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



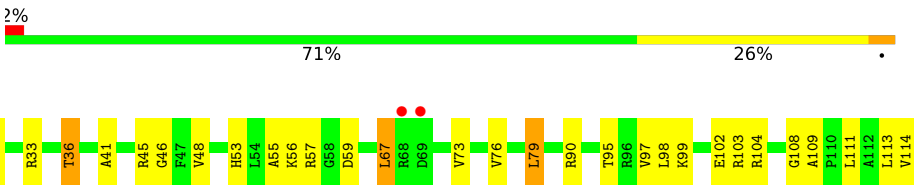
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



• Molecule 13: 50S ribosomal protein L17

Chain 2R:

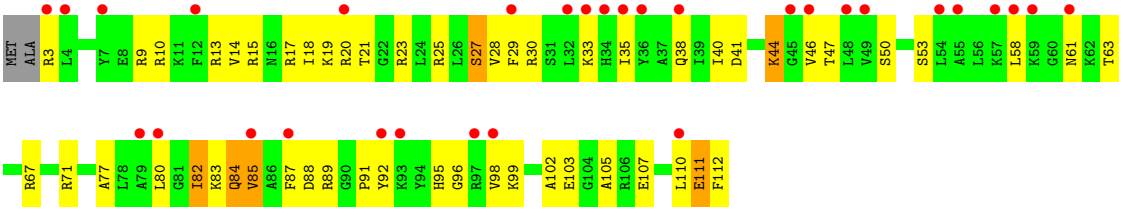


• Molecule 14: 50S ribosomal protein L18

Chain 1S:

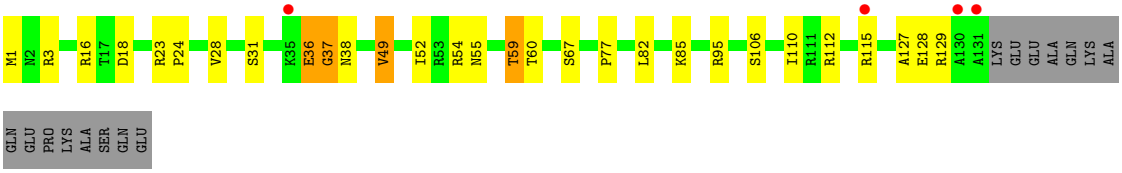
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



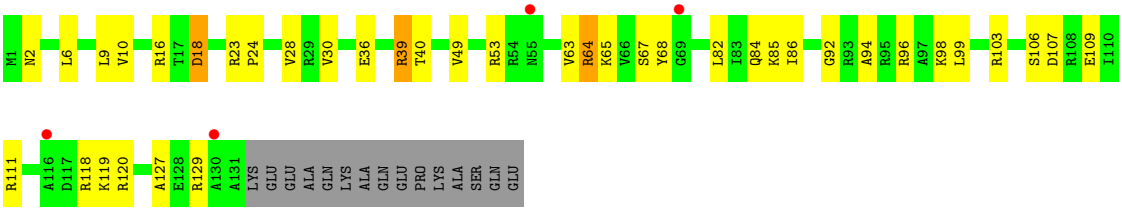
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



• Molecule 15: 50S ribosomal protein L19

Chain 2T:

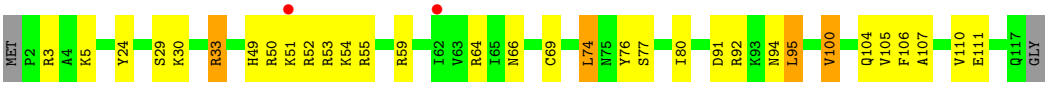


• Molecule 16: 50S ribosomal protein L20

Chain 1U:

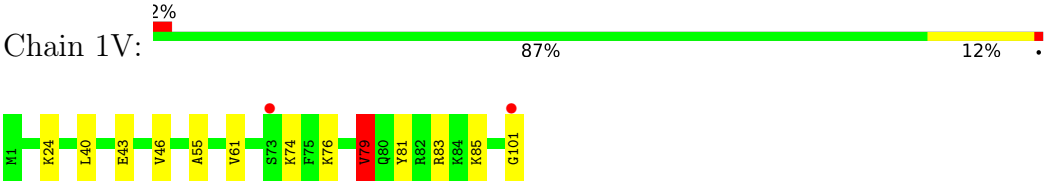
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



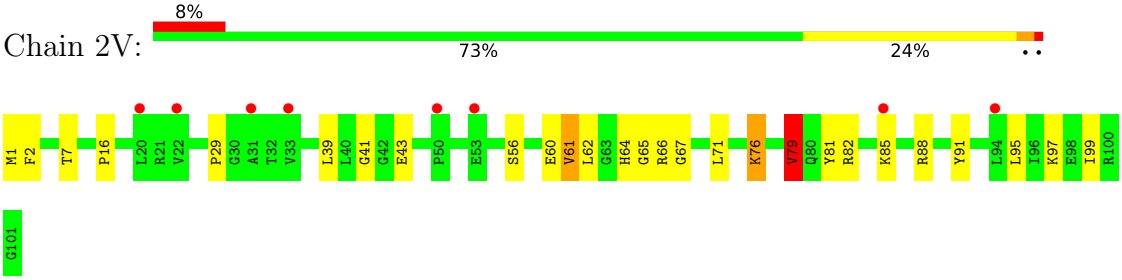
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



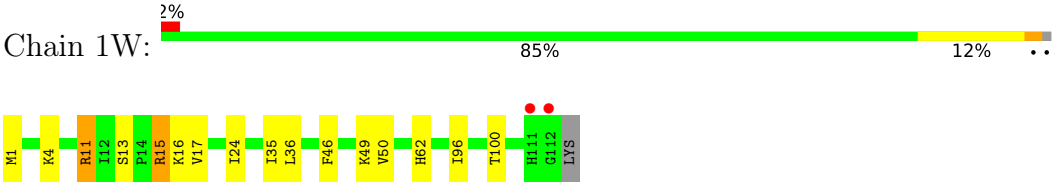
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



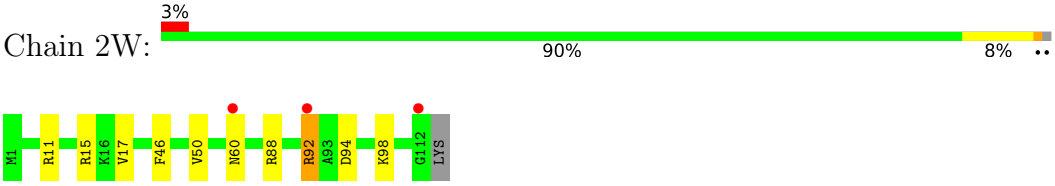
• Molecule 18: 50S ribosomal protein L22

Chain 1W:



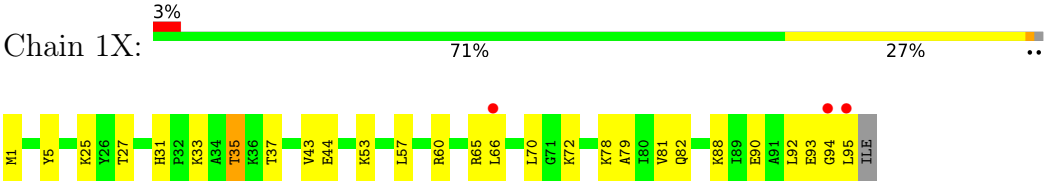
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



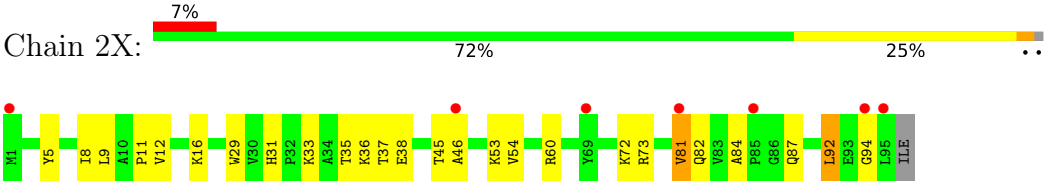
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



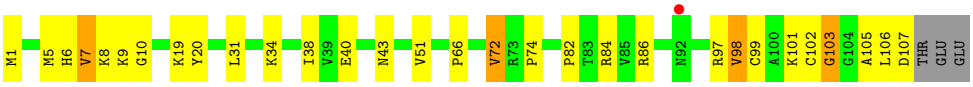
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



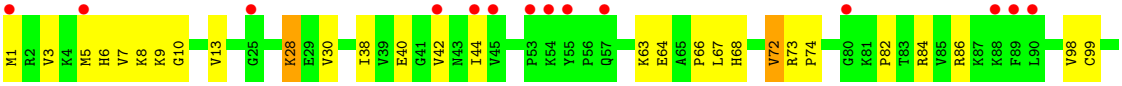
• Molecule 20: 50S ribosomal protein L24

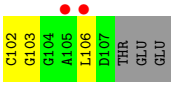
Chain 1Y:



• Molecule 20: 50S ribosomal protein L24

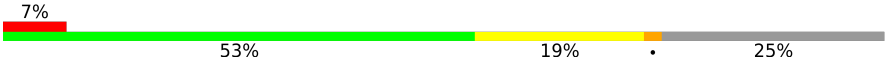
Chain 2Y:

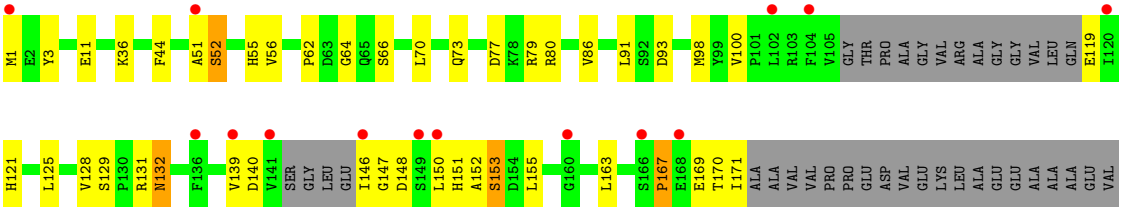




• Molecule 21: 50S ribosomal protein L25

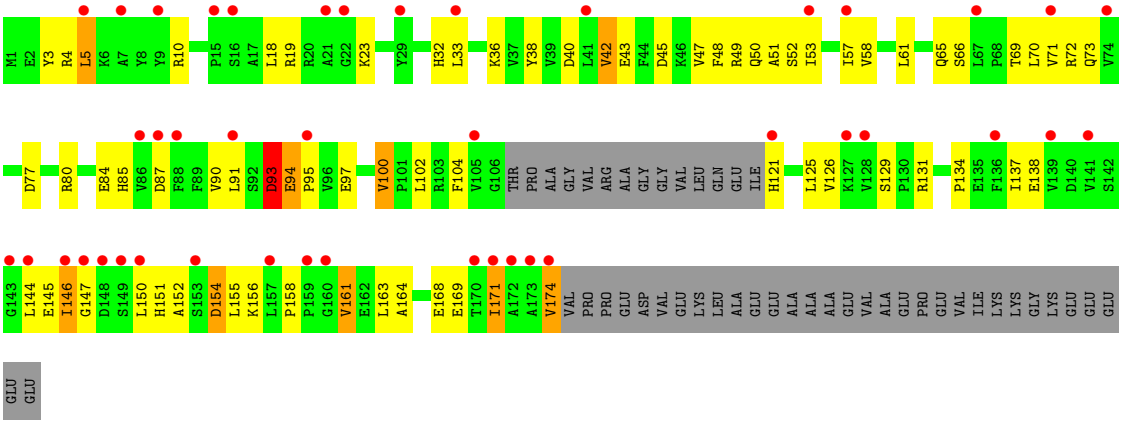
Chain 1Z:





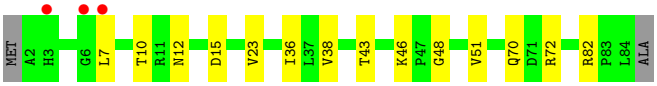
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:

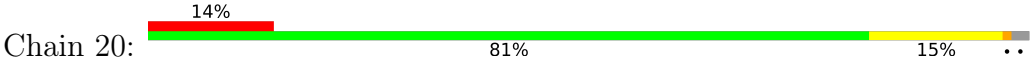


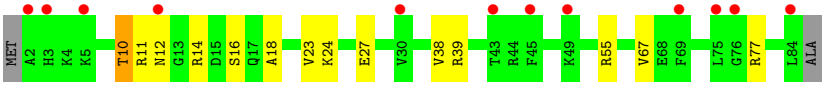
• Molecule 22: 50S ribosomal protein L27

Chain 10:

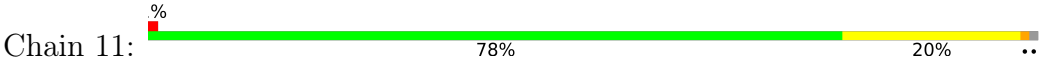


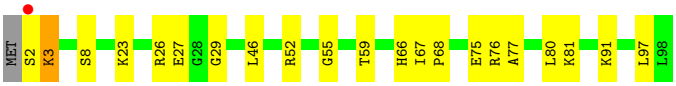
• Molecule 22: 50S ribosomal protein L27



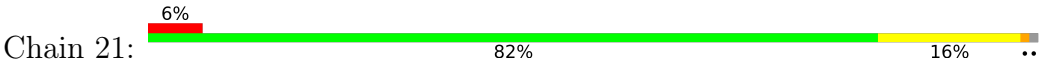


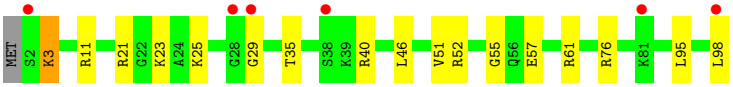
• Molecule 23: 50S ribosomal protein L28



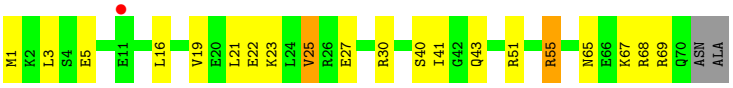


• Molecule 23: 50S ribosomal protein L28

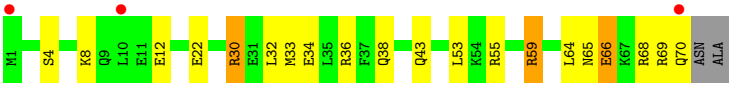




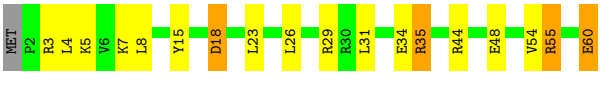
• Molecule 24: 50S ribosomal protein L29



• Molecule 24: 50S ribosomal protein L29

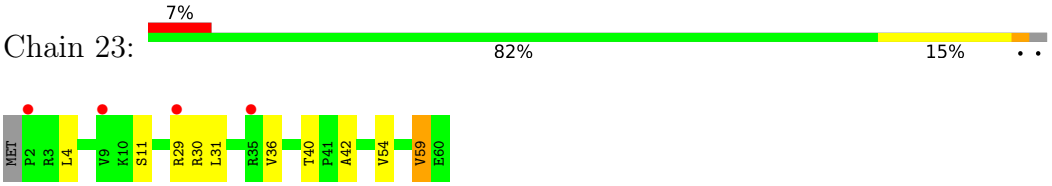


• Molecule 25: 50S ribosomal protein L30



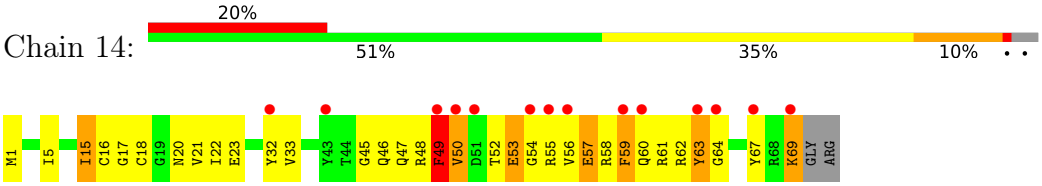
• Molecule 25: 50S ribosomal protein L30

Chain 23:



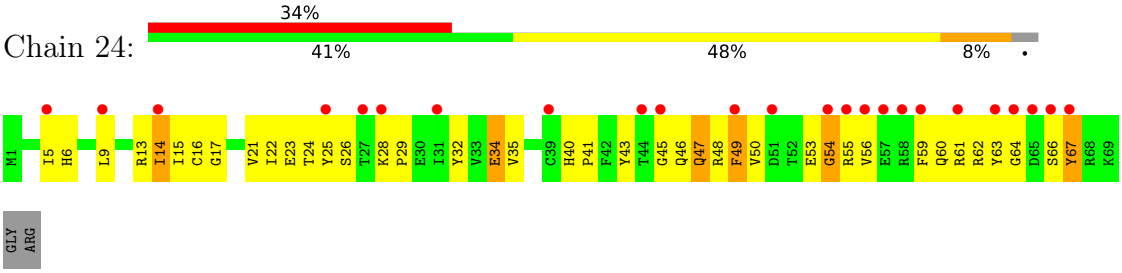
• Molecule 26: 50S ribosomal protein L31

Chain 14:



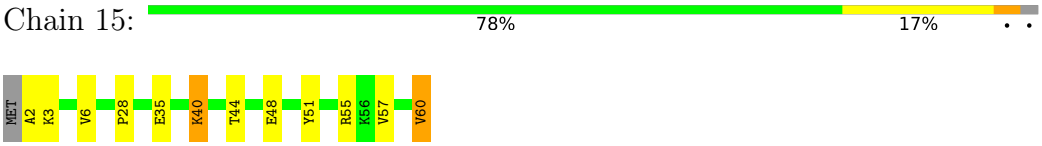
• Molecule 26: 50S ribosomal protein L31

Chain 24:



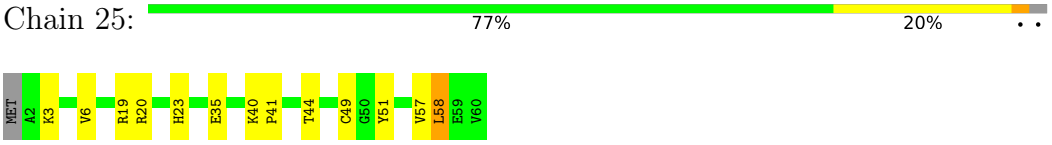
• Molecule 27: 50S ribosomal protein L32

Chain 15:



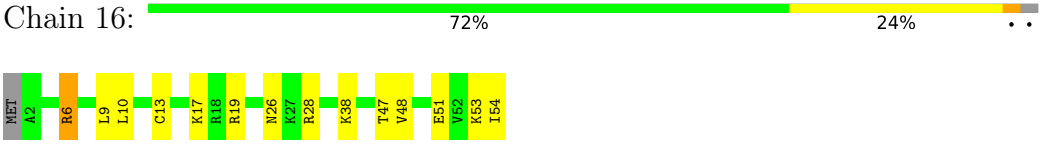
• Molecule 27: 50S ribosomal protein L32

Chain 25:



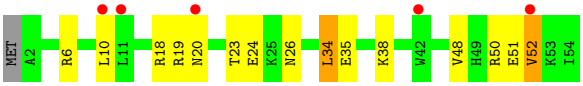
• Molecule 28: 50S ribosomal protein L33

Chain 16:

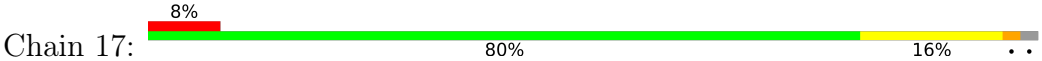


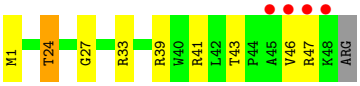
• Molecule 28: 50S ribosomal protein L33

Chain 26:

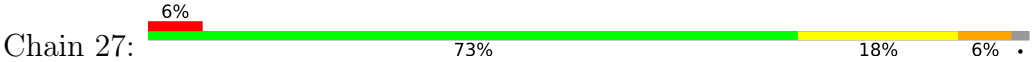


• Molecule 29: 50S ribosomal protein L34

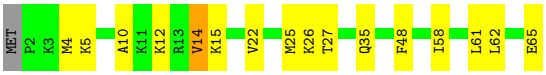




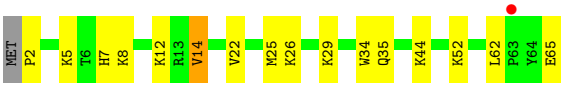
• Molecule 29: 50S ribosomal protein L34



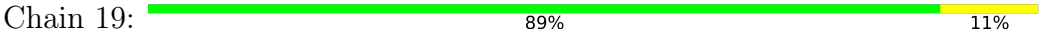
• Molecule 30: 50S ribosomal protein L35



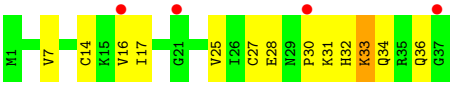
• Molecule 30: 50S ribosomal protein L35



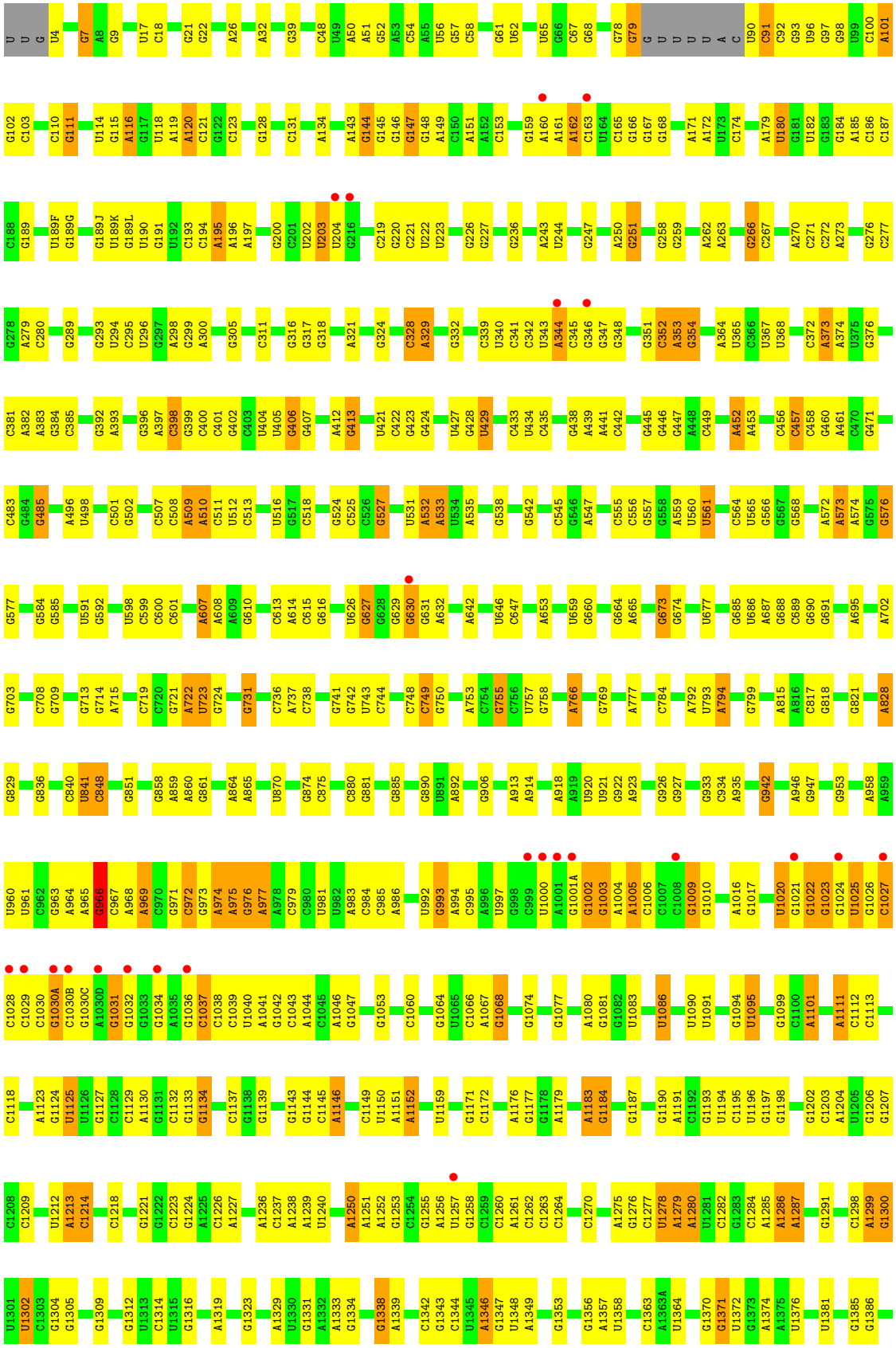
• Molecule 31: 50S ribosomal protein L36

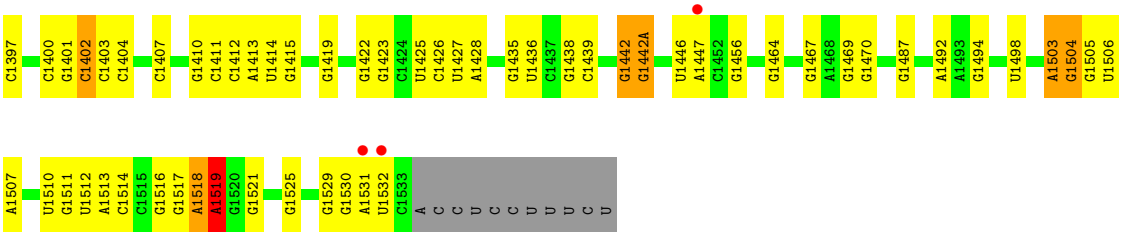


• Molecule 31: 50S ribosomal protein L36



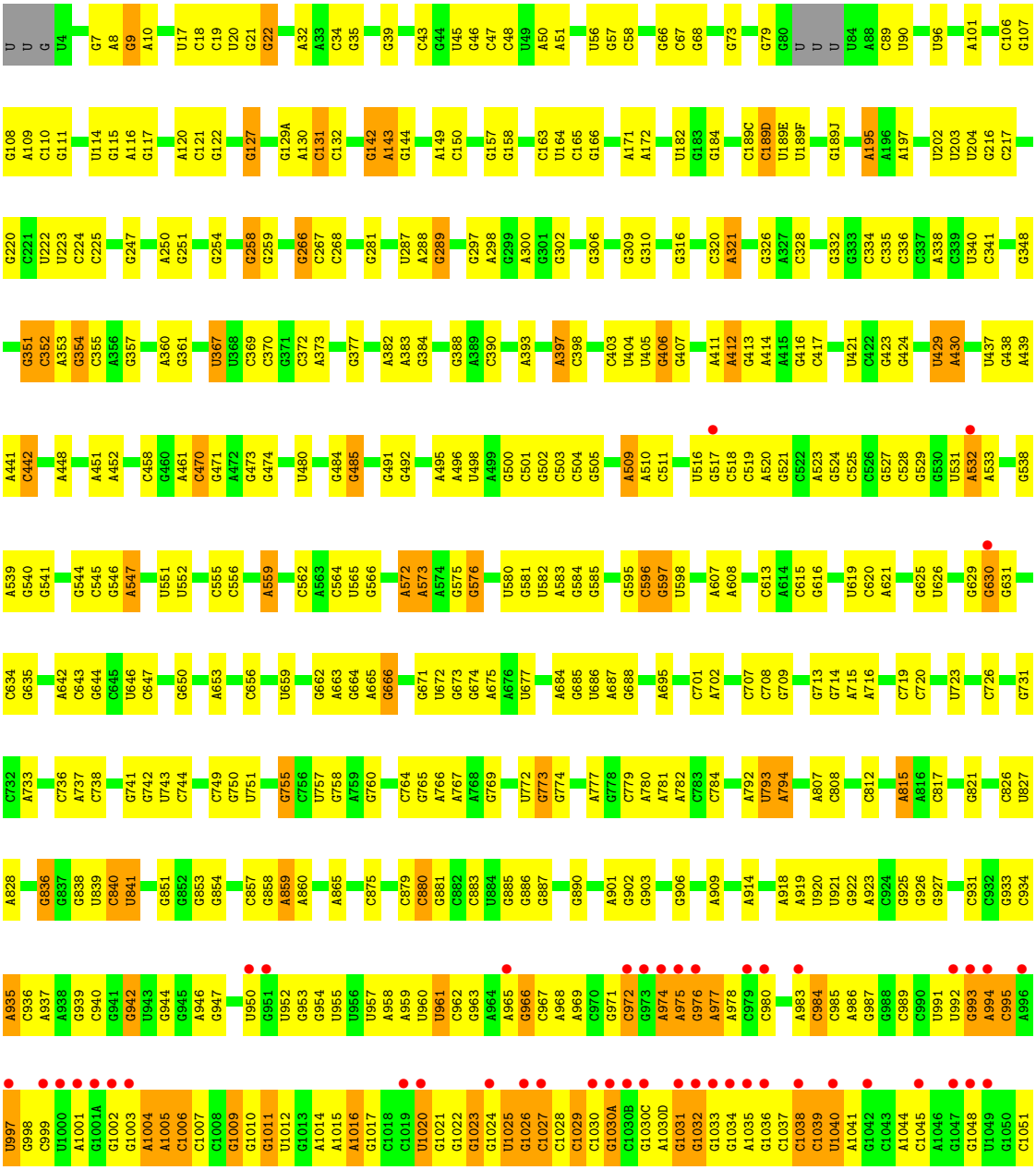
• Molecule 32: 16S Ribosomal RNA

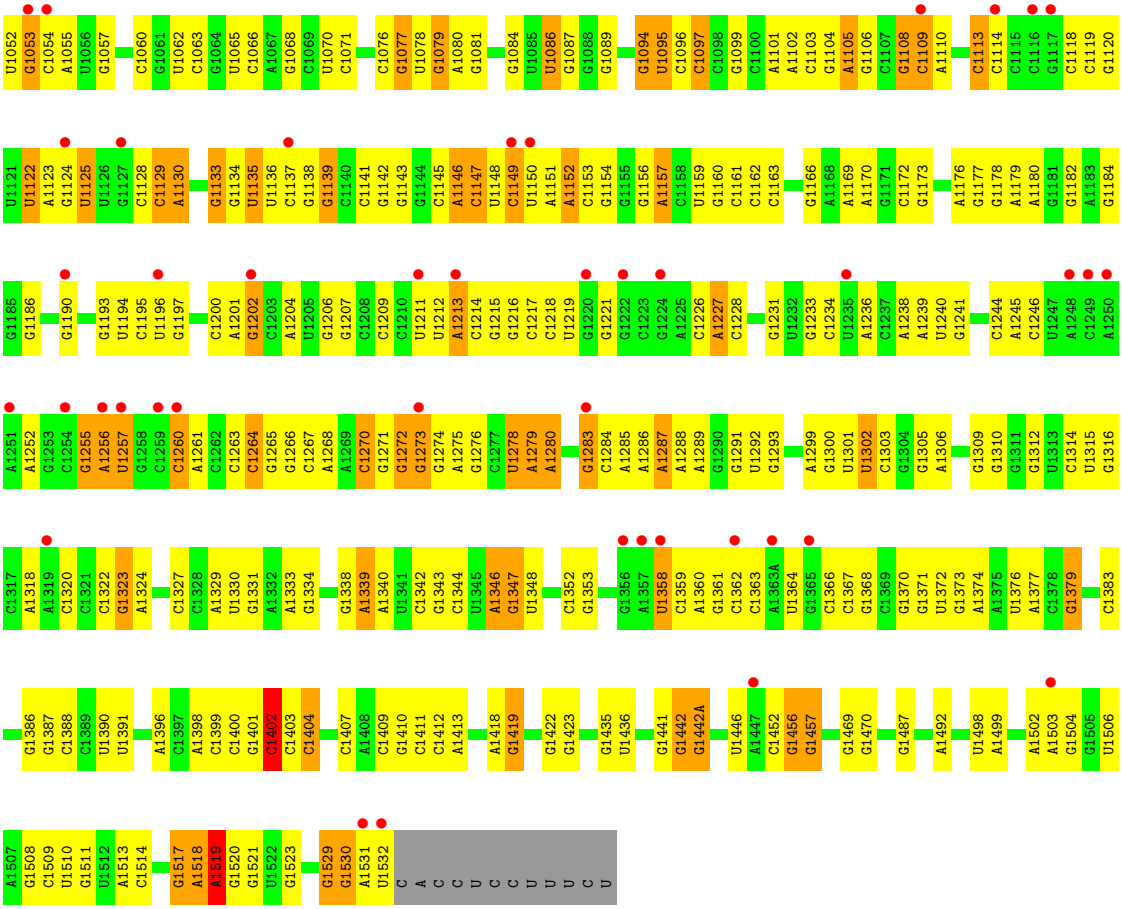




• Molecule 32: 16S Ribosomal RNA

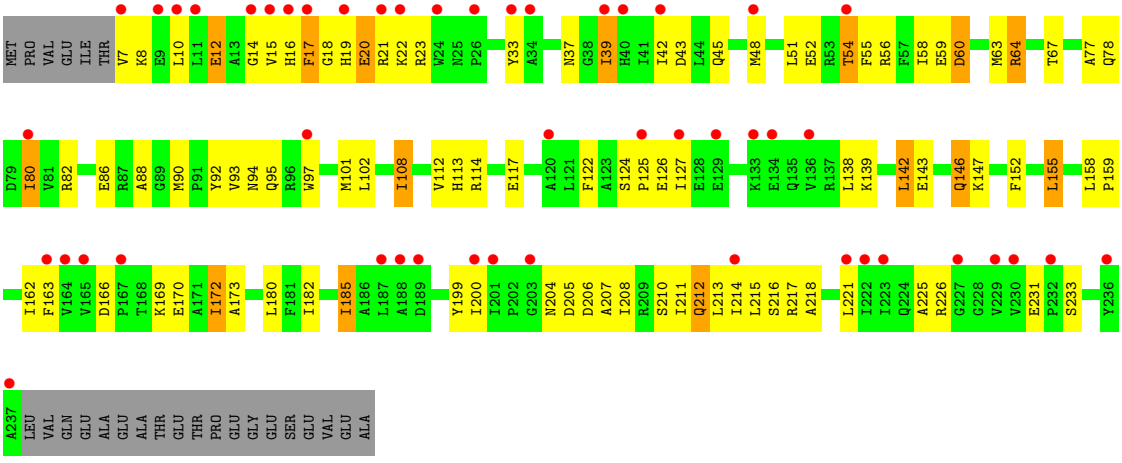
Chain 2a:





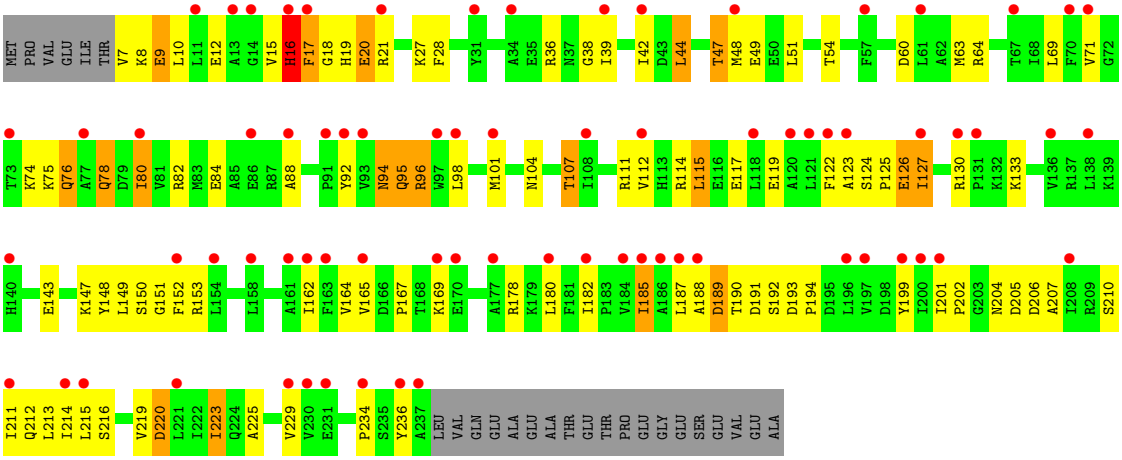
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



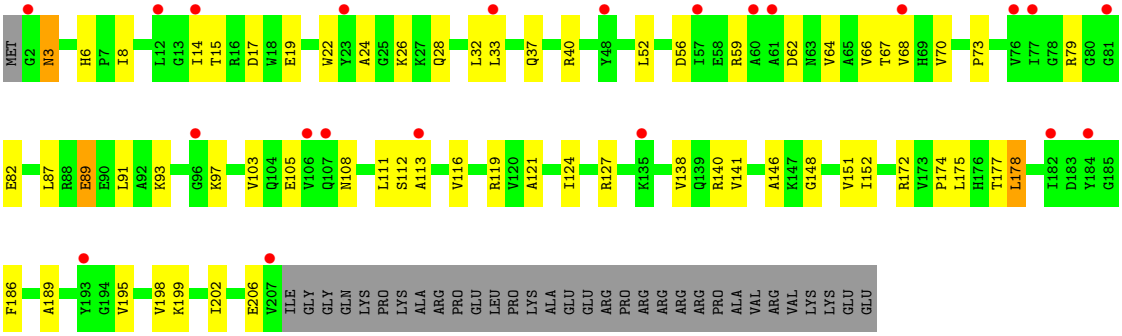
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



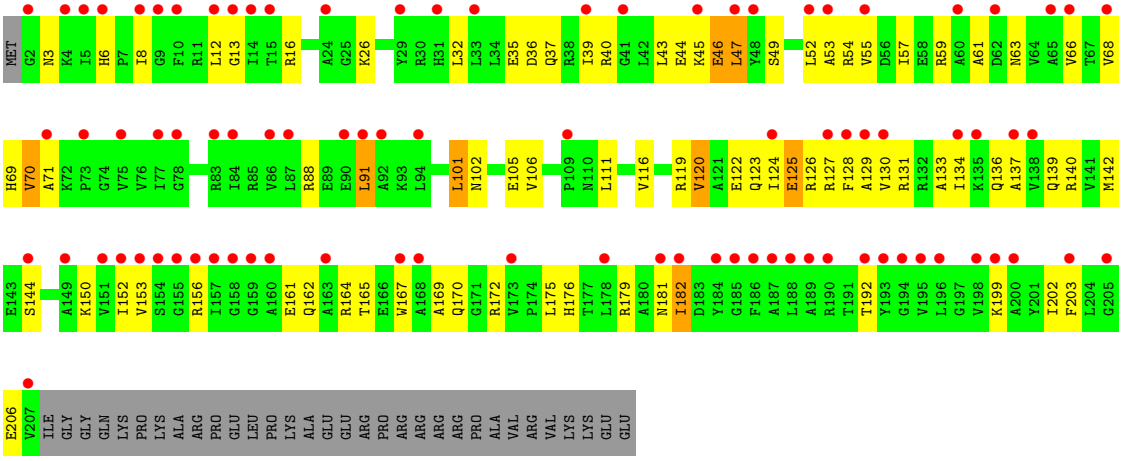
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



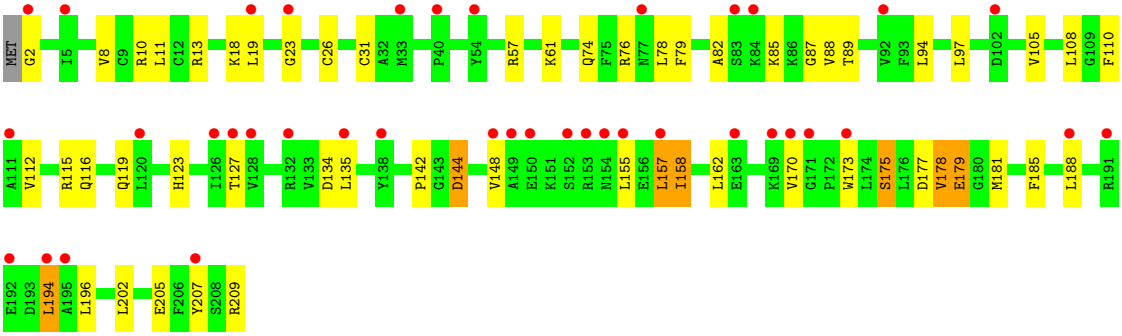
• Molecule 34: 30S ribosomal protein S3

Chain 2c:

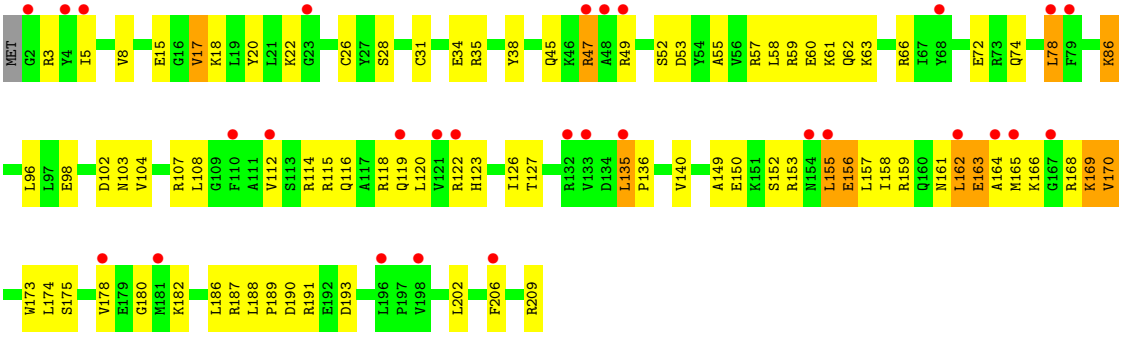


• Molecule 35: 30S ribosomal protein S4

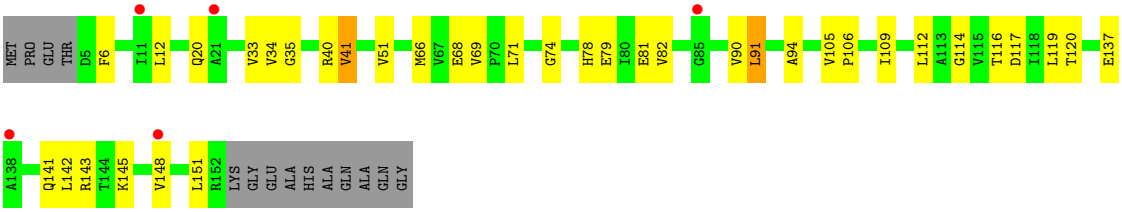
Chain 1d:



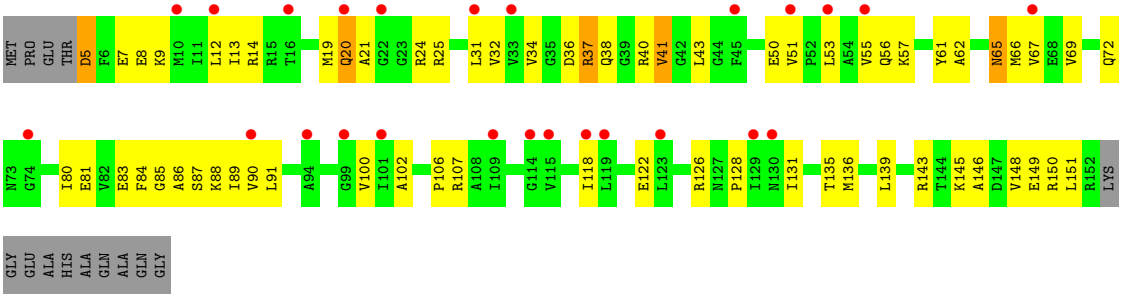
• Molecule 35: 30S ribosomal protein S4



• Molecule 36: 30S ribosomal protein S5

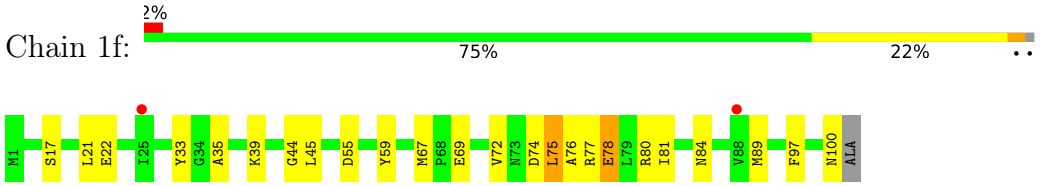


• Molecule 36: 30S ribosomal protein S5



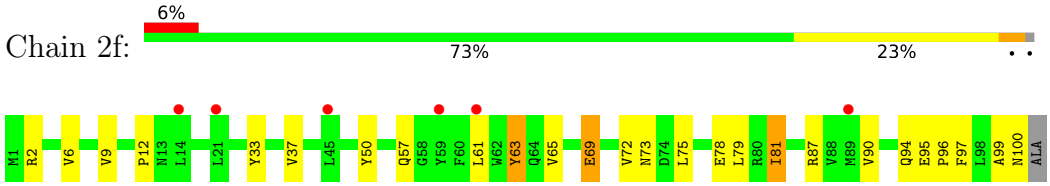
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



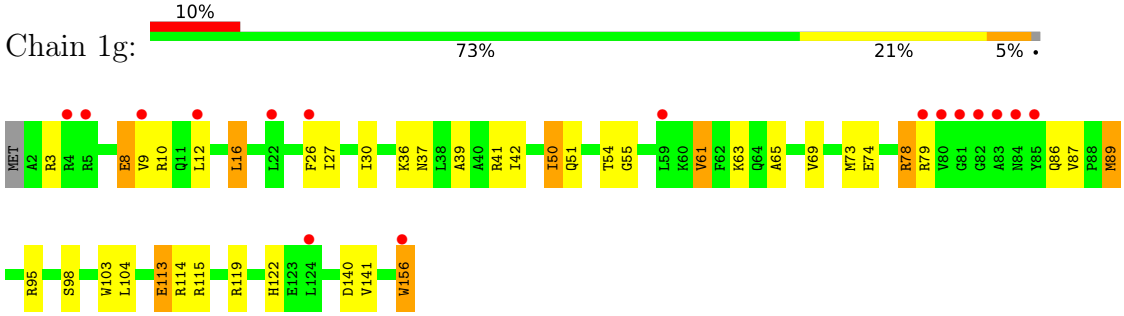
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



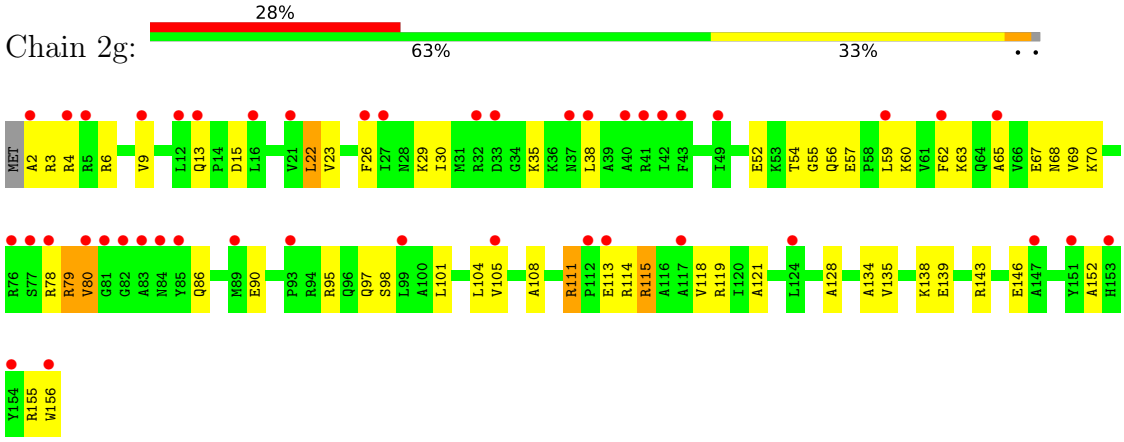
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



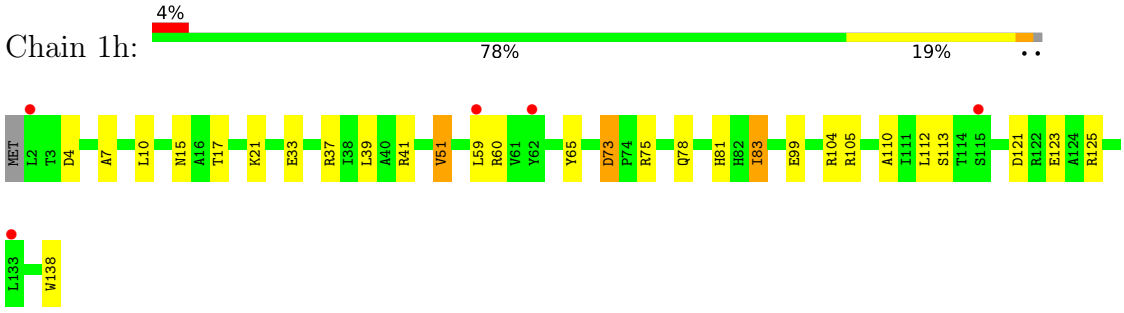
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



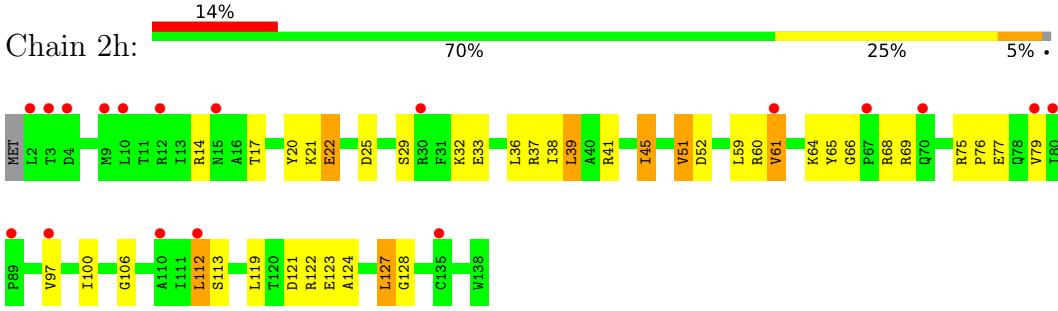
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



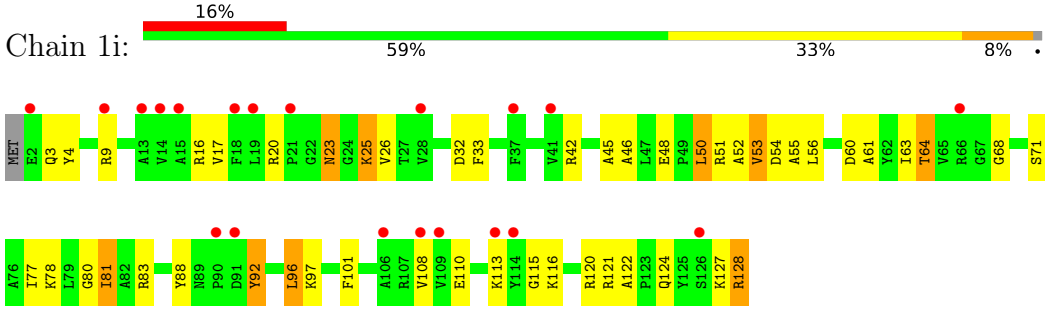
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



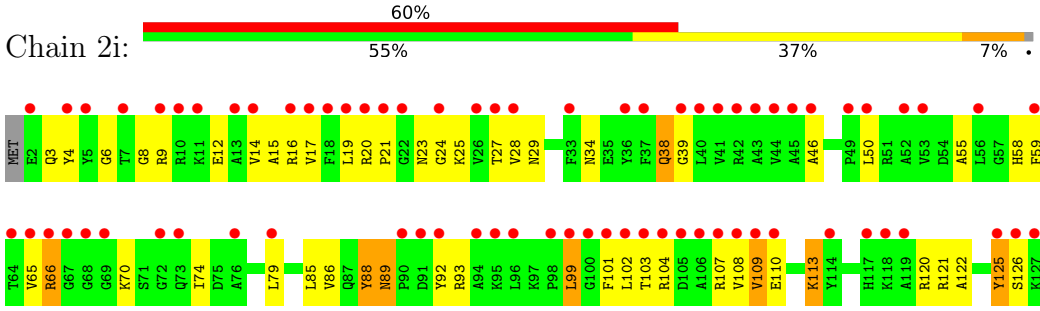
• Molecule 40: 30S ribosomal protein S9

Chain 1i:



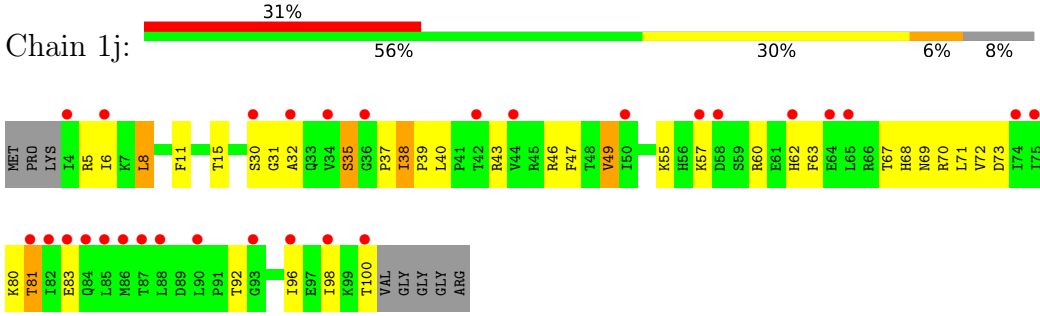
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



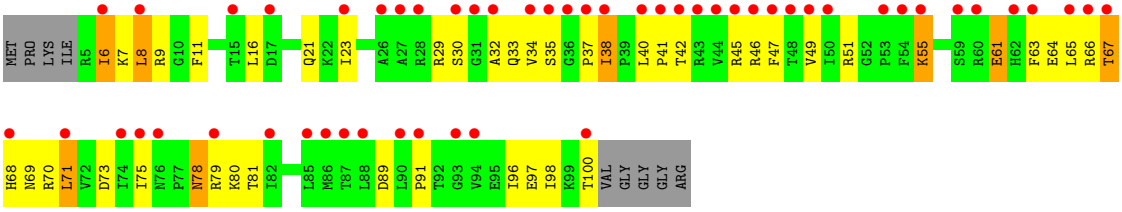
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



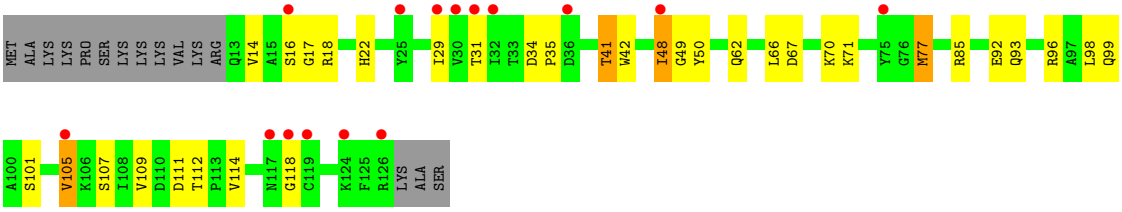
• Molecule 41: 30S ribosomal protein S10

Chain 2j:

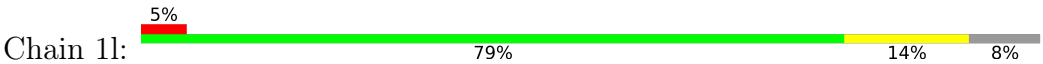


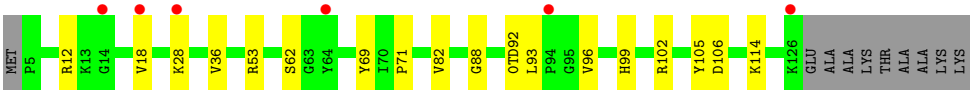
• Molecule 42: 30S ribosomal protein S11

• Molecule 42: 30S ribosomal protein S11

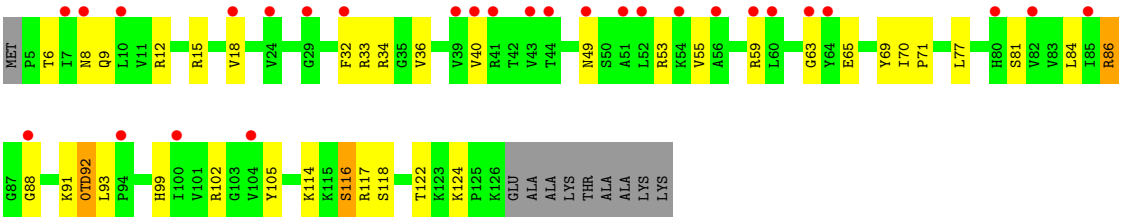


• Molecule 43: 30S ribosomal protein S12



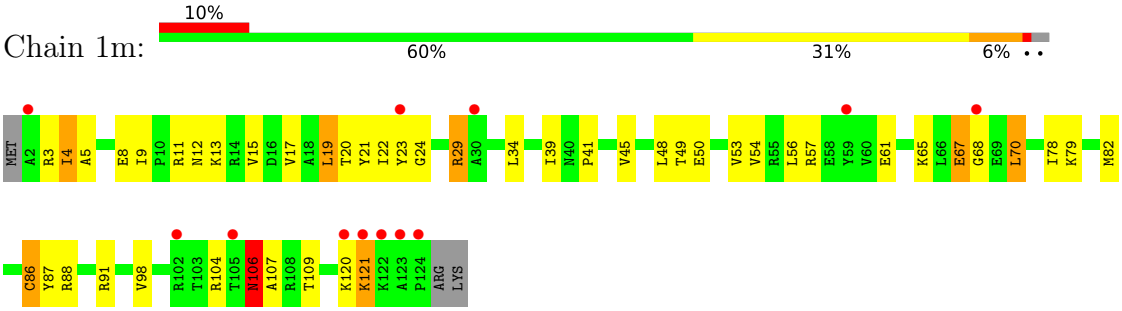


• Molecule 43: 30S ribosomal protein S12



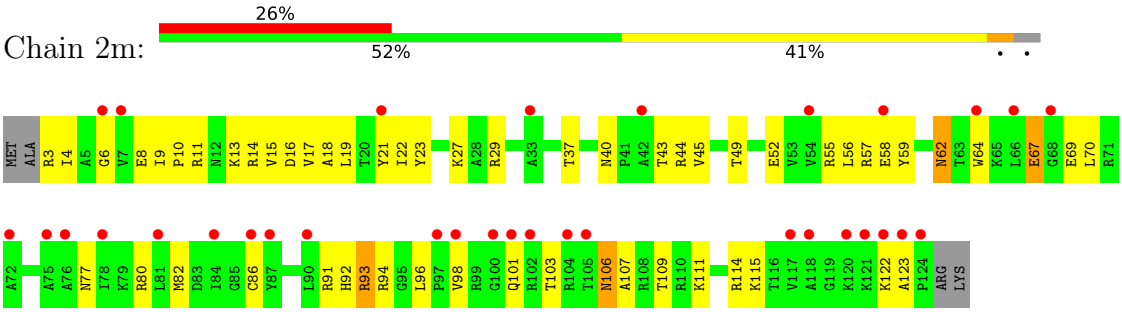
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



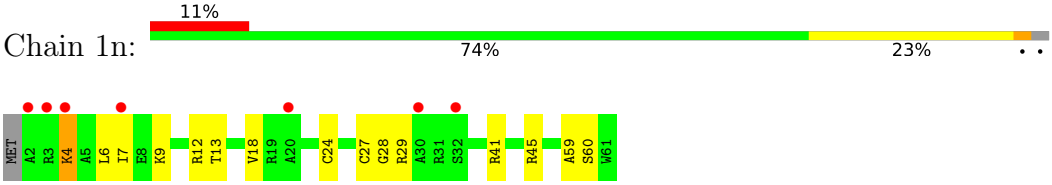
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



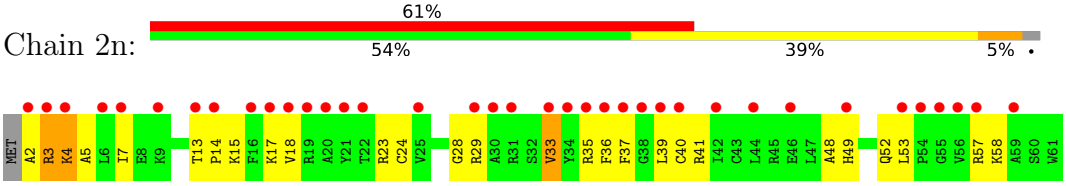
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



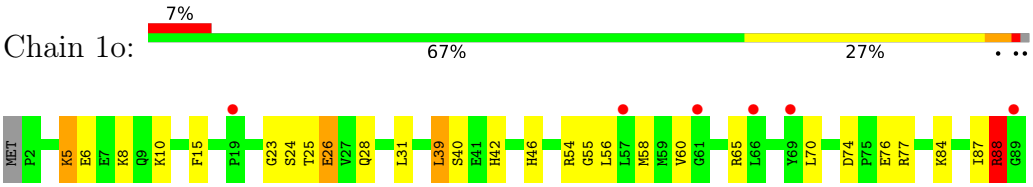
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



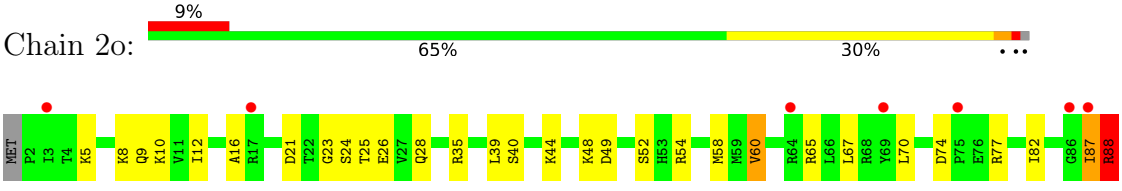
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



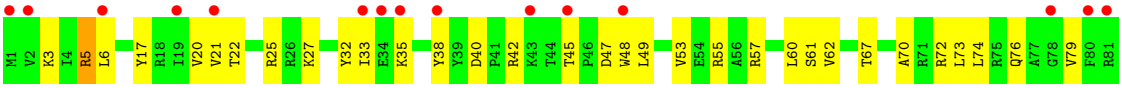
• Molecule 46: 30S ribosomal protein S15

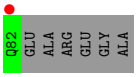
Chain 2o:



• Molecule 47: 30S ribosomal protein S16

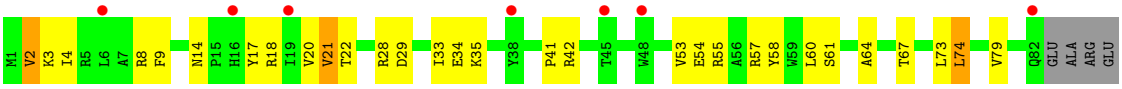
Chain 1p:





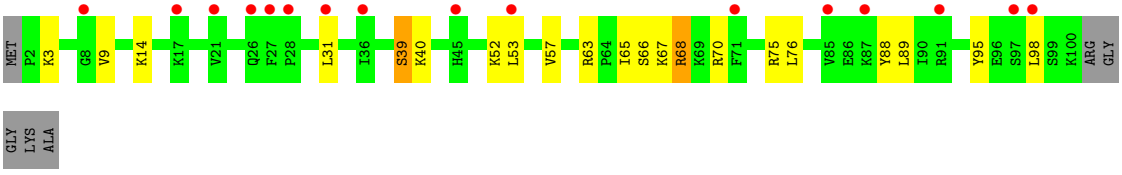
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



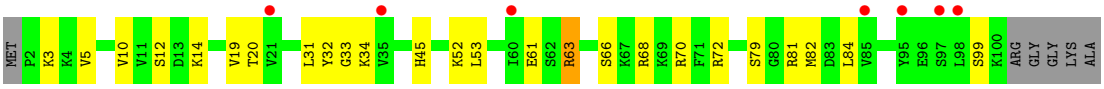
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



• Molecule 48: 30S ribosomal protein S17

Chain 2q:

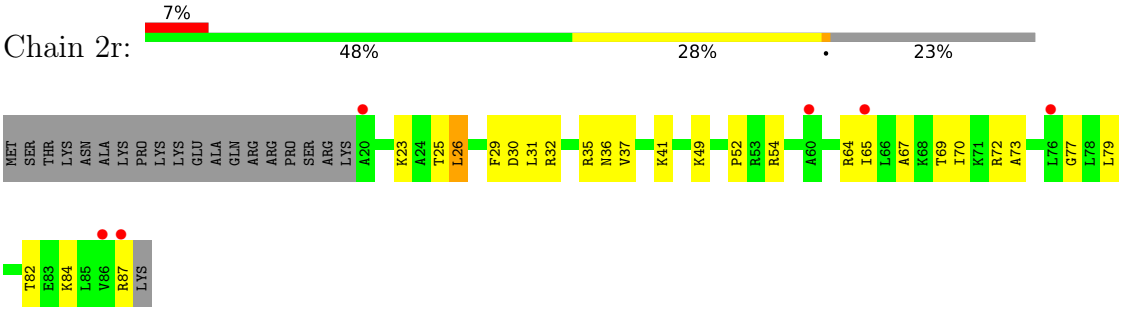


• Molecule 49: 30S ribosomal protein S18

Chain 1r:

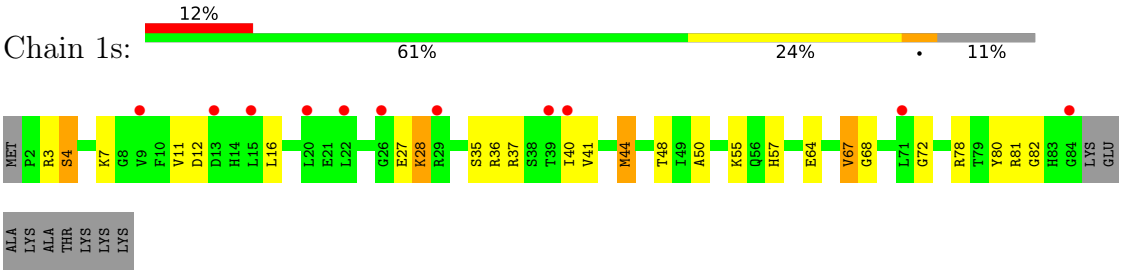
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



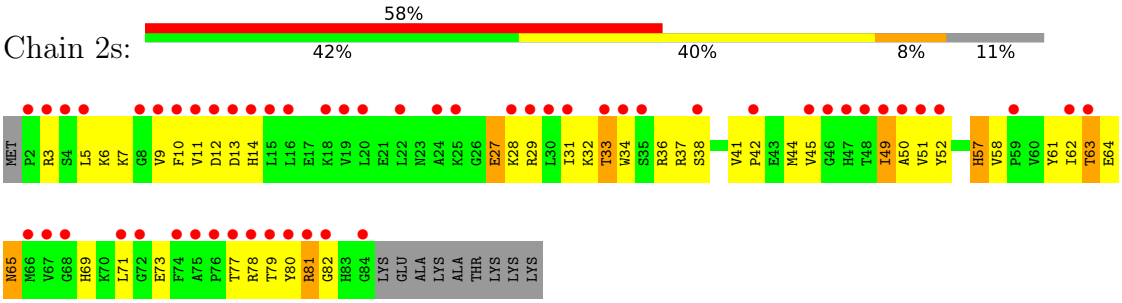
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



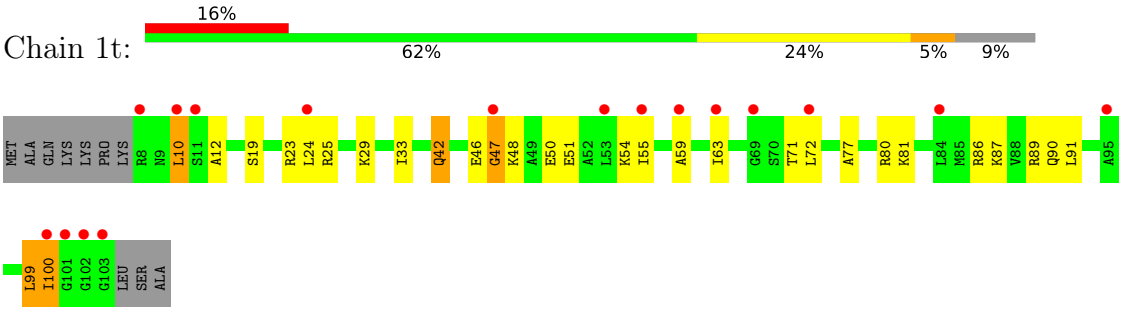
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



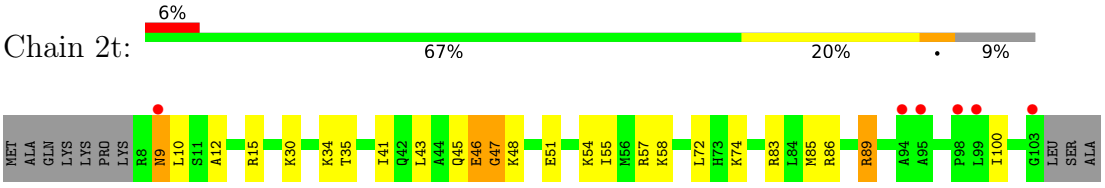
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



• Molecule 51: 30S ribosomal protein S20

Chain 2t:

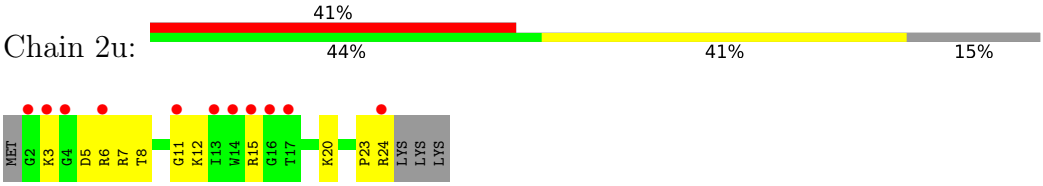


• Molecule 52: 30S ribosomal protein Thx

Chain 1u:

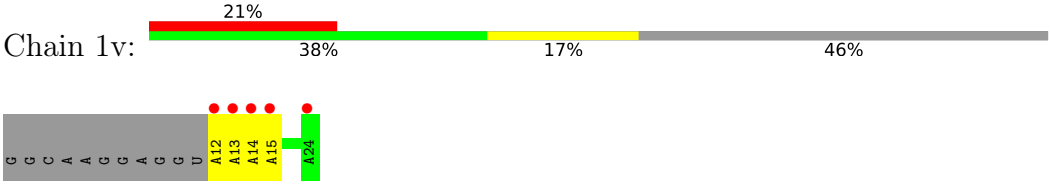
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



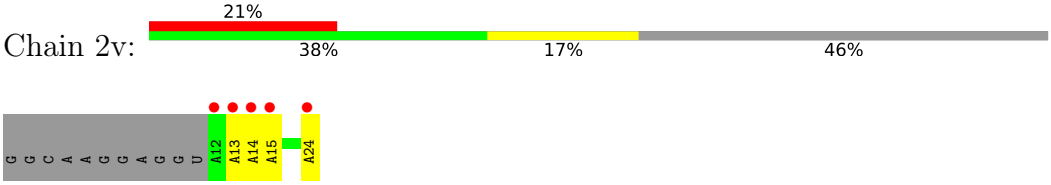
• Molecule 53: MG-mRNA

Chain 1v:



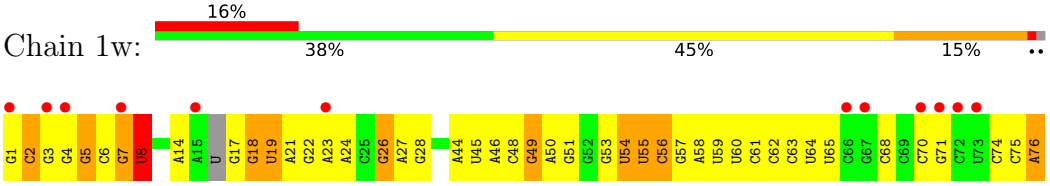
• Molecule 53: MG-mRNA

Chain 2v:



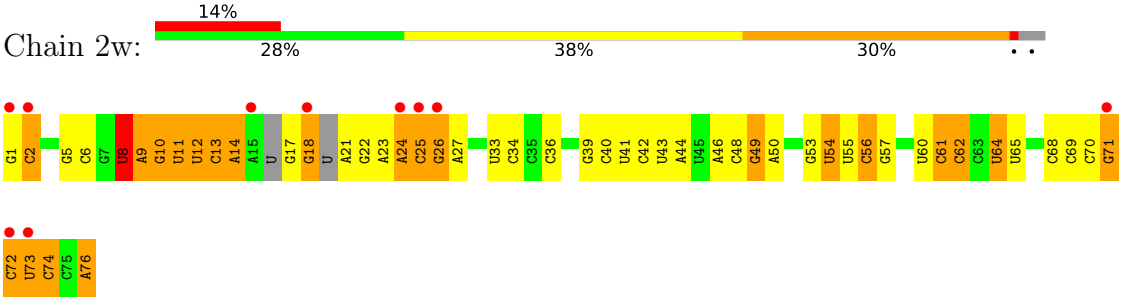
• Molecule 54: A-site Aminoacyl-tRNA Gly-NH-tRNAgly

Chain 1w:



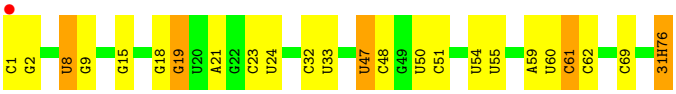
• Molecule 54: A-site Aminoacyl-tRNA Gly-NH-tRNAgly

Chain 2w:

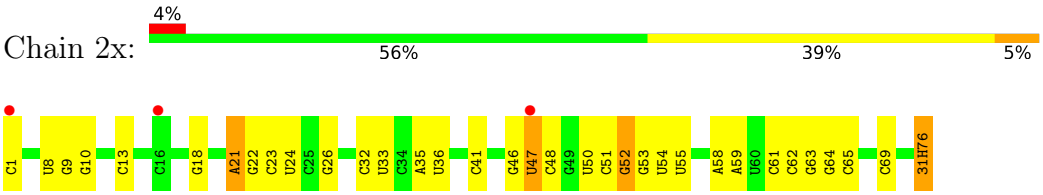


• Molecule 55: P-site Aminoacyl-tRNA fMet-NH-tRNAmet

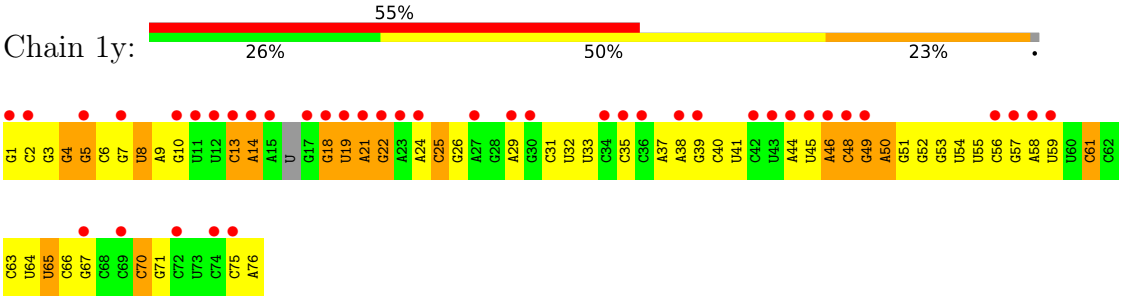
Chain 1x:



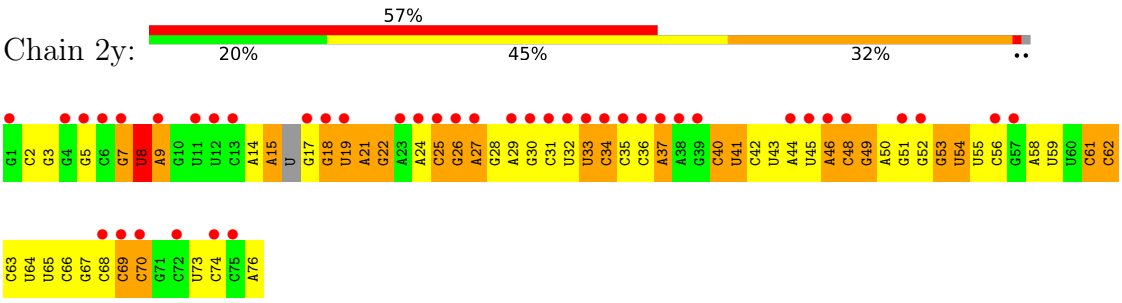
• Molecule 55: P-site Aminoacyl-tRNA fMet-NH-tRNAmet



• Molecule 56: E-site Deacylated tRNAgly



• Molecule 56: E-site Deacylated tRNAgly



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.17Å 450.98Å 624.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.74 – 2.55 153.74 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.4 (153.74-2.55) 99.4 (153.74-2.55)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.223 , 0.268 0.223 , 0.267	Depositor DCC
R_{free} test set	94751 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 63.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	300046	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PSU, 2MA, OMC, CLM, L3X, SF4, 5MU, 5MC, 2MG, K, MA6, M2G, 4SU, MG, G7M, UR3, ZN, OMU, 0TD, 31H, OMG, 4OC

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	0.27	0/69011	0.47	2/107720 (0.0%)
1	2A	0.21	1/67295 (0.0%)	0.41	2/105042 (0.0%)
2	1B	0.21	0/2882	0.40	0/4494
2	2B	0.18	0/2879	0.35	0/4487
3	1D	0.26	0/2186	0.49	0/2944
3	2D	0.21	0/2186	0.47	0/2944
4	1E	0.26	0/1592	0.51	0/2149
4	2E	0.21	0/1592	0.43	0/2149
5	1F	0.26	0/1618	0.46	0/2191
5	2F	0.19	0/1614	0.45	2/2186 (0.1%)
6	1G	0.20	0/1448	0.43	0/1957
6	2G	0.20	0/1453	0.43	0/1963
7	1H	0.21	0/1356	0.42	0/1834
7	2H	0.18	0/1356	0.40	0/1834
8	1I	0.19	0/1112	0.43	0/1514
8	2I	0.19	0/1079	0.41	0/1475
9	1N	0.26	0/1144	0.47	0/1543
9	2N	0.18	0/1144	0.41	0/1543
10	1O	0.25	0/943	0.44	0/1269
10	2O	0.19	0/943	0.44	0/1269
11	1P	0.26	0/1152	0.55	0/1533
11	2P	0.21	0/1152	0.51	0/1533
12	1Q	0.25	0/1143	0.47	0/1527
12	2Q	0.22	0/1143	0.46	0/1527
13	1R	0.28	0/982	0.49	0/1312
13	2R	0.20	0/982	0.44	0/1312
14	1S	0.21	0/883	0.47	0/1176
14	2S	0.21	0/880	0.45	0/1172
15	1T	0.26	0/1105	0.50	0/1477
15	2T	0.21	0/1097	0.43	0/1468
16	1U	0.28	0/977	0.46	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.19	0/977	0.39	0/1301
17	1V	0.25	0/782	0.48	0/1049
17	2V	0.18	0/782	0.41	0/1049
18	1W	0.27	0/897	0.45	0/1205
18	2W	0.21	0/897	0.43	0/1205
19	1X	0.26	0/764	0.53	0/1025
19	2X	0.21	0/764	0.49	2/1025 (0.2%)
20	1Y	0.22	0/819	0.49	0/1095
20	2Y	0.20	0/819	0.46	0/1095
21	1Z	0.21	0/1267	0.46	0/1717
21	2Z	0.22	0/1299	0.47	0/1763
22	10	0.27	0/662	0.49	0/881
22	20	0.19	0/662	0.44	0/881
23	11	0.22	0/762	0.43	0/1014
23	21	0.21	0/762	0.41	0/1014
24	12	0.24	0/590	0.44	0/781
24	22	0.17	0/590	0.35	0/781
25	13	0.26	0/474	0.47	0/635
25	23	0.17	0/469	0.39	0/630
26	14	0.25	0/565	0.60	0/761
26	24	0.24	0/545	0.58	2/737 (0.3%)
27	15	0.26	0/469	0.52	0/635
27	25	0.23	0/469	0.41	0/635
28	16	0.25	0/460	0.46	0/613
28	26	0.20	0/456	0.43	0/608
29	17	0.30	0/426	0.52	0/561
29	27	0.25	0/426	0.47	0/561
30	18	0.25	0/525	0.46	0/691
30	28	0.19	0/525	0.39	0/691
31	19	0.25	0/310	0.45	0/407
31	29	0.19	0/310	0.44	0/407
32	1a	0.19	0/35795	0.39	1/55864 (0.0%)
32	2a	0.19	0/35886	0.38	0/56005
33	1b	0.20	0/1881	0.47	0/2542
33	2b	0.23	0/1860	0.51	0/2518
34	1c	0.20	0/1572	0.39	0/2126
34	2c	0.22	0/1566	0.44	0/2119
35	1d	0.18	0/1685	0.42	0/2262
35	2d	0.19	0/1704	0.44	0/2284
36	1e	0.20	0/1145	0.47	0/1543
36	2e	0.19	0/1149	0.46	0/1548
37	1f	0.18	0/823	0.37	0/1115
37	2f	0.19	0/829	0.42	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.18	0/1250	0.38	0/1679
38	2g	0.19	0/1254	0.40	0/1683
39	1h	0.18	0/1108	0.40	0/1494
39	2h	0.18	0/1108	0.40	0/1494
40	1i	0.19	0/1002	0.47	0/1346
40	2i	0.21	0/997	0.47	0/1343
41	1j	0.18	0/722	0.45	0/982
41	2j	0.22	0/727	0.47	0/988
42	1k	0.21	0/844	0.48	0/1145
42	2k	0.17	0/848	0.39	0/1149
43	1l	0.21	0/937	0.40	0/1260
43	2l	0.21	0/937	0.48	1/1260 (0.1%)
44	1m	0.19	0/969	0.46	0/1302
44	2m	0.20	0/961	0.48	0/1291
45	1n	0.20	0/501	0.42	0/664
45	2n	0.21	0/501	0.45	0/664
46	1o	0.19	0/739	0.37	0/985
46	2o	0.17	0/739	0.42	0/985
47	1p	0.20	0/697	0.47	0/939
47	2p	0.18	0/693	0.45	0/935
48	1q	0.18	0/836	0.44	0/1117
48	2q	0.17	0/836	0.44	0/1117
49	1r	0.19	0/560	0.46	0/746
49	2r	0.20	0/560	0.40	0/746
50	1s	0.20	0/667	0.49	0/900
50	2s	0.24	0/661	0.58	0/893
51	1t	0.20	0/730	0.49	0/965
51	2t	0.20	0/729	0.43	0/965
52	1u	0.19	0/203	0.43	0/266
52	2u	0.20	0/203	0.47	0/266
53	1v	0.20	0/322	0.33	0/501
53	2v	0.20	0/322	0.33	0/501
54	1w	0.27	1/1639 (0.1%)	0.41	0/2548
54	2w	0.27	0/1616	0.43	0/2510
55	1x	0.26	0/1723	0.41	0/2684
55	2x	0.24	0/1723	0.39	0/2684
56	1y	0.29	1/1664 (0.1%)	0.43	0/2587
56	2y	0.30	1/1664 (0.1%)	0.43	0/2587
All	All	0.22	4/316940 (0.0%)	0.43	12/474518 (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
51	1t	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	8	4SU	O3'-P	5.50	1.61	1.56
54	1w	8	4SU	O3'-P	5.22	1.61	1.56
56	1y	8	4SU	O3'-P	5.18	1.61	1.56
1	2A	2552	OMU	O3'-P	5.05	1.61	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1992	G	C2'-C3'-O3'	6.55	119.33	109.50
1	1A	1992	G	C2'-C3'-O3'	6.27	118.91	109.50
26	24	56	VAL	N-CA-C	-5.96	106.69	112.29
26	24	54	GLY	N-CA-C	-5.82	106.93	115.30
43	2l	63	GLY	N-CA-C	-5.40	108.65	115.08
1	2A	1992	G	P-O3'-C3'	5.27	128.11	120.20
5	2F	21	ALA	CA-C-N	5.24	131.13	121.70
5	2F	21	ALA	C-N-CA	5.24	131.13	121.70
19	2X	94	GLY	CA-C-N	5.19	131.05	121.70
19	2X	94	GLY	C-N-CA	5.19	131.05	121.70
32	1a	266	G	C2'-C3'-O3'	5.15	117.22	109.50
1	1A	548	A	P-O3'-C3'	5.10	127.85	120.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	1t	99	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31195	563	0
1	2A	60322	0	30428	638	0
2	1B	2577	0	1305	16	0
2	2B	2575	0	1303	36	0
3	1D	2136	0	2218	33	0
3	2D	2136	0	2218	44	0
4	1E	1559	0	1618	18	0
4	2E	1559	0	1618	30	0
5	1F	1583	0	1625	28	0
5	2F	1579	0	1619	43	0
6	1G	1423	0	1436	31	0
6	2G	1428	0	1438	55	0
7	1H	1330	0	1407	30	0
7	2H	1330	0	1407	27	0
8	1I	1097	0	1140	35	0
8	2I	1064	0	1082	34	1
9	1N	1117	0	1184	12	0
9	2N	1117	0	1184	21	0
10	1O	933	0	996	14	0
10	2O	933	0	996	20	0
11	1P	1135	0	1212	29	0
11	2P	1135	0	1212	33	0
12	1Q	1122	0	1179	22	0
12	2Q	1122	0	1179	26	0
13	1R	968	0	1033	12	0
13	2R	968	0	1033	20	0
14	1S	873	0	927	16	0
14	2S	870	0	923	39	0
15	1T	1091	0	1151	16	0
15	2T	1083	0	1136	26	0
16	1U	959	0	1019	10	0
16	2U	959	0	1019	24	0
17	1V	771	0	830	8	0
17	2V	771	0	830	19	0
18	1W	886	0	940	8	0
18	2W	886	0	940	6	0
19	1X	750	0	814	19	0
19	2X	750	0	814	20	0
20	1Y	806	0	881	19	0
20	2Y	806	0	881	18	0
21	1Z	1240	0	1240	29	0
21	2Z	1271	0	1273	45	0
22	10	653	0	674	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	653	0	674	12	0
23	11	755	0	826	15	0
23	21	755	0	826	11	0
24	12	588	0	643	13	0
24	22	588	0	643	14	0
25	13	469	0	518	10	0
25	23	464	0	514	6	0
26	14	552	0	533	23	0
26	24	532	0	503	38	0
27	15	455	0	465	8	0
27	25	455	0	465	8	0
28	16	453	0	473	10	0
28	26	449	0	469	10	0
29	17	418	0	467	8	0
29	27	418	0	467	9	0
30	18	517	0	582	14	0
30	28	517	0	582	14	0
31	19	307	0	335	2	0
31	29	307	0	335	9	0
32	1a	32246	0	16293	394	1
32	2a	32327	0	16338	528	0
33	1b	1846	0	1867	64	0
33	2b	1825	0	1828	77	0
34	1c	1548	0	1535	39	0
34	2c	1542	0	1517	59	0
35	1d	1655	0	1672	39	0
35	2d	1674	0	1714	60	0
36	1e	1129	0	1185	20	0
36	2e	1133	0	1191	45	0
37	1f	810	0	804	15	0
37	2f	816	0	808	21	0
38	1g	1231	0	1238	25	0
38	2g	1235	0	1249	38	0
39	1h	1088	0	1126	17	0
39	2h	1088	0	1126	27	0
40	1i	983	0	986	34	0
40	2i	978	0	966	44	0
41	1j	709	0	650	21	0
41	2j	714	0	672	30	0
42	1k	829	0	825	15	0
42	2k	833	0	836	18	0
43	1l	932	0	980	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	932	0	980	21	0
44	1m	958	0	1002	34	0
44	2m	950	0	988	45	0
45	1n	492	0	529	9	0
45	2n	492	0	529	25	0
46	1o	728	0	760	21	0
46	2o	728	0	760	19	0
47	1p	681	0	697	25	0
47	2p	677	0	686	19	0
48	1q	823	0	891	13	0
48	2q	823	0	891	10	0
49	1r	555	0	618	14	0
49	2r	555	0	618	19	0
50	1s	652	0	662	21	0
50	2s	646	0	644	41	0
51	1t	728	0	798	20	0
51	2t	727	0	796	17	0
52	1u	199	0	208	6	0
52	2u	199	0	208	8	0
53	1v	286	0	142	1	0
53	2v	286	0	142	1	0
54	1w	1556	0	778	30	0
54	2w	1536	0	770	46	0
55	1x	1656	0	849	15	0
55	2x	1656	0	849	23	0
56	1y	1552	0	791	33	0
56	2y	1552	0	791	51	0
57	10	9	0	0	0	0
57	11	3	0	0	0	0
57	12	2	0	0	0	0
57	13	5	0	0	0	0
57	15	6	0	0	0	0
57	16	2	0	0	0	0
57	17	5	0	0	0	0
57	18	6	0	0	0	0
57	19	1	0	0	0	0
57	1A	1095	0	0	0	0
57	1B	36	0	0	0	0
57	1D	13	0	0	0	0
57	1E	12	0	0	0	0
57	1F	15	0	0	0	0
57	1G	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1I	1	0	0	0	0
57	1N	5	0	0	0	0
57	1O	5	0	0	0	0
57	1P	5	0	0	0	0
57	1Q	7	0	0	0	0
57	1R	7	0	0	0	0
57	1S	3	0	0	0	0
57	1T	3	0	0	0	0
57	1U	10	0	0	0	0
57	1V	7	0	0	0	0
57	1W	7	0	0	0	0
57	1X	7	0	0	0	0
57	1Y	3	0	0	0	0
57	1Z	3	0	0	0	0
57	1a	226	0	0	0	0
57	1b	2	0	0	0	0
57	1e	2	0	0	0	0
57	1f	2	0	0	0	0
57	1h	1	0	0	0	0
57	1l	2	0	0	0	0
57	1m	1	0	0	0	0
57	1n	2	0	0	0	0
57	1s	1	0	0	0	0
57	1t	1	0	0	0	0
57	1v	1	0	0	0	0
57	1w	7	0	0	0	0
57	1x	12	0	0	0	0
57	20	2	0	0	0	0
57	21	1	0	0	0	0
57	23	4	0	0	0	0
57	25	5	0	0	0	0
57	26	1	0	0	0	0
57	27	3	0	0	0	0
57	28	2	0	0	0	0
57	2A	861	0	0	0	0
57	2B	20	0	0	0	0
57	2D	5	0	0	0	0
57	2E	8	0	0	0	0
57	2F	7	0	0	0	0
57	2G	1	0	0	0	0
57	2N	1	0	0	0	0
57	2O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2P	2	0	0	0	0
57	2Q	3	0	0	0	0
57	2R	2	0	0	0	0
57	2T	4	0	0	0	0
57	2U	2	0	0	0	0
57	2V	3	0	0	0	0
57	2W	2	0	0	0	0
57	2X	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	225	0	0	0	0
57	2d	2	0	0	0	0
57	2e	1	0	0	0	0
57	2f	2	0	0	0	0
57	2i	1	0	0	0	0
57	2j	1	0	0	0	0
57	2k	1	0	0	0	0
57	2l	3	0	0	0	0
57	2q	2	0	0	0	0
57	2r	1	0	0	0	0
57	2t	1	0	0	0	0
57	2v	4	0	0	0	0
57	2w	4	0	0	0	0
57	2x	4	0	0	0	0
57	2y	1	0	0	0	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	1A	20	0	11	1	0
59	2A	20	0	11	0	0
60	14	1	0	0	0	0
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2d	8	0	0	1	0
62	10	12	0	0	1	0
62	11	10	0	0	1	0
62	12	3	0	0	1	0
62	13	6	0	0	0	0
62	14	1	0	0	0	0
62	15	6	0	0	0	0
62	16	5	0	0	0	0
62	17	9	0	0	1	0
62	18	10	0	0	0	0
62	1A	2086	0	0	75	0
62	1B	65	0	0	0	0
62	1D	28	0	0	0	0
62	1E	28	0	0	1	0
62	1F	17	0	0	1	0
62	1G	7	0	0	1	0
62	1H	2	0	0	0	0
62	1N	5	0	0	0	0
62	1O	6	0	0	0	0
62	1P	21	0	0	0	0
62	1Q	7	0	0	0	0
62	1R	7	0	0	0	0
62	1S	3	0	0	0	0
62	1T	9	0	0	0	0
62	1U	13	0	0	1	0
62	1V	9	0	0	0	0
62	1W	5	0	0	0	0
62	1X	6	0	0	1	0
62	1Y	3	0	0	1	0
62	1Z	1	0	0	0	0
62	1a	331	0	0	28	0
62	1b	1	0	0	0	0
62	1d	1	0	0	0	0
62	1e	1	0	0	0	0
62	1l	3	0	0	0	0
62	1m	2	0	0	1	0
62	1q	3	0	0	0	0
62	1u	1	0	0	1	0
62	1v	6	0	0	0	0
62	1w	9	0	0	2	0
62	1x	11	0	0	0	0
62	1y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	20	1	0	0	0	0
62	21	8	0	0	0	0
62	23	2	0	0	0	0
62	25	3	0	0	0	0
62	27	5	0	0	0	0
62	28	3	0	0	0	0
62	29	1	0	0	0	0
62	2A	1147	0	0	73	0
62	2B	21	0	0	0	0
62	2D	18	0	0	0	0
62	2E	14	0	0	0	0
62	2F	12	0	0	0	0
62	2I	1	0	0	0	0
62	2N	2	0	0	0	0
62	2O	2	0	0	0	0
62	2P	10	0	0	1	0
62	2Q	1	0	0	0	0
62	2R	5	0	0	0	0
62	2T	3	0	0	0	0
62	2U	3	0	0	0	0
62	2W	4	0	0	0	0
62	2X	5	0	0	0	0
62	2Z	2	0	0	0	0
62	2a	205	0	0	21	0
62	2c	1	0	0	0	0
62	2i	1	0	0	0	0
62	2j	3	0	0	0	0
62	2l	4	0	0	1	0
62	2r	1	0	0	0	0
62	2t	2	0	0	0	0
62	2v	2	0	0	0	0
62	2w	1	0	0	0	0
62	2x	7	0	0	0	0
All	All	300046	0	196682	4057	1

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 (4057) 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	1.25	1.32
1:1A:1054:A:N6	1:1A:1105:U:H3	1.39	1.19
54:1w:50:A:N6	54:1w:64:U:H3	1.43	1.16
54:2w:8:4SU:HN3	54:2w:14:A:H62	1.08	1.02
1:1A:1082:U:O4	1:1A:1086:A:N1	1.95	0.98
32:2a:1029:C:C4	32:2a:1032:G:N1	2.32	0.98
1:1A:1055:G:H1	1:1A:1104:C:H42	0.99	0.98
32:2a:1025:U:H3	32:2a:1036:G:H1	1.08	0.96
1:2A:2138:C:N4	1:2A:2153:G:H1	1.65	0.94
1:2A:1204:A:H2	1:2A:1241:A:H62	1.17	0.93
32:2a:931:C:H42	32:2a:1386:G:H1	1.15	0.93
10:2O:48:PRO:HB3	32:2a:1422:G:H5”	1.48	0.93
1:1A:1798:U:H5’	3:1D:259:THR:HG22	1.50	0.92
1:2A:1798:U:H5’	3:2D:259:THR:HG22	1.50	0.92
1:2A:2138:C:H42	1:2A:2153:G:H1	1.07	0.92
1:1A:2100:G:H1	1:1A:2189:U:H3	0.93	0.92
54:2w:50:A:N6	54:2w:64:U:H3	1.66	0.92
1:1A:2136:C:N3	1:1A:2155:G:C2	2.39	0.90
5:1F:53:THR:HG22	5:1F:55:GLY:H	1.35	0.90
54:2w:49:G:H1	54:2w:65:U:H3	0.92	0.90
32:2a:997:U:H3	32:2a:1044:A:H61	1.18	0.90
1:1A:2427:C:OP1	62:1A:4102:HOH:O	1.91	0.90
54:2w:50:A:H61	54:2w:64:U:H3	1.14	0.90
15:1T:54:ARG:HA	15:1T:59:THR:HB	1.54	0.87
1:2A:2110:G:OP1	1:2A:2118:U:N3	2.06	0.87
41:2j:7:LYS:HG3	41:2j:71:LEU:HD23	1.55	0.87
1:1A:1058:G:H1	1:1A:1080:C:N4	1.72	0.87
33:2b:54:THR:HG22	33:2b:199:TYR:HB3	1.57	0.87
1:2A:2100:G:H1	1:2A:2189:U:H3	0.86	0.86
1:1A:1055:G:H1	1:1A:1104:C:N4	1.72	0.86
1:2A:1670:C:OP1	62:2A:3903:HOH:O	1.93	0.86
54:2w:49:G:N2	54:2w:65:U:O2	2.08	0.85
1:1A:1058:G:N2	1:1A:1080:C:N3	2.25	0.84
32:2a:1089:G:H1	32:2a:1096:C:H42	1.24	0.83
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.25	0.83
1:1A:1065:U:O2	1:1A:1073:A:N6	2.12	0.83
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.61	0.83
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.59	0.83
1:2A:2122:U:H3	1:2A:2176:A:H61	1.24	0.83
1:1A:1469:A:OP2	62:1A:4103:HOH:O	1.95	0.83
1:1A:1811:G:N7	62:1A:4118:HOH:O	2.10	0.83
32:2a:1104:G:H4’	33:2b:111:ARG:HE	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2g:115:ARG:HG2	38:2g:118:VAL:HG12	1.59	0.83
54:2w:14:A:N6	54:2w:21:A:H2	1.77	0.83
1:1A:1332:G:OP1	62:1A:4104:HOH:O	1.97	0.82
40:1i:17:VAL:HG21	40:1i:81:ILE:HG22	1.61	0.82
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.24	0.82
1:2A:2133:G:O2'	1:2A:2157:G:N2	2.12	0.82
1:1A:1058:G:H1	1:1A:1080:C:H42	1.26	0.81
1:1A:1069:A:H5'	1:1A:1070:A:H8	1.45	0.81
1:1A:2499:C:OP1	62:1A:4105:HOH:O	1.98	0.81
1:2A:1671:U:OP2	62:2A:3903:HOH:O	1.99	0.81
1:1A:2822:G:OP2	62:1A:4106:HOH:O	1.99	0.81
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.64	0.80
32:2a:73:G:H1	32:2a:96:U:H3	1.29	0.80
54:2w:8:4SU:HN3	54:2w:14:A:N6	1.78	0.80
32:1a:664:G:H22	32:1a:741:G:H1	1.26	0.80
29:27:24:THR:HG22	29:27:27:GLY:H	1.46	0.79
42:1k:79:SER:HA	42:1k:104:GLN:HB3	1.63	0.79
1:2A:1840:G:OP2	62:2A:3904:HOH:O	2.01	0.79
1:1A:2126:A:N6	1:1A:2163:C:O4'	2.16	0.79
1:1A:2136:C:N4	1:1A:2155:G:C6	2.50	0.79
1:2A:2133:G:HO2'	1:2A:2157:G:N2	1.80	0.79
21:1Z:152:ALA:HB1	21:1Z:163:LEU:HD11	1.65	0.79
1:2A:2134:A:H62	1:2A:2157:G:H4'	1.47	0.79
32:1a:1505:G:OP2	62:1a:1901:HOH:O	2.00	0.79
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.00	0.78
42:1k:48:ILE:HD12	42:1k:63:LEU:HB2	1.63	0.78
36:2e:89:ILE:HG12	36:2e:135:THR:HG22	1.65	0.78
29:17:24:THR:HG22	29:17:27:GLY:H	1.46	0.78
1:1A:2702:U:OP2	62:1A:4107:HOH:O	2.01	0.78
1:1A:307:G:N7	62:1A:4132:HOH:O	2.17	0.78
2:2B:22:U:H3	2:2B:61:G:H1	1.31	0.78
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.16	0.78
40:2i:4:TYR:HB2	40:2i:19:LEU:HB2	1.64	0.78
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.19	0.77
1:2A:2448:A:OP1	62:2A:3905:HOH:O	2.01	0.77
54:2w:14:A:N6	54:2w:21:A:C2	2.50	0.77
1:1A:2550:G:OP1	62:1A:4109:HOH:O	2.02	0.77
1:1A:11:G:H2'	1:1A:12:U:H5'	1.67	0.77
1:1A:736:C:OP1	62:1A:4110:HOH:O	2.03	0.77
56:1y:49:G:H1	56:1y:65:U:H3	0.80	0.77
1:1A:1058:G:N1	1:1A:1080:C:N4	2.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2125:G:N3	1:2A:2173:A:N6	2.33	0.76
11:2P:126:VAL:HG12	11:2P:148:LEU:HD22	1.67	0.76
32:2a:79:G:H1	32:2a:90:U:H3	1.31	0.76
1:1A:1014:U:OP2	62:1A:4108:HOH:O	2.01	0.76
7:1H:3:ARG:HH11	7:1H:5:GLY:H	1.31	0.76
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.18	0.76
1:1A:880:G:H2'	1:1A:881:G:H8	1.50	0.76
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.67	0.76
54:1w:75:C:OP1	62:1w:201:HOH:O	2.03	0.76
50:2s:77:THR:HG23	50:2s:78:ARG:HG3	1.68	0.76
32:1a:975:A:H4'	32:1a:976:G:H5"	1.68	0.76
1:1A:1060:U:H3	1:1A:1088:A:H8	1.31	0.76
32:2a:596:C:OP2	62:2a:1901:HOH:O	2.03	0.76
32:2a:972:C:O2'	41:2j:55:LYS:O	2.03	0.76
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.49	0.76
32:1a:1224:G:OP1	62:1a:1902:HOH:O	2.03	0.76
1:2A:1253:A:OP1	62:2A:3907:HOH:O	2.04	0.75
1:2A:1352:U:OP2	62:2A:3906:HOH:O	2.03	0.75
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	1.68	0.75
42:2k:99:GLN:HG2	42:2k:105:VAL:HG21	1.68	0.75
26:14:16:CYS:SG	26:14:17:GLY:N	2.59	0.75
1:2A:2319:G:H22	14:2S:3:ARG:HH11	1.34	0.75
13:2R:103:ARG:NH1	13:2R:108:GLY:O	2.18	0.75
1:1A:2128:C:N3	1:1A:2160:G:N2	2.33	0.75
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.20	0.75
1:2A:2129:C:N4	1:2A:2159:G:H1	1.85	0.75
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.68	0.75
6:1G:19:LEU:HD13	6:1G:32:PRO:HD2	1.68	0.74
11:1P:126:VAL:HG12	11:1P:148:LEU:HD22	1.66	0.74
3:2D:125:ILE:HB	37:2f:81:ILE:HD11	1.67	0.74
10:2O:49:ARG:NH2	32:2a:1423:G:OP1	2.18	0.74
32:2a:953:G:H5'	32:2a:965:A:H61	1.52	0.74
44:1m:3:ARG:HD2	44:1m:9:ILE:HG12	1.69	0.74
44:2m:37:THR:O	44:2m:55:ARG:NH1	2.20	0.74
32:1a:573:A:OP2	62:1a:1903:HOH:O	2.05	0.74
21:2Z:100:VAL:HG21	21:2Z:134:PRO:HG2	1.69	0.74
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.67	0.74
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.21	0.74
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.70	0.74
32:1a:1198:G:OP1	62:1a:1904:HOH:O	2.06	0.74
1:2A:805:G:OP1	62:2A:3909:HOH:O	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:25:ARG:HB3	14:2S:40:ILE:HB	1.70	0.74
1:1A:2122:U:O4	1:1A:2176:A:N1	2.21	0.74
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.21	0.74
1:1A:2629:A:O2'	1:1A:2630:G:OP2	2.06	0.73
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.68	0.73
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.70	0.73
32:2a:573:A:OP2	62:2a:1902:HOH:O	2.04	0.73
1:1A:2133:G:H1	1:1A:2157:G:H1'	1.52	0.73
1:1A:2810:A:N6	1:1A:2891:G:O2'	2.21	0.73
32:1a:79:G:C6	32:1a:90:U:O2	2.42	0.73
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.20	0.73
6:2G:73:ALA:HB3	6:2G:85:GLY:H	1.52	0.73
41:2j:42:THR:HG22	41:2j:68:HIS:HA	1.70	0.73
54:2w:17:G:O2'	54:2w:57:G:N2	2.19	0.73
1:2A:1689:A:H62	1:2A:1698:A:H2	1.36	0.73
34:2c:156:ARG:HH21	34:2c:161:GLU:HA	1.53	0.73
36:2e:20:GLN:NE2	36:2e:21:ALA:O	2.19	0.73
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.68	0.73
1:2A:1271:G:OP2	62:2A:3910:HOH:O	2.06	0.73
1:2A:1648:C:OP1	62:2A:3910:HOH:O	2.07	0.73
36:1e:78:HIS:HE1	36:1e:143:ARG:H	1.35	0.73
32:2a:1089:G:H1	32:2a:1096:C:N4	1.86	0.73
1:1A:2840:C:OP2	62:1A:4114:HOH:O	2.05	0.73
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.70	0.73
1:2A:1313:U:OP1	62:2A:3908:HOH:O	2.05	0.73
1:1A:1993:U:OP2	62:1A:4111:HOH:O	2.04	0.73
34:2c:123:GLN:HA	34:2c:126:ARG:HD2	1.69	0.73
1:2A:1024:G:OP2	62:2A:3911:HOH:O	2.06	0.73
7:2H:98:LEU:HD11	7:2H:125:VAL:H	1.54	0.73
36:2e:5:ASP:N	36:2e:5:ASP:OD1	2.22	0.73
1:1A:2409:G:O2'	62:1A:4113:HOH:O	2.05	0.72
1:2A:2428:G:N7	62:2A:3951:HOH:O	2.21	0.72
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.22	0.72
35:2d:191:ARG:NH1	35:2d:191:ARG:O	2.22	0.72
1:1A:78:A:N7	62:1A:4153:HOH:O	2.21	0.72
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.71	0.72
1:1A:2407:G:OP1	62:1A:4115:HOH:O	2.06	0.72
1:1A:2128:C:N4	1:1A:2160:G:H1	1.88	0.72
32:1a:123:C:OP1	32:1a:311:C:O2'	2.06	0.72
1:2A:1568:G:N7	62:2A:3957:HOH:O	2.22	0.72
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2135:A:N1	1:2A:2156:G:O2'	2.22	0.72
1:2A:2260:C:OP1	62:2A:3912:HOH:O	2.07	0.72
32:2a:597:G:OP2	62:2a:1901:HOH:O	2.08	0.72
1:2A:2049:G:N7	62:2A:3950:HOH:O	2.21	0.72
32:2a:1029:C:C2	32:2a:1032:G:N2	2.58	0.72
40:2i:121:ARG:NH1	40:2i:122:ALA:O	2.23	0.72
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.72	0.72
32:2a:931:C:N4	32:2a:1386:G:H1	1.86	0.72
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.72	0.72
37:2f:6:VAL:HG13	37:2f:90:VAL:HG22	1.70	0.72
43:2l:71:PRO:O	43:2l:102:ARG:NH1	2.22	0.72
1:2A:2138:C:N3	1:2A:2153:G:N2	2.34	0.72
1:1A:2849:U:OP2	15:1T:95:ARG:NH1	2.23	0.72
1:1A:2096:U:H3	1:1A:2193:G:H1	1.38	0.71
32:1a:1027:C:C2	32:1a:1034:G:N2	2.57	0.71
1:2A:2518:A:OP2	62:2A:3913:HOH:O	2.07	0.71
2:2B:20:C:N4	2:2B:63:G:O6	2.19	0.71
1:1A:2821:A:OP2	62:1A:4106:HOH:O	2.09	0.71
1:2A:2079:U:OP1	23:21:21:ARG:NH2	2.20	0.71
12:2Q:78:PRO:HG2	12:2Q:81:VAL:HG11	1.72	0.71
54:2w:8:4SU:S4	54:2w:14:A:N7	2.63	0.71
1:2A:89:G:H3'	1:2A:90:U:H5"	1.72	0.71
1:1A:2128:C:N4	1:1A:2160:G:N1	2.38	0.71
34:2c:88:ARG:HA	34:2c:91:LEU:HG	1.72	0.71
56:2y:14:A:H61	56:2y:21:A:H2	1.38	0.71
40:1i:53:VAL:O	40:1i:55:ALA:N	2.24	0.71
1:2A:2131:G:OP2	1:2A:2131:G:N2	2.14	0.71
1:1A:630:G:OP2	30:18:15:LYS:NZ	2.21	0.71
1:1A:2749:A:H5"	7:1H:3:ARG:NH2	2.05	0.71
32:2a:1105:A:H2'	32:2a:1106:G:H8	1.55	0.71
32:2a:1226:C:OP2	44:2m:91:ARG:NH1	2.24	0.71
56:2y:48:C:O2'	56:2y:49:G:OP2	2.09	0.71
1:1A:1176:G:N2	1:1A:1178:C:OP2	2.24	0.71
32:1a:79:G:O6	32:1a:90:U:O2	2.08	0.71
21:2Z:5:LEU:HB2	21:2Z:47:VAL:HG21	1.70	0.71
1:1A:387:U:O4	62:1A:4112:HOH:O	2.05	0.71
32:2a:1108:G:O6	62:2a:1903:HOH:O	2.09	0.71
32:2a:1346:A:H61	32:2a:1374:A:H3'	1.55	0.71
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.64	0.70
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.25	0.70
50:2s:49:ILE:HG22	50:2s:62:ILE:HD11	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:956:G:H5"	12:2Q:77:LYS:HD2	1.74	0.70
27:25:40:LYS:NZ	27:25:44:THR:O	2.24	0.70
32:2a:662:G:O2'	32:2a:836:G:OP1	2.08	0.70
32:2a:1119:C:OP2	40:2i:9:ARG:NH2	2.23	0.70
40:2i:3:GLN:HE21	40:2i:20:ARG:HE	1.39	0.70
1:2A:2129:C:N4	1:2A:2159:G:N1	2.40	0.70
40:2i:86:VAL:HG11	40:2i:93:ARG:HE	1.57	0.70
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.25	0.70
56:2y:14:A:N6	56:2y:21:A:H2	1.89	0.70
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.74	0.70
44:1m:3:ARG:HG2	44:1m:8:GLU:HA	1.74	0.70
1:2A:962:G:OP1	62:2A:3915:HOH:O	2.09	0.70
32:2a:562:C:H1'	43:2l:15:ARG:HB3	1.74	0.70
33:2b:48:MET:HA	33:2b:51:LEU:HB2	1.73	0.70
56:1y:53:G:H1	56:1y:61:C:H42	1.39	0.70
41:2j:47:PHE:HB2	41:2j:63:PHE:HB2	1.73	0.70
1:1A:2183:C:H2'	1:1A:2184:G:C8	2.27	0.70
26:14:58:ARG:HE	50:1s:68:GLY:H	1.39	0.70
32:1a:1030(A):G:O2'	32:1a:1031:G:N2	2.24	0.70
1:2A:2122:U:H3	1:2A:2176:A:N6	1.90	0.70
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.73	0.70
36:2e:43:LEU:HD22	36:2e:136:MET:HG3	1.73	0.70
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.73	0.70
32:2a:997:U:H3	32:2a:1044:A:N6	1.87	0.70
32:2a:1316:G:N7	50:2s:7:LYS:NZ	2.40	0.70
6:1G:122:PRO:HB3	6:1G:170:ARG:HH12	1.57	0.70
33:1b:122:PHE:HE2	33:1b:139:LYS:HD2	1.57	0.70
1:2A:1443:G:N7	62:2A:3960:HOH:O	2.24	0.70
15:2T:107:ASP:OD2	15:2T:111:ARG:NH1	2.25	0.70
44:2m:82:MET:HE3	44:2m:93:ARG:HB3	1.73	0.70
1:1A:2134:A:N3	1:1A:2159:G:O2'	2.25	0.70
3:1D:2:ALA:N	3:1D:200:ASP:OD2	2.25	0.70
1:2A:2129:C:N3	1:2A:2159:G:N2	2.35	0.70
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.26	0.70
33:2b:63:MET:HG3	33:2b:225:ALA:HB1	1.74	0.70
32:1a:79:G:O6	32:1a:90:U:C2	2.45	0.69
52:1u:5:ASP:OD2	62:1u:101:HOH:O	2.10	0.69
6:2G:114:ILE:HA	6:2G:140:ILE:HD11	1.74	0.69
8:2I:55:ALA:HA	8:2I:58:LEU:HB3	1.72	0.69
38:2g:78:ARG:HH21	38:2g:79:ARG:HE	1.39	0.69
32:2a:1102:A:O3'	33:2b:96:ARG:NH2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:765:G:H1	32:2a:812:C:HO2'	1.39	0.69
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.73	0.69
7:2H:51:ARG:NH2	7:2H:53:GLU:OE1	2.25	0.69
1:2A:622:G:OP2	11:2P:108:LYS:NZ	2.25	0.69
1:1A:1701:A:OP2	62:1A:4116:HOH:O	2.09	0.69
5:1F:89:VAL:O	62:1F:401:HOH:O	2.11	0.69
1:2A:1365:A:O2'	23:21:11:ARG:NH1	2.26	0.69
14:2S:67:ARG:HG2	14:2S:71:ARG:HD2	1.75	0.69
32:2a:1270:C:OP2	52:2u:24:ARG:NH2	2.26	0.69
1:1A:671:C:N4	62:1A:4173:HOH:O	2.25	0.69
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.25	0.69
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.25	0.69
1:2A:1973:G:OP1	62:2A:3918:HOH:O	2.11	0.69
1:2A:2063:C:OP1	62:2A:3919:HOH:O	2.11	0.69
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.58	0.69
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.57	0.69
35:2d:175:SER:HB3	35:2d:186:LEU:HD11	1.74	0.69
36:2e:8:GLU:HG2	36:2e:34:VAL:HG12	1.75	0.69
43:2l:53:ARG:HG3	43:2l:93:LEU:HD21	1.75	0.69
1:2A:938:G:OP2	30:28:52:LYS:NZ	2.20	0.69
38:2g:152:ALA:O	38:2g:155:ARG:NH1	2.25	0.69
19:1X:88:LYS:NZ	19:1X:90:GLU:OE1	2.26	0.69
32:2a:1521:G:N3	62:2a:1919:HOH:O	2.24	0.69
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.25	0.68
1:1A:2319:G:H1	14:1S:3:ARG:HD3	1.58	0.68
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.11	0.68
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.25	0.68
19:2X:60:ARG:HH22	29:27:47:ARG:HH11	1.39	0.68
32:2a:944:G:OP1	62:2a:1905:HOH:O	2.11	0.68
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.26	0.68
1:2A:2819:G:N7	62:2A:3965:HOH:O	2.26	0.68
1:1A:762:U:OP1	62:1A:4117:HOH:O	2.10	0.68
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.28	0.68
40:1i:110:GLU:OE2	40:1i:113:LYS:NZ	2.26	0.68
1:2A:2697:G:O6	62:2A:3914:HOH:O	2.08	0.68
5:2F:116:ASP:OD2	11:2P:1:MET:N	2.25	0.68
32:2a:1004:A:H5"	32:2a:1024:G:H22	1.57	0.68
32:2a:1396:A:OP2	62:2a:1908:HOH:O	2.12	0.68
41:1j:5:ARG:NH2	41:1j:73:ASP:OD2	2.27	0.68
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.26	0.68
1:2A:2006:C:OP2	62:2A:3921:HOH:O	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.27	0.68
35:2d:157:LEU:O	35:2d:161:ASN:ND2	2.27	0.68
36:2e:100:VAL:O	36:2e:107:ARG:NH2	2.23	0.68
56:2y:8:4SU:O2	56:2y:21:A:C2	2.47	0.68
19:1X:44:GLU:OE2	62:1X:201:HOH:O	2.10	0.68
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.20	0.68
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.27	0.68
1:2A:1023:U:OP2	62:2A:3911:HOH:O	2.11	0.68
1:2A:2206:G:H5"	1:2A:2207:G:N7	2.08	0.68
28:26:19:ARG:HH12	28:26:52:VAL:HG21	1.59	0.68
41:1j:62:HIS:HB3	45:1n:59:ALA:HB3	1.76	0.68
1:1A:382:G:OP2	62:1A:4119:HOH:O	2.12	0.68
1:1A:2120:G:H1	1:1A:2178:C:H42	1.42	0.68
1:2A:1169:G:H1	1:2A:1180:C:H42	1.39	0.68
1:2A:1297:C:OP2	62:2A:3917:HOH:O	2.10	0.68
32:2a:117:G:OP2	62:2a:1904:HOH:O	2.11	0.68
38:2g:113:GLU:HG3	38:2g:118:VAL:HG13	1.76	0.68
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.09	0.68
32:2a:1255:G:OP1	41:2j:45:ARG:NH2	2.27	0.68
1:2A:2060:A:N3	62:2A:3964:HOH:O	2.25	0.67
32:2a:473:G:H2'	32:2a:474:G:H8	1.60	0.67
34:2c:39:ILE:HG22	34:2c:43:LEU:HD11	1.76	0.67
34:2c:40:ARG:HA	34:2c:43:LEU:HD12	1.75	0.67
1:1A:887:A:H2	1:1A:889:C:H3'	1.59	0.67
1:1A:1054:A:H61	1:1A:1105:U:H3	0.72	0.67
32:2a:643:C:H2'	32:2a:644:G:H8	1.60	0.67
1:2A:2134:A:H1'	1:2A:2158:A:C6	2.30	0.67
26:24:40:HIS:HD2	26:24:41:PRO:HD2	1.57	0.67
1:1A:1315:C:OP2	62:1A:4104:HOH:O	2.13	0.67
1:1A:2350:C:OP2	62:1A:4121:HOH:O	2.12	0.67
32:1a:393:A:OP1	62:1a:1905:HOH:O	2.12	0.67
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.77	0.67
1:2A:775:G:O3'	62:2A:3920:HOH:O	2.11	0.67
1:2A:2126:A:N3	1:2A:2127:G:H1'	2.10	0.67
1:2A:2691:C:OP2	62:2A:3924:HOH:O	2.12	0.67
62:1A:4106:HOH:O	4:1E:110:GLY:O	2.13	0.67
26:14:46:GLN:O	26:14:48:ARG:N	2.27	0.67
32:2a:533:A:OP1	62:2a:1907:HOH:O	2.11	0.67
32:2a:903:G:OP1	62:2a:1906:HOH:O	2.11	0.67
1:1A:826:U:OP1	62:1A:4102:HOH:O	2.11	0.67
32:1a:1348:U:H4'	40:1i:120:ARG:HD2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:204:ASN:OD1	33:1b:206:ASP:N	2.25	0.67
1:1A:1071:G:H1'	1:1A:1089:G:H2'	1.76	0.67
34:1c:56:ASP:HB2	34:1c:67:THR:HB	1.77	0.67
55:1x:47:U:H5'	55:1x:48:C:H5'	1.75	0.67
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.27	0.67
35:2d:104:VAL:HG21	35:2d:140:VAL:HG21	1.77	0.67
1:2A:2143:C:H42	1:2A:2148:G:H1	1.41	0.67
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.28	0.67
1:1A:2277:G:OP2	22:10:10:THR:HG21	1.95	0.67
1:2A:2130:U:O2	1:2A:2134:A:O2'	2.12	0.67
33:2b:47:THR:O	33:2b:51:LEU:N	2.28	0.67
1:2A:271(G):C:H2'	1:2A:271(H):G:C8	2.30	0.66
32:1a:324:G:N7	62:1a:1931:HOH:O	2.27	0.66
56:1y:66:C:H2'	56:1y:67:G:C8	2.30	0.66
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.76	0.66
1:1A:1082:U:N3	1:1A:1086:A:N6	2.08	0.66
1:1A:2222:G:OP2	62:1A:4123:HOH:O	2.13	0.66
1:2A:804:A:OP1	62:2A:3909:HOH:O	2.12	0.66
7:2H:9:ILE:HB	7:2H:50:VAL:HG23	1.76	0.66
1:1A:2131:G:OP2	1:1A:2158:A:N6	2.25	0.66
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.10	0.66
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	1.78	0.66
1:2A:248:G:OP1	62:2A:3928:HOH:O	2.14	0.66
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.59	0.66
26:24:46:GLN:HG2	26:24:48:ARG:H	1.59	0.66
35:2d:60:GLU:HG3	35:2d:202:LEU:HD12	1.76	0.66
35:2d:156:GLU:HG3	35:2d:159:ARG:HH21	1.60	0.66
43:2l:117:ARG:HB3	43:2l:122:THR:HB	1.77	0.66
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.61	0.66
2:2B:75:G:N2	21:2Z:87:ASP:OD1	2.28	0.66
50:2s:38:SER:HB2	50:2s:71:LEU:HD22	1.78	0.66
27:15:40:LYS:NZ	27:15:44:THR:O	2.28	0.66
32:1a:236:G:OP1	48:1q:40:LYS:NZ	2.29	0.66
32:2a:1310:G:H5'	44:2m:77:ASN:HD21	1.61	0.66
32:2a:1106:G:H5"	34:2c:172:ARG:HG2	1.77	0.66
9:1N:62:VAL:HG22	9:1N:66:LYS:HD2	1.78	0.66
13:1R:86:ARG:NH2	13:1R:87:TYR:OH	2.27	0.66
32:1a:557:G:OP1	62:1a:1907:HOH:O	2.14	0.66
50:1s:27:GLU:HB2	50:1s:28:LYS:HB3	1.77	0.66
1:2A:854:G:H2'	1:2A:855:G:H8	1.61	0.66
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2625:G:O6	62:2A:3916:HOH:O	2.09	0.66
32:2a:352:C:O2'	32:2a:354:G:OP1	2.09	0.66
44:2m:80:ARG:HH22	50:2s:69:HIS:HE1	1.43	0.66
1:1A:1062:G:H1	1:1A:1077:A:H61	1.43	0.65
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.29	0.65
33:1b:33:TYR:HB2	33:1b:43:ASP:HB2	1.77	0.65
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.13	0.65
1:2A:1952:A:OP1	10:2O:44:LYS:NZ	2.27	0.65
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.29	0.65
35:2d:98:GLU:OE2	35:2d:103:ASN:ND2	2.29	0.65
5:1F:116:ASP:OD2	11:1P:1:MET:N	2.25	0.65
1:2A:1466:G:HO2'	1:2A:1546:C:HO2'	1.41	0.65
32:1a:574:A:OP2	62:1a:1903:HOH:O	2.13	0.65
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.11	0.65
32:2a:975:A:H4'	32:2a:976:G:H5"	1.78	0.65
1:1A:2161:C:HO2'	1:1A:2162:G:H8	1.44	0.65
1:2A:449:A:OP2	62:2A:3929:HOH:O	2.15	0.65
11:2P:87:ASP:O	11:2P:90:ARG:NH1	2.29	0.65
32:2a:157:G:H1	32:2a:164:U:H3	1.43	0.65
1:2A:2114:A:H2	1:2A:2171:A:H61	1.45	0.65
32:2a:977:A:O3'	32:2a:980:C:N4	2.30	0.65
32:2a:1286:A:H8	32:2a:1287:A:H4'	1.60	0.65
34:2c:44:GLU:HA	34:2c:52:LEU:HD23	1.78	0.65
1:1A:1468:C:OP1	62:1A:4125:HOH:O	2.14	0.65
1:1A:2303:G:O6	62:1A:4120:HOH:O	2.12	0.65
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.79	0.65
32:1a:184:G:H2'	32:1a:185:A:H8	1.62	0.65
1:2A:531:C:OP1	1:2A:561:G:N1	2.30	0.65
44:2m:23:TYR:HB3	44:2m:67:GLU:HA	1.76	0.65
46:2o:67:LEU:HD11	46:2o:87:ILE:HD12	1.78	0.65
1:2A:948:G:OP1	62:2A:3915:HOH:O	2.14	0.65
1:2A:2592:G:OP2	62:2A:3927:HOH:O	2.13	0.65
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.78	0.65
32:2a:1125:U:OP1	41:2j:35:SER:OG	2.15	0.65
1:1A:2141:G:O6	1:1A:2150:U:O2	2.15	0.65
33:1b:48:MET:HA	33:1b:51:LEU:HB2	1.79	0.65
41:1j:49:VAL:HB	45:1n:41:ARG:HB2	1.79	0.65
1:2A:300:A:OP2	20:2Y:86:ARG:NH1	2.28	0.65
13:2R:97:VAL:HG22	13:2R:114:VAL:HG12	1.79	0.65
17:2V:1:MET:HE3	17:2V:43:GLU:H	1.61	0.65
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1346:A:N1	32:2a:1374:A:H5”	2.11	0.65
36:1e:74:GLY:HA3	36:1e:116:THR:HG22	1.79	0.65
1:2A:2759:G:OP2	62:2A:3930:HOH:O	2.15	0.65
7:2H:159:GLU:HG3	7:2H:169:VAL:HG11	1.78	0.65
1:1A:1300:U:H4’	1:1A:1301:A:H5”	1.78	0.64
62:1A:4106:HOH:O	13:1R:3:HIS:NE2	2.29	0.64
25:13:55:ARG:C	25:13:55:ARG:HE	2.05	0.64
44:1m:19:LEU:HD21	44:1m:56:LEU:HD21	1.79	0.64
12:2Q:111:GLU:OE2	12:2Q:133:ARG:NH2	2.25	0.64
23:21:52:ARG:HH21	23:21:57:GLU:HB2	1.61	0.64
42:2k:18:ARG:NH2	42:2k:35:PRO:O	2.30	0.64
1:1A:2131:G:N2	1:1A:2133:G:N3	2.46	0.64
32:1a:677:U:H3	32:1a:713:G:H22	1.45	0.64
1:2A:2100:G:H2’	1:2A:2101:G:C8	2.33	0.64
24:22:22:GLU:OE2	24:22:68:ARG:NH2	2.29	0.64
34:2c:6:HIS:HD2	34:2c:8:ILE:H	1.44	0.64
32:1a:421:U:O4	34:1c:127:ARG:NH2	2.27	0.64
32:1a:964:A:OP1	62:1a:1908:HOH:O	2.15	0.64
32:2a:1289:A:O2’	38:2g:35:LYS:NZ	2.30	0.64
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.30	0.64
1:1A:878:A:N6	1:1A:899:A:O2’	2.23	0.64
10:1O:48:PRO:HB3	32:1a:1422:G:H5”	1.79	0.64
32:1a:673:G:H2’	32:1a:674:G:C8	2.32	0.64
33:1b:166:ASP:HB3	33:1b:169:LYS:HB3	1.80	0.64
42:1k:34:ASP:HB2	42:1k:35:PRO:HD2	1.78	0.64
1:2A:855:G:O2’	22:20:27:GLU:OE2	2.14	0.64
6:2G:7:LEU:HD13	6:2G:104:GLU:HA	1.79	0.64
32:2a:1302:U:OP2	44:2m:21:TYR:OH	2.14	0.64
32:2a:1348:U:H4’	40:2i:120:ARG:HD2	1.78	0.64
32:1a:1385:G:N7	62:1a:1939:HOH:O	2.30	0.64
1:1A:376:C:OP1	62:1A:4126:HOH:O	2.14	0.64
32:1a:1436:U:OP1	51:1t:23:ARG:NH2	2.30	0.64
34:2c:37:GLN:NE2	45:2n:52:GLN:OE1	2.22	0.64
50:2s:32:LYS:HB2	50:2s:57:HIS:CD2	2.32	0.64
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.79	0.64
32:2a:664:G:H22	32:2a:741:G:H1	1.44	0.64
32:2a:1139:G:N2	32:2a:1142:G:O6	2.21	0.64
52:1u:17:THR:O	52:1u:22:ARG:NH1	2.31	0.64
6:2G:114:ILE:HB	6:2G:117:PHE:HD1	1.63	0.64
32:1a:532:A:N6	32:1a:1206:G:O2’	2.30	0.64
51:1t:42:GLN:NE2	51:1t:46:GLU:OE2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1647:G:OP1	62:1A:4129:HOH:O	2.15	0.64
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.30	0.64
47:1p:20:VAL:HG21	47:1p:32:TYR:CG	2.33	0.64
1:2A:2318:G:H21	14:2S:3:ARG:NE	1.96	0.64
13:2R:67:LEU:HD13	13:2R:76:VAL:HG21	1.80	0.64
1:1A:1053:C:H42	1:1A:1106:G:H1	1.46	0.63
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.14	0.63
22:20:23:VAL:HG22	22:20:38:VAL:HG22	1.79	0.63
1:1A:2226:C:OP2	62:1A:4130:HOH:O	2.15	0.63
33:1b:52:GLU:OE2	33:1b:56:ARG:NH2	2.31	0.63
47:1p:20:VAL:HG23	47:1p:35:LYS:HA	1.80	0.63
1:2A:2682:U:OP2	62:2A:3931:HOH:O	2.15	0.63
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.33	0.63
9:2N:43:THR:HG23	16:2U:64:ARG:HH11	1.61	0.63
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.31	0.63
41:2j:11:PHE:HE1	41:2j:67:THR:HG22	1.62	0.63
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.33	0.63
32:1a:78:G:C6	32:1a:91:C:N4	2.66	0.63
32:2a:650:G:N7	62:2a:1924:HOH:O	2.30	0.63
1:1A:1991:U:H2'	1:1A:1992:G:H5"	1.81	0.63
12:2Q:135:ASP:OD2	21:2Z:49:ARG:NH1	2.32	0.63
32:2a:984:C:H2'	32:2a:985:C:H6	1.64	0.63
12:1Q:81:VAL:HB	22:10:7:LEU:HD21	1.80	0.63
32:1a:118:U:O4	62:1a:1906:HOH:O	2.14	0.63
32:2a:438:G:N1	32:2a:495:A:OP2	2.24	0.63
49:2r:52:PRO:HB2	49:2r:54:ARG:HG2	1.81	0.63
56:2y:9:A:H5'	56:2y:46:A:C2	2.33	0.63
32:1a:434:U:H2'	32:1a:435:C:C6	2.33	0.63
1:2A:271(U):G:N7	62:2A:3990:HOH:O	2.31	0.63
1:1A:881:G:N2	1:1A:897:C:O2	2.32	0.63
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.34	0.63
1:1A:2469:A:O3'	12:1Q:56:ARG:NH1	2.32	0.63
9:1N:35:ARG:HD3	9:1N:37:LYS:HD2	1.80	0.63
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.32	0.63
42:1k:48:ILE:O	42:1k:50:TYR:N	2.31	0.63
32:1a:429:U:OP1	35:1d:13:ARG:NH1	2.32	0.63
34:1c:52:LEU:HD13	34:1c:68:VAL:HG13	1.79	0.63
35:1d:112:VAL:HG23	35:1d:116:GLN:HE22	1.64	0.63
1:2A:652(T):C:H2'	1:2A:652(U):G:C8	2.33	0.63
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.32	0.63
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:708:C:H2'	32:2a:709:G:H8	1.64	0.63
32:2a:1272:G:N2	32:2a:1273:G:C5	2.67	0.63
39:2h:41:ARG:NH2	39:2h:123:GLU:OE2	2.32	0.63
40:1i:16:ARG:HH11	40:1i:64:THR:HG21	1.63	0.62
32:2a:67:C:H2'	32:2a:68:G:C8	2.33	0.62
32:2a:157:G:N2	32:2a:164:U:O2	2.18	0.62
34:1c:172:ARG:NH2	34:1c:206:GLU:OE2	2.31	0.62
33:2b:98:LEU:HB2	33:2b:101:MET:HE3	1.80	0.62
1:1A:2136:C:C2	1:1A:2155:G:N2	2.67	0.62
32:1a:1291:G:OP1	38:1g:37:ASN:ND2	2.32	0.62
44:1m:104:ARG:NH2	62:1m:3101:HOH:O	2.31	0.62
56:1y:37:A:H2'	56:1y:38:A:C8	2.34	0.62
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.32	0.62
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.18	0.62
1:2A:1633:G:OP2	62:2A:3935:HOH:O	2.16	0.62
14:1S:20:ARG:NH2	22:10:51:VAL:O	2.29	0.62
28:16:53:LYS:NZ	56:1y:1:G:OP1	2.32	0.62
54:1w:2:C:H2'	54:1w:3:G:C8	2.34	0.62
1:2A:852:G:H2'	1:2A:853:G:H8	1.64	0.62
7:2H:84:SER:OG	7:2H:132:ARG:NH1	2.32	0.62
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.35	0.62
35:2d:17:VAL:HG21	35:2d:63:LYS:HD3	1.81	0.62
35:1d:23:GLY:HA3	35:1d:112:VAL:HG12	1.81	0.62
54:1w:27:A:H2'	54:1w:28:G:C8	2.34	0.62
1:2A:921:G:O6	62:2A:3923:HOH:O	2.12	0.62
1:2A:958:U:O2	2:2B:90:A:O2'	2.16	0.62
13:2R:104:ARG:HD2	13:2R:109:ALA:HB3	1.81	0.62
32:2a:412:A:O4'	35:2d:35:ARG:NH2	2.32	0.62
32:2a:839:U:H3'	32:2a:840:C:H5'	1.81	0.62
44:2m:10:PRO:HB2	44:2m:13:LYS:HD2	1.82	0.62
1:1A:493:G:O6	62:1A:4127:HOH:O	2.15	0.62
1:1A:536:A:H2'	1:1A:537:C:C6	2.35	0.62
2:2B:14:U:OP2	2:2B:70:C:O2'	2.15	0.62
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.80	0.62
32:2a:1239:A:H62	32:2a:1299:A:H61	1.48	0.62
42:2k:48:ILE:O	42:2k:50:TYR:N	2.24	0.62
32:2a:259:G:OP2	51:2t:83:ARG:NH1	2.33	0.62
33:2b:78:GLN:O	33:2b:94:ASN:ND2	2.31	0.62
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.34	0.62
33:1b:63:MET:HG2	33:1b:225:ALA:HB1	1.80	0.62
32:2a:1163:C:H42	32:2a:1173:G:H1	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:37:LEU:HD12	3:1D:62:TYR:HB2	1.81	0.61
26:14:58:ARG:HD3	50:1s:67:VAL:H	1.65	0.61
32:2a:1142:G:H3'	32:2a:1143:G:H8	1.65	0.61
36:2e:12:LEU:HB3	36:2e:31:LEU:HB2	1.81	0.61
8:1I:77:LEU:HB3	8:1I:142:VAL:HG12	1.81	0.61
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.31	0.61
21:1Z:150:LEU:HB3	21:1Z:171:ILE:HD11	1.81	0.61
1:2A:1223:G:N2	1:2A:1226:A:OP2	2.29	0.61
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.82	0.61
32:2a:1309:G:O3'	44:2m:77:ASN:ND2	2.33	0.61
33:2b:76:GLN:HE21	33:2b:206:ASP:HA	1.64	0.61
44:2m:22:ILE:HG23	44:2m:67:GLU:HG2	1.82	0.61
8:1I:69:LYS:HG2	8:1I:138:ILE:HG12	1.82	0.61
32:1a:405:U:O4	35:1d:2:GLY:N	2.34	0.61
21:2Z:138:GLU:H	21:2Z:156:LYS:HZ3	1.48	0.61
21:2Z:151:HIS:HB3	21:2Z:168:GLU:HA	1.81	0.61
4:1E:12:THR:HG22	4:1E:13:ARG:H	1.65	0.61
56:1y:22:G:H8	56:1y:46:A:H61	1.47	0.61
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.80	0.61
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.65	0.61
54:2w:11:U:H2'	54:2w:12:U:H6	1.66	0.61
56:2y:51:G:N2	56:2y:64:U:O2	2.33	0.61
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.30	0.61
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.00	0.61
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.34	0.61
1:2A:2156:G:H2'	1:2A:2157:G:C2	2.36	0.61
26:24:46:GLN:C	26:24:48:ARG:H	2.09	0.61
1:1A:1055:G:N2	1:1A:1104:C:N3	2.42	0.61
32:1a:56:U:H2'	32:1a:57:G:C8	2.35	0.61
32:1a:1239:A:H62	32:1a:1299:A:N6	1.99	0.61
36:1e:35:GLY:HA3	36:1e:112:LEU:HB3	1.82	0.61
32:1a:279:A:C5	48:1q:98:LEU:HD23	2.35	0.61
56:1y:37:A:H2'	56:1y:38:A:H8	1.66	0.61
56:2y:42:C:H2'	56:2y:43:U:H6	1.64	0.61
33:1b:114:ARG:NH1	33:1b:117:GLU:OE1	2.27	0.61
1:2A:2176:A:H2'	1:2A:2177:C:H6	1.65	0.61
32:2a:1086:U:H3	32:2a:1099:G:H22	1.47	0.61
1:1A:904:C:O2'	21:1Z:169:GLU:OE2	2.17	0.60
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.32	0.60
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.83	0.60
47:1p:53:VAL:HG13	47:1p:79:VAL:HG22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:113:ARG:NH2	6:2G:139:LEU:O	2.34	0.60
32:2a:952:U:H2'	32:2a:953:G:C8	2.36	0.60
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.36	0.60
1:1A:1168:G:H1	1:1A:1181:C:H42	1.49	0.60
32:1a:858:G:OP2	62:1a:1910:HOH:O	2.17	0.60
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.19	0.60
40:2i:28:VAL:HG22	40:2i:63:ILE:HB	1.83	0.60
44:2m:80:ARG:HH22	50:2s:69:HIS:CE1	2.18	0.60
56:2y:42:C:H2'	56:2y:43:U:C6	2.36	0.60
8:1I:87:LYS:HA	8:1I:122:GLU:HA	1.83	0.60
2:2B:52:A:N6	14:2S:33:LYS:HG2	2.17	0.60
21:2Z:102:LEU:HB2	21:2Z:104:PHE:HE2	1.66	0.60
45:2n:33:VAL:HA	45:2n:40:CYS:HA	1.82	0.60
50:2s:32:LYS:HA	50:2s:50:ALA:HB3	1.82	0.60
32:1a:1402:4OC:HM22	32:1a:1403:C:H5'	1.84	0.60
35:1d:162:LEU:HD13	35:1d:181:MET:HG2	1.84	0.60
1:2A:9:U:OP1	9:2N:115:ARG:NH2	2.33	0.60
1:2A:1011:G:OP2	16:2U:66:ASN:ND2	2.34	0.60
1:2A:2035:G:OP1	62:2A:3933:HOH:O	2.15	0.60
1:2A:2524:G:O6	62:2A:3925:HOH:O	2.13	0.60
3:2D:71:ASP:HB2	3:2D:103:ARG:HH12	1.65	0.60
41:2j:61:GLU:OE2	45:2n:58:LYS:NZ	2.34	0.60
32:1a:946:A:H2'	32:1a:947:G:C8	2.36	0.60
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.17	0.60
32:1a:1442:G:O2'	32:1a:1442(A):G:H5'	2.02	0.60
40:1i:17:VAL:HG23	40:1i:63:ILE:HG12	1.83	0.60
1:2A:332:A:O2'	1:2A:334:C:OP2	2.17	0.60
32:2a:1029:C:C5	32:2a:1032:G:N1	2.61	0.60
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.66	0.60
34:2c:142:MET:HG3	34:2c:170:GLN:HB3	1.82	0.60
1:1A:2120:G:H1	1:1A:2178:C:N4	1.99	0.60
32:2a:297:G:N2	32:2a:300:A:OP2	2.34	0.60
32:1a:159:G:O2'	32:1a:161:A:N7	2.27	0.60
32:1a:972:C:O2'	41:1j:55:LYS:O	2.19	0.60
1:2A:1113:U:H2'	1:2A:1114:G:C8	2.36	0.60
1:2A:2100:G:O6	1:2A:2189:U:O4	2.20	0.60
11:2P:35:HIS:O	62:2P:301:HOH:O	2.16	0.60
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.35	0.60
1:1A:382:G:O6	62:1A:4122:HOH:O	2.13	0.60
1:1A:654:A:OP2	62:1A:4131:HOH:O	2.16	0.60
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:116:GLY:O	11:1P:137:LYS:NZ	2.31	0.60
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.01	0.60
1:2A:2292:C:OP1	14:2S:17:ARG:NH2	2.32	0.60
1:2A:2299:G:H2'	1:2A:2300:G:H8	1.67	0.60
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.36	0.60
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.30	0.60
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.01	0.60
26:24:60:GLN:HB3	26:24:62:ARG:HG2	1.82	0.60
32:2a:393:A:OP1	62:2a:1910:HOH:O	2.17	0.60
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.36	0.60
1:1A:1069:A:H5'	1:1A:1070:A:C8	2.32	0.60
1:1A:2483:C:N3	12:1Q:124:LYS:NZ	2.46	0.60
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.35	0.60
12:1Q:20:ALA:HB2	21:1Z:79:ARG:HG3	1.84	0.60
28:16:10:LEU:HG	28:16:54:ILE:HG13	1.84	0.60
1:1A:2139:C:H2'	1:1A:2140:C:O4'	2.02	0.59
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.20	0.59
39:1h:10:LEU:HB3	39:1h:83:ILE:HG12	1.84	0.59
1:2A:249:C:O2	30:28:12:LYS:NZ	2.34	0.59
1:2A:883:G:N2	1:2A:894:C:O2	2.35	0.59
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.37	0.59
6:2G:170:ARG:NH1	6:2G:174:GLU:OE2	2.34	0.59
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.84	0.59
26:24:53:GLU:HG2	26:24:55:ARG:H	1.67	0.59
44:2m:58:GLU:O	44:2m:62:ASN:ND2	2.20	0.59
54:2w:8:4SU:H4'	54:2w:48:C:H4'	1.83	0.59
1:1A:621:A:OP2	11:1P:108:LYS:NZ	2.35	0.59
1:1A:2379:G:O2'	14:1S:17:ARG:NH2	2.35	0.59
56:1y:6:C:N4	56:1y:7:G:O6	2.35	0.59
14:2S:105:ALA:HB1	14:2S:110:LEU:HD12	1.84	0.59
32:2a:1256:A:H61	32:2a:1278:U:C2'	2.15	0.59
44:2m:122:LYS:HG3	44:2m:123:ALA:H	1.67	0.59
1:1A:1069:A:O4'	1:1A:1096:A:O2'	2.19	0.59
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.84	0.59
1:2A:80:G:H1	1:2A:106:C:H42	1.50	0.59
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.36	0.59
47:2p:28:ARG:NH1	47:2p:29:ASP:OD1	2.35	0.59
32:1a:1414:U:O4	62:1a:1909:HOH:O	2.15	0.59
32:2a:974:A:OP2	45:2n:29:ARG:NH1	2.30	0.59
32:2a:1279:A:H4'	32:2a:1280:A:OP1	2.02	0.59
33:2b:114:ARG:HA	33:2b:117:GLU:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2749:A:H5"	7:1H:3:ARG:HH22	1.68	0.59
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.11	0.59
50:1s:11:VAL:HG11	50:1s:16:LEU:HB2	1.84	0.59
1:2A:839:U:H2'	1:2A:840:C:C6	2.38	0.59
2:2B:48:A:OP1	14:2S:30:ARG:NH2	2.36	0.59
8:2I:93:THR:OG1	8:2I:96:ASP:OD1	2.17	0.59
9:2N:32:THR:HG23	9:2N:37:LYS:HB2	1.84	0.59
32:2a:701:C:OP1	32:2a:702:A:O2'	2.17	0.59
1:1A:2136:C:C4	1:1A:2155:G:C2	2.90	0.59
56:1y:4:G:C2	56:1y:5:G:H1'	2.37	0.59
14:2S:10:ARG:HH21	14:2S:91:PRO:HB2	1.67	0.59
26:24:40:HIS:CD2	26:24:41:PRO:HD2	2.38	0.59
44:2m:3:ARG:HH22	44:2m:11:ARG:HG3	1.67	0.59
56:2y:18:G:C2	56:2y:56:C:C2	2.90	0.59
1:1A:260:G:O6	62:1A:4128:HOH:O	2.15	0.59
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.38	0.59
24:12:55:ARG:NH2	62:12:3801:HOH:O	2.23	0.59
32:1a:576:G:O6	32:1a:880:C:O2'	2.15	0.59
1:2A:2497:A:O2'	62:2A:3934:HOH:O	2.16	0.59
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.21	0.59
32:2a:258:G:OP1	51:2t:86:ARG:NH2	2.33	0.59
32:2a:437:U:H5'	35:2d:155:LEU:HD21	1.84	0.59
32:2a:1257:U:O4	45:2n:17:LYS:NZ	2.34	0.59
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.38	0.59
8:1I:93:THR:H	8:1I:96:ASP:HB2	1.68	0.59
36:1e:78:HIS:CE1	36:1e:143:ARG:H	2.18	0.59
1:2A:307:G:N1	1:2A:310:A:OP2	2.36	0.59
1:2A:2137:C:N4	1:2A:2154:G:H1	2.00	0.59
1:2A:2705:A:OP2	62:2A:3937:HOH:O	2.17	0.59
1:2A:2847:U:OP1	15:2T:98:LYS:NZ	2.36	0.59
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.85	0.59
32:2a:9:G:H2'	32:2a:10:A:H8	1.68	0.59
32:2a:473:G:H2'	32:2a:474:G:C8	2.38	0.59
32:2a:1302:U:OP1	44:2m:13:LYS:NZ	2.35	0.59
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.03	0.59
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.36	0.59
48:1q:67:LYS:HA	48:1q:70:ARG:HH12	1.68	0.59
1:2A:1783:A:HO2'	1:2A:2607:G:HO2'	1.50	0.59
1:2A:2493:U:O2'	12:2Q:80:GLU:OE2	2.17	0.59
1:2A:2782:G:OP2	62:2A:3939:HOH:O	2.17	0.59
33:2b:16:HIS:HB2	33:2b:204:ASN:HD22	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:75:LEU:O	8:1I:141:LYS:NZ	2.35	0.59
32:1a:642:A:N3	39:1h:113:SER:OG	2.26	0.59
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.84	0.59
1:2A:2698:U:O4	62:2A:3926:HOH:O	2.13	0.59
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.36	0.59
32:2a:663:A:O3'	49:2r:64:ARG:NH2	2.31	0.59
34:2c:13:GLY:HA3	45:2n:57:ARG:NH2	2.17	0.59
32:1a:67:C:H2'	32:1a:68:G:C8	2.37	0.58
32:1a:1123:A:O2'	41:1j:37:PRO:O	2.20	0.58
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.38	0.58
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.85	0.58
4:2E:14:ILE:HG13	4:2E:21:VAL:HG13	1.85	0.58
5:2F:113:ALA:HB1	5:2F:186:ILE:HG21	1.84	0.58
21:2Z:154:ASP:OD1	21:2Z:154:ASP:N	2.26	0.58
1:1A:1054:A:N1	1:1A:1105:U:O2	2.36	0.58
1:1A:2100:G:N1	1:1A:2189:U:N3	2.34	0.58
2:1B:66:A:H61	2:1B:109:C:H5'	1.68	0.58
6:1G:49:ASP:N	6:1G:49:ASP:OD1	2.35	0.58
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.85	0.58
56:1y:13:C:H2'	56:1y:14:A:H5"	1.86	0.58
1:2A:2133:G:HO2'	1:2A:2157:G:H22	1.45	0.58
26:14:55:ARG:N	26:14:56:VAL:HA	2.17	0.58
32:1a:92:C:H2'	32:1a:93:G:C8	2.38	0.58
32:2a:222:U:H2'	32:2a:223:U:C6	2.38	0.58
32:2a:224:C:H2'	32:2a:225:C:H6	1.69	0.58
32:2a:504:C:OP1	62:2a:1909:HOH:O	2.17	0.58
32:2a:1095:U:OP2	62:2a:1903:HOH:O	2.17	0.58
50:2s:28:LYS:HB3	50:2s:29:ARG:CB	2.33	0.58
1:1A:1013:C:OP2	62:1A:4108:HOH:O	2.17	0.58
1:1A:2264:C:N4	22:10:15:ASP:OD2	2.31	0.58
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.38	0.58
1:2A:1356:G:OP1	62:2A:3936:HOH:O	2.16	0.58
32:2a:1134:G:C2	32:2a:1135:U:H1'	2.38	0.58
32:2a:1272:G:N2	32:2a:1273:G:N7	2.50	0.58
42:2k:14:VAL:O	42:2k:77:MET:N	2.28	0.58
1:1A:882:G:O6	1:1A:883:G:N2	2.36	0.58
12:1Q:78:PRO:HD3	55:1x:1:C:N3	2.18	0.58
35:1d:194:LEU:HD11	35:1d:196:LEU:HG	1.86	0.58
49:1r:24:ALA:O	49:1r:26:LEU:N	2.35	0.58
1:2A:400:G:O6	62:2A:3932:HOH:O	2.15	0.58
6:2G:36:LYS:HE3	6:2G:160:VAL:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:106:GLY:O	39:2h:122:ARG:NH2	2.36	0.58
39:2h:124:ALA:O	39:2h:128:GLY:N	2.37	0.58
1:1A:760:G:OP1	62:1A:4134:HOH:O	2.17	0.58
1:1A:998:C:OP1	62:1A:4133:HOH:O	2.17	0.58
1:1A:1062:G:H8	1:1A:1070:A:H4'	1.67	0.58
50:1s:12:ASP:OD2	50:1s:35:SER:OG	2.21	0.58
1:2A:652(A):A:H3'	1:2A:652(B):A:H5"	1.86	0.58
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.39	0.58
1:2A:2127:G:C6	1:2A:2161:C:N4	2.72	0.58
8:2I:5:LEU:HD11	8:2I:19:VAL:HG22	1.84	0.58
8:2I:77:LEU:HB3	8:2I:142:VAL:HG13	1.85	0.58
1:1A:1670:C:OP2	62:1A:4109:HOH:O	2.17	0.58
32:1a:111:G:H5"	47:1p:27:LYS:HB3	1.86	0.58
1:2A:106:C:H1'	20:2Y:1:MET:HE2	1.84	0.58
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.36	0.58
3:2D:182:LEU:HB2	3:2D:272:ALA:HB3	1.85	0.58
32:2a:1005:A:H5"	32:2a:1006:C:C5	2.39	0.58
32:2a:1118:C:N3	32:2a:1156:G:N2	2.51	0.58
1:1A:272(J):C:H2'	1:1A:274:G:H8	1.69	0.58
1:1A:2161:C:O2'	1:1A:2162:G:H8	1.87	0.58
12:1Q:136:ALA:HB1	21:1Z:52:SER:HB3	1.85	0.58
1:2A:2135:A:H2	1:2A:2157:G:H5'	1.69	0.58
1:2A:2690:C:OP1	13:2R:17:ARG:NH2	2.37	0.58
11:2P:59:LEU:HG	11:2P:60:MET:HE2	1.86	0.58
37:2f:95:GLU:O	49:2r:32:ARG:NH1	2.36	0.58
40:2i:20:ARG:HH22	40:2i:62:TYR:HB3	1.67	0.58
40:2i:21:PRO:HA	40:2i:59:PHE:HA	1.86	0.58
34:1c:24:ALA:HB1	34:1c:28:GLN:HG3	1.85	0.58
1:2A:81:G:N7	62:2A:3999:HOH:O	2.32	0.58
15:2T:24:PRO:HA	15:2T:49:VAL:HG12	1.84	0.58
32:2a:45:U:H2'	32:2a:46:G:C8	2.39	0.58
1:1A:184:C:H2'	1:1A:185:U:C6	2.38	0.58
1:1A:428:A:OP1	62:1A:4136:HOH:O	2.17	0.58
7:1H:124:GLU:HG2	7:1H:132:ARG:HB3	1.85	0.58
32:1a:1305:G:OP2	52:1u:2:GLY:N	2.37	0.58
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.85	0.58
54:1w:4:G:OP1	62:1w:202:HOH:O	2.17	0.58
1:2A:242:G:C8	30:28:5:LYS:HG2	2.39	0.58
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.36	0.58
5:2F:33:LEU:HB3	11:2P:6:LEU:HD21	1.84	0.58
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1030(A):G:N2	32:2a:1030(D):A:OP2	2.37	0.58
40:1i:121:ARG:NH1	40:1i:122:ALA:O	2.37	0.57
1:2A:854:G:H2'	1:2A:855:G:C8	2.37	0.57
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	1.86	0.57
32:2a:1263:C:N3	32:2a:1272:G:O6	2.37	0.57
50:2s:11:VAL:O	50:2s:13:ASP:N	2.36	0.57
14:1S:20:ARG:NH1	22:10:48:GLY:O	2.32	0.57
42:1k:104:GLN:O	42:1k:104:GLN:HG3	2.03	0.57
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.03	0.57
15:2T:30:VAL:HG22	15:2T:86:ILE:HG12	1.87	0.57
32:2a:165:C:H2'	32:2a:166:G:C8	2.38	0.57
54:1w:27:A:H2'	54:1w:28:G:H8	1.68	0.57
1:2A:2319:G:N2	14:2S:3:ARG:HD2	2.19	0.57
14:2S:77:ALA:HB1	14:2S:82:ILE:HB	1.86	0.57
43:2l:55:VAL:HG12	43:2l:69:TYR:HA	1.87	0.57
56:2y:14:A:N6	56:2y:21:A:C2	2.67	0.57
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.39	0.57
46:1o:5:LYS:H	46:1o:5:LYS:HD2	1.70	0.57
1:2A:1323:U:OP1	18:2W:98:LYS:NZ	2.34	0.57
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.39	0.57
32:2a:1002:G:C6	32:2a:1003:G:H8	2.23	0.57
32:2a:1033:G:H2'	32:2a:1034:G:H8	1.69	0.57
32:2a:1376:U:OP1	38:2g:98:SER:OG	2.20	0.57
36:2e:102:ALA:HB1	36:2e:106:PRO:HB2	1.85	0.57
40:2i:23:ASN:HD21	40:2i:25:LYS:HE2	1.68	0.57
24:12:41:ILE:HG13	24:12:43:GLN:HG3	1.86	0.57
32:1a:78:G:N1	32:1a:91:C:N4	2.53	0.57
32:1a:1144:G:N2	32:1a:1146:A:H62	2.02	0.57
32:1a:1278:U:H5'	32:1a:1279:A:O4'	2.05	0.57
32:2a:1409:C:H2'	32:2a:1410:G:H8	1.69	0.57
33:2b:16:HIS:O	33:2b:18:GLY:N	2.37	0.57
32:1a:258:G:H2'	32:1a:259:G:H8	1.70	0.57
26:24:13:ARG:HG3	26:24:23:GLU:HA	1.86	0.57
38:2g:79:ARG:NH2	38:2g:80:VAL:HA	2.19	0.57
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.19	0.57
1:1A:2753:A:N3	31:19:15:LYS:NZ	2.53	0.57
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	1.86	0.57
1:2A:792:G:O6	62:2A:3922:HOH:O	2.12	0.57
1:2A:1021:A:H62	1:2A:1141:U:H3	1.52	0.57
9:2N:96:GLU:CD	9:2N:96:GLU:H	2.13	0.57
16:2U:29:SER:OG	16:2U:30:LYS:NZ	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:23:LYS:HD3	21:2Z:40:ASP:HA	1.87	0.57
26:24:13:ARG:HD2	26:24:23:GLU:HG2	1.86	0.57
35:2d:108:LEU:HD21	35:2d:174:LEU:HB3	1.85	0.57
15:1T:112:ARG:HG3	15:1T:115:ARG:NH2	2.19	0.57
21:1Z:152:ALA:HB3	21:1Z:167:PRO:HA	1.86	0.57
46:1o:39:LEU:HD13	46:1o:56:LEU:HB2	1.87	0.57
1:2A:1772:G:OP1	62:2A:3944:HOH:O	2.18	0.57
48:2q:45:HIS:HB3	48:2q:72:ARG:HG2	1.85	0.57
54:2w:11:U:H2'	54:2w:12:U:C6	2.39	0.57
1:1A:271(M):G:H21	8:1I:50:ARG:NH2	2.02	0.57
32:1a:966:M2G:O2'	40:1i:127:LYS:O	2.22	0.57
54:1w:58:A:O2'	54:1w:61:C:N4	2.38	0.57
1:2A:752:A:H3'	29:27:1:MET:HE1	1.87	0.57
6:2G:46:ALA:HB2	6:2G:53:LEU:HD23	1.85	0.57
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.38	0.57
32:2a:382:A:H2'	32:2a:383:A:C8	2.40	0.57
32:2a:772:U:H2'	32:2a:773:G:O4'	2.04	0.57
33:2b:185:ILE:HG22	33:2b:199:TYR:HB2	1.87	0.57
45:2n:48:ALA:HB2	45:2n:53:LEU:HD12	1.87	0.57
25:13:3:ARG:NE	25:13:60:GLU:OE1	2.37	0.57
33:1b:12:GLU:O	33:1b:15:VAL:HG22	2.05	0.57
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.87	0.57
33:1b:82:ARG:NH1	33:1b:86:GLU:OE2	2.38	0.57
36:1e:145:LYS:HA	36:1e:148:VAL:HG22	1.85	0.57
44:1m:78:ILE:HG22	44:1m:82:MET:HE2	1.87	0.57
1:2A:1847:A:H3'	1:2A:1848:A:H5'	1.87	0.57
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.03	0.57
5:2F:101:LEU:HD12	5:2F:102:PRO:HD2	1.87	0.57
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.20	0.57
31:29:27:CYS:SG	31:29:28:GLU:N	2.77	0.57
32:2a:34:C:H2'	32:2a:35:G:H8	1.69	0.57
32:2a:171:A:H2'	32:2a:172:A:C8	2.39	0.57
32:1a:702:A:OP2	62:1a:1912:HOH:O	2.18	0.56
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.04	0.56
1:2A:643:A:N1	1:2A:2369:A:O2'	2.35	0.56
1:2A:851:U:O2'	25:23:42:ALA:O	2.23	0.56
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.05	0.56
28:26:35:GLU:HG2	28:26:50:ARG:HD3	1.86	0.56
32:2a:909:A:N3	32:2a:1413:A:O2'	2.32	0.56
34:2c:124:ILE:HG21	34:2c:130:VAL:HG13	1.87	0.56
40:2i:3:GLN:NE2	40:2i:20:ARG:HE	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:99:LEU:HB3	40:2i:101:PHE:CE2	2.40	0.56
46:2o:74:ASP:HB3	46:2o:77:ARG:HB2	1.85	0.56
48:2q:32:TYR:O	48:2q:34:LYS:N	2.33	0.56
32:1a:836:G:OP1	49:1r:61:LYS:NZ	2.28	0.56
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.38	0.56
6:2G:41:GLN:HE22	6:2G:153:ARG:HB3	1.70	0.56
12:2Q:78:PRO:HD3	55:2x:1:C:N3	2.21	0.56
27:25:41:PRO:O	27:25:44:THR:OG1	2.23	0.56
32:2a:673:G:H2'	32:2a:674:G:C8	2.40	0.56
32:2a:1133:G:H1	32:2a:1141:C:H42	1.51	0.56
32:2a:1256:A:N6	32:2a:1278:U:O2'	2.31	0.56
32:2a:1318:A:OP1	50:2s:3:ARG:NH2	2.32	0.56
41:2j:6:ILE:HG12	41:2j:98:ILE:HG12	1.87	0.56
50:2s:61:TYR:HE2	50:2s:63:THR:HG23	1.70	0.56
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.69	0.56
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.40	0.56
9:1N:115:ARG:HA	9:1N:118:LYS:HE3	1.86	0.56
32:1a:184:G:H2'	32:1a:185:A:C8	2.39	0.56
32:1a:1531:A:H8	32:1a:1531:A:O5'	1.88	0.56
33:1b:155:LEU:HD11	33:1b:159:PRO:HG3	1.86	0.56
34:1c:68:VAL:HG12	34:1c:70:VAL:HG23	1.87	0.56
42:1k:59:TYR:CZ	42:1k:63:LEU:HD21	2.41	0.56
45:1n:24:CYS:HB3	45:1n:28:GLY:H	1.70	0.56
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.70	0.56
26:24:60:GLN:O	26:24:62:ARG:NH1	2.37	0.56
32:2a:7:G:H5'	32:2a:298:A:O4'	2.05	0.56
32:2a:130:A:H5'	48:2q:63:ARG:HE	1.70	0.56
32:2a:859:A:H2'	32:2a:860:A:O4'	2.05	0.56
36:2e:143:ARG:NE	39:2h:77:GLU:OE2	2.28	0.56
5:1F:9:ILE:HG12	5:1F:123:LEU:HD23	1.86	0.56
11:1P:98:GLU:O	11:1P:101:VAL:HG12	2.06	0.56
1:2A:330:A:H2	1:2A:1210:A:HO2'	1.53	0.56
1:2A:898:C:H2'	1:2A:899:A:H5'	1.86	0.56
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.69	0.56
32:2a:547:A:OP1	62:2a:1912:HOH:O	2.18	0.56
34:2c:142:MET:HE2	34:2c:170:GLN:HG2	1.88	0.56
41:2j:40:LEU:HB2	41:2j:69:ASN:HB3	1.87	0.56
44:2m:10:PRO:HD2	44:2m:18:ALA:HB1	1.87	0.56
1:1A:278:A:O2'	1:1A:279:C:OP1	2.20	0.56
1:1A:918:A:N3	2:1B:80:U:O2'	2.38	0.56
1:1A:1359:A:H2'	1:1A:1360:A:H5'	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1g:16:LEU:HD11	40:1i:45:ALA:HB2	1.88	0.56
38:1g:89:MET:HE2	38:1g:89:MET:HA	1.86	0.56
47:2p:58:TYR:O	47:2p:61:SER:OG	2.23	0.56
1:1A:1253:A:OP1	62:1A:4138:HOH:O	2.18	0.56
32:1a:165:C:H2'	32:1a:166:G:H8	1.70	0.56
32:1a:719:C:H1'	49:1r:49:LYS:HB3	1.87	0.56
40:1i:17:VAL:HG11	40:1i:80:GLY:C	2.31	0.56
40:1i:96:LEU:HD22	40:1i:101:PHE:HD2	1.71	0.56
44:1m:34:LEU:HD13	44:1m:41:PRO:HA	1.88	0.56
1:2A:2557:G:H2'	1:2A:2558:C:C6	2.41	0.56
33:2b:180:LEU:HB2	33:2b:182:ILE:HG12	1.87	0.56
1:1A:2447:G:OP2	62:1A:4135:HOH:O	2.17	0.56
32:1a:1005:A:OP2	32:1a:1024:G:N2	2.39	0.56
1:2A:131:G:OP1	62:2A:3940:HOH:O	2.18	0.56
1:2A:2743:C:OP1	31:29:33:LYS:NZ	2.37	0.56
32:2a:1133:G:H2'	32:2a:1134:G:H8	1.70	0.56
32:2a:1228:C:OP1	44:2m:115:LYS:NZ	2.37	0.56
32:2a:1256:A:OP1	34:2c:26:LYS:NZ	2.39	0.56
19:1X:5:TYR:CZ	24:12:30:ARG:HB2	2.41	0.56
1:2A:2361:A:OP2	30:28:26:LYS:NZ	2.39	0.56
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.40	0.56
30:28:62:LEU:HB3	30:28:65:GLU:HG3	1.88	0.56
32:2a:737:A:H1'	37:2f:73:ASN:HD21	1.71	0.56
40:2i:99:LEU:HB3	40:2i:101:PHE:HE2	1.70	0.56
54:2w:64:U:H2'	54:2w:65:U:H6	1.70	0.56
1:1A:1595:G:O6	62:1A:4137:HOH:O	2.18	0.56
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.86	0.56
6:1G:18:GLU:HG3	6:1G:22:ARG:HD2	1.86	0.56
7:1H:9:ILE:HB	7:1H:50:VAL:HG23	1.88	0.56
32:1a:1145:C:H4'	32:1a:1146:A:H5'	1.87	0.56
52:1u:6:ARG:HG2	52:1u:15:ARG:HD2	1.88	0.56
1:2A:83:G:H1	1:2A:102:G:HO2'	1.54	0.56
1:2A:1340:U:OP1	19:2X:16:LYS:NZ	2.38	0.56
1:2A:2126:A:N6	1:2A:2163:C:O4'	2.39	0.56
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.41	0.56
32:2a:921:U:O2	36:2e:19:MET:HB2	2.06	0.56
32:2a:953:G:H5'	32:2a:965:A:N6	2.19	0.56
34:2c:35:GLU:OE2	34:2c:59:ARG:NH2	2.39	0.56
36:2e:36:ASP:C	36:2e:38:GLN:H	2.14	0.56
56:2y:66:C:H2'	56:2y:67:G:O4'	2.05	0.56
1:1A:2612:C:OP2	27:15:2:ALA:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.90	0.56
33:1b:204:ASN:OD1	33:1b:205:ASP:N	2.38	0.56
1:2A:625:G:N7	11:2P:107:LYS:NZ	2.43	0.56
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.40	0.56
8:2I:69:LYS:HG3	8:2I:138:ILE:HG12	1.88	0.56
14:2S:15:ARG:O	14:2S:19:LYS:HG2	2.05	0.56
25:23:40:THR:HG22	25:23:42:ALA:H	1.71	0.56
32:2a:67:C:H2'	32:2a:68:G:H8	1.71	0.56
32:2a:1002:G:N1	32:2a:1003:G:H8	2.02	0.56
32:2a:1338:G:H21	55:2x:41:C:H1'	1.72	0.56
34:2c:13:GLY:HA3	45:2n:57:ARG:HH21	1.71	0.56
34:1c:113:ALA:HB2	34:1c:202:ILE:HG13	1.88	0.55
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.23	0.55
2:2B:114:C:H4'	14:2S:46:VAL:HG22	1.89	0.55
8:2I:37:VAL:HG12	8:2I:38:LEU:HD12	1.87	0.55
32:2a:881:G:P	43:2l:12:ARG:HH22	2.29	0.55
40:2i:8:GLY:O	40:2i:15:ALA:N	2.38	0.55
1:1A:1641:A:H2'	1:1A:1642:G:O4'	2.06	0.55
32:1a:427:U:OP1	35:1d:13:ARG:NH2	2.37	0.55
33:1b:10:LEU:HG	33:1b:48:MET:HE1	1.88	0.55
36:1e:6:PHE:HB3	36:1e:34:VAL:HG22	1.88	0.55
1:2A:884:C:H3'	1:2A:885:C:C6	2.41	0.55
1:2A:2106:G:H2'	1:2A:2107:C:O4'	2.06	0.55
21:2Z:69:THR:HG22	21:2Z:90:VAL:HG22	1.89	0.55
32:2a:1029:C:N4	32:2a:1032:G:C6	2.74	0.55
32:2a:1457:G:H5"	51:2t:35:THR:HG21	1.89	0.55
34:2c:6:HIS:CD2	34:2c:8:ILE:H	2.23	0.55
35:2d:173:TRP:CD2	35:2d:189:PRO:HB3	2.41	0.55
54:2w:50:A:N1	54:2w:64:U:O2	2.39	0.55
1:1A:668:G:H5'	1:1A:669:G:OP2	2.06	0.55
1:1A:2805:G:H2'	1:1A:2807:G:C8	2.41	0.55
6:1G:115:ARG:HG2	6:1G:136:ARG:HH22	1.70	0.55
56:1y:2:C:H2'	56:1y:3:G:C8	2.40	0.55
1:2A:652(T):C:H2'	1:2A:652(U):G:H8	1.69	0.55
1:2A:993:G:OP1	16:2U:50:ARG:NH2	2.39	0.55
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.42	0.55
1:2A:1592:C:H2'	1:2A:1593:G:H8	1.71	0.55
32:2a:19:C:H5"	36:2e:86:ALA:HB1	1.87	0.55
32:2a:1004:A:N6	32:2a:1037:C:O2	2.30	0.55
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.39	0.55
33:2b:74:LYS:NZ	33:2b:205:ASP:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2g:115:ARG:HH11	38:2g:118:VAL:HG11	1.71	0.55
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.42	0.55
32:1a:161:A:H2'	32:1a:162:A:C8	2.41	0.55
32:1a:1469:G:H2'	32:1a:1470:G:H8	1.70	0.55
32:1a:1469:G:H2'	32:1a:1470:G:C8	2.40	0.55
37:1f:74:ASP:OD1	37:1f:77:ARG:NH2	2.39	0.55
51:1t:86:ARG:O	51:1t:90:GLN:NE2	2.39	0.55
1:2A:2529:G:O6	31:29:31:LYS:NZ	2.40	0.55
32:2a:17:U:H2'	32:2a:18:C:C6	2.42	0.55
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.41	0.55
47:2p:14:ASN:HA	47:2p:42:ARG:HD2	1.89	0.55
56:2y:8:4SU:O2	56:2y:21:A:H2	1.87	0.55
56:2y:49:G:O6	56:2y:65:U:O2	2.23	0.55
15:2T:92:GLY:O	15:2T:120:ARG:NH2	2.39	0.55
26:24:67:TYR:HD2	50:2s:9:VAL:HB	1.71	0.55
32:2a:142:G:H2'	32:2a:143:A:H8	1.71	0.55
32:2a:890:G:O2'	32:2a:906:G:O6	2.23	0.55
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.21	0.55
35:2d:18:LYS:NZ	35:2d:26:CYS:O	2.40	0.55
37:2f:2:ARG:NE	37:2f:69:GLU:HG2	2.21	0.55
44:2m:40:ASN:HD22	44:2m:43:THR:HG23	1.71	0.55
1:1A:747:U:O2	1:1A:2014:A:H1'	2.05	0.55
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.42	0.55
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.88	0.55
33:2b:84:GLU:HB3	33:2b:219:VAL:HG21	1.89	0.55
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.42	0.55
32:1a:613:C:H2'	32:1a:614:A:H8	1.71	0.55
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.25	0.55
36:1e:137:GLU:HG3	36:1e:141:GLN:HE21	1.72	0.55
47:1p:22:THR:HA	47:1p:33:ILE:HG13	1.88	0.55
1:2A:839:U:H2'	1:2A:840:C:H6	1.71	0.55
1:2A:2049:G:OP2	62:2A:3941:HOH:O	2.18	0.55
24:22:38:GLN:HG3	24:22:43:GLN:HB2	1.87	0.55
33:2b:115:LEU:HD13	33:2b:153:ARG:HD2	1.88	0.55
10:1O:73:ASP:HB2	15:1T:82:LEU:HD13	1.89	0.55
21:1Z:132:ASN:OD1	21:1Z:132:ASN:N	2.37	0.55
32:1a:1129:C:O2	32:1a:1130:A:N6	2.38	0.55
1:2A:796:C:H2'	1:2A:797:C:C6	2.42	0.55
11:2P:35:HIS:O	11:2P:36:LYS:HB2	2.06	0.55
32:2a:671:G:H2'	32:2a:672:U:O4'	2.07	0.55
32:2a:1320:C:N3	50:2s:36:ARG:NH2	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:64:LYS:HD2	39:2h:79:VAL:HG11	1.87	0.55
1:1A:1851:U:H4'	56:1y:71:G:H4'	1.89	0.55
33:1b:12:GLU:HB2	33:1b:213:LEU:HD21	1.88	0.55
54:1w:63:C:H2'	54:1w:64:U:C6	2.41	0.55
1:2A:287:C:H2'	1:2A:288:C:H6	1.71	0.55
1:2A:2166:G:O6	1:2A:2171:A:N6	2.38	0.55
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.41	0.55
2:2B:24:G:H4'	2:2B:25:A:C8	2.42	0.55
6:2G:39:ILE:HG12	6:2G:157:ILE:HG23	1.88	0.55
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.39	0.55
26:24:61:ARG:HG2	50:2s:42:PRO:HG3	1.89	0.55
32:2a:34:C:H2'	32:2a:35:G:C8	2.41	0.55
33:2b:204:ASN:HD21	33:2b:207:ALA:HB3	1.72	0.55
1:1A:818:G:O6	62:1A:4139:HOH:O	2.18	0.55
32:1a:194:C:H2'	32:1a:195:A:H5"	1.88	0.55
32:1a:631:G:H2'	32:1a:632:A:C8	2.42	0.55
32:1a:818:G:OP2	62:1a:1914:HOH:O	2.18	0.55
32:1a:1009:G:O6	32:1a:1020:U:O2	2.25	0.55
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.38	0.55
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.42	0.55
7:2H:8:PRO:HB3	7:2H:51:ARG:HG2	1.88	0.55
9:2N:56:ASN:N	9:2N:125:GLY:O	2.40	0.55
11:2P:85:LEU:HA	11:2P:88:LEU:HD12	1.88	0.55
24:22:8:LYS:HE2	24:22:12:GLU:HG2	1.88	0.55
32:2a:920:U:H2'	32:2a:921:U:C6	2.42	0.55
33:2b:119:GLU:OE1	33:2b:153:ARG:NH1	2.36	0.55
7:1H:33:LEU:HD21	7:1H:136:ILE:HG13	1.89	0.54
8:1I:45:LYS:HA	8:1I:48:GLU:HG3	1.89	0.54
32:1a:757:U:H2'	32:1a:758:G:O4'	2.07	0.54
33:1b:77:ALA:HB2	33:1b:211:ILE:HD13	1.90	0.54
40:1i:23:ASN:OD1	40:1i:23:ASN:N	2.36	0.54
1:2A:1354:A:H5"	3:2D:38:LYS:HD3	1.89	0.54
6:2G:50:ALA:O	6:2G:52:ILE:N	2.33	0.54
10:2O:80:ASP:OD2	15:2T:64:ARG:NH2	2.40	0.54
32:2a:646:U:H2'	32:2a:647:C:C6	2.42	0.54
32:2a:1029:C:N3	32:2a:1032:G:N2	2.55	0.54
32:2a:1097:C:O2'	32:2a:1169:A:N3	2.34	0.54
11:1P:95:VAL:HG22	11:1P:125:VAL:HG12	1.89	0.54
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.08	0.54
32:2a:195:A:N3	32:2a:222:U:O2'	2.39	0.54
32:2a:881:G:OP2	43:2l:12:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1352:C:OP1	52:2u:3:LYS:NZ	2.39	0.54
32:2a:1530:G:OP1	32:2a:1530:G:H4'	2.06	0.54
44:2m:86:CYS:HB2	50:2s:73:GLU:HG2	1.89	0.54
1:1A:764:A:H5"	3:1D:210:GLY:CA	2.37	0.54
1:1A:1648:C:OP1	62:1A:4129:HOH:O	2.18	0.54
9:1N:46:VAL:HG23	9:1N:48:MET:HG2	1.89	0.54
32:1a:78:G:N2	32:1a:91:C:N3	2.55	0.54
32:1a:984:C:H42	32:1a:1221:G:H1	1.55	0.54
33:1b:93:VAL:HG11	33:1b:97:TRP:CD1	2.42	0.54
1:2A:894:C:O2'	1:2A:895:U:H5"	2.07	0.54
1:2A:2867:G:OP2	15:2T:119:LYS:NZ	2.34	0.54
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.07	0.54
26:24:41:PRO:HG3	26:24:49:PHE:CE1	2.43	0.54
35:2d:15:GLU:OE2	35:2d:66:ARG:NH1	2.40	0.54
1:1A:2136:C:C4	1:1A:2155:G:N1	2.75	0.54
10:1O:36:GLY:HA3	10:1O:109:LYS:HD2	1.88	0.54
32:1a:1083:U:OP1	62:1a:1911:HOH:O	2.17	0.54
41:1j:47:PHE:HB2	41:1j:63:PHE:HB2	1.89	0.54
1:2A:2100:G:H2'	1:2A:2101:G:H8	1.72	0.54
32:2a:1330:U:H4'	44:2m:23:TYR:CZ	2.43	0.54
38:2g:57:GLU:HG3	38:2g:60:LYS:H	1.72	0.54
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.41	0.54
1:1A:1364:G:P	23:11:3:LYS:HG3	2.48	0.54
42:1k:15:ALA:O	42:1k:78:GLN:N	2.41	0.54
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.53	0.54
2:2B:7:G:H21	14:2S:38:GLN:NE2	2.02	0.54
15:2T:106:SER:N	15:2T:109:GLU:OE1	2.34	0.54
32:2a:1010:G:H2'	32:2a:1011:G:H8	1.72	0.54
32:2a:1070:U:H2'	32:2a:1071:C:H6	1.72	0.54
38:2g:143:ARG:HH21	56:2y:42:C:H5'	1.73	0.54
42:2k:17:GLY:HA3	42:2k:77:MET:HE1	1.90	0.54
1:1A:764:A:H5"	3:1D:210:GLY:HA2	1.90	0.54
32:1a:865:A:H2	32:1a:918:A:H4'	1.72	0.54
54:1w:49:G:H1	54:1w:65:U:H3	1.56	0.54
1:2A:1420:U:HO2'	1:2A:1421:G:P	2.29	0.54
32:2a:1176:A:H2'	32:2a:1177:G:C8	2.43	0.54
37:2f:37:VAL:HA	37:2f:65:VAL:HG12	1.88	0.54
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.41	0.54
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.03	0.54
8:1I:76:THR:HG23	8:1I:141:LYS:HE2	1.88	0.54
12:1Q:89:ASN:HB2	55:1x:1:C:C4	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:222:A:H3'	1:2A:421:U:H5'	1.89	0.54
8:2I:84:GLY:O	8:2I:86:THR:N	2.37	0.54
36:2e:36:ASP:O	36:2e:38:GLN:N	2.40	0.54
1:1A:388:G:O2'	1:1A:389:G:N7	2.39	0.54
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.23	0.54
1:1A:2448:A:OP1	62:1A:4105:HOH:O	2.19	0.54
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	1.89	0.54
54:1w:50:A:H61	54:1w:64:U:H3	0.66	0.54
1:2A:2299:G:N1	1:2A:2318:G:N7	2.56	0.54
6:2G:69:ALA:HB3	6:2G:91:ARG:NH2	2.23	0.54
21:2Z:47:VAL:O	21:2Z:50:GLN:NE2	2.40	0.54
32:2a:659:U:OP1	46:2o:9:GLN:NE2	2.41	0.54
32:2a:1077:G:N2	32:2a:1080:A:OP2	2.39	0.54
54:2w:17:G:H5'	54:2w:60:U:O2'	2.07	0.54
1:1A:34:C:H5"	1:1A:35:G:OP2	2.07	0.54
1:1A:2104:G:H2'	1:1A:2105:C:C6	2.43	0.54
1:1A:2727:G:O2'	10:1O:70:LYS:NZ	2.40	0.54
5:1F:164:ARG:HD2	5:1F:175:THR:HG23	1.90	0.54
8:1I:42:SER:OG	8:1I:43:ASN:N	2.39	0.54
15:1T:16:ARG:HH21	15:1T:18:ASP:CG	2.16	0.54
15:1T:127:ALA:C	15:1T:129:ARG:H	2.16	0.54
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.89	0.54
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.90	0.54
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.08	0.54
5:2F:165:ARG:HG2	5:2F:168:ARG:NH2	2.23	0.54
13:2R:33:ARG:NH2	13:2R:115:GLU:OE1	2.33	0.54
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.80	0.54
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.12	0.54
42:2k:34:ASP:HB2	42:2k:35:PRO:HD2	1.88	0.54
18:1W:11:ARG:HA	18:1W:100:THR:HG22	1.90	0.54
33:1b:19:HIS:HA	33:1b:39:ILE:HG23	1.90	0.54
43:1l:88:GLY:O	43:1l:99:HIS:HD2	1.90	0.54
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.42	0.54
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.38	0.54
5:2F:192:LEU:HD13	5:2F:194:MET:HE2	1.89	0.54
9:2N:68:GLU:HG3	9:2N:88:GLU:OE2	2.08	0.54
32:2a:266:G:H5"	32:2a:268:C:H41	1.72	0.54
39:2h:64:LYS:HG2	39:2h:79:VAL:HG21	1.90	0.54
1:1A:639:U:H2'	1:1A:640:C:C6	2.43	0.53
1:1A:1448:G:H4'	1:1A:1542:A:OP1	2.08	0.53
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.90	0.53
32:1a:110:C:O2'	47:1p:25:ARG:O	2.26	0.53
32:2a:1010:G:N1	32:2a:1020:U:H1'	2.23	0.53
32:2a:1411:C:H2'	32:2a:1412:C:C6	2.42	0.53
32:1a:316:G:OP2	32:1a:351:G:O2'	2.26	0.53
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.89	0.53
1:2A:55:G:O2'	1:2A:127:A:N1	2.40	0.53
1:2A:2100:G:N2	1:2A:2189:U:O2	2.34	0.53
17:2V:67:GLY:O	17:2V:88:ARG:NE	2.41	0.53
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.42	0.53
32:2a:108:G:C6	51:2t:15:ARG:HG2	2.43	0.53
32:2a:642:A:N3	39:2h:113:SER:OG	2.41	0.53
32:2a:1148:U:O4'	40:2i:16:ARG:HD2	2.08	0.53
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.43	0.53
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.23	0.53
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.42	0.53
32:1a:258:G:H2'	32:1a:259:G:C8	2.42	0.53
32:1a:591:U:H2'	32:1a:592:G:H8	1.73	0.53
32:1a:721:G:H4'	32:1a:722:A:O4'	2.09	0.53
34:1c:108:ASN:HB3	34:1c:111:LEU:HB2	1.90	0.53
41:1j:40:LEU:HD11	41:1j:71:LEU:HB2	1.91	0.53
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.40	0.53
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.43	0.53
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.90	0.53
32:2a:407:G:H5"	35:2d:115:ARG:HB3	1.89	0.53
40:2i:9:ARG:H	40:2i:79:LEU:HD23	1.73	0.53
44:2m:3:ARG:NH2	44:2m:9:ILE:O	2.33	0.53
47:2p:53:VAL:HG13	47:2p:79:VAL:HG22	1.90	0.53
28:16:9:LEU:HD13	28:16:51:GLU:HG3	1.90	0.53
32:1a:219:C:H2'	32:1a:220:G:O4'	2.07	0.53
32:1a:942:G:H21	40:1i:124:GLN:NE2	2.06	0.53
32:1a:963:G:H5'	62:1a:2024:HOH:O	2.09	0.53
1:2A:300:A:P	20:2Y:86:ARG:HH12	2.31	0.53
1:2A:629:G:N3	1:2A:639:U:O2'	2.41	0.53
1:2A:1434:A:H61	1:2A:1558:A:H62	1.55	0.53
1:2A:2637:U:OP1	4:2E:82:ARG:NH1	2.42	0.53
14:2S:10:ARG:NH2	14:2S:91:PRO:O	2.42	0.53
33:2b:187:LEU:HA	33:2b:201:ILE:HB	1.90	0.53
1:1A:271(G):C:H2'	1:1A:271(H):G:H8	1.74	0.53
1:1A:2155:G:H2'	1:1A:2155:G:N3	2.24	0.53
32:1a:159:G:N2	32:1a:162:A:OP2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:381:C:H2'	32:1a:382:A:O4'	2.09	0.53
1:2A:2557:G:H2'	1:2A:2558:C:H6	1.73	0.53
2:2B:87:G:N2	2:2B:90:A:OP2	2.37	0.53
32:2a:142:G:H2'	32:2a:143:A:C8	2.44	0.53
32:2a:524:G:H2'	32:2a:525:C:C6	2.42	0.53
32:2a:954:G:H2'	32:2a:955:U:O4'	2.08	0.53
32:2a:1052:U:O2'	32:2a:1055:A:OP2	2.17	0.53
44:2m:3:ARG:HB3	44:2m:8:GLU:HA	1.89	0.53
54:2w:76:L3X:N	55:2x:76:31H:O2'	2.41	0.53
1:1A:2754:U:OP1	62:1A:4142:HOH:O	2.19	0.53
37:1f:100:ASN:HB2	49:1r:28:GLU:HA	1.91	0.53
55:1x:15:G:N2	55:1x:21:A:N3	2.57	0.53
1:2A:668:G:H5'	1:2A:669:G:OP2	2.08	0.53
5:2F:117:ARG:HH12	11:2P:1:MET:H3	1.56	0.53
32:2a:947:G:O3'	44:2m:109:THR:OG1	2.26	0.53
33:2b:27:LYS:HD2	33:2b:193:ASP:OD1	2.09	0.53
33:2b:47:THR:HG23	33:2b:202:PRO:HG2	1.90	0.53
1:1A:1054:A:N6	1:1A:1105:U:N3	2.22	0.53
1:1A:2105:C:H2'	1:1A:2106:G:H8	1.73	0.53
1:1A:2165:G:H2'	1:1A:2166:G:C8	2.44	0.53
3:1D:275:LYS:HE3	3:1D:275:LYS:H	1.74	0.53
21:1Z:93:ASP:HB3	21:1Z:131:ARG:HH22	1.74	0.53
32:1a:343:U:O2'	32:1a:346:G:O6	2.25	0.53
32:1a:973:G:H3'	32:1a:974:A:H5"	1.91	0.53
50:1s:80:TYR:CZ	50:1s:82:GLY:HA2	2.43	0.53
1:2A:2823:A:OP1	4:2E:159:HIS:NE2	2.41	0.53
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.09	0.53
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.89	0.53
21:2Z:94:GLU:H	21:2Z:94:GLU:CD	2.17	0.53
32:2a:17:U:O2'	32:2a:1079:G:N3	2.42	0.53
32:2a:35:G:O2'	43:2l:118:SER:O	2.24	0.53
32:2a:1080:A:H5'	36:2e:14:ARG:HH21	1.72	0.53
32:2a:1217:C:H2'	32:2a:1218:C:C6	2.44	0.53
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.09	0.53
56:2y:19:U:H1'	56:2y:21:A:H5'	1.90	0.53
1:1A:1045:A:OP1	1:1A:1046:A:H3'	2.08	0.53
6:1G:66:GLN:HG3	26:14:1:MET:HE1	1.90	0.53
32:1a:279:A:OP2	48:1q:95:TYR:OH	2.22	0.53
32:1a:406:G:N3	35:1d:119:GLN:NE2	2.57	0.53
32:1a:714:G:H2'	32:1a:715:A:C8	2.44	0.53
32:1a:1064:G:O2'	32:1a:1190:G:N2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1090:U:H2'	32:1a:1091:U:H6	1.74	0.53
32:1a:1263:C:H2'	32:1a:1264:C:C6	2.43	0.53
32:1a:1467:G:O6	62:1a:1913:HOH:O	2.18	0.53
37:1f:33:TYR:CD2	37:1f:75:LEU:HD23	2.43	0.53
1:2A:2291:U:OP1	1:2A:2380:C:O2'	2.26	0.53
8:2I:45:LYS:O	8:2I:49:ALA:N	2.35	0.53
32:2a:519:C:H2'	32:2a:520:A:O4'	2.09	0.53
32:2a:620:C:H2'	32:2a:621:A:O4'	2.09	0.53
32:2a:1029:C:C4	32:2a:1032:G:C2	2.97	0.53
32:2a:1263:C:C4	32:2a:1272:G:O6	2.62	0.53
36:2e:32:VAL:HG23	36:2e:62:ALA:HB2	1.91	0.53
1:1A:272(A):U:O2'	1:1A:272(B):G:O5'	2.17	0.53
32:1a:975:A:H5'	32:1a:975:A:H8	1.74	0.53
32:1a:1427:U:H2'	32:1a:1428:A:C8	2.44	0.53
38:1g:50:ILE:HG13	38:1g:61:VAL:HG11	1.89	0.53
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.44	0.53
2:2B:41:U:H5	6:2G:70:VAL:H	1.57	0.53
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.23	0.53
40:2i:9:ARG:HG2	40:2i:14:VAL:HA	1.89	0.53
1:1A:882:G:H4'	54:1w:18:G:O6	2.08	0.53
6:1G:125:PHE:O	62:1G:301:HOH:O	2.19	0.53
6:2G:49:ASP:C	6:2G:51:ARG:H	2.16	0.53
32:2a:1005:A:H3'	32:2a:1006:C:C6	2.44	0.53
32:2a:1060:C:H5"	41:2j:51:ARG:HG2	1.91	0.53
32:2a:1273:G:H5'	32:2a:1274:G:OP2	2.09	0.53
32:2a:1348:U:OP2	62:2a:1913:HOH:O	2.18	0.53
56:2y:36:C:H2'	56:2y:37:A:C8	2.44	0.53
5:1F:129:PHE:CD2	5:1F:163:VAL:HG21	2.43	0.52
32:1a:186:C:H2'	32:1a:187:C:C6	2.44	0.52
32:1a:399:G:H2'	32:1a:400:C:C6	2.43	0.52
32:1a:1226:C:H4'	50:1s:80:TYR:OH	2.09	0.52
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.75	0.52
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.42	0.52
1:2A:1474:C:H42	1:2A:1517:G:H1	1.57	0.52
32:2a:224:C:H2'	32:2a:225:C:C6	2.44	0.52
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.91	0.52
32:2a:935:A:N6	38:2g:3:ARG:HG3	2.24	0.52
32:2a:1517:G:N7	32:2a:1518:MA6:H103	2.24	0.52
33:2b:16:HIS:C	33:2b:18:GLY:H	2.16	0.52
34:2c:6:HIS:HB3	45:2n:49:HIS:ND1	2.24	0.52
36:2e:57:LYS:HG2	36:2e:61:TYR:HE2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2g:29:LYS:HB3	38:2g:105:VAL:HG21	1.91	0.52
51:2t:57:ARG:HH12	51:2t:100:ILE:HD12	1.73	0.52
52:2u:6:ARG:HG2	52:2u:15:ARG:HD2	1.90	0.52
15:1T:24:PRO:HA	15:1T:49:VAL:HG22	1.91	0.52
26:14:20:ASN:OD1	26:14:21:VAL:N	2.41	0.52
35:1d:144:ASP:N	35:1d:144:ASP:OD1	2.42	0.52
14:2S:67:ARG:NH1	14:2S:107:GLU:OE2	2.43	0.52
32:2a:815:A:N7	32:2a:1509:C:O2'	2.35	0.52
32:2a:1118:C:OP1	40:2i:104:ARG:NH1	2.41	0.52
36:2e:7:GLU:OE1	36:2e:37:ARG:NH2	2.30	0.52
1:1A:1866:C:H2'	1:1A:1876:A:O4'	2.08	0.52
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.44	0.52
32:1a:148:G:H2'	32:1a:149:A:C8	2.45	0.52
37:1f:33:TYR:OH	37:1f:78:GLU:HG3	2.10	0.52
37:1f:97:PHE:N	49:1r:30:ASP:OD1	2.41	0.52
42:1k:72:ALA:HB1	42:1k:77:MET:HG2	1.91	0.52
56:1y:66:C:H2'	56:1y:67:G:H8	1.73	0.52
1:2A:657:U:H2'	1:2A:658:C:C6	2.44	0.52
1:2A:1541:G:OP2	1:2A:1542:A:O2'	2.26	0.52
32:2a:1216:G:H5"	45:2n:5:ALA:HB2	1.92	0.52
42:2k:92:GLU:O	42:2k:96:ARG:HG2	2.10	0.52
1:1A:670:A:OP2	62:1A:4141:HOH:O	2.18	0.52
32:1a:110:C:H2'	32:1a:111:G:O4'	2.08	0.52
32:1a:1302:U:OP2	44:1m:21:TYR:OH	2.25	0.52
33:1b:54:THR:HG23	33:1b:199:TYR:HB3	1.91	0.52
56:1y:49:G:N2	56:1y:65:U:O2	2.26	0.52
1:2A:2343:C:O2'	1:2A:2373:G:O2'	2.22	0.52
16:2U:49:HIS:HA	16:2U:52:ARG:HB2	1.90	0.52
32:2a:946:A:H2'	32:2a:947:G:C8	2.44	0.52
32:2a:1347:G:H5"	40:2i:107:ARG:HB3	1.92	0.52
33:2b:15:VAL:HG23	33:2b:16:HIS:HD2	1.74	0.52
1:1A:899:A:H2'	1:1A:899:A:N3	2.25	0.52
8:1I:72:LEU:HD12	8:1I:75:LEU:HD21	1.90	0.52
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.75	0.52
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.91	0.52
46:1o:24:SER:O	46:1o:28:GLN:HG3	2.10	0.52
51:1t:63:ILE:HG22	51:1t:77:ALA:HB1	1.90	0.52
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.44	0.52
1:2A:2125:G:H1	1:2A:2172:U:P	2.33	0.52
1:2A:2320:A:H1'	1:2A:2321:G:C2	2.45	0.52
32:2a:165:C:H2'	32:2a:166:G:H8	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1456:G:O6	51:2t:54:LYS:NZ	2.43	0.52
34:2c:52:LEU:HD13	34:2c:68:VAL:HG13	1.91	0.52
56:2y:34:C:H2'	56:2y:35:C:C6	2.45	0.52
1:1A:744:G:OP1	62:1A:4144:HOH:O	2.19	0.52
1:1A:1078:U:H5'	1:1A:1079:C:OP1	2.10	0.52
1:1A:1187:G:H5"	17:1V:81:TYR:CE1	2.45	0.52
1:1A:2147:G:H3'	1:1A:2147:G:N3	2.24	0.52
24:12:16:LEU:O	24:12:67:LYS:NZ	2.43	0.52
32:1a:933:G:O6	38:1g:3:ARG:NH2	2.42	0.52
1:2A:171:G:H2'	1:2A:172:C:C6	2.45	0.52
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.09	0.52
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.10	0.52
32:2a:254:G:OP1	48:2q:66:SER:OG	2.23	0.52
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.45	0.52
50:2s:52:TYR:HB2	50:2s:57:HIS:CE1	2.45	0.52
32:1a:1504:G:OP1	32:1a:1507:A:H4'	2.10	0.52
1:2A:2342:C:O2'	1:2A:2374:C:OP1	2.25	0.52
15:2T:118:ARG:HG2	32:2a:1442(A):G:C8	2.45	0.52
32:2a:107:G:H2'	32:2a:108:G:O4'	2.09	0.52
32:2a:716:A:N3	42:2k:118:GLY:HA2	2.25	0.52
32:2a:737:A:H2'	32:2a:738:C:C6	2.45	0.52
32:2a:1404:5MC:O2	32:2a:1519:MA6:O2'	2.25	0.52
33:2b:19:HIS:ND1	33:2b:20:GLU:OE2	2.39	0.52
1:1A:264:C:O2	62:1A:4124:HOH:O	2.14	0.52
1:1A:271(X):G:OP2	62:1A:4143:HOH:O	2.19	0.52
1:1A:2140:C:H2'	1:1A:2141:G:H8	1.74	0.52
1:1A:2611:U:C4	27:15:3:LYS:HG2	2.45	0.52
17:1V:74:LYS:HB2	17:1V:83:ARG:HB2	1.91	0.52
2:2B:13:A:N1	2:2B:69:G:O2'	2.41	0.52
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.78	0.52
38:2g:67:GLU:OE2	38:2g:70:LYS:NZ	2.36	0.52
1:1A:363(A):A:H2'	1:1A:363(B):G:C8	2.45	0.52
1:1A:1219:G:OP2	16:1U:19:LYS:NZ	2.42	0.52
4:1E:9:VAL:HB	15:1T:3:ARG:HG2	1.91	0.52
27:15:48:GLU:C	27:15:60:VAL:HG11	2.35	0.52
46:1o:74:ASP:HB3	46:1o:77:ARG:HB2	1.91	0.52
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.43	0.52
14:2S:71:ARG:NH1	14:2S:107:GLU:OE1	2.43	0.52
32:2a:1402:4OC:HM22	32:2a:1403:C:H5'	1.91	0.52
1:1A:2820:A:C5	13:1R:4:LEU:HD11	2.45	0.52
33:1b:21:ARG:HB3	33:1b:39:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1h:21:LYS:O	39:1h:65:TYR:OH	2.21	0.52
1:2A:1815:A:P	3:2D:54:ARG:HH22	2.33	0.52
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.28	0.52
19:2X:31:HIS:HD2	19:2X:33:LYS:H	1.55	0.52
32:2a:1271:G:C2	32:2a:1272:G:N7	2.78	0.52
32:2a:1271:G:N1	32:2a:1272:G:N7	2.57	0.52
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	1.91	0.52
33:2b:92:TYR:CE2	33:2b:151:GLY:HA3	2.45	0.52
36:2e:41:VAL:O	36:2e:66:MET:HA	2.08	0.52
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.09	0.51
1:1A:1278:A:OP1	13:1R:36:THR:HG23	2.11	0.51
1:1A:2127:G:H2'	1:1A:2128:C:C6	2.45	0.51
19:1X:92:LEU:O	19:1X:94:GLY:N	2.42	0.51
23:11:76:ARG:HB2	23:11:97:LEU:HD13	1.91	0.51
32:1a:7:G:H5'	32:1a:298:A:O4'	2.10	0.51
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.10	0.51
2:2B:88:C:H2'	2:2B:89:G:O4'	2.10	0.51
21:2Z:61:LEU:HB2	21:2Z:65:GLN:O	2.10	0.51
21:2Z:152:ALA:HB1	21:2Z:163:LEU:HD11	1.91	0.51
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.45	0.51
37:2f:100:ASN:ND2	49:2r:23:LYS:HE3	2.24	0.51
39:2h:17:THR:HA	39:2h:65:TYR:HE1	1.75	0.51
2:1B:14:U:OP2	2:1B:70:C:O2'	2.23	0.51
32:1a:456:C:H2'	32:1a:457:C:C6	2.45	0.51
32:1a:1036:G:H5"	32:1a:1037:C:C5	2.45	0.51
32:1a:1386:G:N7	62:1a:1946:HOH:O	2.34	0.51
34:1c:73:PRO:HB3	34:1c:103:VAL:HG11	1.92	0.51
56:1y:53:G:H1	56:1y:61:C:N4	2.07	0.51
1:2A:1181:C:H2'	1:2A:1182:A:C8	2.45	0.51
1:2A:2134:A:H2'	1:2A:2134:A:N3	2.25	0.51
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.45	0.51
32:2a:1239:A:O2'	38:2g:114:ARG:O	2.28	0.51
33:2b:21:ARG:HA	33:2b:39:ILE:HA	1.93	0.51
40:2i:88:TYR:HD2	40:2i:89:ASN:HB2	1.75	0.51
42:2k:92:GLU:OE2	49:2r:87:ARG:NH1	2.39	0.51
50:2s:64:GLU:CD	50:2s:64:GLU:H	2.17	0.51
56:2y:22:G:C8	56:2y:46:A:N6	2.78	0.51
1:1A:593:G:H4'	30:18:4:MET:HE2	1.91	0.51
1:1A:674:G:O2'	5:1F:74:ARG:HD3	2.10	0.51
1:1A:1359:A:H2	1:1A:1372:U:O4	1.93	0.51
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1346:A:O2'	38:1g:10:ARG:NH2	2.44	0.51
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	1.93	0.51
1:2A:272:G:O2'	1:2A:421:U:OP2	2.19	0.51
1:2A:1156:A:C8	16:2U:51:LYS:HD2	2.45	0.51
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.91	0.51
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.91	0.51
15:2T:18:ASP:OD1	15:2T:18:ASP:N	2.34	0.51
55:2x:50:U:H2'	55:2x:51:C:C6	2.46	0.51
56:2y:61:C:H2'	56:2y:62:C:C6	2.46	0.51
1:1A:2150:U:H2'	1:1A:2151:G:C8	2.45	0.51
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.93	0.51
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.08	0.51
32:1a:861:G:HO2'	32:1a:874:G:HO2'	1.58	0.51
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.46	0.51
40:1i:42:ARG:NH1	40:1i:71:SER:OG	2.41	0.51
51:1t:87:LYS:O	51:1t:91:LEU:HG	2.11	0.51
1:2A:320:A:O2'	1:2A:322:A:OP2	2.26	0.51
1:2A:330:A:H2	1:2A:1210:A:H2'	1.76	0.51
1:2A:922:U:H2'	1:2A:923:C:C6	2.45	0.51
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.92	0.51
37:2f:9:VAL:HB	37:2f:87:ARG:HB2	1.93	0.51
50:2s:32:LYS:HE2	50:2s:57:HIS:HD2	1.74	0.51
1:1A:1271:G:OP2	62:1A:4129:HOH:O	2.19	0.51
7:1H:3:ARG:HG3	7:1H:4:ILE:N	2.23	0.51
20:1Y:38:ILE:HD11	20:1Y:66:PRO:HG3	1.92	0.51
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.45	0.51
46:1o:6:GLU:OE1	46:1o:6:GLU:N	2.38	0.51
1:2A:1019:U:H2'	1:2A:1020:A:H8	1.75	0.51
21:2Z:93:ASP:HA	21:2Z:131:ARG:HH12	1.75	0.51
1:1A:7:G:H2'	1:1A:8:A:O4'	2.11	0.51
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.11	0.51
1:1A:880:G:H2'	1:1A:881:G:C8	2.40	0.51
1:1A:897:C:N3	1:1A:898:C:N4	2.59	0.51
1:1A:1069:A:H2'	1:1A:1073:A:N7	2.26	0.51
1:1A:2552:OMU:OP2	62:1A:4146:HOH:O	2.19	0.51
32:1a:396:G:O2'	32:1a:398:C:OP1	2.20	0.51
1:2A:2134:A:N6	1:2A:2157:G:H4'	2.20	0.51
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.75	0.51
6:2G:167:GLU:OE1	6:2G:167:GLU:N	2.38	0.51
8:2I:58:LEU:O	8:2I:62:LYS:N	2.44	0.51
9:2N:1:MET:HE1	16:2U:94:ASN:ND2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.10	0.51
39:2h:36:LEU:HD22	39:2h:61:VAL:HG11	1.91	0.51
55:2x:21:A:H61	55:2x:46:G:H2'	1.74	0.51
1:1A:2101:G:H2'	1:1A:2102:U:C6	2.45	0.51
1:1A:2123:G:H2'	1:1A:2124:G:C8	2.46	0.51
32:1a:1212:U:H5"	32:1a:1213:A:H5'	1.93	0.51
32:1a:1286:A:C8	32:1a:1287:A:H4'	2.46	0.51
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.46	0.51
1:2A:2137:C:H42	1:2A:2154:G:H1	1.57	0.51
1:2A:2436:G:O2'	62:2A:3946:HOH:O	2.19	0.51
2:2B:3:C:H2'	2:2B:4:C:C6	2.46	0.51
6:2G:122:PRO:HB3	6:2G:170:ARG:HH21	1.76	0.51
8:2I:75:LEU:HD13	8:2I:105:HIS:HD2	1.75	0.51
19:2X:35:THR:HB	19:2X:38:GLU:HB2	1.92	0.51
21:2Z:126:VAL:HB	21:2Z:161:VAL:HG23	1.92	0.51
32:2a:404:U:H5'	35:2d:122:ARG:HE	1.75	0.51
32:2a:539:A:H2'	32:2a:540:G:C8	2.46	0.51
32:2a:1029:C:N4	32:2a:1032:G:N1	2.58	0.51
32:2a:1312:G:H5'	50:2s:5:LEU:HD11	1.92	0.51
33:2b:149:LEU:HD22	33:2b:152:PHE:CD2	2.45	0.51
1:1A:422:A:OP2	62:1A:4149:HOH:O	2.19	0.51
1:1A:796:C:H2'	1:1A:797:C:C6	2.46	0.51
1:1A:1062:G:P	1:1A:1070:A:H1'	2.50	0.51
1:1A:1796:U:H2'	1:1A:1797:C:H6	1.74	0.51
1:1A:2127:G:H2'	1:1A:2128:C:H6	1.75	0.51
1:1A:2308:G:O2'	1:1A:2310:A:N7	2.42	0.51
9:1N:108:PRO:O	9:1N:113:GLY:HA3	2.10	0.51
32:1a:222:U:H2'	32:1a:223:U:C6	2.46	0.51
32:1a:591:U:H2'	32:1a:592:G:C8	2.46	0.51
32:1a:1152:A:OP1	41:1j:68:HIS:ND1	2.43	0.51
35:1d:119:GLN:HG2	35:1d:123:HIS:CD2	2.46	0.51
41:1j:38:ILE:HD12	41:1j:71:LEU:HD23	1.93	0.51
32:2a:1004:A:C6	32:2a:1037:C:H1'	2.46	0.51
54:2w:72:C:C4	54:2w:73:U:H5	2.27	0.51
1:1A:568:U:H5'	1:1A:945:A:N6	2.26	0.51
1:1A:1095:A:N6	1:1A:1097:U:O2	2.42	0.51
32:1a:373:A:H2'	32:1a:374:A:H8	1.76	0.51
32:1a:920:U:H2'	32:1a:921:U:C6	2.46	0.51
1:2A:586:A:N1	1:2A:809:G:O2'	2.39	0.51
32:2a:1053:G:N7	32:2a:1200:C:H5"	2.26	0.51
33:2b:82:ARG:HB3	33:2b:94:ASN:OD1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:169:LYS:O	33:2b:169:LYS:HD3	2.11	0.51
39:2h:119:LEU:HD13	39:2h:127:LEU:HD13	1.93	0.51
50:2s:28:LYS:HB3	50:2s:29:ARG:CA	2.41	0.51
19:1X:57:LEU:HD11	19:1X:78:LYS:HE2	1.93	0.51
25:13:8:LEU:HG	25:13:31:LEU:HD23	1.92	0.51
32:1a:62:U:OP1	32:1a:385:C:O2'	2.26	0.51
34:1c:172:ARG:HG2	34:1c:174:PRO:HD3	1.92	0.51
42:1k:27:ASN:OD1	42:1k:28:THR:N	2.42	0.51
56:1y:49:G:O6	56:1y:65:U:O4	2.29	0.51
1:2A:646:A:H2'	1:2A:647:G:O4'	2.11	0.51
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.23	0.51
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.44	0.51
32:2a:994:A:H2'	32:2a:995:C:H6	1.76	0.51
32:2a:1094:G:O2'	32:2a:1108:G:N1	2.44	0.51
33:2b:212:GLN:NE2	33:2b:234:PRO:O	2.44	0.51
41:2j:30:SER:O	41:2j:81:THR:OG1	2.19	0.51
1:1A:2163:C:OP2	1:1A:2165:G:N2	2.44	0.50
12:1Q:10:ARG:HH11	12:1Q:11:LYS:HE2	1.75	0.50
32:1a:116:A:OP1	62:1a:1915:HOH:O	2.19	0.50
32:1a:262:A:H2'	32:1a:263:A:C8	2.45	0.50
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.26	0.50
44:1m:23:TYR:HB3	44:1m:67:GLU:HA	1.92	0.50
50:1s:41:VAL:O	50:1s:44:MET:HG3	2.11	0.50
56:1y:75:C:HO2'	56:1y:76:A:H8	1.59	0.50
1:2A:39:C:H2'	1:2A:40:C:C6	2.47	0.50
1:2A:881:G:N1	1:2A:897:C:N3	2.60	0.50
1:2A:1019:U:OP1	1:2A:1035:U:O2'	2.28	0.50
14:2S:23:ARG:NH2	14:2S:85:VAL:O	2.36	0.50
31:29:14:CYS:HA	31:29:27:CYS:HB2	1.92	0.50
32:2a:576:G:O6	32:2a:880:C:O2'	2.25	0.50
56:2y:14:A:H3'	56:2y:15:A:H5"	1.93	0.50
1:1A:1484:G:H1	1:1A:1505:C:H42	1.59	0.50
1:1A:2185:C:H2'	1:1A:2186:G:H8	1.76	0.50
32:1a:993:G:H2'	32:1a:995:C:H41	1.76	0.50
32:1a:1095:U:OP2	62:1a:1916:HOH:O	2.20	0.50
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.75	0.50
35:1d:155:LEU:HB3	35:1d:158:ILE:HD11	1.93	0.50
39:1h:73:ASP:OD1	39:1h:75:ARG:NE	2.44	0.50
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.11	0.50
1:2A:852:G:H2'	1:2A:853:G:C8	2.45	0.50
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.25	0.50
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.39	0.50
6:2G:37:VAL:HB	6:2G:94:LEU:HB2	1.92	0.50
18:2W:88:ARG:NH1	18:2W:94:ASP:OD2	2.45	0.50
32:2a:807:A:H2'	32:2a:808:C:C6	2.46	0.50
32:2a:1411:C:H2'	32:2a:1412:C:H6	1.76	0.50
43:2l:86:ARG:NH1	62:2l:302:HOH:O	2.44	0.50
47:2p:28:ARG:HG2	47:2p:29:ASP:OD1	2.12	0.50
56:2y:2:C:H2'	56:2y:3:G:C8	2.45	0.50
1:1A:752:A:H3'	29:17:1:MET:HE1	1.92	0.50
1:1A:800:A:H8	1:1A:800:A:OP1	1.95	0.50
1:1A:2134:A:O2'	1:1A:2135:A:OP1	2.20	0.50
1:1A:2140:C:N3	1:1A:2151:G:O6	2.45	0.50
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	1.92	0.50
32:1a:1149:C:H2'	32:1a:1150:U:C6	2.46	0.50
34:1c:24:ALA:HB2	34:1c:32:LEU:HD12	1.94	0.50
51:1t:99:LEU:O	51:1t:100:ILE:HG23	2.11	0.50
3:2D:73:VAL:HG13	3:2D:120:GLY:HA3	1.93	0.50
5:2F:156:LEU:HD21	5:2F:163:VAL:HG12	1.93	0.50
9:2N:38:HIS:CE1	9:2N:39:ARG:HG3	2.47	0.50
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.12	0.50
47:2p:74:LEU:HD13	47:2p:79:VAL:HG21	1.92	0.50
55:2x:64:G:H2'	55:2x:65:C:C6	2.47	0.50
1:1A:759:G:OP1	62:1A:4145:HOH:O	2.19	0.50
1:1A:1139:G:OP1	9:1N:101:HIS:ND1	2.38	0.50
3:1D:38:LYS:HE2	3:1D:39:LYS:O	2.10	0.50
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.93	0.50
8:1I:109:ILE:HD12	8:1I:130:TYR:CZ	2.46	0.50
28:16:13:CYS:SG	28:16:47:THR:HG21	2.50	0.50
39:1h:121:ASP:OD2	39:1h:125:ARG:NH2	2.45	0.50
4:2E:3:GLY:HA3	4:2E:81:ILE:HD12	1.93	0.50
33:2b:80:ILE:HG12	33:2b:211:ILE:HD13	1.94	0.50
37:2f:94:GLN:HE22	49:2r:72:ARG:HH12	1.60	0.50
38:2g:22:LEU:HG	38:2g:62:PHE:HE2	1.76	0.50
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.94	0.50
1:1A:588:U:H2'	1:1A:589:C:C6	2.46	0.50
1:1A:1093:G:H3'	1:1A:1094:U:H5"	1.93	0.50
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	1.93	0.50
4:1E:77:ILE:HD13	4:1E:195:LEU:HD13	1.94	0.50
5:1F:53:THR:HG22	5:1F:55:GLY:N	2.17	0.50
32:1a:953:G:H5'	32:1a:965:A:H61	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:166:ASP:O	33:1b:170:GLU:N	2.44	0.50
41:1j:57:LYS:O	41:1j:60:ARG:NE	2.43	0.50
56:1y:46:A:O2'	56:1y:48:C:O5'	2.25	0.50
1:2A:271(G):C:H2'	1:2A:271(H):G:H8	1.75	0.50
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.47	0.50
13:2R:57:ARG:NE	13:2R:59:ASP:OD1	2.45	0.50
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.93	0.50
32:2a:407:G:OP1	35:2d:115:ARG:HD3	2.12	0.50
32:2a:976:G:H5'	32:2a:1358:U:O2'	2.11	0.50
32:2a:994:A:H2'	32:2a:995:C:C6	2.46	0.50
34:2c:152:ILE:HG22	34:2c:167:TRP:HB3	1.93	0.50
1:1A:2136:C:C2	1:1A:2155:G:C2	2.99	0.50
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.93	0.50
20:1Y:82:PRO:O	20:1Y:101:LYS:NZ	2.35	0.50
22:10:23:VAL:HG22	22:10:38:VAL:HG22	1.92	0.50
29:17:33:ARG:NH2	62:17:201:HOH:O	2.39	0.50
32:1a:600:C:H2'	32:1a:601:C:C6	2.46	0.50
1:2A:555:U:O2'	1:2A:556:G:N7	2.38	0.50
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.45	0.50
1:2A:2290:G:O6	62:2A:3938:HOH:O	2.17	0.50
1:2A:2875:C:O2'	15:2T:2:ASN:OD1	2.20	0.50
10:2O:71:ARG:NE	10:2O:105:GLU:OE2	2.44	0.50
21:2Z:23:LYS:HB3	21:2Z:38:TYR:CD1	2.47	0.50
32:2a:613:C:H4'	35:2d:86:LYS:HZ1	1.76	0.50
32:2a:1133:G:H2'	32:2a:1134:G:C8	2.47	0.50
32:2a:1233:G:H2'	32:2a:1234:C:C6	2.47	0.50
32:2a:1261:A:H5'	32:2a:1283:G:O3'	2.11	0.50
50:2s:11:VAL:C	50:2s:13:ASP:H	2.18	0.50
1:1A:81:G:H21	20:1Y:1:MET:HE2	1.75	0.50
1:1A:2131:G:N2	1:1A:2158:A:N1	2.59	0.50
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.46	0.50
29:17:24:THR:CG2	29:17:27:GLY:H	2.18	0.50
32:1a:193:C:H2'	32:1a:194:C:H6	1.75	0.50
32:1a:1223:C:OP2	50:1s:78:ARG:NH2	2.44	0.50
1:2A:570:G:H2'	1:2A:2030:A:C5	2.47	0.50
1:2A:856:C:N4	62:2A:3923:HOH:O	2.40	0.50
1:2A:1665:A:H4'	10:2O:67:LYS:HB2	1.93	0.50
1:2A:1805:U:O2	3:2D:50:THR:HB	2.11	0.50
1:2A:2112:G:C6	56:2y:18:G:C2	2.99	0.50
10:2O:49:ARG:NH1	32:2a:1422:G:O3'	2.44	0.50
32:2a:382:A:H2'	32:2a:383:A:H8	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:674:G:H2'	32:2a:675:A:H8	1.77	0.50
32:2a:685:G:C2	32:2a:686:U:C4	3.00	0.50
1:1A:272(J):C:H2'	1:1A:274:G:C8	2.47	0.50
1:1A:881:G:C2	1:1A:882:G:H1'	2.45	0.50
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.12	0.50
11:1P:94:GLU:HG3	11:1P:124:LYS:HD2	1.92	0.50
32:1a:1513:A:H2'	32:1a:1514:C:C6	2.46	0.50
33:1b:16:HIS:HB3	33:1b:210:SER:CB	2.41	0.50
54:1w:5:G:H2'	54:1w:6:C:C6	2.47	0.50
1:2A:2278:A:OP2	22:20:12:ASN:ND2	2.44	0.50
5:2F:164:ARG:O	5:2F:168:ARG:HB2	2.12	0.50
7:2H:101:ARG:HH12	7:2H:122:THR:HG23	1.76	0.50
11:2P:84:ASN:HB3	11:2P:86:LYS:HG2	1.93	0.50
19:2X:35:THR:HG22	19:2X:37:THR:N	2.26	0.50
21:2Z:45:ASP:OD1	21:2Z:49:ARG:NE	2.45	0.50
33:2b:104:ASN:OD1	33:2b:107:THR:OG1	2.28	0.50
36:2e:84:PHE:O	36:2e:86:ALA:N	2.44	0.50
43:2l:70:ILE:HD13	43:2l:77:LEU:HD12	1.93	0.50
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.47	0.50
1:1A:1859:A:N6	1:1A:1883:G:O2'	2.44	0.50
32:1a:750:G:N3	46:1o:23:GLY:HA3	2.27	0.50
32:1a:958:A:C2	50:1s:55:LYS:HB2	2.47	0.50
44:1m:50:GLU:HA	44:1m:53:VAL:HG12	1.93	0.50
1:2A:30:G:H2'	1:2A:31:C:C6	2.47	0.50
1:2A:1032:A:H2	1:2A:1122:G:H22	1.60	0.50
6:2G:32:PRO:HB2	6:2G:172:LEU:HD22	1.92	0.50
19:2X:46:ALA:HB1	24:22:33:MET:HE1	1.93	0.50
32:2a:544:G:OP1	35:2d:62:GLN:NE2	2.40	0.50
32:2a:1095:U:H2'	32:2a:1096:C:O4'	2.12	0.50
32:2a:1244:C:H42	32:2a:1293:G:H1	1.60	0.50
32:2a:1366:C:H2'	32:2a:1367:C:C6	2.47	0.50
34:2c:120:VAL:HG21	34:2c:137:ALA:HB2	1.93	0.50
43:2l:88:GLY:O	43:2l:99:HIS:HD2	1.95	0.50
1:1A:55:G:O2'	1:1A:127:A:N1	2.41	0.49
1:1A:484:C:OP1	20:1Y:51:VAL:HG22	2.12	0.49
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.76	0.49
1:1A:1075:C:H2'	1:1A:1076:C:H2'	1.94	0.49
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.93	0.49
1:1A:2889:C:H2'	1:1A:2891:G:O4'	2.11	0.49
6:1G:34:LEU:HD23	6:1G:161:THR:HG22	1.92	0.49
32:1a:864:A:H2'	32:1a:865:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.11	0.49
1:2A:1847:A:H4'	1:2A:1848:A:OP2	2.12	0.49
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.93	0.49
6:2G:150:ASP:OD1	6:2G:150:ASP:N	2.39	0.49
26:24:45:GLY:C	26:24:47:GLN:H	2.19	0.49
32:2a:936:C:H2'	32:2a:937:A:O4'	2.12	0.49
32:2a:1518:MA6:H93	32:2a:1519:MA6:H92	1.93	0.49
33:2b:15:VAL:O	33:2b:17:PHE:N	2.45	0.49
35:2d:22:LYS:HB2	35:2d:26:CYS:SG	2.52	0.49
37:2f:75:LEU:O	37:2f:79:LEU:HG	2.12	0.49
38:2g:54:THR:O	38:2g:56:GLN:N	2.45	0.49
1:1A:1179:C:H2'	1:1A:1180:C:H6	1.77	0.49
6:1G:115:ARG:HG2	6:1G:136:ARG:NH2	2.27	0.49
13:1R:2:ARG:HG2	13:1R:5:LYS:HB2	1.94	0.49
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.93	0.49
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.47	0.49
54:1w:1:G:H2'	54:1w:2:C:C6	2.46	0.49
1:2A:84:A:N1	1:2A:98:G:O2'	2.41	0.49
1:2A:715:G:O4'	46:2o:60:VAL:HG11	2.12	0.49
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.12	0.49
1:2A:2065:C:H2'	1:2A:2066:C:H6	1.77	0.49
1:2A:2125:G:N2	1:2A:2173:A:N7	2.60	0.49
1:2A:2540:C:H2'	1:2A:2541:A:O4'	2.12	0.49
4:2E:54:GLN:OE1	4:2E:55:ASN:N	2.45	0.49
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.95	0.49
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	1.94	0.49
15:2T:39:ARG:HG3	15:2T:40:THR:N	2.26	0.49
32:2a:9:G:H2'	32:2a:10:A:C8	2.45	0.49
32:2a:619:U:C2	35:2d:135:LEU:HD21	2.47	0.49
32:2a:976:G:OP2	32:2a:1358:U:O2'	2.27	0.49
32:2a:1004:A:N1	32:2a:1037:C:C2	2.80	0.49
32:2a:1026:G:H5'	32:2a:1027:C:O5'	2.12	0.49
32:2a:1279:A:H5"	41:2j:9:ARG:NH2	2.27	0.49
33:2b:51:LEU:HA	33:2b:54:THR:OG1	2.12	0.49
36:2e:43:LEU:H	36:2e:65:ASN:HB3	1.76	0.49
1:1A:1584:C:O2'	1:1A:1586:A:H5'	2.12	0.49
32:1a:344:A:O2'	32:1a:346:G:O6	2.24	0.49
44:1m:88:ARG:HG2	44:1m:98:VAL:HG13	1.94	0.49
55:1x:59:A:H2'	55:1x:60:U:H5'	1.93	0.49
56:1y:38:A:H2'	56:1y:39:G:O4'	2.12	0.49
1:2A:1496:A:N3	1:2A:1577:C:O2'	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2695:C:H2'	1:2A:2696:U:H6	1.76	0.49
20:2Y:40:GLU:O	20:2Y:42:VAL:HG23	2.12	0.49
32:2a:923:A:OP1	36:2e:21:ALA:HB2	2.12	0.49
32:2a:1003:G:H2'	32:2a:1004:A:O4'	2.12	0.49
33:2b:216:SER:O	33:2b:220:ASP:N	2.34	0.49
34:2c:45:LYS:HG3	34:2c:46:GLU:H	1.76	0.49
50:2s:80:TYR:O	50:2s:82:GLY:N	2.44	0.49
55:2x:61:C:H2'	55:2x:62:C:H6	1.76	0.49
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.12	0.49
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.47	0.49
1:1A:2049:G:N7	62:1A:4226:HOH:O	2.34	0.49
18:1W:1:MET:HE2	18:1W:62:HIS:HB3	1.93	0.49
32:1a:560:U:O2'	32:1a:561:U:OP2	2.28	0.49
32:1a:748:C:H4'	32:1a:749:C:O5'	2.12	0.49
1:2A:700:G:O2'	1:2A:1632:A:N3	2.40	0.49
1:2A:1482:G:H1	1:2A:1506:C:H42	1.60	0.49
1:2A:1782:C:H1'	1:2A:2609:U:H5"	1.94	0.49
1:2A:2156:G:H2'	1:2A:2157:G:N1	2.27	0.49
15:2T:127:ALA:C	15:2T:129:ARG:H	2.20	0.49
32:2a:573:A:N3	32:2a:883:C:O2'	2.43	0.49
32:2a:986:A:H2'	32:2a:987:G:O4'	2.12	0.49
32:2a:1108:G:H5'	34:2c:176:HIS:CD2	2.46	0.49
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.28	0.49
33:2b:44:LEU:O	33:2b:47:THR:OG1	2.26	0.49
40:2i:9:ARG:HG2	40:2i:14:VAL:HG12	1.94	0.49
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.45	0.49
33:1b:60:ASP:OD1	33:1b:64:ARG:NH2	2.38	0.49
38:1g:78:ARG:HG2	38:1g:156:TRP:CZ3	2.47	0.49
40:1i:77:ILE:O	40:1i:81:ILE:HG23	2.13	0.49
1:2A:11:G:C2'	1:2A:12:U:H5'	2.42	0.49
1:2A:247:G:H4'	1:2A:386:G:C5	2.48	0.49
1:2A:903:C:H2'	1:2A:904:C:C6	2.47	0.49
32:2a:222:U:H2'	32:2a:223:U:H6	1.78	0.49
32:2a:1104:G:O2'	33:2b:111:ARG:NH2	2.46	0.49
1:1A:1452:A:OP2	62:1A:4150:HOH:O	2.20	0.49
19:1X:43:VAL:HG21	19:1X:81:VAL:HG11	1.93	0.49
33:1b:142:LEU:HG	33:1b:146:GLN:HE22	1.77	0.49
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.59	0.49
1:2A:11:G:H2'	1:2A:12:U:H5'	1.95	0.49
1:2A:1193:G:OP1	11:2P:14:LYS:NZ	2.33	0.49
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.38	0.49
8:2I:77:LEU:HD13	8:2I:79:ILE:HD11	1.95	0.49
32:2a:1023:G:H3'	32:2a:1024:G:H8	1.77	0.49
32:2a:1133:G:H1	32:2a:1141:C:N4	2.10	0.49
38:2g:65:ALA:O	38:2g:69:VAL:HG23	2.13	0.49
1:1A:2319:G:H1	14:1S:3:ARG:HA	1.77	0.49
5:1F:178:PRO:O	5:1F:205:ARG:NH2	2.45	0.49
22:10:10:THR:HG22	22:10:12:ASN:H	1.77	0.49
32:1a:4:U:O4	39:1h:105:ARG:HD3	2.12	0.49
33:1b:59:GLU:HG3	33:1b:225:ALA:HB2	1.95	0.49
1:2A:2304:G:OP1	6:2G:124:SER:HB2	2.12	0.49
1:2A:2363:C:O2	22:20:39:ARG:NH2	2.44	0.49
9:2N:56:ASN:OD1	9:2N:59:LYS:NZ	2.46	0.49
14:2S:19:LYS:C	14:2S:21:THR:H	2.20	0.49
33:2b:27:LYS:HB2	33:2b:194:PRO:HD2	1.94	0.49
33:2b:219:VAL:O	33:2b:223:ILE:HG12	2.13	0.49
34:2c:131:ARG:NH2	36:2e:50:GLU:HG3	2.27	0.49
34:2c:150:LYS:HG3	34:2c:169:ALA:HB2	1.94	0.49
41:2j:33:GLN:HG2	41:2j:34:VAL:H	1.78	0.49
1:1A:8:A:H2'	1:1A:9:U:C6	2.48	0.49
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.45	0.49
1:1A:1714:G:H1	1:1A:1745(A):C:H42	1.61	0.49
1:1A:2107:C:H2'	1:1A:2108:C:O4'	2.13	0.49
1:1A:2139:C:H42	1:1A:2152:G:H1	1.59	0.49
2:1B:1:U:H2'	2:1B:2:C:C6	2.48	0.49
7:1H:46:GLU:OE1	7:1H:51:ARG:NE	2.40	0.49
20:1Y:98:VAL:HG12	20:1Y:105:ALA:HA	1.94	0.49
43:1l:82:VAL:O	43:1l:106:ASP:HB2	2.13	0.49
44:1m:20:THR:C	44:1m:22:ILE:H	2.21	0.49
1:2A:2127:G:N1	1:2A:2161:C:N4	2.60	0.49
17:2V:29:PRO:HG3	17:2V:64:HIS:CD2	2.47	0.49
40:2i:23:ASN:HD21	40:2i:25:LYS:CE	2.25	0.49
47:2p:17:TYR:HE2	47:2p:41:PRO:HG3	1.76	0.49
1:1A:143:G:H4'	19:1X:35:THR:HG21	1.95	0.49
1:1A:1057:A:N6	1:1A:1087:G:OP1	2.45	0.49
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.48	0.49
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.47	0.49
32:1a:339:C:H2'	32:1a:340:U:C6	2.47	0.49
32:1a:1223:C:P	50:1s:78:ARG:HH21	2.36	0.49
8:2I:81:VAL:HG21	8:2I:88:ILE:HG12	1.95	0.49
15:2T:94:ALA:HB1	15:2T:99:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:24:THR:OG1	26:24:25:TYR:N	2.44	0.49
34:2c:36:ASP:HA	34:2c:39:ILE:HD12	1.95	0.49
36:2e:145:LYS:O	36:2e:149:GLU:HB2	2.13	0.49
38:2g:26:PHE:HB2	38:2g:101:LEU:HD22	1.94	0.49
38:2g:108:ALA:HA	38:2g:111:ARG:HD2	1.95	0.49
38:2g:114:ARG:HB2	38:2g:115:ARG:NH2	2.28	0.49
44:2m:14:ARG:HA	44:2m:44:ARG:HA	1.95	0.49
44:2m:15:VAL:O	44:2m:19:LEU:HG	2.13	0.49
44:2m:29:ARG:HB3	44:2m:64:TRP:CZ3	2.47	0.49
1:1A:11:G:C2'	1:1A:12:U:H5'	2.41	0.49
1:1A:1399:C:OP1	19:1X:25:LYS:NZ	2.46	0.49
1:1A:2146:C:H5"	1:1A:2147:G:C5	2.48	0.49
7:1H:20:ALA:HB3	7:1H:23:ARG:HG3	1.95	0.49
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.48	0.49
24:12:23:LYS:O	24:12:27:GLU:HG3	2.13	0.49
32:1a:21:G:H2'	32:1a:22:G:C8	2.48	0.49
32:1a:190:U:H2'	32:1a:191:G:H8	1.75	0.49
32:1a:890:G:O2'	32:1a:906:G:O6	2.30	0.49
32:1a:1143:G:H2'	32:1a:1144:G:H8	1.78	0.49
37:1f:76:ALA:O	37:1f:80:ARG:HG3	2.13	0.49
1:2A:93:G:H2'	1:2A:94:C:C6	2.47	0.49
1:2A:900:A:O2'	1:2A:901:A:OP1	2.31	0.49
4:2E:50:GLY:HA3	4:2E:75:VAL:HG21	1.95	0.49
5:2F:33:LEU:HD12	5:2F:183:VAL:HG11	1.94	0.49
6:2G:124:SER:O	6:2G:124:SER:OG	2.21	0.49
32:2a:978:A:O2'	32:2a:1322:C:N3	2.42	0.49
33:2b:165:VAL:HA	33:2b:187:LEU:HB3	1.95	0.49
41:2j:40:LEU:HB2	41:2j:69:ASN:CB	2.42	0.49
54:2w:9:A:O2'	54:2w:10:G:N7	2.44	0.49
1:1A:1528:A:OP2	62:1A:4140:HOH:O	2.18	0.48
32:1a:401:C:H2'	32:1a:402:G:H8	1.78	0.48
32:1a:1309:G:OP1	44:1m:88:ARG:NH2	2.37	0.48
39:1h:17:THR:O	39:1h:78:GLN:NE2	2.34	0.48
49:1r:52:PRO:HB2	49:1r:54:ARG:HG2	1.95	0.48
1:2A:2096:U:H2'	1:2A:2097:C:C6	2.48	0.48
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.95	0.48
6:2G:3:LEU:O	6:2G:8:LYS:NZ	2.28	0.48
7:2H:5:GLY:HA3	7:2H:65:HIS:ND1	2.28	0.48
23:21:3:LYS:HB2	23:21:61:ARG:HH22	1.77	0.48
28:26:23:THR:OG1	28:26:24:GLU:N	2.46	0.48
32:2a:501:C:H2'	32:2a:502:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1216:G:OP1	45:2n:2:ALA:HA	2.13	0.48
32:2a:1327:C:OP2	52:2u:12:LYS:NZ	2.39	0.48
32:2a:1370:G:N7	40:2i:109:VAL:HG11	2.28	0.48
38:2g:90:GLU:H	38:2g:90:GLU:CD	2.20	0.48
1:1A:84:A:H5'	20:1Y:8:LYS:HG2	1.95	0.48
1:1A:2126:A:H62	1:1A:2163:C:C4'	2.25	0.48
1:1A:2417:C:OP1	11:1P:65:ARG:NH2	2.45	0.48
12:1Q:10:ARG:NH1	12:1Q:90:VAL:H	2.11	0.48
21:1Z:153:SER:HA	21:1Z:167:PRO:HB3	1.95	0.48
32:1a:509:A:O2'	32:1a:510:A:OP1	2.23	0.48
32:1a:1212:U:H4'	32:1a:1213:A:C8	2.48	0.48
35:1d:8:VAL:HA	35:1d:11:LEU:HD13	1.94	0.48
39:1h:110:ALA:HB3	39:1h:121:ASP:HB3	1.94	0.48
1:2A:2114:A:H2	1:2A:2171:A:N6	2.09	0.48
1:2A:2277:G:OP2	22:20:10:THR:HG21	2.12	0.48
2:2B:2:C:H2'	2:2B:3:C:C6	2.48	0.48
32:2a:957:U:O2'	32:2a:959:A:N7	2.27	0.48
32:2a:1265:G:H2'	32:2a:1266:G:C8	2.48	0.48
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.29	0.48
32:2a:1371:G:OP1	40:2i:12:GLU:HB3	2.13	0.48
37:2f:96:PRO:HB3	49:2r:30:ASP:CG	2.38	0.48
51:2t:9:ASN:OD1	51:2t:9:ASN:N	2.46	0.48
1:1A:1412:A:H2'	1:1A:1413:G:C8	2.49	0.48
6:1G:5:VAL:HG22	6:1G:8:LYS:H	1.78	0.48
7:1H:101:ARG:HH12	7:1H:122:THR:HG23	1.79	0.48
14:1S:77:ALA:HB3	14:1S:110:LEU:HD11	1.94	0.48
32:1a:128:G:H4'	48:1q:3:LYS:HG2	1.96	0.48
32:1a:538:G:H5"	43:1l:114:LYS:HB2	1.95	0.48
46:1o:84:LYS:O	46:1o:84:LYS:HD3	2.13	0.48
56:1y:31:C:H2'	56:1y:32:U:O4'	2.12	0.48
1:2A:35:G:H2'	1:2A:36:G:O4'	2.13	0.48
1:2A:2305:A:H5"	6:2G:134:GLY:HA3	1.96	0.48
1:2A:2391:G:O6	1:2A:2425:A:H8	1.96	0.48
6:2G:44:GLY:N	6:2G:88:ILE:O	2.42	0.48
32:2a:677:U:H3	32:2a:713:G:H22	1.59	0.48
32:2a:946:A:O2'	32:2a:1333:A:N3	2.39	0.48
32:2a:994:A:N7	32:2a:1216:G:H4'	2.29	0.48
33:2b:167:PRO:HD3	33:2b:187:LEU:O	2.13	0.48
35:2d:22:LYS:HG2	61:2d:303:SF4:S4	2.53	0.48
42:2k:41:THR:HG21	42:2k:71:LYS:HB2	1.95	0.48
43:2l:59:ARG:HG3	43:2l:65:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:969:U:H2'	1:1A:970:C:C6	2.48	0.48
1:1A:1669:A:OP2	62:1A:4109:HOH:O	2.20	0.48
24:12:22:GLU:OE2	24:12:68:ARG:NH2	2.46	0.48
32:1a:271:C:H2'	32:1a:272:C:H6	1.78	0.48
32:1a:1090:U:H2'	32:1a:1091:U:C6	2.48	0.48
32:1a:1305:G:H5"	52:1u:4:GLY:HA3	1.96	0.48
34:1c:148:GLY:HA3	34:1c:172:ARG:H	1.78	0.48
36:1e:81:GLU:HG2	36:1e:90:VAL:HG22	1.96	0.48
54:1w:1:G:H2'	54:1w:2:C:C5	2.48	0.48
1:2A:307:G:H21	1:2A:330:A:H62	1.62	0.48
1:2A:1589:C:H2'	1:2A:1590:U:H6	1.78	0.48
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.14	0.48
9:2N:110:GLY:O	9:2N:114:ARG:HG3	2.13	0.48
12:2Q:78:PRO:HD3	55:2x:1:C:C2	2.48	0.48
32:2a:950:U:H3	32:2a:1231:G:H1	1.62	0.48
32:2a:1070:U:H2'	32:2a:1071:C:C6	2.48	0.48
32:2a:1275:A:H2'	32:2a:1276:G:O4'	2.13	0.48
56:2y:18:G:N2	56:2y:56:C:C2	2.81	0.48
56:2y:26:G:H2'	56:2y:27:A:H5'	1.96	0.48
1:1A:1753:G:N1	1:1A:1756:G:OP2	2.46	0.48
3:1D:17:THR:HG1	3:1D:205:VAL:H	1.59	0.48
13:1R:38:VAL:HG12	13:1R:42:LYS:HE3	1.94	0.48
20:1Y:97:ARG:HH11	20:1Y:107:ASP:C	2.22	0.48
34:1c:19:GLU:O	34:1c:40:ARG:NH2	2.46	0.48
34:1c:89:GLU:O	34:1c:93:LYS:N	2.42	0.48
44:1m:120:LYS:HG2	44:1m:121:LYS:H	1.78	0.48
48:1q:67:LYS:O	48:1q:68:ARG:HB2	2.13	0.48
1:2A:287:C:H2'	1:2A:288:C:C6	2.48	0.48
1:2A:492:A:H2'	1:2A:493:G:O4'	2.14	0.48
1:2A:597:U:H2'	1:2A:598:G:C8	2.48	0.48
2:2B:51:G:OP2	14:2S:61:ASN:HA	2.13	0.48
14:2S:84:GLN:H	14:2S:111:GLU:HB2	1.78	0.48
21:2Z:48:PHE:CE1	21:2Z:52:SER:HA	2.48	0.48
32:2a:738:C:OP1	37:2f:2:ARG:NH1	2.46	0.48
32:2a:1006:C:H2'	32:2a:1007:C:O4'	2.13	0.48
32:2a:1310:G:H5'	44:2m:77:ASN:ND2	2.26	0.48
34:2c:119:ARG:NH1	34:2c:123:GLN:HE21	2.12	0.48
40:2i:34:ASN:O	40:2i:38:GLN:HB2	2.13	0.48
40:2i:128:ARG:NH2	55:2x:33:U:OP2	2.47	0.48
54:2w:49:G:O6	54:2w:65:U:O4	2.31	0.48
1:1A:2511:U:O2'	4:1E:138:PRO:O	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:127:GLU:O	7:1H:129:THR:N	2.47	0.48
32:1a:179:A:H2'	32:1a:180:U:C6	2.48	0.48
32:1a:631:G:H2'	32:1a:632:A:H8	1.78	0.48
1:2A:8:A:H2'	1:2A:9:U:C6	2.47	0.48
1:2A:208:C:H2'	1:2A:209:C:C6	2.48	0.48
1:2A:1630:G:H2'	1:2A:1631:C:C6	2.48	0.48
1:2A:2127:G:N2	1:2A:2161:C:N3	2.62	0.48
2:2B:17:C:H2'	2:2B:18:G:O4'	2.13	0.48
8:2I:40:THR:O	8:2I:44:LEU:HB2	2.13	0.48
32:2a:572:A:OP1	62:2a:1914:HOH:O	2.20	0.48
32:2a:1105:A:H2'	32:2a:1106:G:C8	2.41	0.48
32:2a:1292:U:H5'	40:2i:38:GLN:HE21	1.78	0.48
33:2b:74:LYS:NZ	33:2b:206:ASP:OD1	2.46	0.48
52:2u:5:ASP:O	52:2u:11:GLY:HA3	2.14	0.48
1:1A:1800:C:OP1	3:1D:260:ARG:NH2	2.47	0.48
1:1A:2319:G:H22	14:1S:3:ARG:HD3	1.79	0.48
2:1B:33:G:H5'	6:1G:2:PRO:HD3	1.95	0.48
2:1B:84:C:OP1	25:13:15:TYR:OH	2.19	0.48
32:1a:1372:U:OP1	40:1i:72:GLY:N	2.45	0.48
1:2A:184:C:H2'	1:2A:185:U:C6	2.49	0.48
1:2A:884:C:H3'	1:2A:885:C:H6	1.77	0.48
1:2A:992:C:O4'	17:2V:85:LYS:NZ	2.47	0.48
1:2A:2837:G:H21	13:2R:45:ARG:HH12	1.61	0.48
1:2A:2879:C:OP2	62:2A:3948:HOH:O	2.20	0.48
15:2T:36:GLU:O	15:2T:39:ARG:HB3	2.14	0.48
32:2a:1010:G:N2	32:2a:1020:U:HO2'	2.11	0.48
32:2a:1347:G:H22	32:2a:1374:A:P	2.37	0.48
32:2a:1469:G:H2'	32:2a:1470:G:C8	2.48	0.48
33:2b:178:ARG:HH22	39:2h:68:ARG:HH12	1.60	0.48
1:1A:882:G:H4'	54:1w:18:G:C6	2.49	0.48
1:1A:1607:C:H4'	1:1A:1608:A:O5'	2.14	0.48
1:1A:2130:U:H2'	1:1A:2158:A:N1	2.29	0.48
1:1A:2136:C:N3	1:1A:2155:G:N3	2.61	0.48
6:1G:56:ALA:O	6:1G:59:GLU:HG2	2.13	0.48
14:1S:39:ILE:HB	14:1S:49:VAL:HG12	1.95	0.48
1:2A:918:A:N3	2:2B:80:U:O2'	2.40	0.48
1:2A:2070:G:H2'	1:2A:2071:A:C8	2.48	0.48
3:2D:121:PRO:HB3	3:2D:135:PHE:CE2	2.49	0.48
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	1.95	0.48
32:2a:1005:A:H5"	32:2a:1006:C:H5	1.79	0.48
32:2a:1010:G:N2	32:2a:1020:U:O2'	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:85:LEU:O	40:2i:88:TYR:HB3	2.14	0.48
1:1A:484:C:H2'	1:1A:485:C:C6	2.49	0.48
1:1A:857:C:N4	1:1A:858:U:O4	2.47	0.48
1:1A:886:C:OP1	1:1A:886:C:H4'	2.14	0.48
1:1A:2145:C:H3'	1:1A:2146:C:H5'	1.96	0.48
6:1G:38:VAL:HG22	6:1G:93:THR:HG22	1.96	0.48
26:14:15:ILE:O	26:14:33:VAL:N	2.33	0.48
32:1a:736:C:H2'	32:1a:737:A:C8	2.48	0.48
32:1a:828:A:H2'	32:1a:829:G:O4'	2.12	0.48
38:1g:26:PHE:CE2	38:1g:30:ILE:HD11	2.48	0.48
1:2A:744:G:OP1	4:2E:132:HIS:ND1	2.44	0.48
1:2A:1037:G:H2'	1:2A:1038:C:O4'	2.14	0.48
1:2A:1830:C:OP2	62:2A:3945:HOH:O	2.19	0.48
1:2A:2287:A:O2'	1:2A:2288:A:H5"	2.13	0.48
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.48	0.48
32:2a:129(A):G:C6	32:2a:189(E):U:H4'	2.49	0.48
32:2a:952:U:H2'	32:2a:953:G:H8	1.79	0.48
33:2b:28:PHE:CD2	33:2b:190:THR:HA	2.49	0.48
33:2b:92:TYR:CZ	33:2b:151:GLY:HA3	2.49	0.48
35:2d:98:GLU:OE1	35:2d:107:ARG:NH1	2.47	0.48
1:1A:604:G:OP2	11:1P:90:ARG:NH1	2.47	0.48
1:1A:2287:A:O2'	1:1A:2289:G:N7	2.41	0.48
6:1G:116:ASP:OD2	44:1m:68:GLY:HA3	2.13	0.48
32:1a:985:C:H2'	32:1a:986:A:H8	1.78	0.48
32:1a:1111:A:N1	34:1c:177:THR:OG1	2.44	0.48
46:1o:6:GLU:O	46:1o:10:LYS:HG3	2.14	0.48
1:2A:674:G:O2'	5:2F:74:ARG:HD3	2.14	0.48
1:2A:1452:A:OP2	62:2A:3947:HOH:O	2.20	0.48
1:2A:2394:C:N3	56:2y:76:A:O2'	2.31	0.48
32:2a:1260:C:P	32:2a:1284:C:H4'	2.54	0.48
41:2j:47:PHE:N	41:2j:63:PHE:O	2.29	0.48
50:2s:64:GLU:OE2	50:2s:65:ASN:ND2	2.47	0.48
1:1A:383:U:H2'	1:1A:385:C:H5	1.79	0.47
1:1A:883:G:H21	1:1A:893:C:H42	1.62	0.47
1:1A:1252:G:N7	16:1U:36:ARG:NH1	2.62	0.47
1:1A:2143:C:H2'	1:1A:2144:U:O4'	2.14	0.47
8:1I:109:ILE:HD13	8:1I:109:ILE:HA	1.73	0.47
25:13:44:ARG:O	25:13:48:GLU:HG3	2.12	0.47
32:1a:78:G:N1	32:1a:91:C:C4	2.82	0.47
32:1a:1284:C:H3'	32:1a:1285:A:C8	2.48	0.47
32:1a:1381:U:H1'	38:1g:79:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1h:51:VAL:HG11	39:1h:60:ARG:NH1	2.29	0.47
1:2A:71:A:H5"	1:2A:73:A:C8	2.49	0.47
1:2A:886:C:H2'	1:2A:887:A:O4'	2.14	0.47
1:2A:2064:C:H2'	1:2A:2065:C:C6	2.49	0.47
1:2A:2143:C:N4	1:2A:2148:G:H1	2.08	0.47
4:2E:52:LEU:HB3	4:2E:76:ARG:HD3	1.96	0.47
5:2F:123:LEU:HD13	5:2F:192:LEU:HB3	1.96	0.47
32:2a:58:C:O2'	32:2a:388:G:N7	2.39	0.47
32:2a:1040:U:H2'	32:2a:1041:A:H8	1.79	0.47
32:2a:1316:G:N2	32:2a:1318:A:H3'	2.29	0.47
32:2a:1333:A:H2'	32:2a:1334:G:O4'	2.14	0.47
33:2b:74:LYS:O	33:2b:78:GLN:HG2	2.14	0.47
40:2i:125:TYR:HD2	40:2i:126:SER:N	2.12	0.47
42:2k:31:THR:HG23	42:2k:42:TRP:HB3	1.95	0.47
43:2l:8:ASN:O	43:2l:12:ARG:HG3	2.13	0.47
1:1A:41:C:H2'	1:1A:42:G:O4'	2.14	0.47
1:1A:839:U:H2'	1:1A:840:C:C6	2.49	0.47
4:1E:101:ARG:CZ	4:1E:171:GLU:HB2	2.44	0.47
32:1a:841:U:C4	32:1a:848:C:H1'	2.49	0.47
34:1c:66:VAL:HG21	34:1c:91:LEU:HD21	1.95	0.47
35:1d:76:ARG:HA	35:1d:79:PHE:HB3	1.96	0.47
46:1o:88:ARG:HD2	46:1o:88:ARG:HA	1.63	0.47
1:2A:994:C:OP2	16:2U:54:LYS:NZ	2.47	0.47
1:2A:1592:C:H2'	1:2A:1593:G:C8	2.49	0.47
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.49	0.47
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.53	0.47
32:2a:501:C:H2'	32:2a:502:G:H8	1.79	0.47
32:2a:625:G:H2'	32:2a:626:U:H6	1.79	0.47
32:2a:984:C:H2'	32:2a:985:C:C6	2.46	0.47
32:2a:1039:C:C2	32:2a:1040:U:H1'	2.49	0.47
32:2a:1149:C:O2'	32:2a:1280:A:N1	2.36	0.47
38:2g:35:LYS:HD3	38:2g:38:LEU:HD23	1.96	0.47
55:2x:64:G:H2'	55:2x:65:C:H6	1.79	0.47
1:1A:10:G:H1'	1:1A:2801(A):A:C6	2.49	0.47
1:1A:1047:G:H2'	1:1A:1110:G:N2	2.29	0.47
32:1a:1370:G:C2	32:1a:1371:G:C8	3.02	0.47
35:1d:155:LEU:HG	35:1d:157:LEU:H	1.79	0.47
47:1p:40:ASP:HB3	47:1p:48:TRP:HB2	1.96	0.47
54:1w:50:A:N1	54:1w:64:U:O2	2.47	0.47
1:2A:10:G:H2'	1:2A:11:G:C8	2.49	0.47
1:2A:2203:U:H2'	1:2A:2205:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:23:4:LEU:O	25:23:36:VAL:HA	2.15	0.47
28:26:34:LEU:HB2	28:26:51:GLU:HB2	1.95	0.47
32:2a:1409:C:H2'	32:2a:1410:G:C8	2.49	0.47
35:2d:163:GLU:O	35:2d:165:MET:N	2.46	0.47
39:2h:20:TYR:CE1	39:2h:76:PRO:HG2	2.49	0.47
44:2m:59:TYR:O	44:2m:62:ASN:ND2	2.47	0.47
46:2o:82:ILE:HB	46:2o:87:ILE:HB	1.97	0.47
48:2q:12:SER:HB3	48:2q:20:THR:HB	1.96	0.47
50:2s:61:TYR:CE2	50:2s:63:THR:HG23	2.49	0.47
1:1A:1075:C:C2'	1:1A:1076:C:H5'	2.44	0.47
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.50	0.47
6:1G:67:LYS:HD3	26:14:5:ILE:HD12	1.95	0.47
8:1I:72:LEU:HD11	8:1I:107:VAL:HG21	1.95	0.47
21:1Z:3:TYR:CE2	21:1Z:51:ALA:HB2	2.49	0.47
1:2A:882:G:H22	1:2A:894:C:N4	2.13	0.47
1:2A:1762:A:N1	62:2A:4013:HOH:O	2.35	0.47
1:2A:2186:G:C2	1:2A:2187:G:C8	3.03	0.47
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.47	0.47
5:2F:12:LEU:HD12	5:2F:124:LEU:HD21	1.96	0.47
8:2I:72:LEU:HD21	8:2I:107:VAL:HG21	1.96	0.47
9:2N:108:PRO:O	9:2N:113:GLY:HA3	2.14	0.47
15:2T:23:ARG:HD3	15:2T:120:ARG:NH1	2.29	0.47
32:2a:565:U:OP2	32:2a:566:G:O2'	2.28	0.47
32:2a:1109:C:H2'	32:2a:1110:A:O4'	2.15	0.47
36:2e:146:ALA:O	36:2e:150:ARG:HG2	2.15	0.47
54:2w:76:L3X:N	55:2x:76:31H:N3'	2.62	0.47
1:1A:1851:U:H2'	1:1A:1852:C:O4'	2.14	0.47
1:1A:2789:C:O2	1:1A:2894:G:N2	2.46	0.47
1:1A:2804:C:H2'	1:1A:2805:G:C8	2.49	0.47
12:1Q:78:PRO:HG2	12:1Q:81:VAL:HG11	1.96	0.47
32:1a:438:G:H4'	35:1d:123:HIS:CE1	2.49	0.47
1:2A:271(K):U:H4'	1:2A:271(L):U:OP1	2.14	0.47
1:2A:1589:C:H2'	1:2A:1590:U:C6	2.49	0.47
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.32	0.47
32:2a:127:G:OP1	32:2a:635:G:H1'	2.14	0.47
32:2a:532:A:N6	32:2a:1206:G:O2'	2.48	0.47
32:2a:1030(A):G:N3	32:2a:1030(C):G:C8	2.82	0.47
39:2h:39:LEU:HB3	39:2h:45:ILE:HG12	1.96	0.47
39:2h:121:ASP:N	39:2h:121:ASP:OD1	2.47	0.47
1:1A:9:U:O4	1:1A:2629:A:H2	1.97	0.47
1:1A:278:A:H2'	1:1A:279:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.15	0.47
1:1A:2771:C:H2'	1:1A:2772:C:C6	2.49	0.47
3:1D:8:PRO:HB3	3:1D:14:ARG:HG3	1.97	0.47
20:1Y:86:ARG:HB2	20:1Y:98:VAL:HG23	1.96	0.47
26:14:54:GLY:N	26:14:55:ARG:HA	2.29	0.47
28:16:26:ASN:HD21	28:16:28:ARG:NH2	2.12	0.47
32:1a:406:G:H21	35:1d:119:GLN:HE22	1.63	0.47
32:1a:1002:G:H3'	32:1a:1003:G:C4'	2.44	0.47
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.96	0.47
38:1g:78:ARG:HG3	38:1g:87:VAL:HG21	1.97	0.47
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.50	0.47
1:2A:2781:A:H5"	1:2A:2782:G:H5'	1.96	0.47
3:2D:6:PHE:HE2	3:2D:18:VAL:HG13	1.79	0.47
5:2F:117:ARG:HH12	11:2P:1:MET:N	2.12	0.47
6:2G:103:LEU:O	6:2G:107:LEU:HG	2.14	0.47
9:2N:138:LEU:HB3	9:2N:140:VAL:HG13	1.97	0.47
12:2Q:12:GLN:NE2	12:2Q:72:LYS:HG3	2.30	0.47
32:2a:1151:A:O2'	32:2a:1152:A:O5'	2.26	0.47
32:2a:1316:G:H5"	45:2n:17:LYS:HE3	1.97	0.47
33:2b:18:GLY:HA2	33:2b:42:ILE:HG13	1.96	0.47
34:2c:12:LEU:HD23	34:2c:16:ARG:HB3	1.96	0.47
35:2d:158:ILE:O	35:2d:162:LEU:HB2	2.14	0.47
38:2g:108:ALA:O	38:2g:119:ARG:HD2	2.15	0.47
44:2m:6:GLY:HA3	44:2m:67:GLU:HG3	1.96	0.47
49:2r:35:ARG:O	49:2r:37:VAL:N	2.47	0.47
55:2x:21:A:N6	55:2x:46:G:H2'	2.30	0.47
1:1A:271(H):G:H5'	23:11:81:LYS:HE2	1.97	0.47
1:1A:922:U:H2'	1:1A:923:C:C6	2.50	0.47
1:1A:1062:G:C8	1:1A:1070:A:H4'	2.48	0.47
1:1A:1166:C:H2'	1:1A:1167:U:C6	2.49	0.47
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.50	0.47
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.14	0.47
1:1A:2038:G:O6	62:1A:4148:HOH:O	2.19	0.47
11:1P:59:LEU:HD11	30:18:10:ALA:HA	1.97	0.47
12:1Q:29:PHE:HB3	12:1Q:65:PHE:CE1	2.50	0.47
24:12:21:LEU:O	24:12:25:VAL:HG13	2.14	0.47
25:13:4:LEU:HD21	25:13:44:ARG:HH21	1.78	0.47
27:15:35:GLU:HG3	27:15:51:TYR:CD1	2.50	0.47
32:1a:407:G:H5"	35:1d:115:ARG:HB3	1.96	0.47
35:1d:94:LEU:HA	35:1d:97:LEU:HD12	1.95	0.47
46:1o:70:LEU:HD11	46:1o:77:ARG:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:597:U:H2'	1:2A:598:G:H8	1.80	0.47
1:2A:1022:G:N7	9:2N:66:LYS:HE2	2.30	0.47
1:2A:1803:A:HO2'	3:2D:259:THR:HG21	1.80	0.47
1:2A:2218:U:N3	23:21:55:GLY:O	2.48	0.47
1:2A:2390:U:P	30:28:35:GLN:HE22	2.38	0.47
3:2D:36:PRO:HA	3:2D:61:LEU:HD23	1.96	0.47
3:2D:146:GLU:HG2	3:2D:152:GLY:C	2.39	0.47
6:2G:151:ALA:HB3	6:2G:153:ARG:HH12	1.79	0.47
9:2N:67:LEU:HB3	9:2N:88:GLU:HG3	1.96	0.47
32:2a:634:C:H2'	32:2a:635:G:H8	1.80	0.47
32:2a:1024:G:O3'	32:2a:1025:U:H4'	2.14	0.47
32:2a:1193:G:O2'	36:2e:25:ARG:NH2	2.48	0.47
32:2a:1299:A:H2'	32:2a:1299:A:N3	2.30	0.47
32:2a:1401:G:C2	32:2a:1402:4OC:H1'	2.49	0.47
35:2d:163:GLU:C	35:2d:165:MET:H	2.22	0.47
40:2i:4:TYR:CE1	40:2i:88:TYR:HA	2.49	0.47
50:2s:51:VAL:O	50:2s:58:VAL:N	2.35	0.47
56:2y:21:A:C6	56:2y:48:C:C4	3.03	0.47
56:2y:32:U:H2'	56:2y:33:U:O2	2.14	0.47
1:1A:2233:U:H2'	1:1A:2234:G:C8	2.50	0.47
20:1Y:5:MET:HE2	20:1Y:5:MET:HB2	1.70	0.47
25:13:18:ASP:OD1	25:13:18:ASP:N	2.46	0.47
28:16:38:LYS:HE3	28:16:38:LYS:HB3	1.72	0.47
32:1a:328:C:H4'	32:1a:329:A:H5"	1.95	0.47
32:1a:447:G:H2'	32:1a:485:G:N2	2.30	0.47
32:1a:985:C:H2'	32:1a:986:A:C8	2.50	0.47
32:1a:1198:G:N7	62:1a:1949:HOH:O	2.35	0.47
41:1j:78:ASN:O	41:1j:80:LYS:N	2.48	0.47
1:2A:882:G:H22	1:2A:894:C:H42	1.62	0.47
1:2A:918:A:C2	2:2B:81:G:H5'	2.50	0.47
1:2A:1183:G:H5"	25:23:30:ARG:NH2	2.30	0.47
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.80	0.47
6:2G:70:VAL:HA	6:2G:90:LEU:HD23	1.97	0.47
8:2I:96:ASP:OD1	8:2I:96:ASP:N	2.48	0.47
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HE2	1.97	0.47
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.50	0.47
32:2a:503:C:OP2	43:2l:116:SER:HB3	2.15	0.47
32:2a:545:C:H5'	35:2d:72:GLU:HB2	1.97	0.47
32:2a:983:A:H3'	32:2a:983:A:N3	2.29	0.47
32:2a:1129:C:O2'	32:2a:1130:A:N7	2.48	0.47
33:2b:82:ARG:HB2	33:2b:92:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:61:C:H3'	54:2w:62:C:H5"	1.95	0.47
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.14	0.47
1:1A:2805:G:H2'	1:1A:2807:G:H8	1.77	0.47
3:1D:180:GLY:HA3	3:1D:275:LYS:HE2	1.97	0.47
5:1F:135:LYS:HB2	5:1F:138:GLU:HG3	1.97	0.47
8:1I:4:ILE:HB	8:1I:37:VAL:HG23	1.97	0.47
26:14:58:ARG:NE	50:1s:68:GLY:H	2.10	0.47
32:1a:243:A:H4'	32:1a:244:U:H5"	1.97	0.47
32:1a:1209:C:O2'	32:1a:1214:C:N4	2.48	0.47
32:1a:1316:G:N1	32:1a:1319:A:OP2	2.48	0.47
38:1g:27:ILE:HA	38:1g:30:ILE:HD12	1.97	0.47
38:1g:74:GLU:OE2	38:1g:95:ARG:NE	2.43	0.47
50:1s:36:ARG:NH2	50:1s:72:GLY:O	2.48	0.47
1:2A:286:C:H2'	1:2A:287:C:H6	1.80	0.47
1:2A:1837:C:O2'	1:2A:1927:A:N3	2.34	0.47
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	1.97	0.47
21:2Z:146:ILE:HA	21:2Z:174:VAL:O	2.15	0.47
26:24:53:GLU:HG2	26:24:54:GLY:N	2.30	0.47
32:2a:1150:U:H4'	41:2j:41:PRO:HG3	1.97	0.47
33:2b:213:LEU:HD22	33:2b:214:ILE:HD13	1.97	0.47
34:2c:111:LEU:HD11	34:2c:144:SER:O	2.15	0.47
34:2c:164:ARG:HG2	34:2c:165:THR:H	1.80	0.47
38:2g:70:LYS:O	38:2g:138:LYS:HD2	2.15	0.47
54:2w:43:U:H2'	54:2w:44:A:C8	2.50	0.47
1:1A:992:C:OP1	17:1V:74:LYS:NZ	2.35	0.47
1:1A:2241:A:O2'	1:1A:2242:G:H5'	2.15	0.47
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.50	0.47
1:1A:2820:A:OP2	13:1R:2:ARG:NH2	2.48	0.47
7:1H:3:ARG:CD	7:1H:6:ARG:HG3	2.44	0.47
32:1a:17:U:H2'	32:1a:18:C:C6	2.50	0.47
32:1a:1277:C:H1'	32:1a:1282:C:O2	2.15	0.47
33:1b:15:VAL:HG21	33:1b:213:LEU:HD23	1.97	0.47
33:1b:20:GLU:HG2	33:1b:23:ARG:HH11	1.80	0.47
47:1p:47:ASP:OD1	47:1p:47:ASP:N	2.48	0.47
1:2A:271(Y):U:O3'	1:2A:271(Z):C:H6	1.98	0.47
1:2A:2127:G:C2	1:2A:2161:C:N3	2.83	0.47
2:2B:24:G:N3	2:2B:26:A:N6	2.62	0.47
3:2D:206:LEU:HD22	3:2D:211:ARG:HG2	1.97	0.47
10:2O:68:GLU:OE1	10:2O:78:ARG:NH1	2.48	0.47
21:2Z:95:PRO:HA	21:2Z:129:SER:HA	1.97	0.47
21:2Z:138:GLU:N	21:2Z:156:LYS:HZ3	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:187:LEU:HD23	33:2b:188:ALA:N	2.30	0.47
34:2c:61:ALA:N	34:2c:63:ASN:OD1	2.36	0.47
38:2g:69:VAL:HG11	38:2g:134:ALA:HB1	1.97	0.47
49:2r:26:LEU:HB3	49:2r:29:PHE:HE2	1.80	0.47
1:1A:2116:G:H2'	1:1A:2117:A:C5	2.50	0.46
1:1A:2140:C:H2'	1:1A:2141:G:C8	2.50	0.46
11:1P:39:LYS:HB2	11:1P:45:LEU:HD13	1.97	0.46
20:1Y:6:HIS:HE1	20:1Y:72:VAL:O	1.97	0.46
32:1a:102:G:O2'	32:1a:151:A:N3	2.44	0.46
32:1a:452:A:O2'	32:1a:453:A:OP2	2.25	0.46
32:1a:545:C:OP1	35:1d:61:LYS:NZ	2.43	0.46
55:1x:61:C:H2'	55:1x:62:C:C6	2.50	0.46
1:2A:828:U:H4'	1:2A:831:G:N1	2.30	0.46
1:2A:1445(A):C:H2'	1:2A:1446:C:C6	2.50	0.46
1:2A:2611:U:H6	1:2A:2611:U:H5'	1.79	0.46
3:2D:182:LEU:HD23	3:2D:182:LEU:HA	1.81	0.46
10:2O:119:PRO:HB2	15:2T:68:TYR:CZ	2.50	0.46
17:2V:16:PRO:HD3	17:2V:99:ILE:HD11	1.97	0.46
32:2a:114:U:O2'	32:2a:115:G:H5'	2.15	0.46
32:2a:1287:A:N6	32:2a:1371:G:O4'	2.40	0.46
56:2y:65:U:H2'	56:2y:66:C:C6	2.50	0.46
1:1A:271(G):C:H2'	1:1A:271(H):G:C8	2.51	0.46
1:1A:548:A:O2'	1:1A:549:G:OP1	2.28	0.46
1:1A:1183:G:O2'	25:13:29:ARG:NH1	2.48	0.46
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.97	0.46
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.16	0.46
32:1a:78:G:C2	32:1a:91:C:N3	2.84	0.46
32:1a:413:G:N2	32:1a:428:G:H1'	2.29	0.46
32:1a:738:C:H5"	37:1f:69:GLU:HB2	1.97	0.46
32:1a:859:A:H2'	32:1a:860:A:O4'	2.15	0.46
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.15	0.46
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.30	0.46
1:2A:2816:C:O3'	13:2R:99:LYS:NZ	2.48	0.46
1:2A:2837:G:H21	13:2R:45:ARG:NH1	2.13	0.46
2:2B:14:U:O3'	2:2B:108:U:O2'	2.32	0.46
14:2S:41:ASP:OD1	14:2S:44:LYS:N	2.48	0.46
17:2V:1:MET:HG2	17:2V:43:GLU:OE1	2.15	0.46
26:24:9:LEU:HA	26:24:26:SER:O	2.15	0.46
1:1A:2331:G:O2'	22:10:43:THR:HG22	2.15	0.46
1:1A:2722:G:H5'	13:1R:4:LEU:HD12	1.97	0.46
19:1X:60:ARG:HH22	29:17:47:ARG:HH12	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:250:A:H4'	32:1a:251:G:O5'	2.15	0.46
32:1a:352:C:O2'	32:1a:354:G:OP1	2.30	0.46
32:1a:737:A:H2'	32:1a:738:C:C6	2.50	0.46
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.31	0.46
32:1a:1236:A:H4'	32:1a:1304:G:H4'	1.96	0.46
35:1d:134:ASP:OD1	35:1d:134:ASP:N	2.47	0.46
38:1g:8:GLU:H	38:1g:8:GLU:HG3	1.50	0.46
54:1w:76:L3X:N	55:1x:76:31H:N3'	2.63	0.46
1:2A:730:C:H3'	62:2A:4340:HOH:O	2.14	0.46
1:2A:882:G:H2'	1:2A:883:G:C8	2.50	0.46
1:2A:1263:U:C4	1:2A:1264:G:C6	3.04	0.46
1:2A:1316:U:H2'	1:2A:1317:A:H8	1.81	0.46
4:2E:181:LEU:HD12	4:2E:181:LEU:HA	1.81	0.46
11:2P:7:ARG:HH21	11:2P:7:ARG:HB3	1.79	0.46
19:2X:60:ARG:HH22	29:27:47:ARG:NH1	2.10	0.46
31:29:16:VAL:HG22	31:29:25:VAL:HG22	1.97	0.46
32:2a:1227:A:OP1	50:2s:80:TYR:OH	2.26	0.46
32:2a:1264:C:C4	32:2a:1272:G:O6	2.68	0.46
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.50	0.46
1:1A:271(K):U:H4'	1:1A:271(L):U:OP2	2.14	0.46
1:1A:375:C:H5"	62:1A:4209:HOH:O	2.16	0.46
1:1A:576:U:H2'	1:1A:577:G:C8	2.50	0.46
1:1A:2304:G:H22	1:1A:2312:U:H3	1.63	0.46
1:1A:2557:G:H2'	1:1A:2558:C:C6	2.51	0.46
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.50	0.46
1:1A:2693:A:H2'	1:1A:2694:G:C8	2.51	0.46
1:1A:2879:C:OP2	62:1A:4151:HOH:O	2.20	0.46
8:1I:48:GLU:HB3	8:1I:52:ARG:NH1	2.31	0.46
21:1Z:70:LEU:HG	21:1Z:91:LEU:HD11	1.97	0.46
32:1a:149:A:N1	32:1a:172:A:N6	2.63	0.46
32:1a:1151:A:O2'	32:1a:1152:A:H8	1.98	0.46
42:1k:20:TYR:HB2	42:1k:31:THR:HG23	1.98	0.46
54:1w:60:U:H5"	54:1w:61:C:H5	1.81	0.46
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.31	0.46
1:2A:686:G:N2	1:2A:788:A:H61	2.14	0.46
1:2A:991:C:H42	1:2A:1163:G:H1	1.62	0.46
1:2A:1462:C:H4'	1:2A:2703:C:H5'	1.98	0.46
1:2A:2165:G:H2'	1:2A:2166:G:O4'	2.15	0.46
1:2A:2802:G:C4	1:2A:2803:C:H1'	2.50	0.46
2:2B:80:U:H2'	2:2B:81:G:C8	2.50	0.46
21:2Z:144:LEU:HD23	21:2Z:174:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:14:ILE:O	26:24:21:VAL:HA	2.15	0.46
26:24:62:ARG:HA	26:24:62:ARG:NE	2.30	0.46
32:2a:56:U:H2'	32:2a:57:G:C8	2.51	0.46
32:2a:643:C:H2'	32:2a:644:G:C8	2.47	0.46
32:2a:1508:G:H2'	32:2a:1509:C:C6	2.51	0.46
38:2g:78:ARG:HG3	38:2g:156:TRP:CZ3	2.50	0.46
40:2i:8:GLY:HA2	40:2i:79:LEU:HD23	1.98	0.46
43:2l:49:ASN:HD22	43:2l:53:ARG:HH12	1.62	0.46
44:2m:13:LYS:HA	44:2m:44:ARG:HH11	1.79	0.46
1:1A:198:C:H5'	1:1A:2244:U:OP1	2.15	0.46
1:1A:2175:C:H2'	1:1A:2176:A:C8	2.50	0.46
1:1A:2336:A:H61	22:10:43:THR:CG2	2.29	0.46
7:1H:101:ARG:HH22	7:1H:122:THR:HA	1.80	0.46
32:1a:1187:G:N3	45:1n:60:SER:OG	2.48	0.46
32:1a:1284:C:H3'	32:1a:1285:A:H8	1.79	0.46
32:1a:1343:G:H2'	32:1a:1344:C:C6	2.50	0.46
33:1b:78:GLN:NE2	33:1b:94:ASN:O	2.48	0.46
37:1f:22:GLU:OE1	37:1f:84:ASN:HB2	2.16	0.46
44:1m:79:LYS:HA	44:1m:82:MET:HE3	1.96	0.46
56:1y:8:4SU:O2'	56:1y:48:C:H1'	2.16	0.46
1:2A:86:C:H4'	1:2A:104:U:H1'	1.98	0.46
2:2B:7:G:H2'	2:2B:8:U:O4'	2.15	0.46
4:2E:56:PRO:HA	4:2E:59:VAL:HG22	1.98	0.46
27:25:35:GLU:HG3	27:25:51:TYR:CD1	2.51	0.46
32:2a:781:A:H5'	32:2a:782:A:OP2	2.15	0.46
32:2a:1209:C:O2'	32:2a:1214:C:N4	2.41	0.46
44:2m:91:ARG:HD2	44:2m:96:LEU:HB2	1.97	0.46
45:2n:24:CYS:HB2	45:2n:40:CYS:HB3	1.97	0.46
50:2s:33:THR:HG21	50:2s:49:ILE:HD11	1.96	0.46
54:2w:18:G:H1	54:2w:56:C:H42	1.64	0.46
1:1A:184:C:H2'	1:1A:185:U:H6	1.78	0.46
1:1A:1164:G:H2'	1:1A:1165:U:C6	2.51	0.46
1:1A:1693:U:H1'	3:1D:14:ARG:NH1	2.31	0.46
3:1D:37:LEU:HD13	3:1D:87:ASN:ND2	2.30	0.46
3:1D:71:ASP:HB2	3:1D:103:ARG:HH12	1.80	0.46
6:1G:111:LEU:HD13	6:1G:120:LEU:HD11	1.98	0.46
22:10:10:THR:HA	62:10:211:HOH:O	2.15	0.46
32:1a:1239:A:H62	32:1a:1299:A:H62	1.63	0.46
35:1d:112:VAL:H	35:1d:116:GLN:NE2	2.14	0.46
35:1d:202:LEU:HA	35:1d:205:GLU:HB2	1.97	0.46
38:1g:113:GLU:OE1	38:1g:122:HIS:ND1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:1l:69:TYR:HB2	43:1l:96:VAL:HG11	1.98	0.46
1:2A:1598:C:H2'	1:2A:1599:C:C6	2.50	0.46
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.96	0.46
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	1.97	0.46
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.16	0.46
14:2S:29:PHE:O	14:2S:35:ILE:HA	2.15	0.46
21:2Z:93:ASP:HA	21:2Z:131:ARG:HH22	1.81	0.46
32:2a:189(D):C:H2'	32:2a:189(E):U:O4'	2.16	0.46
32:2a:448:A:OP2	32:2a:485:G:N2	2.39	0.46
32:2a:662:G:H2'	32:2a:663:A:C8	2.51	0.46
32:2a:742:G:OP2	46:2o:35:ARG:NH2	2.49	0.46
32:2a:1004:A:N3	32:2a:1038:C:C2	2.83	0.46
32:2a:1128:C:O2'	32:2a:1147:C:N3	2.43	0.46
32:2a:1190:G:O2'	34:2c:3:ASN:HB2	2.16	0.46
34:2c:47:LEU:HB3	34:2c:52:LEU:HB2	1.97	0.46
34:2c:182:ILE:HG22	34:2c:203:PHE:HA	1.98	0.46
36:2e:43:LEU:O	36:2e:65:ASN:ND2	2.49	0.46
40:2i:102:LEU:HD12	40:2i:103:THR:HG22	1.97	0.46
46:2o:8:LYS:O	46:2o:12:ILE:HG13	2.15	0.46
1:1A:1837:C:OP1	32:1a:784:C:H4'	2.16	0.46
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.15	0.46
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.51	0.46
4:1E:29:GLY:HA3	62:1E:412:HOH:O	2.14	0.46
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.51	0.46
10:1O:26:LYS:HB3	10:1O:26:LYS:HE3	1.83	0.46
28:16:47:THR:HG22	28:16:48:VAL:O	2.15	0.46
32:1a:1532:U:O5'	32:1a:1532:U:H6	1.97	0.46
33:1b:122:PHE:CE2	33:1b:139:LYS:HD2	2.45	0.46
41:1j:11:PHE:HE1	41:1j:67:THR:HG22	1.80	0.46
44:1m:86:CYS:SG	44:1m:87:TYR:N	2.88	0.46
54:1w:55:PSU:N3	54:1w:57:G:H5"	2.31	0.46
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.15	0.46
1:2A:1580:A:H8	1:2A:1580:A:OP2	1.98	0.46
7:2H:3:ARG:HG2	7:2H:6:ARG:HG2	1.97	0.46
13:2R:55:ALA:HB2	13:2R:79:LEU:HD13	1.96	0.46
32:2a:875:C:O2'	39:2h:14:ARG:HD2	2.16	0.46
32:2a:1239:A:H62	32:2a:1299:A:N6	2.13	0.46
32:2a:1343:G:H2'	32:2a:1344:C:C6	2.50	0.46
33:2b:12:GLU:O	33:2b:15:VAL:HG22	2.15	0.46
34:2c:70:VAL:O	34:2c:106:VAL:N	2.43	0.46
49:2r:37:VAL:O	49:2r:41:LYS:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:2s:41:VAL:HG12	50:2s:44:MET:SD	2.55	0.46
56:2y:17:G:O2'	56:2y:18:G:H5'	2.15	0.46
1:1A:884:C:C5	1:1A:885:C:H1'	2.50	0.46
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.51	0.46
32:1a:195:A:H2'	32:1a:196:A:C4	2.51	0.46
32:1a:964:A:N3	32:1a:969:A:O2'	2.47	0.46
35:1d:76:ARG:HD2	35:1d:207:TYR:CE1	2.51	0.46
50:1s:40:ILE:HB	50:1s:67:VAL:O	2.16	0.46
1:2A:1830:C:H2'	1:2A:1831:G:H8	1.81	0.46
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.51	0.46
1:2A:2378:A:H4'	14:2S:23:ARG:CZ	2.46	0.46
1:2A:2402:C:H1'	1:2A:2403:C:H5	1.80	0.46
3:2D:232:PRO:HB3	3:2D:244:ARG:CZ	2.46	0.46
5:2F:116:ASP:O	5:2F:120:GLU:HG2	2.16	0.46
26:24:64:GLY:C	26:24:66:SER:H	2.24	0.46
32:2a:120:A:C6	32:2a:122:G:C2	3.04	0.46
32:2a:341:C:O2	32:2a:348:G:N2	2.34	0.46
32:2a:1124:G:H4'	41:2j:38:ILE:HD12	1.96	0.46
41:2j:69:ASN:O	41:2j:70:ARG:NH1	2.41	0.46
48:2q:3:LYS:HD3	48:2q:61:GLU:O	2.16	0.46
49:2r:73:ALA:HB3	49:2r:79:LEU:HD12	1.98	0.46
54:2w:64:U:H2'	54:2w:65:U:C6	2.50	0.46
1:1A:81:G:HO2'	1:1A:295:G:HO2'	1.64	0.46
1:1A:271(D):G:H2'	1:1A:271(E):U:C6	2.51	0.46
1:1A:1070:A:N6	1:1A:1097:U:H4'	2.31	0.46
1:1A:1508:A:O2'	1:1A:1509:C:H5"	2.15	0.46
1:1A:2285:C:OP2	28:16:6:ARG:NH1	2.46	0.46
1:1A:2406:U:H2'	1:1A:2406:U:OP2	2.16	0.46
26:14:53:GLU:HG3	26:14:54:GLY:H	1.81	0.46
33:1b:37:ASN:C	33:1b:39:ILE:H	2.24	0.46
55:1x:61:C:H2'	55:1x:62:C:H6	1.80	0.46
1:2A:1530:C:O2'	1:2A:1531:C:O5'	2.27	0.46
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.51	0.46
19:2X:35:THR:HG22	19:2X:37:THR:H	1.80	0.46
32:2a:736:C:H2'	32:2a:737:A:C8	2.51	0.46
32:2a:1014:A:H2'	32:2a:1015:A:C8	2.51	0.46
32:2a:1260:C:O5'	32:2a:1284:C:H4'	2.15	0.46
32:2a:1518:MA6:H93	32:2a:1519:MA6:C9	2.46	0.46
44:2m:107:ALA:HB3	44:2m:111:LYS:HE3	1.97	0.46
1:1A:1055:G:H2'	1:1A:1056:G:O4'	2.16	0.46
5:1F:150:GLY:HA2	5:1F:172:TRP:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:731:G:H5'	32:1a:766:A:H4'	1.97	0.46
32:1a:1086:U:H3	32:1a:1099:G:H22	1.63	0.46
34:1c:119:ARG:HE	34:1c:140:ARG:CZ	2.28	0.46
44:1m:3:ARG:HG3	44:1m:4:ILE:H	1.81	0.46
51:1t:47:GLY:N	51:1t:48:LYS:HB2	2.31	0.46
1:2A:27:G:O2'	1:2A:28:A:OP2	2.29	0.46
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.51	0.46
1:2A:153:C:H2'	1:2A:154:G:O4'	2.16	0.46
1:2A:171:G:H2'	1:2A:172:C:H6	1.79	0.46
1:2A:907:U:HO2'	12:2Q:101:ARG:HH22	1.60	0.46
5:2F:133:ASN:OD1	5:2F:133:ASN:N	2.49	0.46
7:2H:91:GLY:HA2	7:2H:160:LYS:HG2	1.98	0.46
9:2N:4:TYR:O	16:2U:64:ARG:NH2	2.45	0.46
32:2a:316:G:OP2	32:2a:351:G:O2'	2.33	0.46
32:2a:429:U:H1'	32:2a:430:A:H5"	1.98	0.46
32:2a:792:A:O2'	32:2a:794:A:N7	2.43	0.46
32:2a:939:G:P	38:2g:95:ARG:HH22	2.39	0.46
32:2a:1291:G:O3'	40:2i:39:GLY:HA3	2.16	0.46
32:2a:1412:C:H2'	32:2a:1413:A:H8	1.81	0.46
35:2d:169:LYS:HG3	35:2d:170:VAL:H	1.80	0.46
55:2x:23:C:H2'	55:2x:24:U:C6	2.50	0.46
1:1A:247:G:H4'	1:1A:386:G:C5	2.51	0.45
1:1A:483:A:H3'	1:1A:484:C:C6	2.51	0.45
1:1A:1268:A:C2	1:1A:2013:A:C4	3.04	0.45
8:1I:87:LYS:HB2	8:1I:87:LYS:NZ	2.31	0.45
15:1T:1:MET:HE2	15:1T:3:ARG:HG3	1.97	0.45
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	1.98	0.45
32:1a:555:C:H2'	32:1a:556:C:C6	2.51	0.45
32:1a:1376:U:OP1	38:1g:98:SER:OG	2.28	0.45
8:2I:59:ALA:HA	8:2I:62:LYS:HD2	1.97	0.45
20:2Y:7:VAL:HG21	20:2Y:72:VAL:HG12	1.98	0.45
32:2a:1004:A:C8	32:2a:1005:A:H4'	2.51	0.45
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.16	0.45
35:2d:3:ARG:NH1	35:2d:5:ILE:HG22	2.31	0.45
37:2f:33:TYR:HE2	37:2f:78:GLU:HG2	1.82	0.45
56:2y:40:C:H2'	56:2y:41:U:C6	2.51	0.45
1:1A:414:C:H2'	1:1A:415:A:C8	2.51	0.45
1:1A:1045:A:OP1	1:1A:1045:A:H4'	2.16	0.45
8:1I:38:LEU:HD21	23:11:75:GLU:CD	2.41	0.45
27:15:35:GLU:HG3	27:15:51:TYR:CG	2.51	0.45
34:1c:121:ALA:HB1	34:1c:189:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1f:97:PHE:O	49:1r:31:LEU:HD23	2.16	0.45
38:1g:51:GLN:O	38:1g:55:GLY:HA2	2.16	0.45
49:1r:26:LEU:HB3	49:1r:29:PHE:HE2	1.82	0.45
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.16	0.45
1:2A:335:C:H4'	20:2Y:73:ARG:HD2	1.98	0.45
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.17	0.45
10:2O:26:LYS:O	10:2O:30:ALA:HB2	2.17	0.45
21:2Z:40:ASP:OD2	21:2Z:43:GLU:N	2.36	0.45
26:24:16:CYS:SG	26:24:17:GLY:N	2.90	0.45
32:2a:598:U:O4	62:2a:1901:HOH:O	2.19	0.45
32:2a:1265:G:H2'	32:2a:1266:G:H8	1.81	0.45
34:2c:162:GLN:NE2	53:2v:24:A:O3'	2.48	0.45
41:2j:47:PHE:CE1	45:2n:37:PHE:HE2	2.34	0.45
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.97	0.45
52:2u:5:ASP:O	52:2u:8:THR:OG1	2.30	0.45
1:1A:1406:U:H2'	1:1A:1407:C:H6	1.80	0.45
1:1A:2320:A:H2'	1:1A:2320:A:N3	2.32	0.45
2:1B:66:A:H61	2:1B:108:U:H2'	1.82	0.45
8:1I:4:ILE:HG12	8:1I:18:VAL:HG12	1.97	0.45
26:14:63:TYR:N	26:14:64:GLY:HA2	2.30	0.45
40:1i:25:LYS:N	40:1i:60:ASP:OD1	2.44	0.45
41:1j:8:LEU:HD22	41:1j:96:ILE:HG22	1.99	0.45
1:2A:568:U:H5'	1:2A:945:A:N1	2.31	0.45
1:2A:2552:OMU:H2'	1:2A:2554:U:OP2	2.16	0.45
1:2A:2626:C:H2'	1:2A:2627:G:O4'	2.17	0.45
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.28	0.45
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.97	0.45
17:2V:2:PHE:CZ	17:2V:41:GLY:HA3	2.52	0.45
32:2a:1338:G:N2	55:2x:41:C:O2	2.50	0.45
33:2b:150:SER:OG	33:2b:151:GLY:N	2.48	0.45
40:2i:14:VAL:HG23	40:2i:66:ARG:HG3	1.97	0.45
50:2s:31:ILE:O	50:2s:50:ALA:N	2.46	0.45
50:2s:32:LYS:HD3	50:2s:34:TRP:CH2	2.51	0.45
4:1E:181:LEU:HD12	4:1E:181:LEU:HA	1.84	0.45
6:1G:27:ASN:HB3	6:1G:30:GLU:HG3	1.98	0.45
12:1Q:54:MET:HG2	12:1Q:117:ALA:HB1	1.98	0.45
32:1a:317:G:C6	32:1a:318:G:C5	3.05	0.45
33:1b:152:PHE:CE1	33:1b:155:LEU:HD23	2.51	0.45
43:1l:28:LYS:HD2	43:1l:62:SER:HB2	1.99	0.45
1:2A:812:C:H2'	1:2A:813:U:H6	1.81	0.45
1:2A:815:C:H2'	1:2A:816:C:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1785:A:N6	62:2A:4043:HOH:O	2.49	0.45
21:2Z:125:LEU:HG	21:2Z:164:ALA:HB3	1.98	0.45
32:2a:528:C:H5'	32:2a:529:G:OP2	2.17	0.45
32:2a:538:G:H5"	43:2l:114:LYS:HB2	1.97	0.45
35:2d:119:GLN:HG2	35:2d:123:HIS:CD2	2.51	0.45
38:2g:26:PHE:O	38:2g:30:ILE:HG12	2.17	0.45
47:2p:18:ARG:HG2	47:2p:35:LYS:HE3	1.99	0.45
1:1A:357:A:H2'	1:1A:358:U:O4'	2.17	0.45
1:1A:848:G:H2'	1:1A:849:A:C8	2.51	0.45
1:1A:1364:G:OP2	23:11:3:LYS:HG3	2.17	0.45
1:1A:1968:G:OP1	62:1A:4156:HOH:O	2.21	0.45
11:1P:101:VAL:HG21	11:1P:108:LYS:HG2	1.98	0.45
21:1Z:146:ILE:N	21:1Z:148:ASP:H	2.14	0.45
23:11:52:ARG:HH11	23:11:55:GLY:HA2	1.82	0.45
26:14:53:GLU:HB2	26:14:55:ARG:O	2.16	0.45
32:1a:598:U:H2'	32:1a:599:C:C6	2.51	0.45
32:1a:1027:C:N4	32:1a:1034:G:H1	2.15	0.45
32:1a:1425:U:H2'	32:1a:1426:C:C6	2.51	0.45
44:1m:4:ILE:HA	44:1m:5:ALA:HA	1.73	0.45
44:1m:106:ASN:HB2	44:1m:107:ALA:H	1.51	0.45
48:1q:88:TYR:HD2	48:1q:89:LEU:HD23	1.81	0.45
1:2A:27:G:N2	1:2A:512:G:H1'	2.32	0.45
1:2A:825:C:O2	11:2P:55:ARG:NH1	2.46	0.45
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.98	0.45
1:2A:2271:G:OP1	22:20:18:ALA:HB1	2.17	0.45
1:2A:2314:C:H2'	1:2A:2315:G:C8	2.52	0.45
4:2E:18:ASP:HB3	15:2T:82:LEU:HD21	1.97	0.45
4:2E:195:LEU:HG	4:2E:196:VAL:N	2.32	0.45
7:2H:127:GLU:C	7:2H:129:THR:H	2.23	0.45
11:2P:121:LYS:O	11:2P:123:LEU:N	2.49	0.45
19:2X:11:PRO:HB3	19:2X:92:LEU:HD11	1.98	0.45
21:2Z:40:ASP:OD2	21:2Z:42:VAL:HG13	2.15	0.45
32:2a:397:A:H3'	32:2a:397:A:N3	2.32	0.45
32:2a:416:G:C5	32:2a:417:C:C4	3.04	0.45
32:2a:853:G:C2	32:2a:854:G:C8	3.05	0.45
32:2a:1054:C:C5	54:2w:34:C:H1'	2.52	0.45
33:2b:95:GLN:HB3	33:2b:148:TYR:HD1	1.82	0.45
35:2d:155:LEU:O	35:2d:159:ARG:HG3	2.16	0.45
56:2y:19:U:O2	56:2y:21:A:H4'	2.17	0.45
1:1A:1062:G:H22	1:1A:1077:A:H61	1.65	0.45
29:17:24:THR:HG22	29:17:27:GLY:N	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1039:C:H2'	32:1a:1040:U:C6	2.51	0.45
32:1a:1134:G:N3	32:1a:1134:G:H2'	2.31	0.45
33:1b:102:LEU:HB3	33:1b:180:LEU:HD12	1.99	0.45
35:1d:74:GLN:O	35:1d:78:LEU:HG	2.17	0.45
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.99	0.45
1:2A:1186:G:C2	1:2A:1187:G:H1'	2.52	0.45
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.51	0.45
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.32	0.45
1:2A:2330:G:H2'	1:2A:2331:G:O4'	2.17	0.45
1:2A:2579:C:H4'	4:2E:134:ILE:HG12	1.97	0.45
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.82	0.45
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.17	0.45
25:23:11:SER:HA	25:23:31:LEU:HD11	1.97	0.45
32:2a:1076:C:H2'	32:2a:1077:G:H5"	1.98	0.45
34:2c:45:LYS:HG3	34:2c:46:GLU:N	2.32	0.45
38:2g:22:LEU:HD13	38:2g:97:GLN:OE1	2.16	0.45
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.41	0.45
1:1A:84:A:H5"	20:1Y:8:LYS:HE3	1.98	0.45
1:1A:127:A:H5"	1:1A:128:C:C6	2.52	0.45
1:1A:1062:G:H22	1:1A:1077:A:N6	2.15	0.45
1:1A:1720:U:H2'	1:1A:1721:G:O4'	2.16	0.45
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.38	0.45
4:1E:101:ARG:NH2	4:1E:171:GLU:HB2	2.32	0.45
8:1I:12:LEU:HD22	8:1I:19:VAL:HG21	1.99	0.45
9:1N:96:GLU:H	9:1N:96:GLU:CD	2.24	0.45
12:1Q:59:ARG:C	12:1Q:61:GLY:H	2.24	0.45
26:14:58:ARG:HG2	50:1s:67:VAL:HB	1.98	0.45
32:1a:92:C:H2'	32:1a:93:G:H8	1.81	0.45
32:1a:1066:C:O2'	32:1a:1067:A:H5'	2.17	0.45
32:1a:1401:G:C2	32:1a:1402:4OC:H1'	2.52	0.45
40:1i:46:ALA:HA	40:1i:78:LYS:HB2	1.98	0.45
40:1i:75:ASP:HA	40:1i:78:LYS:HB3	1.99	0.45
40:1i:92:TYR:O	40:1i:96:LEU:HB2	2.16	0.45
41:1j:6:ILE:O	41:1j:72:VAL:N	2.49	0.45
47:1p:49:LEU:HD13	47:1p:73:LEU:HD22	1.99	0.45
47:1p:55:ARG:HA	47:1p:55:ARG:HD2	1.73	0.45
1:2A:724:U:H2'	1:2A:725:G:O4'	2.17	0.45
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.31	0.45
1:2A:1952:A:OP1	10:2O:42:SER:OG	2.31	0.45
21:2Z:4:ARG:HA	21:2Z:58:VAL:H	1.82	0.45
32:2a:20:U:H2'	32:2a:21:G:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:757:U:H2'	32:2a:758:G:O4'	2.17	0.45
35:2d:102:ASP:HB3	35:2d:136:PRO:HB3	1.98	0.45
1:1A:593:G:C4'	30:18:4:MET:HE2	2.46	0.45
1:1A:763:G:OP1	62:1A:4152:HOH:O	2.21	0.45
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.17	0.45
32:1a:445:G:H2'	32:1a:446:G:C8	2.52	0.45
32:1a:1030(B):C:O2	32:1a:1030(B):C:H2'	2.16	0.45
43:1l:53:ARG:HB3	43:1l:69:TYR:HE1	1.82	0.45
1:2A:848:G:H2'	1:2A:849:A:C8	2.52	0.45
1:2A:1532:C:H42	1:2A:1537:G:H1	1.65	0.45
16:2U:92:ARG:HA	16:2U:95:LEU:HB2	1.98	0.45
32:2a:629:G:H2'	32:2a:630:G:O4'	2.17	0.45
35:2d:173:TRP:CG	35:2d:189:PRO:HB3	2.52	0.45
39:2h:33:GLU:HG3	39:2h:59:LEU:HD21	1.99	0.45
41:2j:46:ARG:HA	41:2j:64:GLU:HA	1.98	0.45
56:2y:51:G:H8	56:2y:51:G:O5'	1.99	0.45
1:1A:226:G:N2	1:1A:228:A:H62	2.14	0.45
1:1A:1506:C:H2'	1:1A:1507:A:C8	2.52	0.45
1:1A:2572:A:N7	4:1E:145:LYS:HB2	2.31	0.45
5:1F:64:ILE:HG21	5:1F:78:ILE:HG23	1.99	0.45
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.98	0.45
11:1P:101:VAL:HG23	11:1P:106:LEU:O	2.17	0.45
32:1a:736:C:H2'	32:1a:737:A:H8	1.82	0.45
32:1a:865:A:C2	32:1a:918:A:H4'	2.51	0.45
32:1a:1143:G:H2'	32:1a:1144:G:C8	2.51	0.45
32:1a:1525:G:OP1	42:1k:120:ARG:NH2	2.50	0.45
34:1c:79:ARG:O	34:1c:82:GLU:HG2	2.16	0.45
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.42	0.45
1:2A:328:U:H4'	20:2Y:68:HIS:CD2	2.52	0.45
6:2G:138:GLN:OE1	6:2G:153:ARG:N	2.42	0.45
10:2O:25:LEU:HD12	10:2O:38:VAL:HG12	1.99	0.45
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.55	0.45
32:2a:130:A:O2'	32:2a:131:C:O5'	2.35	0.45
32:2a:334:C:H2'	32:2a:335:C:H6	1.82	0.45
32:2a:939:G:H1	32:2a:1344:C:H42	1.65	0.45
32:2a:942:G:C2	32:2a:1342:C:C2	3.05	0.45
32:2a:1201:A:H4'	32:2a:1202:G:O5'	2.17	0.45
34:2c:116:VAL:HG21	34:2c:202:ILE:HD11	1.99	0.45
35:2d:57:ARG:HB2	35:2d:206:PHE:HD1	1.82	0.45
35:2d:163:GLU:O	35:2d:166:LYS:N	2.49	0.45
35:2d:187:ARG:NH1	35:2d:193:ASP:OD2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:2p:3:LYS:O	47:2p:21:VAL:HA	2.17	0.45
55:2x:50:U:H2'	55:2x:51:C:H6	1.82	0.45
1:1A:2028:U:H2'	1:1A:2029:G:O4'	2.16	0.45
1:1A:2218:U:O4'	23:11:52:ARG:NH2	2.50	0.45
1:1A:2390:U:P	30:18:35:GLN:HE22	2.40	0.45
1:1A:2492:U:H2'	1:1A:2493:U:C6	2.52	0.45
1:1A:2693:A:H2'	1:1A:2694:G:H8	1.81	0.45
14:1S:61:ASN:HB3	14:1S:64:GLU:HB2	1.99	0.45
21:1Z:129:SER:HB2	21:1Z:132:ASN:OD1	2.17	0.45
32:1a:270:A:H2'	32:1a:271:C:C6	2.52	0.45
33:1b:60:ASP:HA	33:1b:63:MET:HG3	1.99	0.45
50:1s:27:GLU:HB2	50:1s:28:LYS:CB	2.46	0.45
1:2A:468:G:N7	29:27:39:ARG:NH2	2.62	0.45
1:2A:1254:A:OP2	62:2A:3949:HOH:O	2.21	0.45
1:2A:2572:A:OP1	1:2A:2574:G:O2'	2.34	0.45
8:2I:88:ILE:HD11	8:2I:144:VAL:HG11	1.98	0.45
32:2a:377:G:OP1	47:2p:3:LYS:HE2	2.16	0.45
32:2a:500:G:N2	32:2a:546:G:H1'	2.32	0.45
32:2a:1134:G:N1	32:2a:1135:U:H1'	2.32	0.45
32:2a:1264:C:N4	32:2a:1272:G:O6	2.50	0.45
33:2b:60:ASP:O	33:2b:64:ARG:HG2	2.17	0.45
35:2d:149:ALA:HB3	35:2d:152:SER:HB2	1.99	0.45
44:2m:27:LYS:HD2	44:2m:27:LYS:HA	1.78	0.45
45:2n:24:CYS:HB3	45:2n:28:GLY:H	1.82	0.45
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.32	0.44
17:1V:24:LYS:HB3	17:1V:24:LYS:HE3	1.85	0.44
19:1X:66:LEU:HD12	19:1X:66:LEU:HA	1.79	0.44
24:12:51:ARG:O	24:12:55:ARG:HG2	2.17	0.44
32:1a:100:C:H2'	32:1a:101:A:C8	2.52	0.44
32:1a:160:A:H2'	32:1a:161:A:O4'	2.17	0.44
32:1a:1329:A:OP1	44:1m:29:ARG:HB2	2.17	0.44
39:1h:81:HIS:N	39:1h:138:TRP:O	2.50	0.44
44:1m:121:LYS:NZ	44:1m:121:LYS:HB3	2.32	0.44
1:2A:250:G:H2'	1:2A:251:A:C8	2.52	0.44
1:2A:1614:A:N6	18:2W:92:ARG:O	2.48	0.44
4:2E:9:VAL:HG13	4:2E:25:VAL:O	2.17	0.44
32:2a:826:C:H2'	32:2a:827:U:C6	2.52	0.44
34:2c:52:LEU:HD12	34:2c:53:ALA:H	1.82	0.44
35:2d:156:GLU:HG3	35:2d:159:ARG:NH2	2.28	0.44
41:2j:32:ALA:HA	41:2j:33:GLN:HA	1.70	0.44
56:2y:63:C:H2'	56:2y:64:U:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:279:C:H42	1:1A:361:G:H1	1.63	0.44
1:1A:1882:C:H2'	1:1A:1883:G:O4'	2.16	0.44
1:1A:2347:C:H2'	1:1A:2348:U:C6	2.53	0.44
3:1D:145:VAL:HG12	3:1D:146:GLU:O	2.16	0.44
8:1I:121:LYS:HB3	8:1I:121:LYS:HE3	1.78	0.44
15:1T:106:SER:O	15:1T:110:ILE:HG13	2.17	0.44
21:1Z:1:MET:N	21:1Z:55:HIS:HB3	2.32	0.44
30:18:58:ILE:HA	30:18:61:LEU:HD12	1.98	0.44
32:1a:305:G:H5"	62:1a:2173:HOH:O	2.18	0.44
32:1a:646:U:H2'	32:1a:647:C:C6	2.52	0.44
32:1a:1025:U:C2	32:1a:1036:G:O6	2.71	0.44
33:1b:19:HIS:HA	33:1b:39:ILE:CG2	2.47	0.44
33:1b:88:ALA:O	33:1b:226:ARG:NH1	2.51	0.44
44:1m:57:ARG:O	44:1m:61:GLU:HG3	2.17	0.44
46:1o:26:GLU:H	46:1o:26:GLU:HG2	1.37	0.44
54:1w:18:G:H4'	54:1w:19:U:OP2	2.14	0.44
1:2A:690:G:H2'	1:2A:691:C:C6	2.52	0.44
1:2A:1359:A:H2	1:2A:1372:U:O4	2.00	0.44
1:2A:2070:G:H2'	1:2A:2071:A:H8	1.82	0.44
8:2I:83:ALA:HB3	8:2I:123:LEU:HD11	2.00	0.44
8:2I:87:LYS:HB2	8:2I:87:LYS:HE3	1.74	0.44
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.51	0.44
12:2Q:89:ASN:HB2	55:2x:1:C:C4	2.52	0.44
22:20:11:ARG:O	22:20:14:ARG:NH2	2.39	0.44
26:24:13:ARG:HA	26:24:22:ILE:O	2.18	0.44
27:25:57:VAL:HG12	27:25:58:LEU:HD13	1.99	0.44
32:2a:685:G:N1	32:2a:686:U:O4	2.50	0.44
32:2a:743:U:H2'	32:2a:744:C:C6	2.52	0.44
32:2a:1014:A:H5'	50:2s:14:HIS:CE1	2.51	0.44
32:2a:1233:G:H2'	32:2a:1234:C:H6	1.82	0.44
33:2b:92:TYR:N	33:2b:151:GLY:O	2.32	0.44
38:2g:63:LYS:HE3	38:2g:63:LYS:HB2	1.87	0.44
45:2n:37:PHE:C	45:2n:39:LEU:H	2.25	0.44
54:2w:18:G:N2	54:2w:57:G:H1'	2.33	0.44
56:2y:53:G:H3'	56:2y:54:5MU:H73	1.99	0.44
9:1N:67:LEU:O	9:1N:88:GLU:HG3	2.17	0.44
16:1U:34:LYS:HA	16:1U:34:LYS:HD2	1.72	0.44
21:1Z:44:PHE:CZ	21:1Z:86:VAL:HG11	2.53	0.44
23:11:59:THR:O	23:11:91:LYS:NZ	2.39	0.44
32:1a:401:C:H2'	32:1a:402:G:C8	2.53	0.44
47:1p:6:LEU:HB3	47:1p:17:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:1y:10:G:N2	56:1y:26:G:H1'	2.33	0.44
1:2A:706:A:H2'	1:2A:707:G:O4'	2.18	0.44
1:2A:731:C:H5"	62:2A:3981:HOH:O	2.17	0.44
1:2A:774:A:H2'	1:2A:774:A:N3	2.32	0.44
1:2A:1372:U:H2'	1:2A:1373:A:O4'	2.17	0.44
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.52	0.44
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.51	0.44
26:24:40:HIS:HB3	26:24:43:TYR:HB2	1.99	0.44
26:24:62:ARG:HB3	26:24:63:TYR:CD2	2.52	0.44
32:2a:289:G:OP2	62:2a:1904:HOH:O	2.21	0.44
32:2a:625:G:OP1	47:2p:9:PHE:HB3	2.17	0.44
32:2a:976:G:C8	32:2a:1358:U:C2	3.05	0.44
32:2a:993:G:N3	32:2a:993:G:H2'	2.32	0.44
32:2a:1360:A:OP2	45:2n:35:ARG:NH2	2.51	0.44
34:2c:101:LEU:HD13	34:2c:102:ASN:N	2.31	0.44
35:2d:122:ARG:HA	35:2d:122:ARG:HD2	1.71	0.44
38:2g:69:VAL:HG21	38:2g:104:LEU:HD21	1.98	0.44
54:2w:41:U:H2'	54:2w:42:C:C6	2.52	0.44
1:1A:194:G:H3'	62:1A:4234:HOH:O	2.16	0.44
1:1A:284:U:H2'	1:1A:285:C:C6	2.52	0.44
1:1A:582:G:H2'	1:1A:583:G:C8	2.52	0.44
1:1A:1506:C:H2'	1:1A:1507:A:H8	1.83	0.44
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.52	0.44
1:1A:2801(A):A:N3	1:1A:2895:U:H1'	2.33	0.44
3:1D:71:ASP:CB	3:1D:103:ARG:HH12	2.30	0.44
32:1a:299:G:O5'	32:1a:299:G:H8	2.00	0.44
32:1a:799:G:OP2	62:1a:1918:HOH:O	2.21	0.44
36:1e:142:LEU:O	36:1e:143:ARG:NH1	2.49	0.44
54:1w:8:4SU:O5'	54:1w:8:4SU:H6	2.17	0.44
54:1w:64:U:O5'	54:1w:64:U:H6	2.01	0.44
1:2A:740:U:H2'	1:2A:741:G:C8	2.52	0.44
1:2A:1799:G:N2	3:2D:155:LEU:HD12	2.32	0.44
1:2A:2127:G:N1	1:2A:2161:C:C4	2.85	0.44
4:2E:203:LYS:HD3	4:2E:203:LYS:HA	1.82	0.44
7:2H:127:GLU:OE2	7:2H:130:ARG:NH2	2.44	0.44
8:2I:128:LEU:HD23	8:2I:128:LEU:HA	1.81	0.44
9:2N:61:ARG:HD3	9:2N:61:ARG:HA	1.75	0.44
16:2U:107:ALA:O	16:2U:111:GLU:HG2	2.18	0.44
32:2a:1390:U:H2'	32:2a:1391:U:C6	2.52	0.44
35:2d:114:ARG:O	35:2d:118:ARG:N	2.49	0.44
1:1A:626:U:O4	11:1P:107:LYS:HE2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1053:C:N4	1:1A:1106:G:H1	2.12	0.44
1:1A:1371:G:O6	62:1A:4147:HOH:O	2.19	0.44
1:1A:1477:A:C2	1:1A:1515:G:C2	3.06	0.44
1:1A:1484:G:H1	1:1A:1505:C:N4	2.14	0.44
1:1A:1503:U:H2'	1:1A:1504:C:C6	2.53	0.44
1:1A:1774:C:O5'	1:1A:1774:C:H6	2.01	0.44
32:1a:629:G:H2'	32:1a:630:G:O4'	2.18	0.44
32:1a:1144:G:H21	32:1a:1146:A:H62	1.64	0.44
32:1a:1237:C:O2'	32:1a:1300:G:N2	2.41	0.44
33:1b:59:GLU:HB2	33:1b:221:LEU:HD21	1.99	0.44
37:1f:69:GLU:H	37:1f:69:GLU:CD	2.25	0.44
40:1i:3:GLN:HE21	40:1i:20:ARG:CZ	2.30	0.44
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	2.00	0.44
47:1p:20:VAL:HG21	47:1p:32:TYR:CD2	2.52	0.44
1:2A:856:C:HO2'	1:2A:857:C:P	2.40	0.44
1:2A:2406:U:C2	11:2P:72:PRO:HG2	2.53	0.44
3:2D:275:LYS:H	3:2D:275:LYS:CE	2.30	0.44
5:2F:20:LEU:HD12	5:2F:20:LEU:HA	1.76	0.44
28:26:6:ARG:NE	28:26:24:GLU:OE2	2.30	0.44
29:27:24:THR:HG22	29:27:27:GLY:N	2.24	0.44
30:28:29:LYS:HD2	30:28:44:LYS:HB3	1.99	0.44
32:2a:630:G:H2'	32:2a:631:G:C8	2.53	0.44
32:2a:684:A:C6	32:2a:685:G:C6	3.05	0.44
32:2a:1004:A:N6	32:2a:1037:C:H1'	2.32	0.44
32:2a:1012:U:O2	32:2a:1017:G:O6	2.35	0.44
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.80	0.44
34:2c:129:ALA:O	34:2c:133:ALA:N	2.45	0.44
35:2d:47:ARG:NH1	35:2d:49:ARG:HA	2.33	0.44
35:2d:180:GLY:O	35:2d:182:LYS:HG3	2.17	0.44
43:2l:59:ARG:HA	43:2l:65:GLU:HA	1.98	0.44
44:2m:16:ASP:OD1	44:2m:17:VAL:N	2.51	0.44
54:2w:13:C:O2'	54:2w:14:A:H8	2.00	0.44
2:1B:88:C:H2'	2:1B:89:G:O4'	2.18	0.44
19:1X:65:ARG:HH11	19:1X:70:LEU:HD21	1.82	0.44
32:1a:404:U:H2'	32:1a:405:U:C6	2.53	0.44
32:1a:1003:G:H2'	32:1a:1004:A:N3	2.33	0.44
32:1a:1410:G:H2'	32:1a:1411:C:C6	2.52	0.44
34:1c:22:TRP:HB3	34:1c:59:ARG:HB2	2.00	0.44
35:1d:18:LYS:NZ	35:1d:26:CYS:O	2.51	0.44
36:1e:94:ALA:HB2	36:1e:119:LEU:HG	1.98	0.44
56:1y:50:A:H8	56:1y:50:A:OP2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:271(O):C:H4'	8:2I:49:ALA:HB1	2.00	0.44
1:2A:323:G:H2'	5:2F:169:ASN:OD1	2.16	0.44
1:2A:1598:C:H2'	1:2A:1599:C:H6	1.83	0.44
1:2A:1991:U:H2'	1:2A:1992:G:H5"	1.98	0.44
1:2A:2348:U:O4	1:2A:2382:G:N1	2.51	0.44
1:2A:2356:C:OP1	22:20:24:LYS:NZ	2.40	0.44
2:2B:11:C:H3'	2:2B:12:C:C6	2.53	0.44
5:2F:150:GLY:HA2	5:2F:172:TRP:CE3	2.53	0.44
6:2G:25:TYR:HB3	6:2G:30:GLU:HB3	1.98	0.44
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.82	0.44
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	1.98	0.44
21:2Z:70:LEU:HD12	21:2Z:70:LEU:HA	1.87	0.44
21:2Z:77:ASP:CG	21:2Z:80:ARG:HH11	2.25	0.44
32:2a:114:U:H2'	32:2a:115:G:C8	2.53	0.44
32:2a:901:A:O2'	32:2a:1513:A:OP1	2.28	0.44
35:2d:155:LEU:HD23	35:2d:156:GLU:H	1.83	0.44
1:1A:788:A:OP1	1:1A:791:C:N4	2.43	0.44
1:1A:1005:C:H5"	62:1A:5823:HOH:O	2.17	0.44
1:1A:1065:U:H5"	1:1A:1066:U:OP2	2.18	0.44
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.17	0.44
1:1A:2747:G:O6	1:1A:2755:C:H5"	2.16	0.44
6:1G:18:GLU:HG2	6:1G:175:LEU:HD21	1.99	0.44
7:1H:87:LEU:HD23	7:1H:164:TYR:HA	2.00	0.44
22:10:82:ARG:HE	22:10:82:ARG:HB2	1.56	0.44
26:14:69:LYS:HE3	26:14:69:LYS:HA	1.99	0.44
32:1a:102:G:H2'	32:1a:103:C:H6	1.82	0.44
32:1a:449:C:O2	47:1p:42:ARG:NH1	2.50	0.44
32:1a:1346:A:N1	32:1a:1374:A:H5"	2.32	0.44
36:1e:78:HIS:CD2	39:1h:104:ARG:HD2	2.53	0.44
38:1g:37:ASN:O	38:1g:41:ARG:HG3	2.17	0.44
1:2A:446:G:OP1	16:2U:3:ARG:NH1	2.51	0.44
1:2A:795:C:H2'	1:2A:796:C:C6	2.53	0.44
1:2A:1003:G:O2'	1:2A:1010:A:N1	2.42	0.44
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.17	0.44
6:2G:112:PRO:HG3	26:24:43:TYR:CZ	2.52	0.44
12:2Q:43:THR:HA	12:2Q:94:VAL:HG12	1.99	0.44
19:2X:84:ALA:HB3	19:2X:87:GLN:NE2	2.32	0.44
24:22:32:LEU:HD13	24:22:53:LEU:HB3	1.99	0.44
30:28:8:LYS:HD3	30:28:8:LYS:HA	1.81	0.44
32:2a:1006:C:C4	32:2a:1007:C:C4	3.06	0.44
39:2h:51:VAL:HG11	39:2h:60:ARG:HH12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:45:ARG:HH11	45:2n:36:PHE:HD1	1.65	0.44
44:2m:13:LYS:O	44:2m:45:VAL:N	2.34	0.44
47:2p:2:VAL:HG22	47:2p:64:ALA:HA	2.00	0.44
1:1A:2751:G:C4	7:1H:2:SER:HA	2.53	0.44
15:1T:36:GLU:O	15:1T:38:ASN:N	2.51	0.44
21:1Z:62:PRO:C	21:1Z:64:GLY:H	2.25	0.44
21:1Z:77:ASP:OD2	21:1Z:80:ARG:HB2	2.17	0.44
23:11:67:ILE:N	23:11:68:PRO:HD2	2.32	0.44
32:1a:280:C:N3	48:1q:39:SER:OG	2.51	0.44
32:1a:1025:U:O2	32:1a:1036:G:C6	2.71	0.44
32:1a:1456:G:H22	51:1t:51:GLU:CD	2.26	0.44
36:1e:35:GLY:HA2	36:1e:40:ARG:O	2.17	0.44
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	2.00	0.44
44:1m:45:VAL:HA	44:1m:48:LEU:HD13	1.99	0.44
1:2A:84:A:H5'	20:2Y:8:LYS:HG2	2.00	0.44
1:2A:2409:G:H2'	1:2A:2410:G:O4'	2.18	0.44
1:2A:2846:G:H2'	1:2A:2847:U:O4'	2.18	0.44
2:2B:114:C:O2'	14:2S:46:VAL:HG13	2.18	0.44
8:2I:77:LEU:HD23	8:2I:77:LEU:HA	1.84	0.44
32:2a:755:G:OP2	46:2o:65:ARG:HD2	2.17	0.44
32:2a:792:A:H4'	32:2a:793:U:H5"	2.00	0.44
32:2a:935:A:O2'	32:2a:1383:C:N3	2.48	0.44
32:2a:1004:A:N6	32:2a:1036:G:C5	2.86	0.44
32:2a:1323:G:H2'	32:2a:1324:A:H8	1.81	0.44
32:2a:1529:G:H4'	32:2a:1530:G:OP2	2.18	0.44
33:2b:188:ALA:HB1	33:2b:192:SER:HB2	1.99	0.44
34:2c:120:VAL:HG11	34:2c:134:ILE:HG22	2.00	0.44
37:2f:50:TYR:CE2	49:2r:77:GLY:HA2	2.53	0.44
50:2s:52:TYR:HB2	50:2s:57:HIS:HE1	1.83	0.44
54:2w:17:G:O2'	54:2w:18:G:OP2	2.33	0.44
1:1A:818:G:H5'	1:1A:839:U:OP1	2.17	0.44
1:1A:1359:A:C2	1:1A:1372:U:O4	2.71	0.44
1:1A:1814:G:C6	1:1A:1815:A:C6	3.06	0.44
1:1A:2110:G:C2	1:1A:2120:G:H1'	2.52	0.44
1:1A:2131:G:C2	1:1A:2133:G:C2	3.06	0.44
11:1P:2:LYS:HG2	11:1P:3:LEU:N	2.32	0.44
32:1a:994:A:N1	32:1a:1047:G:H4'	2.33	0.44
45:1n:27:CYS:SG	45:1n:29:ARG:HB2	2.58	0.44
47:1p:74:LEU:HD23	47:1p:79:VAL:HG11	1.99	0.44
1:2A:75:G:H4'	24:22:55:ARG:NH2	2.33	0.44
1:2A:652(U):G:H2'	1:2A:652(V):C:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:811:U:H2'	11:2P:21:ARG:HA	2.00	0.44
1:2A:2788:C:N3	1:2A:2789:C:N4	2.65	0.44
10:2O:70:LYS:HB3	10:2O:70:LYS:HE2	1.77	0.44
32:2a:1145:C:H4'	32:2a:1146:A:H5'	1.99	0.44
32:2a:1245:A:H2'	32:2a:1246:C:C6	2.53	0.44
33:2b:75:LYS:HA	33:2b:78:GLN:HG2	2.00	0.44
34:2c:6:HIS:ND1	45:2n:49:HIS:HB3	2.33	0.44
48:2q:53:LEU:HD23	48:2q:82:MET:HE1	1.99	0.44
54:2w:33:U:N3	54:2w:36:C:OP2	2.51	0.44
1:1A:207:A:H2'	1:1A:208:C:O4'	2.17	0.43
1:1A:1790:C:H5"	1:1A:1791:A:OP1	2.17	0.43
1:1A:2097:C:H2'	1:1A:2098:U:C6	2.53	0.43
1:1A:2167:U:O2	1:1A:2167:U:H2'	2.18	0.43
2:1B:66:A:N6	2:1B:109:C:H5'	2.33	0.43
6:1G:11:TYR:OH	6:1G:32:PRO:O	2.29	0.43
7:1H:154:PRO:HB3	7:1H:163:TYR:CE1	2.53	0.43
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.61	0.43
24:12:1:MET:HE3	24:12:5:GLU:HB3	1.99	0.43
32:1a:1240:U:OP1	38:1g:119:ARG:NH2	2.39	0.43
33:1b:55:PHE:CD1	33:1b:221:LEU:HD22	2.52	0.43
39:1h:51:VAL:HG21	39:1h:60:ARG:HB2	2.00	0.43
42:1k:104:GLN:O	42:1k:105:VAL:C	2.60	0.43
1:2A:600:G:H2'	1:2A:601:C:C6	2.53	0.43
1:2A:666:G:H2'	1:2A:667:U:C6	2.53	0.43
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.53	0.43
1:2A:2785:C:O2'	4:2E:66:HIS:ND1	2.41	0.43
7:2H:20:ALA:HB1	7:2H:21:PRO:HD2	2.00	0.43
11:2P:133:SER:HA	11:2P:136:GLU:OE1	2.18	0.43
16:2U:104:GLN:NE2	16:2U:105:VAL:HG23	2.33	0.43
20:2Y:74:PRO:O	20:2Y:82:PRO:HA	2.18	0.43
32:2a:131:C:H2'	32:2a:132:C:C6	2.53	0.43
32:2a:630:G:H2'	32:2a:631:G:H8	1.83	0.43
32:2a:1129:C:H1'	32:2a:1146:A:H61	1.83	0.43
32:2a:1221:G:O3'	50:2s:77:THR:OG1	2.31	0.43
47:2p:57:ARG:HA	47:2p:60:LEU:HD12	1.99	0.43
50:2s:80:TYR:C	50:2s:82:GLY:H	2.27	0.43
51:2t:10:LEU:HD23	51:2t:12:ALA:HB2	2.00	0.43
1:1A:75:G:H4'	24:12:55:ARG:NH2	2.33	0.43
1:1A:2136:C:N4	1:1A:2155:G:N1	2.67	0.43
1:1A:2315:G:H2'	1:1A:2316:C:C6	2.53	0.43
1:1A:2354:G:H21	22:10:36:ILE:HD11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:1:U:H2'	2:1B:2:C:H6	1.83	0.43
32:1a:171:A:H2'	32:1a:172:A:C8	2.53	0.43
32:1a:433:C:H2'	32:1a:434:U:H6	1.82	0.43
32:1a:769:G:H4'	32:1a:1513:A:H4'	2.00	0.43
33:1b:139:LYS:O	33:1b:143:GLU:HG3	2.17	0.43
36:1e:71:LEU:HD21	36:1e:114:GLY:C	2.43	0.43
51:1t:29:LYS:O	51:1t:33:ILE:HG13	2.18	0.43
51:1t:89:ARG:HA	51:1t:89:ARG:HD2	1.82	0.43
1:2A:994:C:O2'	1:2A:996:A:OP1	2.35	0.43
1:2A:1599:C:OP1	19:2X:36:LYS:HG3	2.17	0.43
1:2A:1654:A:OP1	13:2R:1:MET:N	2.47	0.43
1:2A:2497:A:H5"	62:2A:4030:HOH:O	2.19	0.43
2:2B:24:G:N7	2:2B:56:G:H2'	2.32	0.43
4:2E:178:GLU:H	4:2E:178:GLU:CD	2.26	0.43
6:2G:135:LEU:HD11	6:2G:157:ILE:HD11	1.99	0.43
10:2O:19:ILE:HG22	10:2O:43:VAL:HA	2.00	0.43
14:2S:87:PHE:CE1	14:2S:102:ALA:HB2	2.53	0.43
32:2a:110:C:H2'	32:2a:111:G:O4'	2.17	0.43
32:2a:1113:C:H2'	32:2a:1114:C:H6	1.83	0.43
32:2a:1288:A:N1	32:2a:1371:G:H1'	2.32	0.43
35:2d:74:GLN:O	35:2d:78:LEU:HB2	2.18	0.43
36:2e:9:LYS:HD2	36:2e:9:LYS:HA	1.79	0.43
43:2l:117:ARG:NH2	43:2l:124:LYS:HB2	2.32	0.43
47:2p:8:ARG:HB3	47:2p:28:ARG:NH1	2.32	0.43
56:2y:26:G:N1	56:2y:44:A:N6	2.66	0.43
1:1A:271(B):C:H42	1:1A:271(V):G:H1	1.65	0.43
1:1A:303:U:O4	62:1A:4158:HOH:O	2.21	0.43
1:1A:489:G:N7	18:1W:49:LYS:NZ	2.65	0.43
1:1A:715:G:C2	46:1o:56:LEU:HD21	2.54	0.43
1:1A:774:A:N3	1:1A:774:A:H2'	2.33	0.43
1:1A:1092:C:C2'	1:1A:1093:G:H5'	2.47	0.43
1:1A:2185:C:H2'	1:1A:2186:G:C8	2.54	0.43
3:1D:2:ALA:O	3:1D:20:ASP:HB3	2.18	0.43
5:1F:34:TRP:CE2	11:1P:8:PRO:HD3	2.54	0.43
5:1F:89:VAL:HG12	5:1F:90:PHE:CD2	2.54	0.43
21:1Z:119:GLU:N	21:1Z:171:ILE:O	2.50	0.43
32:1a:501:C:H2'	32:1a:502:G:C8	2.53	0.43
32:1a:600:C:H2'	32:1a:601:C:H6	1.84	0.43
56:1y:63:C:H2'	56:1y:64:U:O4'	2.18	0.43
1:2A:191:A:H2'	1:2A:192:C:C6	2.52	0.43
1:2A:975:C:OP1	62:2A:3952:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1283:G:O2'	1:2A:1285:G:N7	2.50	0.43
1:2A:2065:C:H2'	1:2A:2066:C:C6	2.52	0.43
1:2A:2080:G:H5'	23:21:35:THR:O	2.17	0.43
1:2A:2161:C:H2'	1:2A:2162:G:O4'	2.17	0.43
1:2A:2657:A:O3'	7:2H:160:LYS:NZ	2.52	0.43
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	1.99	0.43
32:2a:403:C:O2'	35:2d:122:ARG:NH2	2.51	0.43
32:2a:1048:G:OP1	45:2n:3:ARG:HB3	2.17	0.43
32:2a:1213:A:C8	32:2a:1215:G:C5	3.06	0.43
32:2a:1329:A:OP2	52:2u:7:ARG:NH1	2.50	0.43
33:2b:126:GLU:CD	33:2b:126:GLU:H	2.26	0.43
35:2d:61:LYS:HE2	35:2d:61:LYS:HB3	1.90	0.43
49:2r:67:ALA:HA	49:2r:70:ILE:HD12	2.00	0.43
54:2w:24:A:H5'	54:2w:25:C:OP2	2.18	0.43
55:2x:61:C:H2'	55:2x:62:C:C6	2.52	0.43
56:2y:67:G:H2'	56:2y:68:C:C6	2.53	0.43
1:1A:192:C:OP1	62:1A:4154:HOH:O	2.21	0.43
1:1A:278:A:P	1:1A:278:A:H8	2.42	0.43
1:1A:1054:A:H3'	1:1A:1055:G:C8	2.54	0.43
3:1D:38:LYS:HA	3:1D:38:LYS:HD2	1.93	0.43
3:1D:206:LEU:HD23	3:1D:206:LEU:HA	1.68	0.43
21:1Z:150:LEU:HG	21:1Z:151:HIS:H	1.82	0.43
32:1a:22:G:H4'	32:1a:885:G:C8	2.54	0.43
32:1a:148:G:H2'	32:1a:149:A:H8	1.81	0.43
32:1a:202:U:H3'	32:1a:203:U:C5	2.54	0.43
32:1a:221:C:H2'	32:1a:222:U:C6	2.54	0.43
32:1a:743:U:H2'	32:1a:744:C:C6	2.53	0.43
32:1a:1218:C:OP2	45:1n:9:LYS:NZ	2.45	0.43
32:1a:1333:A:H2'	32:1a:1334:G:O4'	2.19	0.43
32:1a:1456:G:C4	51:1t:55:ILE:HD11	2.53	0.43
34:1c:152:ILE:HB	34:1c:199:LYS:HB2	2.00	0.43
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	2.00	0.43
41:1j:5:ARG:HD3	41:1j:71:LEU:HD11	2.01	0.43
44:1m:54:VAL:HG12	44:1m:57:ARG:HH12	1.84	0.43
51:1t:25:ARG:HG2	51:1t:29:LYS:NZ	2.33	0.43
1:2A:154:G:C6	1:2A:154(A):C:C4	3.05	0.43
1:2A:299:A:N1	1:2A:322:A:O2'	2.38	0.43
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.54	0.43
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.33	0.43
1:2A:2232:U:P	23:21:40:ARG:HH12	2.41	0.43
1:2A:2305:A:H2'	1:2A:2306:C:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:1:U:H2'	2:2B:2:C:C6	2.54	0.43
2:2B:34:U:H4'	2:2B:35:U:H5	1.83	0.43
12:2Q:30:GLY:HA2	12:2Q:107:ALA:HB2	1.99	0.43
17:2V:29:PRO:HA	17:2V:61:VAL:HG22	2.00	0.43
21:2Z:158:PRO:O	21:2Z:161:VAL:HG12	2.18	0.43
32:2a:509:A:H5"	35:2d:55:ALA:HB2	2.01	0.43
32:2a:961:U:H2'	32:2a:962:C:O4'	2.18	0.43
32:2a:1123:A:H1'	41:2j:37:PRO:O	2.18	0.43
32:2a:1271:G:C2	32:2a:1272:G:C8	3.06	0.43
34:2c:179:ARG:NH1	34:2c:206:GLU:HB2	2.33	0.43
35:2d:120:LEU:HB3	35:2d:126:ILE:CD1	2.48	0.43
47:2p:4:ILE:HG13	47:2p:64:ALA:HB1	1.99	0.43
1:1A:271(T):C:H2'	1:1A:271(U):G:H8	1.83	0.43
1:1A:305:U:H2'	1:1A:306:U:C6	2.54	0.43
1:1A:1063:G:H2'	1:1A:1064:C:C6	2.53	0.43
1:1A:1805:U:O2	3:1D:50:THR:HB	2.18	0.43
1:1A:2537:U:H2'	1:1A:2538:C:C6	2.54	0.43
1:1A:2788:C:P	4:1E:61:ARG:HH21	2.40	0.43
1:1A:2896:C:H2'	1:1A:2897:U:C6	2.54	0.43
6:1G:53:LEU:HD11	6:1G:87:PRO:HB2	2.00	0.43
6:1G:146:TYR:O	6:1G:149:VAL:HG12	2.19	0.43
7:1H:9:ILE:HD11	7:1H:69:ARG:HG2	2.00	0.43
7:1H:27:LYS:HG2	7:1H:32:GLU:HB3	2.00	0.43
10:1O:107:ARG:HD3	15:1T:37:GLY:H	1.83	0.43
11:1P:97:PRO:HD3	11:1P:126:VAL:O	2.18	0.43
32:1a:146:G:C2	32:1a:147:G:C4	3.06	0.43
32:1a:584:G:H2'	32:1a:585:G:C8	2.52	0.43
32:1a:1286:A:H8	32:1a:1287:A:H4'	1.83	0.43
32:1a:1302:U:C5	44:1m:17:VAL:HG21	2.54	0.43
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.54	0.43
35:1d:175:SER:O	35:1d:175:SER:OG	2.33	0.43
49:1r:65:ILE:H	49:1r:65:ILE:HG12	1.26	0.43
54:1w:53:G:H2'	54:1w:54:5MU:C6	2.53	0.43
1:2A:1837:C:OP1	32:2a:784:C:H4'	2.18	0.43
1:2A:2138:C:H2'	1:2A:2139:C:O4'	2.18	0.43
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.18	0.43
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.54	0.43
6:2G:7:LEU:HD11	6:2G:107:LEU:HD12	2.00	0.43
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	2.00	0.43
11:2P:29:LYS:HD3	11:2P:30:THR:HG23	1.99	0.43
11:2P:92:GLU:OE1	11:2P:121:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:26:10:LEU:HB2	28:26:52:VAL:HG12	2.01	0.43
30:28:14:VAL:HG13	30:28:22:VAL:HG13	1.99	0.43
32:2a:184:G:HO2'	51:2t:74:LYS:HZ1	1.61	0.43
32:2a:406:G:H5'	35:2d:5:ILE:HD13	2.01	0.43
32:2a:523:A:H61	43:2l:92:0TD:CG	2.30	0.43
32:2a:615:C:H2'	32:2a:616:G:O4'	2.19	0.43
32:2a:1040:U:C2	32:2a:1041:A:C8	3.07	0.43
1:1A:957:A:N1	1:1A:2458:G:H4'	2.33	0.43
1:1A:1372:U:H2'	1:1A:1373:A:O4'	2.19	0.43
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.33	0.43
1:1A:1779:U:H2'	62:1A:4248:HOH:O	2.17	0.43
1:1A:1827:C:C2'	1:1A:1828:G:H5'	2.49	0.43
1:1A:2111:C:N4	1:1A:2148:G:H21	2.17	0.43
1:1A:2117:A:O2'	1:1A:2118:U:H5"	2.18	0.43
1:1A:2791:C:H2'	1:1A:2792:G:H8	1.83	0.43
3:1D:232:PRO:HB3	3:1D:244:ARG:CZ	2.48	0.43
32:1a:143:A:O2'	32:1a:144:G:OP2	2.34	0.43
32:1a:1521:G:N3	62:1a:1954:HOH:O	2.36	0.43
33:1b:82:ARG:HD2	33:1b:92:TYR:OH	2.18	0.43
34:1c:6:HIS:NE2	34:1c:8:ILE:HB	2.33	0.43
38:1g:86:GLN:HE22	56:1y:32:U:H4'	1.83	0.43
40:1i:63:ILE:HG21	40:1i:77:ILE:HG12	1.98	0.43
51:1t:50:GLU:HA	51:1t:100:ILE:HG12	1.99	0.43
1:2A:76:C:O3'	24:22:59:ARG:HG3	2.18	0.43
1:2A:2130:U:H2'	1:2A:2158:A:H61	1.82	0.43
7:2H:175:LYS:HE3	7:2H:175:LYS:HB3	1.74	0.43
8:2I:123:LEU:HD23	8:2I:144:VAL:HG12	2.00	0.43
10:2O:20:MET:HE3	10:2O:44:LYS:HE2	2.00	0.43
21:2Z:3:TYR:HB2	21:2Z:57:ILE:HD13	2.01	0.43
21:2Z:145:GLU:HG3	21:2Z:146:ILE:N	2.34	0.43
32:2a:189(C):C:H2'	32:2a:189(D):C:O4'	2.19	0.43
32:2a:840:C:H4'	32:2a:841:U:OP1	2.19	0.43
32:2a:931:C:N3	32:2a:1386:G:N2	2.55	0.43
34:2c:39:ILE:O	34:2c:43:LEU:HG	2.19	0.43
36:2e:80:ILE:HG22	36:2e:91:LEU:HB2	2.00	0.43
36:2e:84:PHE:N	36:2e:87:SER:O	2.51	0.43
47:2p:21:VAL:CG2	47:2p:33:ILE:HB	2.48	0.43
47:2p:22:THR:HA	47:2p:33:ILE:HG13	2.01	0.43
48:2q:10:VAL:HG13	48:2q:19:VAL:HB	2.01	0.43
1:1A:218:A:C2	1:1A:235:U:H4'	2.53	0.43
1:1A:897:C:H4'	54:1w:55:PSU:O3'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:24:VAL:HG11	7:1H:43:VAL:HG11	2.00	0.43
8:1I:38:LEU:H	8:1I:38:LEU:CD2	2.31	0.43
32:1a:115:G:H4'	32:1a:116:A:O5'	2.19	0.43
32:1a:977:A:O2'	32:1a:979:C:OP2	2.35	0.43
32:1a:1112:C:N3	34:1c:178:LEU:HB2	2.34	0.43
35:1d:142:PRO:HA	35:1d:185:PHE:HD2	1.83	0.43
38:1g:78:ARG:HE	38:1g:79:ARG:HG3	1.83	0.43
51:1t:71:THR:HG22	51:1t:72:LEU:HG	2.00	0.43
1:2A:729:G:C6	3:2D:208:LYS:HB2	2.53	0.43
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.54	0.43
1:2A:2499:C:OP1	62:2A:3905:HOH:O	2.21	0.43
5:2F:24:LEU:HB3	5:2F:115:ALA:HB2	2.00	0.43
6:2G:101:ILE:HD13	26:24:25:TYR:HB2	1.99	0.43
7:2H:137:ASP:HB3	7:2H:140:LYS:CB	2.49	0.43
8:2I:65:ALA:O	8:2I:69:LYS:N	2.52	0.43
16:2U:24:TYR:HB2	16:2U:29:SER:HB3	1.99	0.43
21:2Z:53:ILE:HG22	21:2Z:71:VAL:O	2.18	0.43
24:22:64:LEU:HD11	24:22:68:ARG:NH2	2.34	0.43
32:2a:583:A:H2'	32:2a:584:G:O4'	2.18	0.43
33:2b:133:LYS:H	33:2b:133:LYS:HG3	1.70	0.43
38:2g:86:GLN:HE21	38:2g:86:GLN:HA	1.84	0.43
38:2g:135:VAL:O	38:2g:139:GLU:HG3	2.18	0.43
40:2i:28:VAL:HA	40:2i:63:ILE:O	2.19	0.43
44:2m:101:GLN:OE1	44:2m:101:GLN:N	2.49	0.43
56:2y:21:A:C6	56:2y:48:C:C5	3.07	0.43
1:1A:620:G:H2'	1:1A:620:G:N3	2.32	0.43
1:1A:1044:G:H5'	1:1A:1045:A:OP2	2.19	0.43
1:1A:1762:A:H2'	62:1A:5976:HOH:O	2.18	0.43
1:1A:2121:G:H2'	1:1A:2122:U:O4'	2.19	0.43
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.18	0.43
10:1O:111:PHE:O	10:1O:115:VAL:HG23	2.19	0.43
11:1P:1:MET:HE3	11:1P:1:MET:HB2	1.62	0.43
15:1T:31:SER:HB2	15:1T:85:LYS:HG2	2.00	0.43
21:1Z:155:LEU:HD23	21:1Z:155:LEU:HA	1.91	0.43
32:1a:615:C:C2	32:1a:616:G:C8	3.07	0.43
32:1a:1021:G:HO2'	32:1a:1022:G:P	2.37	0.43
32:1a:1356:G:H2'	32:1a:1357:A:H8	1.84	0.43
32:1a:1503:A:C2	53:1v:12:A:H2	2.36	0.43
35:1d:112:VAL:HG23	35:1d:116:GLN:NE2	2.33	0.43
38:1g:103:TRP:CH2	38:1g:141:VAL:HG21	2.54	0.43
40:1i:32:ASP:OD1	40:1i:33:PHE:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1k:33:THR:HA	42:1k:39:PRO:HA	1.99	0.43
44:1m:24:GLY:O	44:1m:29:ARG:NH1	2.51	0.43
46:1o:42:HIS:CE1	46:1o:46:HIS:HD2	2.37	0.43
1:2A:118:A:N3	1:2A:178:G:H1'	2.34	0.43
1:2A:579:G:H2'	1:2A:580:C:C6	2.53	0.43
1:2A:1037:G:C2	1:2A:1119:C:C2	3.07	0.43
1:2A:2163:C:H3'	1:2A:2164:C:C6	2.54	0.43
1:2A:2251:OMG:HM23	1:2A:2251:OMG:H1'	1.79	0.43
1:2A:2734:A:H2'	1:2A:2735:G:O4'	2.19	0.43
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	2.01	0.43
3:2D:147:LEU:HD13	3:2D:155:LEU:HD21	2.01	0.43
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	1.99	0.43
35:2d:38:TYR:CE1	35:2d:45:GLN:HG3	2.54	0.43
36:2e:12:LEU:HD22	36:2e:128:PRO:HB2	1.99	0.43
37:2f:100:ASN:HD21	49:2r:23:LYS:HE3	1.84	0.43
39:2h:21:LYS:O	39:2h:65:TYR:OH	2.32	0.43
46:2o:49:ASP:CG	46:2o:52:SER:HB2	2.44	0.43
54:2w:1:G:O2'	54:2w:2:C:O5'	2.34	0.43
1:1A:2712:U:O2'	1:1A:2713:A:H5'	2.19	0.43
5:1F:192:LEU:HD13	5:1F:194:MET:HE2	2.01	0.43
8:1I:2:LYS:HA	8:1I:19:VAL:O	2.19	0.43
11:1P:85:LEU:HD13	11:1P:120:ALA:HB2	2.01	0.43
12:1Q:45:GLN:OE1	12:1Q:45:GLN:N	2.47	0.43
23:11:26:ARG:HG3	23:11:27:GLU:HG3	2.01	0.43
32:1a:226:G:H2'	32:1a:227:G:O4'	2.19	0.43
32:1a:456:C:H2'	32:1a:457:C:H6	1.84	0.43
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.87	0.43
34:1c:87:LEU:O	34:1c:91:LEU:HB2	2.17	0.43
36:1e:105:VAL:HB	36:1e:106:PRO:HD3	2.00	0.43
38:1g:65:ALA:O	38:1g:69:VAL:HG23	2.19	0.43
1:2A:882:G:H1	1:2A:894:C:H42	1.67	0.43
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.66	0.43
1:2A:1790:C:H5"	1:2A:1791:A:OP1	2.19	0.43
1:2A:2059:A:H2'	1:2A:2503:2MA:HM23	2.00	0.43
1:2A:2175:C:H2'	1:2A:2176:A:C8	2.54	0.43
1:2A:2591:C:H2'	1:2A:2592:G:C8	2.54	0.43
2:2B:105:A:H5'	2:2B:106:G:OP2	2.18	0.43
4:2E:35:GLN:OE1	4:2E:66:HIS:HE1	2.02	0.43
8:2I:77:LEU:HD12	8:2I:97:ILE:HG23	2.01	0.43
32:2a:664:G:P	49:2r:64:ARG:HH21	2.40	0.43
34:2c:137:ALA:HA	34:2c:140:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:61:LYS:NZ	35:2d:72:GLU:OE1	2.43	0.43
36:2e:7:GLU:CD	36:2e:37:ARG:HH21	2.20	0.43
37:2f:69:GLU:CD	37:2f:69:GLU:H	2.25	0.43
45:2n:24:CYS:HB3	45:2n:29:ARG:H	1.84	0.43
54:2w:8:4SU:H1'	54:2w:21:A:N1	2.34	0.43
1:1A:904:C:H4'	21:1Z:169:GLU:OE1	2.19	0.43
1:1A:1010:A:N3	1:1A:1153:C:H1'	2.33	0.43
1:1A:1048:A:N1	1:1A:1112:G:O2'	2.36	0.43
1:1A:1864:U:OP1	1:1A:2410:G:O2'	2.30	0.43
5:1F:13:SER:HB2	5:1F:127:GLU:HG3	2.00	0.43
8:1I:116:LEU:HD11	8:1I:120:ILE:HG13	2.01	0.43
10:1O:2:ILE:HG13	10:1O:8:LEU:HD21	2.01	0.43
12:1Q:63:LYS:HD2	12:1Q:65:PHE:CZ	2.53	0.43
14:1S:25:ARG:HB3	14:1S:25:ARG:HH11	1.84	0.43
32:1a:664:G:N2	32:1a:741:G:H1	2.06	0.43
34:1c:91:LEU:HD12	34:1c:91:LEU:HA	1.89	0.43
1:2A:448:U:O4	1:2A:583:G:H1'	2.19	0.43
1:2A:479:A:N3	1:2A:481:G:H5"	2.33	0.43
1:2A:1001:A:H2'	1:2A:1002:G:O4'	2.19	0.43
1:2A:1923:U:OP1	55:2x:24:U:O2'	2.35	0.43
1:2A:2166:G:H3'	1:2A:2167:U:H5"	2.01	0.43
1:2A:2280:G:O6	22:20:14:ARG:HD2	2.19	0.43
5:2F:125:LEU:HD22	5:2F:196:LEU:HD12	2.01	0.43
16:2U:69:CYS:HB3	16:2U:74:LEU:HD13	2.00	0.43
26:24:15:ILE:HD13	26:24:32:TYR:CE1	2.54	0.43
32:2a:1087:G:N2	32:2a:1099:G:H1'	2.34	0.43
32:2a:1122:U:C4	32:2a:1123:A:N7	2.87	0.43
32:2a:1217:C:H2'	32:2a:1218:C:H6	1.84	0.43
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.54	0.43
41:2j:8:LEU:HD12	41:2j:16:LEU:HD22	2.00	0.43
41:2j:38:ILE:H	41:2j:38:ILE:HG12	1.58	0.43
1:1A:253:C:OP2	30:18:5:LYS:NZ	2.37	0.42
1:1A:1054:A:H3'	1:1A:1055:G:H8	1.84	0.42
1:1A:1957:C:H2'	1:1A:1958:C:C6	2.54	0.42
1:1A:2746:U:OP1	7:1H:85:LYS:NZ	2.51	0.42
32:1a:276:G:O3'	48:1q:68:ARG:NH1	2.50	0.42
32:1a:690:G:C6	32:1a:691:G:C6	3.07	0.42
32:1a:713:G:H2'	32:1a:714:G:C8	2.53	0.42
32:1a:875:C:H1'	39:1h:15:ASN:HD21	1.84	0.42
32:1a:1198:G:H5"	62:1a:1904:HOH:O	2.18	0.42
32:1a:1250:A:H4'	40:1i:68:GLY:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:180:LEU:HB2	33:1b:182:ILE:HD12	2.01	0.42
35:1d:82:ALA:O	35:1d:89:THR:HG22	2.19	0.42
37:1f:89:MET:HE1	49:1r:72:ARG:HB3	2.00	0.42
46:1o:56:LEU:O	46:1o:60:VAL:HG23	2.19	0.42
54:1w:7:G:O2'	54:1w:49:G:OP2	2.27	0.42
56:1y:19:U:P	56:1y:19:U:H3'	2.58	0.42
1:2A:208:C:H2'	1:2A:209:C:H6	1.82	0.42
1:2A:262:A:H2'	1:2A:263:C:O4'	2.19	0.42
1:2A:764:A:H5'	3:2D:210:GLY:CA	2.49	0.42
1:2A:1155:A:H5"	16:2U:55:ARG:NE	2.34	0.42
1:2A:2111:C:N4	1:2A:2144:U:O2'	2.51	0.42
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.49	0.42
6:2G:67:LYS:H	26:24:6:HIS:CE1	2.37	0.42
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.55	0.42
10:2O:2:ILE:HB	10:2O:33:ALA:HB3	2.00	0.42
13:2R:41:ALA:HB1	13:2R:114:VAL:HG13	1.99	0.42
17:2V:66:ARG:NH2	17:2V:88:ARG:HD3	2.34	0.42
32:2a:8:A:N6	35:2d:209:ARG:HB2	2.34	0.42
32:2a:357:G:OP1	32:2a:367:U:H5"	2.19	0.42
32:2a:491:G:H2'	32:2a:492:G:O4'	2.19	0.42
32:2a:714:G:H2'	32:2a:715:A:C8	2.53	0.42
32:2a:1157:A:H61	32:2a:1178:G:H21	1.65	0.42
42:2k:22:HIS:HD2	42:2k:29:ILE:HD13	1.84	0.42
1:1A:601:C:O2'	1:1A:605:C:H5"	2.19	0.42
5:1F:143:ALA:HB1	5:1F:148:LEU:HB2	2.01	0.42
6:1G:136:ARG:HG3	6:1G:137:GLU:HG3	2.01	0.42
10:1O:87:ILE:HD12	10:1O:91:LEU:HA	2.01	0.42
23:11:8:SER:HB3	23:11:66:HIS:CD2	2.54	0.42
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.34	0.42
32:1a:189:G:C6	32:1a:189(L):G:C6	3.07	0.42
32:1a:565:U:H3'	32:1a:566:G:H2'	2.01	0.42
32:1a:741:G:H2'	32:1a:742:G:O4'	2.19	0.42
32:1a:1277:C:O2'	32:1a:1279:A:H8	2.03	0.42
33:1b:80:ILE:HD12	33:1b:212:GLN:HA	2.01	0.42
33:1b:207:ALA:O	33:1b:211:ILE:HG13	2.19	0.42
1:2A:893:C:H2'	1:2A:894:C:C5	2.53	0.42
1:2A:996:A:H4'	16:2U:91:ASP:OD2	2.19	0.42
1:2A:2183:C:H2'	1:2A:2184:G:C8	2.48	0.42
1:2A:2396:G:OP1	23:21:25:LYS:NZ	2.42	0.42
1:2A:2555:U:O2	54:2w:74:C:C2	2.72	0.42
1:2A:2749:A:H5"	7:2H:3:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:48:GLN:NE2	4:2E:78:LEU:HD13	2.34	0.42
26:24:45:GLY:O	26:24:47:GLN:N	2.47	0.42
30:28:34:TRP:CG	30:28:35:GLN:N	2.87	0.42
32:2a:1244:C:N4	32:2a:1293:G:H1	2.17	0.42
32:2a:1291:G:H2'	32:2a:1292:U:C6	2.55	0.42
34:2c:71:ALA:HB2	34:2c:106:VAL:HB	2.00	0.42
56:2y:30:G:H2'	56:2y:31:C:H6	1.85	0.42
1:1A:1289:C:H2'	1:1A:1290:C:C6	2.54	0.42
1:1A:2093:G:C6	1:1A:2225:A:C8	3.07	0.42
1:1A:2239:G:H5'	3:1D:251:GLY:HA3	2.01	0.42
1:1A:2619:C:H4'	4:1E:151:TYR:O	2.19	0.42
2:1B:75:G:H22	21:1Z:73:GLN:NE2	2.17	0.42
8:1I:48:GLU:HB3	8:1I:52:ARG:HH12	1.84	0.42
15:1T:127:ALA:C	15:1T:129:ARG:N	2.77	0.42
22:10:43:THR:O	22:10:43:THR:HG23	2.19	0.42
26:14:59:PHE:HD2	50:1s:64:GLU:HB3	1.82	0.42
32:1a:1176:A:H2'	32:1a:1177:G:C8	2.53	0.42
32:1a:1438:G:H2'	32:1a:1439:C:C6	2.55	0.42
34:1c:6:HIS:HD2	34:1c:8:ILE:N	2.16	0.42
34:1c:68:VAL:CG1	34:1c:70:VAL:HG23	2.47	0.42
35:1d:110:PHE:CD2	35:1d:148:VAL:HG23	2.54	0.42
1:2A:302:C:N4	62:2A:4127:HOH:O	2.51	0.42
1:2A:878:A:H61	1:2A:899:A:H1'	1.84	0.42
1:2A:1031:G:H21	31:29:36:GLN:HE22	1.66	0.42
1:2A:1354:A:O3'	3:2D:38:LYS:NZ	2.48	0.42
2:2B:19:G:H2'	2:2B:20:C:O4'	2.18	0.42
2:2B:75:G:N3	21:2Z:85:HIS:CE1	2.88	0.42
3:2D:166:GLN:NE2	3:2D:176:ARG:HH22	2.16	0.42
6:2G:173:LEU:HB3	6:2G:178:PHE:CD1	2.54	0.42
21:2Z:69:THR:HA	21:2Z:90:VAL:HA	1.99	0.42
26:24:46:GLN:C	26:24:48:ARG:N	2.75	0.42
32:2a:838:G:N2	32:2a:840:C:H5"	2.34	0.42
32:2a:989:C:H1'	32:2a:1016:A:H2	1.84	0.42
32:2a:991:U:C4	32:2a:1212:U:H1'	2.54	0.42
32:2a:1161:C:H2'	32:2a:1162:C:C6	2.54	0.42
32:2a:1163:C:N4	32:2a:1173:G:H1	2.14	0.42
33:2b:9:GLU:HB3	33:2b:10:LEU:H	1.68	0.42
33:2b:15:VAL:HG23	33:2b:16:HIS:CD2	2.53	0.42
33:2b:36:ARG:C	33:2b:38:GLY:H	2.27	0.42
35:2d:18:LYS:HE3	35:2d:20:TYR:OH	2.19	0.42
52:2u:20:LYS:O	52:2u:23:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:39:G:H2'	54:2w:40:C:C6	2.55	0.42
1:1A:468:G:N7	29:17:39:ARG:NH2	2.63	0.42
1:1A:764:A:H5"	3:1D:210:GLY:HA3	2.02	0.42
1:1A:1095:A:C8	1:1A:1096:A:C8	3.07	0.42
1:1A:2629:A:HO2'	1:1A:2630:G:P	2.37	0.42
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	2.01	0.42
11:1P:95:VAL:HA	11:1P:99:LEU:HD23	2.01	0.42
12:1Q:130:LYS:HB3	12:1Q:130:LYS:HE2	1.79	0.42
19:1X:1:MET:HE3	19:1X:1:MET:HB2	1.79	0.42
26:14:18:CYS:SG	26:14:20:ASN:HB2	2.59	0.42
31:19:17:ILE:HD13	31:19:26:ILE:HD13	2.01	0.42
32:1a:262:A:C6	32:1a:263:A:C6	3.07	0.42
32:1a:1251:A:H2'	32:1a:1252:A:O4'	2.18	0.42
40:1i:50:LEU:HB3	40:1i:55:ALA:HB3	2.01	0.42
44:1m:54:VAL:HG12	44:1m:57:ARG:NH1	2.35	0.42
45:1n:4:LYS:HA	45:1n:7:ILE:HD12	2.01	0.42
47:1p:67:THR:HB	47:1p:70:ALA:H	1.84	0.42
1:2A:288:C:H2'	1:2A:289:A:C8	2.54	0.42
1:2A:330:A:H2	1:2A:1210:A:C2'	2.32	0.42
1:2A:514:A:N3	1:2A:581:C:O2'	2.44	0.42
1:2A:608:A:H2'	1:2A:609:A:C8	2.54	0.42
1:2A:675:A:OP1	5:2F:63:LYS:NZ	2.51	0.42
1:2A:829:A:N7	1:2A:2248:C:H5'	2.34	0.42
1:2A:832:G:H5'	11:2P:45:LEU:HD11	2.01	0.42
1:2A:1359:A:C2	1:2A:1372:U:O4	2.73	0.42
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.55	0.42
1:2A:2331:G:O2'	1:2A:2336:A:N1	2.51	0.42
1:2A:2401:U:OP1	28:26:18:ARG:NH2	2.48	0.42
1:2A:2817:G:O2'	1:2A:2836:U:O2	2.30	0.42
14:2S:92:TYR:HB3	14:2S:98:VAL:HG21	2.01	0.42
15:2T:64:ARG:NH1	15:2T:103:ARG:HA	2.33	0.42
21:2Z:51:ALA:HB1	21:2Z:57:ILE:HD11	2.01	0.42
32:2a:411:A:C6	32:2a:429:U:C4	3.07	0.42
32:2a:765:G:N1	32:2a:812:C:O2'	2.46	0.42
32:2a:918:A:H2'	32:2a:919:A:C8	2.54	0.42
32:2a:1129:C:H2'	32:2a:1139:G:N7	2.34	0.42
34:2c:54:ARG:O	34:2c:69:HIS:ND1	2.51	0.42
34:2c:123:GLN:O	34:2c:128:PHE:HB2	2.19	0.42
42:2k:16:SER:O	42:2k:35:PRO:HD3	2.18	0.42
56:2y:26:G:H1	56:2y:44:A:N6	2.16	0.42
1:1A:445:C:OP1	16:1U:2:PRO:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1105:U:O5'	1:1A:1105:U:H6	2.02	0.42
1:1A:1509(A):A:H2'	1:1A:1509(B):A:O4'	2.19	0.42
1:1A:1588:C:H2'	1:1A:1589:C:C6	2.54	0.42
1:1A:2128:C:H1'	1:1A:2174:C:H4'	2.00	0.42
1:1A:2406:U:H2'	1:1A:2406:U:H6	1.69	0.42
10:1O:49:ARG:HH12	32:1a:1423:G:P	2.43	0.42
32:1a:300:A:O2'	32:1a:564:C:N3	2.45	0.42
32:1a:1025:U:O2	32:1a:1036:G:O6	2.38	0.42
33:1b:163:PHE:HA	33:1b:185:ILE:HG12	2.00	0.42
47:1p:40:ASP:HB3	47:1p:48:TRP:CB	2.49	0.42
1:2A:363:G:H2'	1:2A:363(A):A:H8	1.84	0.42
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.36	0.42
1:2A:1400:G:H2'	1:2A:1401:G:C8	2.53	0.42
3:2D:16:MET:HE3	3:2D:16:MET:HB2	1.94	0.42
5:2F:123:LEU:HD11	5:2F:194:MET:HE3	2.00	0.42
6:2G:107:LEU:HD13	6:2G:177:GLY:O	2.19	0.42
12:2Q:16:ARG:HG2	12:2Q:18:LYS:HE2	2.02	0.42
26:24:62:ARG:HA	26:24:62:ARG:CZ	2.49	0.42
32:2a:925:G:H1'	32:2a:1502:A:C4	2.55	0.42
32:2a:1031:G:C8	32:2a:1032:G:N7	2.87	0.42
32:2a:1323:G:HO2'	32:2a:1362:C:HO2'	1.58	0.42
51:2t:30:LYS:O	51:2t:34:LYS:HG3	2.20	0.42
56:2y:22:G:H8	56:2y:46:A:N6	2.18	0.42
1:1A:2259:G:C8	1:1A:2427:C:C4	3.07	0.42
1:1A:2354:G:H21	22:10:36:ILE:CD1	2.33	0.42
2:1B:78:A:C2	2:1B:100:A:C4	3.07	0.42
2:1B:78:A:H2'	2:1B:79:C:O4'	2.20	0.42
5:1F:184:TYR:O	5:1F:188:ARG:HG3	2.19	0.42
7:1H:7:LEU:HD23	7:1H:69:ARG:NH2	2.34	0.42
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.20	0.42
30:18:62:LEU:HB3	30:18:65:GLU:CG	2.49	0.42
32:1a:1145:C:H4'	32:1a:1146:A:H8	1.83	0.42
32:1a:1194:U:H2'	32:1a:1195:C:C6	2.54	0.42
34:1c:33:LEU:O	34:1c:37:GLN:HG2	2.19	0.42
49:1r:55:ARG:HD2	49:1r:55:ARG:HA	1.87	0.42
51:1t:59:ALA:O	51:1t:63:ILE:HG13	2.19	0.42
56:1y:48:C:O2'	56:1y:49:G:OP2	2.30	0.42
1:2A:26:G:C6	1:2A:27:G:N1	2.88	0.42
1:2A:229:A:H5'	1:2A:230:U:OP1	2.19	0.42
1:2A:460:A:OP1	29:27:41:ARG:NH2	2.52	0.42
1:2A:528:A:H8	9:2N:114:ARG:CZ	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:42:GLY:O	6:2G:44:GLY:N	2.52	0.42
14:2S:87:PHE:HB2	14:2S:112:PHE:CE1	2.54	0.42
19:2X:72:LYS:HE2	19:2X:73:ARG:O	2.20	0.42
20:2Y:38:ILE:HD13	20:2Y:66:PRO:HA	2.01	0.42
32:2a:540:G:C4	32:2a:541:G:C8	3.08	0.42
32:2a:957:U:H4'	50:2s:79:THR:HG23	2.02	0.42
32:2a:1252:A:H61	32:2a:1285:A:H61	1.65	0.42
32:2a:1322:C:O2'	32:2a:1323:G:OP2	2.31	0.42
32:2a:1371:G:C6	32:2a:1372:U:C4	3.08	0.42
33:2b:143:GLU:O	33:2b:147:LYS:HB2	2.20	0.42
35:2d:163:GLU:C	35:2d:165:MET:N	2.77	0.42
36:2e:19:MET:SD	36:2e:24:ARG:HG2	2.59	0.42
51:2t:43:LEU:HD13	51:2t:51:GLU:HB3	2.01	0.42
54:2w:10:G:H2'	54:2w:11:U:C6	2.53	0.42
56:2y:67:G:H2'	56:2y:68:C:H6	1.84	0.42
56:2y:69:C:H2'	56:2y:70:C:O4'	2.19	0.42
1:1A:479:A:N3	1:1A:481:G:H5"	2.34	0.42
1:1A:614(C):A:C4	5:1F:180:GLY:HA2	2.55	0.42
1:1A:2163:C:H2'	1:1A:2164:C:O4'	2.19	0.42
1:1A:2228:G:C5	1:1A:2229:C:C4	3.08	0.42
1:1A:2732:G:H3'	1:1A:2733:A:O4'	2.19	0.42
13:1R:98:LEU:HD12	27:15:57:VAL:HG11	2.01	0.42
32:1a:533:A:O2'	32:1a:535:A:OP2	2.30	0.42
32:1a:708:C:H2'	32:1a:709:G:H8	1.85	0.42
32:1a:755:G:OP2	46:1o:65:ARG:HD2	2.18	0.42
32:1a:881:G:P	43:1l:12:ARG:HH22	2.42	0.42
32:1a:1203:C:H2'	32:1a:1204:A:O4'	2.20	0.42
33:1b:158:LEU:HA	33:1b:159:PRO:HD3	1.93	0.42
34:1c:62:ASP:O	34:1c:97:LYS:HB3	2.19	0.42
34:1c:121:ALA:O	34:1c:124:ILE:HG12	2.20	0.42
51:1t:77:ALA:O	51:1t:81:LYS:HG3	2.18	0.42
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.54	0.42
1:2A:1005:C:H2'	1:2A:1006:C:H6	1.82	0.42
1:2A:1252:G:N3	16:2U:33:ARG:HG2	2.35	0.42
1:2A:1913:A:H4'	1:2A:1914:C:O5'	2.18	0.42
1:2A:2119:A:N1	1:2A:2170:A:H2'	2.34	0.42
6:2G:96:ARG:N	6:2G:99:MET:HE2	2.35	0.42
12:2Q:57:HIS:HD2	12:2Q:117:ALA:HB2	1.85	0.42
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.19	0.42
21:2Z:171:ILE:H	21:2Z:171:ILE:HG13	1.65	0.42
31:29:32:HIS:O	31:29:34:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:886:G:H2'	32:2a:887:G:O4'	2.19	0.42
34:2c:57:ILE:HG13	34:2c:66:VAL:HG22	2.01	0.42
34:2c:127:ARG:NH2	34:2c:192:THR:OG1	2.53	0.42
34:2c:136:GLN:O	34:2c:140:ARG:HG3	2.18	0.42
35:2d:112:VAL:HG22	35:2d:116:GLN:NE2	2.34	0.42
36:2e:100:VAL:HA	36:2e:118:ILE:HG22	2.02	0.42
37:2f:12:PRO:HG3	37:2f:57:GLN:O	2.19	0.42
42:2k:85:ARG:HG2	42:2k:111:ASP:O	2.20	0.42
1:1A:992:C:OP1	16:1U:47:TYR:OH	2.36	0.42
1:1A:1006:C:C2	1:1A:1138:G:N2	2.87	0.42
1:1A:1386:C:H2'	1:1A:1387:C:C6	2.55	0.42
1:1A:2168:G:N1	1:1A:2171:A:N7	2.68	0.42
1:1A:2633:G:H2'	1:1A:2634:G:O4'	2.20	0.42
8:1I:38:LEU:H	8:1I:38:LEU:HD23	1.84	0.42
11:1P:46:LYS:HB3	11:1P:46:LYS:HE3	1.78	0.42
23:11:80:LEU:HD11	23:11:97:LEU:HD11	2.01	0.42
32:1a:119:A:H4'	32:1a:120:A:C8	2.54	0.42
32:1a:376:G:H4'	47:1p:5:ARG:NH2	2.34	0.42
32:1a:977:A:O2'	32:1a:981:U:N3	2.49	0.42
32:1a:1309:G:P	44:1m:88:ARG:HH21	2.41	0.42
32:1a:1511:G:H2'	32:1a:1512:U:O4'	2.20	0.42
33:1b:172:ILE:H	33:1b:172:ILE:HG13	1.66	0.42
36:1e:78:HIS:CE1	36:1e:142:LEU:HA	2.55	0.42
39:1h:4:ASP:OD1	39:1h:7:ALA:N	2.34	0.42
44:1m:57:ARG:HG3	44:1m:61:GLU:OE2	2.20	0.42
54:1w:4:G:H2'	54:1w:5:G:H5'	2.02	0.42
55:1x:8:4SU:O2	55:1x:21:A:H2	2.03	0.42
1:2A:214:G:O2'	1:2A:216:A:O2'	2.23	0.42
1:2A:955:C:OP1	12:2Q:87:LYS:NZ	2.44	0.42
1:2A:1243:G:O2'	11:2P:7:ARG:NH2	2.52	0.42
1:2A:2128:C:H6	1:2A:2128:C:O5'	2.03	0.42
1:2A:2238:G:H5"	62:2A:4453:HOH:O	2.19	0.42
1:2A:2445:G:OP1	5:2F:74:ARG:NH2	2.52	0.42
3:2D:24:ILE:HD13	3:2D:84:TYR:HB2	2.01	0.42
9:2N:123:TYR:CZ	9:2N:129:PRO:HD2	2.54	0.42
10:2O:60:ALA:HB1	10:2O:84:ALA:HB1	2.01	0.42
16:2U:106:PHE:O	16:2U:110:VAL:HG23	2.20	0.42
17:2V:62:LEU:HD21	17:2V:95:LEU:HD12	2.02	0.42
32:2a:1318:A:H4'	50:2s:10:PHE:CD2	2.54	0.42
33:2b:188:ALA:O	33:2b:202:PRO:HA	2.20	0.42
35:2d:165:MET:HE2	35:2d:168:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:24:GLY:O	40:2i:25:LYS:HD3	2.19	0.42
1:1A:438:G:H2'	1:1A:440:G:C8	2.55	0.42
1:1A:762:U:H5"	62:1A:4332:HOH:O	2.20	0.42
1:1A:2120:G:N2	1:1A:2178:C:N3	2.58	0.42
1:1A:2124:G:H3'	1:1A:2125:G:C8	2.55	0.42
5:1F:18:ARG:NH2	5:1F:127:GLU:OE2	2.52	0.42
8:1I:38:LEU:HG	8:1I:40:THR:HG23	2.02	0.42
12:1Q:51:ARG:HD3	12:1Q:66:ILE:HD11	2.02	0.42
20:1Y:7:VAL:HG23	20:1Y:74:PRO:HD3	2.02	0.42
32:1a:222:U:H2'	32:1a:223:U:H6	1.84	0.42
32:1a:512:U:H2'	32:1a:513:C:C6	2.55	0.42
32:1a:1041:A:H2'	32:1a:1042:G:O4'	2.20	0.42
33:1b:97:TRP:CH2	33:1b:173:ALA:HA	2.55	0.42
33:1b:101:MET:HG3	33:1b:108:ILE:HD12	2.02	0.42
38:1g:39:ALA:HA	38:1g:42:ILE:HD12	2.02	0.42
40:1i:52:ALA:HB2	40:1i:101:PHE:HE2	1.85	0.42
41:1j:81:THR:C	41:1j:83:GLU:N	2.78	0.42
1:2A:821:A:N1	62:2A:4023:HOH:O	2.37	0.42
1:2A:2484:G:C2	1:2A:2485:G:C8	3.07	0.42
8:2I:40:THR:OG1	8:2I:41:GLU:N	2.53	0.42
13:2R:53:HIS:HA	13:2R:56:LYS:HD3	2.01	0.42
15:2T:65:LYS:HE3	15:2T:67:SER:HB2	2.02	0.42
17:2V:60:GLU:HB2	17:2V:97:LYS:HE2	2.01	0.42
32:2a:595:G:H1'	32:2a:596:C:H5	1.85	0.42
32:2a:779:C:H2'	32:2a:780:A:O4'	2.20	0.42
32:2a:1338:G:C6	32:2a:1339:A:C6	3.07	0.42
32:2a:1348:U:OP1	40:2i:110:GLU:HB2	2.19	0.42
36:2e:131:ILE:O	36:2e:135:THR:HG23	2.19	0.42
37:2f:97:PHE:CD2	49:2r:31:LEU:HD21	2.55	0.42
38:2g:29:LYS:HD3	38:2g:29:LYS:HA	1.92	0.42
43:2l:6:THR:HG23	43:2l:9:GLN:OE1	2.20	0.42
54:2w:71:G:H5'	54:2w:72:C:OP2	2.20	0.42
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.55	0.42
1:1A:1104:C:H2'	1:1A:1105:U:C6	2.55	0.42
1:1A:1914:C:H2'	1:1A:1915:5MU:O4'	2.19	0.42
1:1A:2110:G:C6	1:1A:2120:G:C4	3.08	0.42
1:1A:2705:A:O2'	1:1A:2852:G:OP1	2.31	0.42
3:1D:218:ARG:HB3	3:1D:219:PRO:HD2	2.02	0.42
4:1E:54:GLN:NE2	4:1E:76:ARG:HG2	2.35	0.42
11:1P:63:PRO:HG2	30:18:25:MET:HB2	2.02	0.42
19:1X:35:THR:HG22	19:1X:37:THR:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.70	0.42
30:18:26:LYS:HD3	30:18:48:PHE:HB3	2.02	0.42
32:1a:376:G:OP2	47:1p:67:THR:HG21	2.20	0.42
32:1a:1255:G:O3'	32:1a:1258:G:H1'	2.20	0.42
33:1b:16:HIS:HB2	33:1b:204:ASN:CB	2.50	0.42
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.20	0.42
1:2A:141:A:C8	1:2A:1408:C:O2'	2.63	0.42
1:2A:1456:G:OP2	62:2A:3954:HOH:O	2.22	0.42
1:2A:2262:U:OP2	22:20:16:SER:OG	2.35	0.42
1:2A:2639:A:H2'	1:2A:2640:G:O4'	2.20	0.42
5:2F:197:ASP:O	5:2F:200:GLU:HB3	2.18	0.42
12:2Q:38:GLU:HB2	12:2Q:127:ILE:HB	2.01	0.42
25:23:29:ARG:HE	25:23:29:ARG:HB2	1.71	0.42
26:24:50:VAL:HG11	44:2m:64:TRP:O	2.19	0.42
32:2a:302:G:N3	32:2a:556:C:H4'	2.35	0.42
32:2a:1054:C:C4	54:2w:34:C:H1'	2.55	0.42
33:2b:98:LEU:HB2	33:2b:101:MET:HG3	2.01	0.42
44:2m:94:ARG:HH12	50:2s:81:ARG:HA	1.85	0.42
45:2n:23:ARG:NH1	45:2n:28:GLY:O	2.48	0.42
54:2w:53:G:H2'	54:2w:54:5MU:C6	2.54	0.42
1:1A:272(I):U:H2'	1:1A:272(J):C:C6	2.55	0.41
1:1A:581:C:H5"	62:1U:308:HOH:O	2.20	0.41
1:1A:1342:A:O2'	1:1A:1344:G:OP2	2.34	0.41
1:1A:1427:A:H4'	1:1A:1428:C:O4'	2.19	0.41
1:1A:1803:A:H4'	3:1D:259:THR:HG23	2.01	0.41
1:1A:2439:A:N6	55:1x:76:31H:OP1	2.53	0.41
5:1F:65:TRP:CZ2	5:1F:75:HIS:HD2	2.38	0.41
11:1P:95:VAL:O	11:1P:126:VAL:HG23	2.20	0.41
32:1a:160:A:H1'	32:1a:344:A:C5	2.55	0.41
32:1a:294:U:OP1	32:1a:610:G:O2'	2.36	0.41
32:1a:406:G:N2	35:1d:119:GLN:HE22	2.18	0.41
32:1a:660:G:N7	62:1a:1955:HOH:O	2.37	0.41
32:1a:794:A:OP2	62:1a:1919:HOH:O	2.21	0.41
32:1a:841:U:OP2	32:1a:841:U:H6	2.03	0.41
32:1a:1009:G:N2	32:1a:1010:G:H1'	2.35	0.41
33:1b:113:HIS:O	33:1b:117:GLU:N	2.50	0.41
51:1t:33:ILE:HG23	51:1t:63:ILE:HG12	2.01	0.41
1:2A:271(X):G:C2	1:2A:271(Y):U:O4	2.73	0.41
1:2A:566:U:H5"	11:2P:29:LYS:HE3	2.02	0.41
1:2A:887:A:O2'	1:2A:889:C:OP2	2.33	0.41
1:2A:2155:G:N7	1:2A:2156:G:H1'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:179:GLU:HG3	15:2T:9:LEU:HD21	2.00	0.41
6:2G:166:ASP:O	6:2G:170:ARG:N	2.51	0.41
6:2G:179:PRO:HG3	26:24:43:TYR:CZ	2.55	0.41
12:2Q:130:LYS:HE2	12:2Q:130:LYS:HB3	1.78	0.41
14:2S:10:ARG:HA	14:2S:13:ARG:HD3	2.02	0.41
18:2W:88:ARG:HB2	18:2W:92:ARG:HB3	2.01	0.41
19:2X:9:LEU:HA	24:22:36:ARG:HH21	1.85	0.41
20:2Y:6:HIS:H	20:2Y:6:HIS:CD2	2.37	0.41
32:2a:287:U:H2'	32:2a:288:A:C8	2.55	0.41
32:2a:369:C:H2'	32:2a:370:C:H6	1.85	0.41
32:2a:461:A:O2'	32:2a:470:C:H5'	2.20	0.41
32:2a:555:C:H2'	32:2a:556:C:C6	2.55	0.41
32:2a:1057:G:C4	32:2a:1204:A:C2	3.08	0.41
32:2a:1261:A:H62	32:2a:1274:G:H21	1.68	0.41
38:2g:22:LEU:HD12	38:2g:22:LEU:O	2.20	0.41
42:2k:67:ASP:OD2	42:2k:71:LYS:HE3	2.19	0.41
44:2m:49:THR:HG23	44:2m:52:GLU:OE2	2.20	0.41
51:2t:43:LEU:HD12	51:2t:55:ILE:HG13	2.02	0.41
55:2x:58:A:H4'	55:2x:59:A:OP1	2.19	0.41
56:2y:21:A:N6	56:2y:46:A:C4	2.87	0.41
1:1A:2114:A:C2	1:1A:2168:G:H1'	2.55	0.41
1:1A:2131:G:H5'	1:1A:2133:G:C8	2.55	0.41
1:1A:2818:G:O2'	1:1A:2819:G:H5'	2.20	0.41
3:1D:72:LYS:HB3	3:1D:75:ILE:HD12	2.01	0.41
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	2.00	0.41
7:1H:118:PRO:HD2	7:1H:121:ILE:HB	2.02	0.41
12:1Q:10:ARG:HH12	12:1Q:89:ASN:HA	1.85	0.41
18:1W:13:SER:HB3	18:1W:16:LYS:HD2	2.02	0.41
20:1Y:19:LYS:HB3	20:1Y:19:LYS:HE2	1.83	0.41
22:10:70:GLN:HE21	22:10:72:ARG:CG	2.33	0.41
32:1a:272:C:H2'	32:1a:273:A:C8	2.55	0.41
33:1b:95:GLN:HG3	33:1b:147:LYS:O	2.20	0.41
55:1x:19:G:H5"	55:1x:60:U:O4	2.20	0.41
1:2A:667:U:O2	30:28:2:PRO:HD2	2.20	0.41
1:2A:848:G:C2	1:2A:933:A:H1'	2.56	0.41
1:2A:1027:A:C2	1:2A:2488:A:H5'	2.55	0.41
1:2A:1198:U:H2'	1:2A:1199:U:C6	2.55	0.41
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.20	0.41
1:2A:1528(A):A:H2'	1:2A:1529:G:O4'	2.20	0.41
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.21	0.41
1:2A:2821:A:H2'	1:2A:2822:G:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:101:ILE:HG21	26:24:25:TYR:HB2	2.02	0.41
6:2G:122:PRO:HG3	6:2G:182:LYS:C	2.45	0.41
32:2a:551:U:H2'	32:2a:552:U:C6	2.55	0.41
32:2a:1387:G:H2'	32:2a:1388:C:H6	1.85	0.41
34:2c:43:LEU:HD13	34:2c:55:VAL:HG21	2.02	0.41
35:2d:31:CYS:O	35:2d:35:ARG:HG3	2.20	0.41
45:2n:4:LYS:HG3	45:2n:7:ILE:HD12	2.02	0.41
46:2o:88:ARG:HD2	46:2o:88:ARG:HA	1.68	0.41
1:1A:249:C:O2	30:18:12:LYS:NZ	2.45	0.41
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.85	0.41
1:1A:1939:5MU:OP1	1:1A:2604:U:O2'	2.37	0.41
1:1A:2155:G:H3'	1:1A:2156:G:H5'	2.02	0.41
1:1A:2552:OMU:O5'	1:1A:2552:OMU:H6	2.20	0.41
6:1G:83:ARG:O	6:1G:86:MET:HG3	2.21	0.41
8:1I:95:LYS:NZ	8:1I:99:GLU:OE2	2.53	0.41
20:1Y:34:LYS:NZ	62:1Y:301:HOH:O	2.21	0.41
26:14:57:GLU:OE1	26:14:58:ARG:NH1	2.53	0.41
30:18:14:VAL:HG13	30:18:22:VAL:HG13	2.02	0.41
32:1a:277:C:P	48:1q:68:ARG:HH12	2.44	0.41
32:1a:405:U:H3'	32:1a:406:G:H5'	2.02	0.41
34:1c:6:HIS:CD2	34:1c:8:ILE:HB	2.56	0.41
34:1c:138:VAL:HG23	34:1c:151:VAL:HG23	2.02	0.41
37:1f:39:LYS:HE3	37:1f:39:LYS:HB3	1.77	0.41
45:1n:12:ARG:HG2	45:1n:13:THR:N	2.35	0.41
49:1r:31:LEU:HD23	49:1r:31:LEU:H	1.84	0.41
56:1y:70:C:H3'	56:1y:71:G:H8	1.85	0.41
1:2A:184:C:H2'	1:2A:185:U:H6	1.84	0.41
1:2A:1035:U:H5"	7:2H:59:ARG:HD3	2.02	0.41
1:2A:1539:G:H2'	1:2A:1540:U:O4'	2.20	0.41
1:2A:2228:G:C5	1:2A:2229:C:C4	3.08	0.41
1:2A:2786:U:OP1	4:2E:69:LYS:NZ	2.37	0.41
14:2S:99:LYS:HE3	14:2S:103:GLU:OE2	2.20	0.41
17:2V:76:LYS:HB2	17:2V:81:TYR:HD2	1.86	0.41
32:2a:340:U:H2'	32:2a:341:C:C6	2.55	0.41
32:2a:664:G:N2	32:2a:741:G:H1	2.15	0.41
32:2a:1157:A:H61	32:2a:1178:G:N2	2.18	0.41
32:2a:1261:A:H5'	32:2a:1284:C:P	2.60	0.41
32:2a:1441:G:H8	32:2a:1441:G:O5'	2.03	0.41
42:2k:62:GLN:OE1	42:2k:93:GLN:NE2	2.53	0.41
54:2w:8:4SU:S4	54:2w:14:A:C8	3.14	0.41
1:1A:286:C:H2'	1:1A:287:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1056:G:H1'	1:1A:1103:A:H61	1.86	0.41
1:1A:2088:G:C6	1:1A:2089:U:C4	3.09	0.41
1:1A:2492:U:H2'	1:1A:2493:U:H6	1.86	0.41
6:1G:47:LYS:O	6:1G:86:MET:HE2	2.20	0.41
8:1I:12:LEU:O	8:1I:19:VAL:HG11	2.20	0.41
21:1Z:121:HIS:HE2	21:1Z:169:GLU:HG2	1.84	0.41
32:1a:114:U:H1'	32:1a:353:A:H1'	2.02	0.41
32:1a:279:A:C4	48:1q:98:LEU:HD23	2.56	0.41
32:1a:689:C:OP1	42:1k:27:ASN:ND2	2.48	0.41
32:1a:1456:G:O6	51:1t:54:LYS:NZ	2.40	0.41
33:1b:12:GLU:C	33:1b:14:GLY:H	2.27	0.41
33:1b:185:ILE:HG22	33:1b:199:TYR:HD2	1.86	0.41
49:1r:38:GLU:HA	49:1r:41:LYS:HE2	2.02	0.41
56:1y:14:A:C6	56:1y:22:G:C4	3.08	0.41
1:2A:477:A:OP2	62:2A:3953:HOH:O	2.21	0.41
1:2A:479:A:O2'	1:2A:481:G:H5'	2.21	0.41
1:2A:729:G:C8	3:2D:208:LYS:HD2	2.55	0.41
1:2A:893:C:H2'	1:2A:894:C:C4	2.55	0.41
1:2A:1815:A:H8	1:2A:1815:A:OP1	2.02	0.41
1:2A:2170:A:H8	1:2A:2170:A:O5'	2.04	0.41
1:2A:2245:U:H5"	1:2A:2246:G:H5'	2.02	0.41
1:2A:2507:C:H5"	1:2A:2573:C:N4	2.36	0.41
1:2A:2849:U:O4	15:2T:23:ARG:NH2	2.50	0.41
5:2F:184:TYR:O	5:2F:188:ARG:HG3	2.20	0.41
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.55	0.41
8:2I:3:VAL:O	8:2I:18:VAL:HA	2.20	0.41
11:2P:77:ARG:HB2	11:2P:78:PRO:HD2	2.01	0.41
17:2V:71:LEU:HD23	17:2V:71:LEU:HA	1.85	0.41
32:2a:390:C:O3'	47:2p:28:ARG:NH2	2.54	0.41
32:2a:404:U:H2'	32:2a:405:U:H6	1.85	0.41
32:2a:1212:U:H5'	32:2a:1213:A:C8	2.56	0.41
33:2b:185:ILE:HG22	33:2b:199:TYR:HD2	1.86	0.41
36:2e:36:ASP:C	36:2e:38:GLN:N	2.78	0.41
46:2o:16:ALA:HB1	46:2o:21:ASP:HB3	2.01	0.41
50:2s:27:GLU:OE1	50:2s:28:LYS:NZ	2.50	0.41
55:2x:35:A:H2'	55:2x:36:U:C6	2.56	0.41
1:1A:918:A:H5"	2:1B:98:G:O2'	2.21	0.41
1:1A:1059:G:OP2	1:1A:1060:U:H3'	2.20	0.41
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.55	0.41
1:1A:2156:G:C8	1:1A:2156:G:OP2	2.73	0.41
6:1G:7:LEU:HD12	6:1G:104:GLU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:28:VAL:O	6:1G:31:VAL:HG13	2.19	0.41
11:1P:38:GLN:O	11:1P:40:SER:N	2.46	0.41
12:1Q:6:ARG:C	12:1Q:7:MET:HG2	2.45	0.41
15:1T:24:PRO:HD3	15:1T:52:ILE:HD12	2.01	0.41
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.56	0.41
23:11:2:SER:OG	62:11:201:HOH:O	2.19	0.41
28:16:17:LYS:HB3	28:16:17:LYS:HE3	1.82	0.41
32:1a:626:U:H2'	32:1a:627:G:C8	2.55	0.41
32:1a:626:U:H2'	32:1a:627:G:H8	1.84	0.41
32:1a:1067:A:H1'	32:1a:1068:G:O4'	2.20	0.41
32:1a:1314:C:OP2	50:1s:4:SER:OG	2.19	0.41
32:1a:1525:G:P	42:1k:120:ARG:HH22	2.43	0.41
33:1b:54:THR:O	33:1b:58:ILE:HG13	2.20	0.41
35:1d:57:ARG:HD3	35:1d:205:GLU:HB3	2.03	0.41
37:1f:17:SER:O	37:1f:21:LEU:HG	2.20	0.41
40:1i:115:GLY:O	40:1i:116:LYS:HD3	2.20	0.41
50:1s:3:ARG:NH2	50:1s:7:LYS:HE2	2.35	0.41
55:1x:50:U:H2'	55:1x:51:C:C6	2.56	0.41
1:2A:286:C:H2'	1:2A:287:C:C6	2.56	0.41
1:2A:340:A:H2'	1:2A:341:G:O4'	2.20	0.41
1:2A:500:G:N2	1:2A:502:A:H3'	2.35	0.41
1:2A:2156:G:H4'	1:2A:2157:G:OP1	2.21	0.41
3:2D:75:ILE:HG21	3:2D:99:ASP:HB2	2.01	0.41
11:2P:1:MET:HE3	11:2P:1:MET:HB2	1.91	0.41
27:25:49:CYS:SG	27:25:51:TYR:HB2	2.61	0.41
32:2a:22:G:H4'	32:2a:885:G:C8	2.55	0.41
32:2a:149:A:H2'	32:2a:150:C:C6	2.55	0.41
32:2a:320:C:H2'	32:2a:321:A:O4'	2.20	0.41
32:2a:1469:G:H2'	32:2a:1470:G:H8	1.84	0.41
36:2e:7:GLU:O	36:2e:34:VAL:HA	2.20	0.41
36:2e:36:ASP:OD2	36:2e:40:ARG:HB2	2.20	0.41
36:2e:40:ARG:HD3	36:2e:67:VAL:O	2.20	0.41
38:2g:118:VAL:HA	38:2g:121:ALA:HB3	2.03	0.41
41:2j:78:ASN:O	41:2j:80:LYS:N	2.53	0.41
54:2w:6:C:H6	54:2w:6:C:O5'	2.04	0.41
1:1A:709:U:H2'	1:1A:710:G:C8	2.55	0.41
1:1A:740:U:H2'	1:1A:741:G:C8	2.55	0.41
1:1A:813:U:H2'	1:1A:814:C:C6	2.56	0.41
1:1A:1680:U:H2'	1:1A:1681:G:O4'	2.21	0.41
1:1A:2137:C:H2'	1:1A:2138:C:C6	2.55	0.41
6:1G:18:GLU:CG	6:1G:22:ARG:HH11	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1N:1:MET:HE1	16:1U:94:ASN:ND2	2.35	0.41
11:1P:38:GLN:O	11:1P:39:LYS:HB3	2.20	0.41
18:1W:46:PHE:O	18:1W:50:VAL:HG23	2.20	0.41
21:1Z:70:LEU:HD23	21:1Z:70:LEU:HA	1.91	0.41
26:14:15:ILE:HD12	26:14:32:TYR:CE1	2.55	0.41
29:17:1:MET:HE2	29:17:1:MET:HB3	1.94	0.41
32:1a:613:C:H2'	32:1a:614:A:C8	2.54	0.41
32:1a:659:U:C2	32:1a:660:G:C8	3.09	0.41
32:1a:1023:G:H5'	32:1a:1024:G:OP2	2.20	0.41
32:1a:1516:G:H2'	32:1a:1518:MA6:OP2	2.21	0.41
36:1e:91:LEU:HD12	36:1e:120:THR:HG22	2.02	0.41
40:1i:3:GLN:HE21	40:1i:20:ARG:NE	2.19	0.41
46:1o:8:LYS:HE3	46:1o:31:LEU:HD22	2.01	0.41
46:1o:15:PHE:CZ	46:1o:84:LYS:HD2	2.56	0.41
46:1o:74:ASP:OD2	46:1o:77:ARG:HD3	2.21	0.41
1:2A:402:A:H2'	1:2A:403:U:H5'	2.02	0.41
1:2A:800:A:H8	1:2A:800:A:OP1	2.04	0.41
1:2A:1927:A:C6	1:2A:1928:A:C6	3.09	0.41
1:2A:1983:C:H4'	1:2A:2606:C:H4'	2.02	0.41
5:2F:202:PHE:O	5:2F:206:ILE:HG12	2.20	0.41
26:24:9:LEU:HA	26:24:9:LEU:HD23	1.90	0.41
32:2a:287:U:H2'	32:2a:288:A:H8	1.86	0.41
32:2a:451:A:N6	32:2a:480:U:H2'	2.36	0.41
32:2a:580:U:H2'	32:2a:581:G:O4'	2.21	0.41
32:2a:865:A:H5'	32:2a:1078:U:C5	2.55	0.41
32:2a:1273:G:H3'	32:2a:1274:G:H8	1.86	0.41
39:2h:33:GLU:HA	39:2h:36:LEU:HD12	2.02	0.41
40:2i:6:GLY:N	40:2i:17:VAL:O	2.53	0.41
40:2i:93:ARG:HA	40:2i:93:ARG:HD3	1.89	0.41
51:2t:72:LEU:HD12	51:2t:72:LEU:HA	1.86	0.41
56:2y:27:A:H2'	56:2y:28:G:C8	2.55	0.41
1:1A:271(J):C:O3'	1:1A:271(K):U:H3'	2.20	0.41
1:1A:359:A:H2'	1:1A:360:G:O4'	2.20	0.41
1:1A:817:C:H4'	1:1A:932:G:C5	2.56	0.41
1:1A:858:U:O2	1:1A:2268:A:H2'	2.21	0.41
1:1A:1828:G:OP2	1:1A:1828:G:H8	2.04	0.41
1:1A:2040:C:H2'	1:1A:2041:U:O4'	2.21	0.41
1:1A:2126:A:H61	1:1A:2162:G:C2'	2.34	0.41
2:1B:14:U:O2	2:1B:108:U:H4'	2.21	0.41
8:1I:117:GLU:HG3	8:1I:118:LYS:H	1.85	0.41
16:1U:16:LYS:HB3	16:1U:16:LYS:HE2	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:189:G:C5	32:1a:189(L):G:N1	2.89	0.41
32:1a:607:A:H2'	32:1a:608:A:C8	2.56	0.41
32:1a:659:U:H2'	32:1a:660:G:C8	2.55	0.41
32:1a:723:U:O2'	32:1a:724:G:H5'	2.21	0.41
33:1b:16:HIS:HB2	33:1b:204:ASN:HB2	2.02	0.41
35:1d:110:PHE:CE2	35:1d:148:VAL:HG23	2.56	0.41
43:1l:53:ARG:HG3	43:1l:93:LEU:HD21	2.01	0.41
1:2A:612:C:C2	1:2A:616:G:N2	2.89	0.41
1:2A:991:C:N4	1:2A:1163:G:H1	2.19	0.41
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.20	0.41
1:2A:2274:A:C5	1:2A:2276:G:C8	3.08	0.41
3:2D:276:LYS:HE3	3:2D:276:LYS:HB3	1.92	0.41
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.21	0.41
21:2Z:10:ARG:HG3	21:2Z:36:LYS:HB3	2.02	0.41
32:2a:106:C:N4	62:2a:1946:HOH:O	2.53	0.41
32:2a:360:A:H2'	32:2a:361:G:C8	2.55	0.41
32:2a:766:A:H2'	32:2a:767:A:O4'	2.21	0.41
32:2a:841:U:O2	32:2a:841:U:H2'	2.20	0.41
32:2a:1403:C:H2'	32:2a:1404:5MC:HM53	2.03	0.41
32:2a:1418:A:H5"	32:2a:1419:G:OP2	2.20	0.41
46:2o:48:LYS:HA	46:2o:48:LYS:HD3	1.87	0.41
56:2y:24:A:H5'	56:2y:25:C:OP2	2.20	0.41
56:2y:48:C:HO2'	56:2y:49:G:P	2.38	0.41
1:1A:818:G:H4'	1:1A:838:C:O3'	2.19	0.41
1:1A:1166:C:H2'	1:1A:1167:U:H6	1.86	0.41
1:1A:1915:5MU:H71	1:1A:1915:5MU:OP2	2.20	0.41
1:1A:2031:A:C6	1:1A:2498:C:H1'	2.56	0.41
1:1A:2804:C:H2'	1:1A:2805:G:H8	1.86	0.41
5:1F:172:TRP:CD1	5:1F:172:TRP:H	2.38	0.41
8:1I:129:THR:HG22	8:1I:139:GLN:HE22	1.85	0.41
19:1X:5:TYR:CD1	24:12:30:ARG:HA	2.56	0.41
25:13:5:LYS:HG2	25:13:55:ARG:HH12	1.86	0.41
32:1a:57:G:H2'	32:1a:58:C:C6	2.56	0.41
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.52	0.41
32:1a:1149:C:H2'	32:1a:1150:U:H6	1.84	0.41
32:1a:1183:A:O2'	32:1a:1184:G:OP1	2.36	0.41
35:1d:105:VAL:HG13	35:1d:110:PHE:HB2	2.03	0.41
48:1q:57:VAL:HG12	48:1q:76:LEU:HA	2.02	0.41
56:1y:8:4SU:O2'	56:1y:21:A:N1	2.44	0.41
1:2A:69:C:H2'	1:2A:70:G:C8	2.56	0.41
1:2A:265:A:H1'	1:2A:266:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:272:G:H4'	1:2A:272(A):U:H5"	2.03	0.41
1:2A:533:G:H5'	16:2U:24:TYR:CE1	2.56	0.41
1:2A:815:C:H2'	1:2A:816:C:C6	2.56	0.41
1:2A:1416:G:H1'	1:2A:1417:C:C5	2.56	0.41
1:2A:1547:C:H2'	1:2A:1548:C:H6	1.86	0.41
6:2G:138:GLN:OE1	6:2G:138:GLN:N	2.53	0.41
7:2H:149:ARG:NH1	7:2H:167:GLU:OE1	2.53	0.41
19:2X:5:TYR:CZ	24:22:30:ARG:HB2	2.55	0.41
32:2a:266:G:H2'	32:2a:266:G:N3	2.36	0.41
32:2a:1103:C:P	33:2b:96:ARG:HH22	2.43	0.41
32:2a:1265:G:C4	32:2a:1271:G:N2	2.89	0.41
33:2b:124:SER:HB3	33:2b:125:PRO:HD3	2.02	0.41
35:2d:187:ARG:HH12	35:2d:190:ASP:HB2	1.85	0.41
37:2f:61:LEU:HB3	37:2f:63:TYR:CE2	2.55	0.41
37:2f:99:ALA:HB1	49:2r:23:LYS:NZ	2.35	0.41
40:2i:70:LYS:O	40:2i:74:ILE:HG13	2.20	0.41
42:2k:66:LEU:O	42:2k:70:LYS:HG3	2.20	0.41
46:2o:10:LYS:HE2	46:2o:10:LYS:HB3	1.89	0.41
56:2y:2:C:H2'	56:2y:3:G:H8	1.85	0.41
56:2y:7:G:C6	56:2y:67:G:C2	3.08	0.41
56:2y:51:G:N2	56:2y:64:U:C2	2.89	0.41
1:1A:154(A):C:O5'	1:1A:154(A):C:H6	2.04	0.41
1:1A:1022:G:N7	9:1N:66:LYS:HE2	2.36	0.41
1:1A:1153:C:H2'	1:1A:1154:G:O4'	2.21	0.41
1:1A:1899:G:H2'	1:1A:1899:G:N3	2.36	0.41
1:1A:2124:G:H3'	1:1A:2125:G:H8	1.86	0.41
1:1A:2854:G:H2'	1:1A:2855:C:C6	2.56	0.41
7:1H:148:ILE:HA	7:1H:151:ILE:HD12	2.03	0.41
17:1V:40:LEU:HD12	17:1V:46:VAL:HB	2.02	0.41
18:1W:35:ILE:HG23	27:15:28:PRO:HD2	2.02	0.41
18:1W:36:LEU:HD23	18:1W:36:LEU:HA	1.91	0.41
32:1a:116:A:O5'	32:1a:116:A:H8	2.04	0.41
32:1a:134:A:H61	47:1p:25:ARG:HH12	1.68	0.41
32:1a:165:C:H2'	32:1a:166:G:C8	2.54	0.41
32:1a:685:G:C2	32:1a:686:U:C4	3.09	0.41
32:1a:942:G:C2	32:1a:1342:C:C2	3.09	0.41
32:1a:1030(A):G:H1'	32:1a:1031:G:H1	1.86	0.41
32:1a:1113:C:O2'	34:1c:14:ILE:HD11	2.21	0.41
32:1a:1171:G:H2'	32:1a:1172:C:C6	2.56	0.41
32:1a:1261:A:H3'	32:1a:1262:C:C6	2.56	0.41
33:1b:155:LEU:HD12	33:1b:155:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:212:GLN:NE2	33:1b:216:SER:HB3	2.35	0.41
33:1b:214:ILE:O	33:1b:218:ALA:HB2	2.21	0.41
34:1c:186:PHE:HD1	34:1c:199:LYS:HG2	1.86	0.41
39:1h:33:GLU:O	39:1h:37:ARG:N	2.46	0.41
40:1i:48:GLU:HA	40:1i:51:ARG:HD3	2.02	0.41
54:1w:26:G:O6	54:1w:44:A:N1	2.53	0.41
1:2A:127:A:H5"	1:2A:128:C:C6	2.56	0.41
1:2A:245:G:O6	30:28:8:LYS:NZ	2.51	0.41
1:2A:272:G:H4'	1:2A:272(A):U:C5'	2.50	0.41
1:2A:645:C:H5"	1:2A:646:A:OP2	2.20	0.41
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.53	0.41
1:2A:955:C:OP2	12:2Q:14:ARG:HG3	2.21	0.41
1:2A:1009:A:O4'	16:2U:59:ARG:HD2	2.21	0.41
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.55	0.41
1:2A:1468:C:H42	1:2A:1524:G:H1	1.68	0.41
1:2A:1803:A:H4'	3:2D:259:THR:CG2	2.50	0.41
1:2A:2037:G:H2'	1:2A:2038:G:C8	2.56	0.41
1:2A:2059:A:O2'	5:2F:69:HIS:HD2	2.04	0.41
1:2A:2125:G:N1	1:2A:2172:U:OP1	2.54	0.41
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.56	0.41
1:2A:2404:C:O3'	11:2P:77:ARG:NH2	2.54	0.41
1:2A:2453:A:OP1	62:2A:3955:HOH:O	2.22	0.41
1:2A:2527:C:H5"	31:29:30:PRO:HB3	2.03	0.41
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.46	0.41
5:2F:178:PRO:HB3	5:2F:198:ALA:HA	2.03	0.41
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.53	0.41
13:2R:98:LEU:HB2	13:2R:113:LEU:HG	2.02	0.41
14:2S:15:ARG:HB3	14:2S:19:LYS:NZ	2.36	0.41
17:2V:65:GLY:HA3	17:2V:91:TYR:CZ	2.56	0.41
23:21:95:LEU:O	23:21:98:LEU:HB2	2.20	0.41
26:24:28:LYS:HA	26:24:29:PRO:HD3	1.91	0.41
27:25:20:ARG:HG2	27:25:23:HIS:ND1	2.36	0.41
32:2a:10:A:OP2	36:2e:126:ARG:HD2	2.21	0.41
32:2a:109:A:C6	32:2a:326:G:C6	3.09	0.41
32:2a:335:C:H2'	32:2a:336:C:C6	2.56	0.41
32:2a:338:A:H2	32:2a:351:G:H22	1.68	0.41
32:2a:416:G:H2'	32:2a:417:C:C6	2.56	0.41
32:2a:751:U:H4'	46:2o:24:SER:HA	2.03	0.41
32:2a:939:G:H2'	32:2a:940:C:C6	2.55	0.41
32:2a:1029:C:C4	32:2a:1032:G:C6	3.05	0.41
32:2a:1084:G:H5'	32:2a:1102:A:OP2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1186:G:O3'	40:2i:113:LYS:NZ	2.53	0.41
32:2a:1252:A:H61	32:2a:1285:A:N6	2.18	0.41
34:2c:122:GLU:HA	34:2c:125:GLU:OE1	2.21	0.41
37:2f:2:ARG:CZ	37:2f:69:GLU:HG2	2.51	0.41
40:2i:55:ALA:HA	40:2i:58:HIS:CD2	2.56	0.41
40:2i:85:LEU:HB3	40:2i:92:TYR:HD2	1.86	0.41
44:2m:49:THR:OG1	44:2m:52:GLU:HG3	2.21	0.41
51:2t:58:LYS:HA	51:2t:58:LYS:HD2	1.86	0.41
55:2x:10:G:N2	55:2x:26:G:H1'	2.36	0.41
1:1A:875:G:O2'	21:1Z:151:HIS:HE1	2.04	0.41
1:1A:1066:U:H2'	1:1A:1068:G:OP2	2.21	0.41
1:1A:1301:A:C8	1:1A:1303:G:C8	3.08	0.41
1:1A:2274:A:OP2	62:1A:4157:HOH:O	2.21	0.41
1:1A:2506:U:O4'	59:1A:4097:CLM:H8	2.21	0.41
12:1Q:32:TYR:OH	12:1Q:111:GLU:OE2	2.21	0.41
21:1Z:77:ASP:OD2	21:1Z:80:ARG:HD2	2.21	0.41
25:13:26:LEU:O	25:13:35:ARG:NE	2.41	0.41
26:14:49:PHE:HB3	26:14:50:VAL:H	1.54	0.41
32:1a:167:G:H2'	32:1a:168:G:H8	1.85	0.41
32:1a:458:C:H2'	32:1a:460:G:O4'	2.21	0.41
32:1a:1349:A:C2	32:1a:1374:A:C4	3.09	0.41
47:1p:53:VAL:O	47:1p:57:ARG:HG3	2.21	0.41
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.20	0.41
1:2A:1831:G:H2'	1:2A:1832:C:C6	2.55	0.41
1:2A:1907:G:C2	1:2A:1908:C:C2	3.09	0.41
1:2A:2370:G:C6	1:2A:2371:G:C6	3.09	0.41
1:2A:2406:U:H6	1:2A:2406:U:H2'	1.76	0.41
5:2F:131:GLY:O	5:2F:138:GLU:HB3	2.21	0.41
6:2G:123:ASN:C	6:2G:125:PHE:H	2.27	0.41
7:2H:144:VAL:O	7:2H:148:ILE:HG13	2.20	0.41
8:2I:4:ILE:HD11	8:2I:44:LEU:HD12	2.02	0.41
15:2T:84:GLN:HG2	15:2T:85:LYS:HG2	2.03	0.41
23:21:23:LYS:HE2	56:2y:74:C:H4'	2.01	0.41
24:22:8:LYS:HA	24:22:8:LYS:HD2	1.80	0.41
32:2a:334:C:H2'	32:2a:335:C:C6	2.56	0.41
32:2a:585:G:O2'	32:2a:879:C:OP1	2.35	0.41
32:2a:620:C:C2	35:2d:135:LEU:HG	2.56	0.41
32:2a:707:C:H2'	32:2a:708:C:C6	2.56	0.41
32:2a:923:A:O2'	32:2a:1399:C:OP2	2.30	0.41
32:2a:1009:G:H2'	32:2a:1010:G:H5'	2.02	0.41
32:2a:1030(A):G:N2	32:2a:1030(C):G:H3'	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1152:A:C6	32:2a:1153:C:C4	3.08	0.41
32:2a:1314:C:OP2	50:2s:6:LYS:HD2	2.21	0.41
33:2b:122:PHE:CE1	33:2b:127:ILE:HD12	2.56	0.41
34:2c:32:LEU:O	34:2c:36:ASP:HB2	2.21	0.41
34:2c:136:GLN:O	34:2c:139:GLN:N	2.54	0.41
36:2e:135:THR:O	36:2e:139:LEU:N	2.40	0.41
39:2h:69:ARG:NE	39:2h:75:ARG:O	2.53	0.41
42:2k:98:LEU:O	42:2k:101:SER:OG	2.37	0.41
54:2w:26:G:H1	54:2w:44:A:H61	1.69	0.41
1:1A:503:A:H4'	1:1A:504:U:H5"	2.03	0.40
1:1A:555:U:O2'	1:1A:556:G:N7	2.49	0.40
1:1A:590:A:H2'	1:1A:591:C:O4'	2.21	0.40
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.21	0.40
12:1Q:115:MET:HE3	12:1Q:115:MET:HB3	1.99	0.40
21:1Z:98:MET:O	21:1Z:125:LEU:HA	2.20	0.40
23:11:77:ALA:HA	23:11:80:LEU:HD12	2.02	0.40
32:1a:96:U:H2'	32:1a:97:G:C8	2.57	0.40
32:1a:507:C:OP2	32:1a:508:C:O2'	2.30	0.40
32:1a:1410:G:H2'	32:1a:1411:C:H6	1.86	0.40
34:1c:141:VAL:HG12	34:1c:146:ALA:HB3	2.02	0.40
35:1d:10:ARG:HG3	35:1d:11:LEU:HD12	2.02	0.40
36:1e:41:VAL:O	36:1e:66:MET:HA	2.21	0.40
37:1f:35:ALA:HA	37:1f:67:MET:HB3	2.03	0.40
44:1m:11:ARG:C	44:1m:13:LYS:H	2.29	0.40
50:1s:80:TYR:O	50:1s:81:ARG:HB2	2.21	0.40
1:2A:328:U:H4'	20:2Y:68:HIS:CG	2.56	0.40
1:2A:467:G:OP1	29:27:33:ARG:HD2	2.21	0.40
1:2A:601:C:O2	1:2A:605:C:H4'	2.20	0.40
1:2A:729:G:C5	3:2D:208:LYS:HB2	2.56	0.40
1:2A:760:G:H2'	1:2A:761:A:O4'	2.20	0.40
1:2A:855:G:C6	1:2A:856:C:C4	3.09	0.40
1:2A:1780:A:N6	62:2A:4162:HOH:O	2.54	0.40
1:2A:1951:U:O2	1:2A:1953:A:H8	2.04	0.40
1:2A:2082:A:H2'	1:2A:2083:G:O4'	2.20	0.40
1:2A:2431:U:O2'	1:2A:2433:A:N7	2.44	0.40
1:2A:2651:C:H2'	1:2A:2652:C:H6	1.85	0.40
5:2F:53:THR:HG22	5:2F:56:GLU:CD	2.46	0.40
6:2G:171:ALA:O	6:2G:175:LEU:HG	2.21	0.40
15:2T:16:ARG:HB3	15:2T:18:ASP:OD1	2.21	0.40
29:27:8:ASN:HB3	29:27:11:LYS:HB3	2.01	0.40
32:2a:607:A:H2'	32:2a:608:A:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1314:C:P	50:2s:6:LYS:HD2	2.61	0.40
34:2c:182:ILE:H	34:2c:182:ILE:HG13	1.63	0.40
46:2o:40:SER:O	46:2o:44:LYS:HG3	2.21	0.40
47:2p:34:GLU:OE1	47:2p:55:ARG:NH2	2.39	0.40
48:2q:81:ARG:HH21	48:2q:84:LEU:HD21	1.86	0.40
51:2t:46:GLU:H	51:2t:46:GLU:HG3	1.57	0.40
1:1A:196:A:O2'	1:1A:805:G:O6	2.30	0.40
1:1A:530:G:N1	1:1A:2023:G:OP1	2.36	0.40
1:1A:829:A:N7	1:1A:2248:C:H5'	2.35	0.40
1:1A:1113:U:H2'	1:1A:1114:G:H8	1.87	0.40
1:1A:1179:C:H2'	1:1A:1180:C:C6	2.56	0.40
1:1A:1858:G:N2	1:1A:1883:G:H2'	2.35	0.40
3:1D:132:PRO:HD3	3:1D:190:TYR:CZ	2.56	0.40
6:1G:66:GLN:HG3	26:14:1:MET:CE	2.51	0.40
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.67	0.40
24:12:3:LEU:HD23	24:12:3:LEU:HA	1.78	0.40
32:1a:26:A:O2'	35:1d:209:ARG:NH2	2.52	0.40
32:1a:993:G:H2'	32:1a:993:G:N3	2.35	0.40
32:1a:1016:A:H2'	32:1a:1017:G:O4'	2.22	0.40
32:1a:1038:C:H2'	32:1a:1039:C:C6	2.56	0.40
32:1a:1149:C:O2'	32:1a:1280:A:N1	2.51	0.40
32:1a:1338:G:H2'	32:1a:1339:A:C8	2.57	0.40
38:1g:79:ARG:HD2	38:1g:79:ARG:C	2.46	0.40
40:1i:4:TYR:CD1	40:1i:88:TYR:HA	2.56	0.40
41:1j:31:GLY:HA3	41:1j:32:ALA:HA	1.90	0.40
47:1p:3:LYS:HE3	47:1p:3:LYS:HB3	1.95	0.40
47:1p:6:LEU:HD23	47:1p:17:TYR:CG	2.56	0.40
47:1p:38:TYR:O	47:1p:49:LEU:HD12	2.20	0.40
55:1x:23:C:H2'	55:1x:24:U:C6	2.56	0.40
1:2A:118:A:C8	1:2A:119:A:C8	3.09	0.40
1:2A:900:A:C4	1:2A:901:A:C8	3.10	0.40
1:2A:1756:G:H4'	1:2A:1758:G:O4'	2.21	0.40
3:2D:5:LYS:HG2	3:2D:17:THR:HG22	2.03	0.40
4:2E:32:PRO:HD2	4:2E:50:GLY:O	2.20	0.40
24:22:66:GLU:H	24:22:66:GLU:HG3	1.61	0.40
32:2a:43:C:OP1	62:2a:1916:HOH:O	2.22	0.40
32:2a:1194:U:H2'	32:2a:1195:C:C6	2.56	0.40
32:2a:1273:G:C6	32:2a:1274:G:C4	3.10	0.40
32:2a:1291:G:C6	32:2a:1292:U:C4	3.10	0.40
33:2b:165:VAL:HG23	33:2b:187:LEU:HD13	2.02	0.40
38:2g:68:ASN:HD22	38:2g:128:ALA:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:37:ARG:NH2	39:2h:38:ILE:HG12	2.36	0.40
41:2j:89:ASP:O	41:2j:91:PRO:HD3	2.21	0.40
51:2t:85:MET:O	51:2t:89:ARG:HB2	2.22	0.40
54:2w:25:C:H2'	54:2w:26:G:H5'	2.02	0.40
1:1A:264:C:O2'	1:1A:265:A:H2'	2.21	0.40
1:1A:897:C:H5'	54:1w:56:C:OP1	2.20	0.40
1:1A:945:A:C4	1:1A:2448:A:C2	3.09	0.40
1:1A:1069:A:H4'	1:1A:1070:A:H5"	2.03	0.40
1:1A:1141:U:H4'	1:1A:1142(A):A:O4'	2.22	0.40
1:1A:1712:C:H2'	1:1A:1713:U:O4'	2.22	0.40
1:1A:2126:A:H4'	1:1A:2127:G:OP1	2.19	0.40
19:1X:27:THR:HA	19:1X:79:ALA:O	2.22	0.40
32:1a:293:G:H5'	32:1a:610:G:N2	2.36	0.40
32:1a:1191:A:OP2	34:1c:3:ASN:ND2	2.55	0.40
33:1b:12:GLU:C	33:1b:14:GLY:N	2.78	0.40
33:1b:142:LEU:HG	33:1b:146:GLN:NE2	2.36	0.40
33:1b:162:ILE:O	33:1b:185:ILE:HG12	2.21	0.40
34:1c:112:SER:O	34:1c:116:VAL:HG23	2.22	0.40
35:1d:178:VAL:HG12	35:1d:179:GLU:H	1.87	0.40
40:1i:16:ARG:NH1	40:1i:64:THR:HG21	2.33	0.40
44:1m:65:LYS:O	44:1m:70:LEU:HG	2.21	0.40
44:1m:70:LEU:HA	44:1m:70:LEU:HD23	1.86	0.40
1:2A:315:G:H2'	1:2A:316:C:C6	2.56	0.40
1:2A:636:G:OP1	11:2P:132:LYS:HE2	2.21	0.40
1:2A:1374:G:H2'	1:2A:1375:C:C6	2.56	0.40
4:2E:33:VAL:HG13	4:2E:47:VAL:HG23	2.02	0.40
6:2G:91:ARG:CZ	6:2G:91:ARG:HB3	2.51	0.40
12:2Q:37:LEU:HD11	12:2Q:130:LYS:HB2	2.03	0.40
20:2Y:28:LYS:NZ	20:2Y:64:GLU:OE1	2.52	0.40
26:24:34:GLU:HB2	44:2m:57:ARG:HE	1.87	0.40
26:24:50:VAL:HG11	44:2m:64:TRP:C	2.46	0.40
32:2a:438:G:H4'	35:2d:123:HIS:CE1	2.56	0.40
32:2a:666:G:H5'	32:2a:726:C:H1'	2.02	0.40
32:2a:1048:G:OP1	45:2n:4:LYS:HE3	2.22	0.40
36:2e:53:LEU:HA	36:2e:56:GLN:HB2	2.03	0.40
39:2h:29:SER:HB3	39:2h:32:LYS:HB2	2.04	0.40
39:2h:100:ILE:H	39:2h:100:ILE:HG13	1.73	0.40
41:2j:23:ILE:HD13	41:2j:23:ILE:HA	1.94	0.40
44:2m:19:LEU:HD11	44:2m:56:LEU:HD21	2.03	0.40
54:2w:8:4SU:N3	54:2w:14:A:N6	2.52	0.40
55:2x:52:G:C4	55:2x:53:G:C8	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2561:A:H2'	1:1A:2562:U:O4'	2.22	0.40
5:1F:183:VAL:O	5:1F:187:VAL:HG23	2.20	0.40
6:1G:39:ILE:HD12	6:1G:64:THR:HG21	2.03	0.40
22:10:43:THR:OG1	22:10:46:LYS:HG2	2.21	0.40
26:14:58:ARG:O	26:14:61:ARG:HB3	2.21	0.40
32:1a:295:C:H2'	32:1a:296:U:O4'	2.21	0.40
32:1a:364:A:H2'	32:1a:365:U:O2	2.22	0.40
32:1a:892:A:O2'	32:1a:1415:G:H4'	2.21	0.40
32:1a:1060:C:OP1	45:1n:45:ARG:NH2	2.49	0.40
36:1e:116:THR:HG23	36:1e:117:ASP:OD2	2.22	0.40
37:1f:44:GLY:HA2	37:1f:59:TYR:CD2	2.56	0.40
51:1t:10:LEU:HD12	51:1t:12:ALA:H	1.86	0.40
54:1w:17:G:O6	54:1w:55:PSU:H1'	2.22	0.40
56:1y:18:G:C5'	56:1y:57:G:H1	2.34	0.40
1:2A:234:C:H2'	1:2A:235:U:C6	2.55	0.40
1:2A:311:A:C6	1:2A:328:U:C4	3.09	0.40
1:2A:565:C:OP1	17:2V:82:ARG:NH2	2.46	0.40
1:2A:2506:U:C2	1:2A:2585:U:O4	2.74	0.40
1:2A:2752:C:OP2	7:2H:4:ILE:HD11	2.22	0.40
4:2E:101:ARG:NH2	4:2E:171:GLU:HB2	2.36	0.40
8:2I:82:ARG:H	8:2I:82:ARG:HG2	1.71	0.40
12:2Q:18:LYS:O	12:2Q:98:LYS:NZ	2.29	0.40
19:2X:54:VAL:HG22	19:2X:81:VAL:HG12	2.02	0.40
21:2Z:151:HIS:HA	21:2Z:169:GLU:O	2.21	0.40
32:2a:157:G:H2'	32:2a:158:G:H8	1.85	0.40
32:2a:441:A:H3'	32:2a:442:C:C6	2.57	0.40
32:2a:582:U:C2	32:2a:760:G:C6	3.10	0.40
32:2a:922:G:C6	32:2a:923:A:C6	3.10	0.40
32:2a:1314:C:H2'	32:2a:1315:U:C6	2.57	0.40
32:2a:1361:G:H2'	32:2a:1362:C:O4'	2.22	0.40
36:2e:83:GLU:HA	36:2e:88:LYS:HA	2.04	0.40
39:2h:66:GLY:N	39:2h:77:GLU:O	2.49	0.40
1:1A:395:U:O2'	1:1A:396:G:N7	2.45	0.40
1:1A:548:A:H1'	1:1A:549:G:OP1	2.22	0.40
1:1A:579:G:H2'	1:1A:580:C:C6	2.57	0.40
1:1A:686:G:N2	1:1A:788:A:H61	2.20	0.40
1:1A:821:A:H2'	1:1A:946:G:H5"	2.04	0.40
1:1A:910:A:N1	1:1A:2277:G:H1'	2.35	0.40
1:1A:1074:G:N1	1:1A:1075:C:H1'	2.36	0.40
1:1A:1092:C:H2'	1:1A:1093:G:H5'	2.03	0.40
1:1A:2482:G:O3'	54:1w:64:U:H4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:29:A:H2'	2:1B:30:C:C6	2.57	0.40
3:1D:147:LEU:HD13	3:1D:155:LEU:HD11	2.02	0.40
5:1F:150:GLY:HA2	5:1F:172:TRP:CE3	2.56	0.40
7:1H:127:GLU:HG3	7:1H:130:ARG:HB2	2.03	0.40
8:1I:90:GLY:O	8:1I:121:LYS:HD2	2.21	0.40
11:1P:124:LYS:HA	11:1P:144:GLU:HB3	2.03	0.40
14:1S:11:LYS:O	14:1S:15:ARG:HB2	2.21	0.40
32:1a:272:C:H2'	32:1a:273:A:H8	1.85	0.40
32:1a:452:A:H4'	47:1p:72:ARG:NH1	2.37	0.40
32:1a:524:G:H2'	32:1a:525:C:C6	2.56	0.40
32:1a:708:C:H2'	32:1a:709:G:C8	2.56	0.40
32:1a:922:G:C6	32:1a:923:A:C6	3.10	0.40
32:1a:983:A:H2	32:1a:984:C:C6	2.39	0.40
32:1a:1001(A):G:H2'	32:1a:1002:G:O4'	2.22	0.40
32:1a:1276:G:H2'	32:1a:1277:C:O4'	2.22	0.40
32:1a:1298:C:C5	38:1g:114:ARG:HD3	2.57	0.40
36:1e:78:HIS:HE1	36:1e:142:LEU:HA	1.87	0.40
56:1y:24:A:H2'	56:1y:25:C:O4'	2.22	0.40
56:1y:51:G:H2'	56:1y:52:G:C8	2.56	0.40
1:2A:460:A:H2'	1:2A:461:C:O4'	2.21	0.40
1:2A:954:G:H5"	12:2Q:13:GLN:HB3	2.02	0.40
1:2A:2018:G:H2'	1:2A:2019:A:C8	2.57	0.40
1:2A:2331:G:C6	1:2A:2332:U:C4	3.10	0.40
7:2H:140:LYS:HE3	7:2H:140:LYS:HB2	1.81	0.40
14:2S:14:VAL:HG11	14:2S:89:ARG:HG2	2.04	0.40
28:26:38:LYS:HE3	28:26:38:LYS:HB3	1.91	0.40
32:2a:309:G:H2'	32:2a:310:G:H8	1.87	0.40
32:2a:858:G:H8	32:2a:858:G:OP2	2.04	0.40
32:2a:1108:G:OP1	34:2c:175:LEU:HB2	2.22	0.40
32:2a:1379:G:O6	38:2g:2:ALA:HB3	2.22	0.40
34:2c:152:ILE:HG13	34:2c:199:LYS:HB2	2.03	0.40
39:2h:106:GLY:CA	39:2h:122:ARG:HH22	2.35	0.40
39:2h:112:LEU:HD11	39:2h:124:ALA:HB2	2.03	0.40
44:2m:23:TYR:HE2	44:2m:70:LEU:HD22	1.86	0.40
44:2m:62:ASN:ND2	44:2m:62:ASN:H	2.19	0.40
54:2w:53:G:H3'	54:2w:54:5MU:H73	2.02	0.40
55:2x:47:U:H5'	55:2x:48:C:H5'	2.03	0.40
56:2y:26:G:N1	56:2y:44:A:C6	2.81	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:368:U:O4	8:2I:82:ARG:NE[2_655]	2.18	0.02

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%)	256 (94%)	16 (6%)	1 (0%)	30 39
3	2D	273/276 (99%)	256 (94%)	16 (6%)	1 (0%)	30 39
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	24 34
4	2E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	24 34
5	1F	200/210 (95%)	193 (96%)	6 (3%)	1 (0%)	24 34
5	2F	200/210 (95%)	187 (94%)	12 (6%)	1 (0%)	24 34
6	1G	179/182 (98%)	166 (93%)	11 (6%)	2 (1%)	11 15
6	2G	179/182 (98%)	150 (84%)	25 (14%)	4 (2%)	5 5
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	21 29
7	2H	172/180 (96%)	155 (90%)	17 (10%)	0	100 100
8	1I	144/148 (97%)	128 (89%)	15 (10%)	1 (1%)	18 25
8	2I	144/148 (97%)	120 (83%)	22 (15%)	2 (1%)	9 11
9	1N	138/140 (99%)	130 (94%)	8 (6%)	0	100 100
9	2N	138/140 (99%)	132 (96%)	6 (4%)	0	100 100
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100 100
10	2O	120/122 (98%)	110 (92%)	9 (8%)	1 (1%)	16 22
11	1P	147/150 (98%)	133 (90%)	12 (8%)	2 (1%)	9 11
11	2P	147/150 (98%)	131 (89%)	12 (8%)	4 (3%)	4 3
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100 100
12	2Q	139/141 (99%)	127 (91%)	12 (9%)	0	100 100
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100 100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100 100
14	2S	108/112 (96%)	100 (93%)	4 (4%)	4 (4%)	2 1
15	1T	129/146 (88%)	123 (95%)	4 (3%)	2 (2%)	7 9
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100 100
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%)	2 (2%)	2 (2%)	6 6
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12 17
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
19	1X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	11 15
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100 100
20	1Y	105/110 (96%)	99 (94%)	5 (5%)	1 (1%)	12 17
20	2Y	105/110 (96%)	97 (92%)	8 (8%)	0	100 100
21	1Z	148/206 (72%)	133 (90%)	13 (9%)	2 (1%)	9 11
21	2Z	156/206 (76%)	119 (76%)	34 (22%)	3 (2%)	6 7
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100 100
22	20	81/85 (95%)	78 (96%)	3 (4%)	0	100 100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11 15
23	21	95/98 (97%)	90 (95%)	4 (4%)	1 (1%)	11 15
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
24	22	68/72 (94%)	68 (100%)	0	0	100 100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
25	23	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	6 7
26	14	67/71 (94%)	52 (78%)	9 (13%)	6 (9%)	0 0
26	24	67/71 (94%)	50 (75%)	15 (22%)	2 (3%)	3 2
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100 100
28	26	51/54 (94%)	46 (90%)	5 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	61 (98%)	1 (2%)	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%)	188 (82%)	32 (14%)	9 (4%)	2	1
33	2b	229/256 (90%)	184 (80%)	37 (16%)	8 (4%)	3	1
34	1c	204/239 (85%)	193 (95%)	11 (5%)	0	100	100
34	2c	204/239 (85%)	176 (86%)	26 (13%)	2 (1%)	12	17
35	1d	206/209 (99%)	189 (92%)	16 (8%)	1 (0%)	24	34
35	2d	206/209 (99%)	190 (92%)	15 (7%)	1 (0%)	24	34
36	1e	146/162 (90%)	131 (90%)	14 (10%)	1 (1%)	18	25
36	2e	146/162 (90%)	127 (87%)	15 (10%)	4 (3%)	4	3
37	1f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
37	2f	98/101 (97%)	98 (100%)	0	0	100	100
38	1g	153/156 (98%)	140 (92%)	12 (8%)	1 (1%)	18	25
38	2g	153/156 (98%)	139 (91%)	10 (6%)	4 (3%)	4	3
39	1h	135/138 (98%)	126 (93%)	8 (6%)	1 (1%)	18	25
39	2h	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	18	25
40	1i	125/128 (98%)	111 (89%)	12 (10%)	2 (2%)	7	9
40	2i	125/128 (98%)	108 (86%)	16 (13%)	1 (1%)	16	22
41	1j	95/105 (90%)	76 (80%)	16 (17%)	3 (3%)	3	2
41	2j	94/105 (90%)	79 (84%)	12 (13%)	3 (3%)	3	2
42	1k	112/129 (87%)	106 (95%)	3 (3%)	3 (3%)	4	3
42	2k	112/129 (87%)	101 (90%)	9 (8%)	2 (2%)	6	7
43	1l	119/132 (90%)	113 (95%)	5 (4%)	1 (1%)	16	22
43	2l	119/132 (90%)	109 (92%)	8 (7%)	2 (2%)	7	8
44	1m	121/126 (96%)	105 (87%)	14 (12%)	2 (2%)	7	8
44	2m	120/126 (95%)	107 (89%)	11 (9%)	2 (2%)	7	8
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
45	2n	58/61 (95%)	53 (91%)	3 (5%)	2 (3%)	3 1
46	1o	86/89 (97%)	82 (95%)	2 (2%)	2 (2%)	5 4
46	2o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10 13
47	1p	80/88 (91%)	70 (88%)	10 (12%)	0	100 100
47	2p	80/88 (91%)	73 (91%)	7 (9%)	0	100 100
48	1q	97/105 (92%)	90 (93%)	6 (6%)	1 (1%)	12 17
48	2q	97/105 (92%)	86 (89%)	9 (9%)	2 (2%)	5 5
49	1r	66/88 (75%)	61 (92%)	4 (6%)	1 (2%)	8 10
49	2r	66/88 (75%)	59 (89%)	6 (9%)	1 (2%)	8 10
50	1s	81/93 (87%)	74 (91%)	7 (9%)	0	100 100
50	2s	81/93 (87%)	65 (80%)	14 (17%)	2 (2%)	4 4
51	1t	94/106 (89%)	84 (89%)	8 (8%)	2 (2%)	5 5
51	2t	94/106 (89%)	83 (88%)	10 (11%)	1 (1%)	11 15
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100 100
All	All	11368/12128 (94%)	10432 (92%)	817 (7%)	119 (1%)	12 17

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	43	LEU
19	1X	93	GLU
21	1Z	52	SER
26	14	47	GLN
26	14	62	ARG
33	1b	17	PHE
40	1i	54	ASP
42	1k	105	VAL
44	1m	67	GLU
44	1m	106	ASN
11	2P	36	LYS
11	2P	45	LEU
23	21	3	LYS
33	2b	17	PHE
33	2b	123	ALA
38	2g	55	GLY

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Mol	Chain	Res	Type
38	2g	80	VAL
44	2m	67	GLU
46	2o	88	ARG
50	2s	81	ARG
11	1P	38	GLN
15	1T	37	GLY
17	1V	79	VAL
23	11	3	LYS
26	14	49	PHE
33	1b	155	LEU
41	1j	79	ARG
42	1k	49	GLY
42	1k	77	MET
48	1q	68	ARG
49	1r	25	THR
6	2G	84	LYS
6	2G	126	ASP
14	2S	96	GLY
17	2V	79	VAL
21	2Z	93	ASP
33	2b	8	LYS
33	2b	20	GLU
33	2b	126	GLU
35	2d	164	ALA
36	2e	65	ASN
36	2e	85	GLY
38	2g	52	GLU
41	2j	75	ILE
42	2k	49	GLY
48	2q	68	ARG
49	2r	36	ASN
50	2s	12	ASP
26	14	45	GLY
40	1i	56	LEU
41	1j	78	ASN
46	1o	87	ILE
51	1t	47	GLY
51	1t	100	ILE
5	2F	130	ALA
6	2G	47	LYS
8	2I	10	GLU
14	2S	84	GLN

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Mol	Chain	Res	Type
26	24	49	PHE
33	2b	16	HIS
34	2c	91	LEU
36	2e	37	ARG
38	2g	4	ARG
42	2k	77	MET
43	2l	91	LYS
3	1D	262	ARG
4	1E	52	LEU
11	1P	29	LYS
15	1T	55	ASN
33	1b	22	LYS
41	1j	30	SER
4	2E	52	LEU
10	2O	5	GLN
14	2S	20	ARG
14	2S	111	GLU
33	2b	78	GLN
39	2h	22	GLU
40	2i	88	TYR
41	2j	78	ASN
44	2m	106	ASN
6	1G	181	ARG
17	1V	43	GLU
26	14	53	GLU
33	1b	124	SER
33	1b	126	GLU
33	1b	231	GLU
38	1g	54	THR
43	1l	105	TYR
46	1o	88	ARG
6	2G	43	LEU
11	2P	136	GLU
21	2Z	146	ILE
33	2b	9	GLU
34	2c	181	ASN
45	2n	3	ARG
48	2q	33	GLY
51	2t	47	GLY
7	1H	174	GLY
8	1I	10	GLU
20	1Y	103	GLY

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Mol	Chain	Res	Type
26	14	57	GLU
33	1b	8	LYS
33	1b	20	GLU
36	1e	69	VAL
8	2I	40	THR
26	24	47	GLN
41	2j	79	ARG
43	2l	105	TYR
21	2Z	147	GLY
35	1d	87	GLY
3	2D	125	ILE
36	2e	69	VAL
45	2n	14	PRO
39	1h	73	ASP
25	23	59	VAL
21	1Z	167	PRO
11	2P	44	GLY
33	1b	125	PRO

5.3.2 Protein sidechains (i)

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%)	207 (96%)	8 (4%)	30 45
3	2D	215/218 (99%)	200 (93%)	15 (7%)	14 19
4	1E	164/166 (99%)	155 (94%)	9 (6%)	19 29
4	2E	164/166 (99%)	155 (94%)	9 (6%)	19 29
5	1F	160/166 (96%)	142 (89%)	18 (11%)	5 6
5	2F	159/166 (96%)	144 (91%)	15 (9%)	8 10
6	1G	143/156 (92%)	128 (90%)	15 (10%)	6 8
6	2G	143/156 (92%)	127 (89%)	16 (11%)	6 6
7	1H	144/148 (97%)	132 (92%)	12 (8%)	10 14
7	2H	144/148 (97%)	128 (89%)	16 (11%)	6 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	1I	113/124 (91%)	94 (83%)	19 (17%)	2 2
8	2I	105/124 (85%)	91 (87%)	14 (13%)	4 4
9	1N	118/119 (99%)	108 (92%)	10 (8%)	10 13
9	2N	118/119 (99%)	106 (90%)	12 (10%)	7 8
10	1O	100/100 (100%)	95 (95%)	5 (5%)	22 33
10	2O	100/100 (100%)	97 (97%)	3 (3%)	36 53
11	1P	115/116 (99%)	105 (91%)	10 (9%)	9 13
11	2P	115/116 (99%)	106 (92%)	9 (8%)	11 16
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	39 58
12	2Q	111/111 (100%)	105 (95%)	6 (5%)	20 30
13	1R	101/101 (100%)	93 (92%)	8 (8%)	11 16
13	2R	101/101 (100%)	94 (93%)	7 (7%)	14 20
14	1S	86/88 (98%)	79 (92%)	7 (8%)	11 15
14	2S	85/88 (97%)	74 (87%)	11 (13%)	4 4
15	1T	115/127 (91%)	108 (94%)	7 (6%)	17 25
15	2T	113/127 (89%)	107 (95%)	6 (5%)	20 31
16	1U	93/94 (99%)	88 (95%)	5 (5%)	20 30
16	2U	93/94 (99%)	87 (94%)	6 (6%)	15 22
17	1V	80/82 (98%)	77 (96%)	3 (4%)	29 44
17	2V	80/82 (98%)	74 (92%)	6 (8%)	12 17
18	1W	90/92 (98%)	84 (93%)	6 (7%)	15 21
18	2W	90/92 (98%)	86 (96%)	4 (4%)	25 38
19	1X	77/78 (99%)	75 (97%)	2 (3%)	40 59
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28 43
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	18 27
20	2Y	85/91 (93%)	76 (89%)	9 (11%)	6 7
21	1Z	135/179 (75%)	126 (93%)	9 (7%)	15 21
21	2Z	137/179 (76%)	120 (88%)	17 (12%)	4 4
22	10	65/67 (97%)	65 (100%)	0	100 100
22	20	65/67 (97%)	63 (97%)	2 (3%)	35 53
23	11	80/83 (96%)	79 (99%)	1 (1%)	61 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	21	80/83 (96%)	77 (96%)	3 (4%)	29 44
24	12	65/67 (97%)	61 (94%)	4 (6%)	16 24
24	22	65/67 (97%)	59 (91%)	6 (9%)	8 10
25	13	51/52 (98%)	43 (84%)	8 (16%)	2 2
25	23	50/52 (96%)	48 (96%)	2 (4%)	28 42
26	14	59/63 (94%)	48 (81%)	11 (19%)	1 1
26	24	53/63 (84%)	47 (89%)	6 (11%)	5 6
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%)	49 (96%)	2 (4%)	28 43
28	26	50/52 (96%)	46 (92%)	4 (8%)	11 15
29	17	41/42 (98%)	37 (90%)	4 (10%)	7 9
29	27	41/42 (98%)	35 (85%)	6 (15%)	3 2
30	18	54/55 (98%)	53 (98%)	1 (2%)	50 69
30	28	54/55 (98%)	53 (98%)	1 (2%)	50 69
31	19	34/34 (100%)	33 (97%)	1 (3%)	37 55
31	29	34/34 (100%)	31 (91%)	3 (9%)	9 12
33	1b	192/220 (87%)	168 (88%)	24 (12%)	4 4
33	2b	187/220 (85%)	162 (87%)	25 (13%)	4 3
34	1c	142/188 (76%)	131 (92%)	11 (8%)	12 17
34	2c	140/188 (74%)	130 (93%)	10 (7%)	13 19
35	1d	169/181 (93%)	152 (90%)	17 (10%)	7 8
35	2d	173/181 (96%)	149 (86%)	24 (14%)	3 3
36	1e	113/123 (92%)	104 (92%)	9 (8%)	11 15
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8 9
37	1f	84/90 (93%)	78 (93%)	6 (7%)	13 19
37	2f	85/90 (94%)	81 (95%)	4 (5%)	23 36
38	1g	119/127 (94%)	103 (87%)	16 (13%)	4 3
38	2g	120/127 (94%)	109 (91%)	11 (9%)	8 10
39	1h	114/119 (96%)	108 (95%)	6 (5%)	20 31
39	2h	114/119 (96%)	104 (91%)	10 (9%)	9 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	1i	90/99 (91%)	76 (84%)	14 (16%)	2 2
40	2i	89/99 (90%)	76 (85%)	13 (15%)	3 2
41	1j	66/92 (72%)	55 (83%)	11 (17%)	2 2
41	2j	69/92 (75%)	54 (78%)	15 (22%)	1 1
42	1k	82/99 (83%)	73 (89%)	9 (11%)	6 6
42	2k	83/99 (84%)	76 (92%)	7 (8%)	10 14
43	1l	96/108 (89%)	94 (98%)	2 (2%)	47 66
43	2l	96/108 (89%)	88 (92%)	8 (8%)	10 14
44	1m	93/101 (92%)	81 (87%)	12 (13%)	4 4
44	2m	92/101 (91%)	83 (90%)	9 (10%)	7 9
45	1n	49/50 (98%)	46 (94%)	3 (6%)	17 25
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7 8
46	1o	78/80 (98%)	72 (92%)	6 (8%)	12 17
46	2o	78/80 (98%)	72 (92%)	6 (8%)	12 17
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7 8
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%)	87 (93%)	7 (7%)	13 17
49	1r	59/77 (77%)	57 (97%)	2 (3%)	32 48
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%)	59 (88%)	8 (12%)	5 5
51	1t	70/82 (85%)	65 (93%)	5 (7%)	13 19
51	2t	70/82 (85%)	65 (93%)	5 (7%)	13 19
52	1u	18/22 (82%)	18 (100%)	0	100 100
52	2u	18/22 (82%)	18 (100%)	0	100 100
All	All	9303/10064 (92%)	8522 (92%)	781 (8%)	10 14

All (781) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	142	VAL

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Mol	Chain	Res	Type
3	1D	155	LEU
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	273	ARG
3	1D	275	LYS
4	1E	9	VAL
4	1E	21	VAL
4	1E	38	THR
4	1E	41	LYS
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	28	ILE
5	1F	53	THR
5	1F	57	VAL
5	1F	70	THR
5	1F	74	ARG
5	1F	88	VAL
5	1F	95	ARG
5	1F	106	ARG
5	1F	127	GLU
5	1F	158	THR
5	1F	162	LEU
5	1F	168	ARG
5	1F	175	THR
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	3	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	28	VAL
6	1G	31	VAL
6	1G	35	GLU
6	1G	43	LEU
6	1G	49	ASP
6	1G	60	LEU

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Mol	Chain	Res	Type
6	1G	81	LYS
6	1G	82	LEU
6	1G	139	LEU
6	1G	140	ILE
6	1G	149	VAL
6	1G	159	VAL
7	1H	3	ARG
7	1H	7	LEU
7	1H	15	VAL
7	1H	33	LEU
7	1H	67	LEU
7	1H	92	ILE
7	1H	107	VAL
7	1H	116	GLU
7	1H	124	GLU
7	1H	129	THR
7	1H	141	VAL
7	1H	155	SER
8	1I	5	LEU
8	1I	10	GLU
8	1I	12	LEU
8	1I	20	ASP
8	1I	38	LEU
8	1I	41	GLU
8	1I	44	LEU
8	1I	47	LEU
8	1I	69	LYS
8	1I	72	LEU
8	1I	75	LEU
8	1I	76	THR
8	1I	87	LYS
8	1I	108	THR
8	1I	109	ILE
8	1I	125	GLU
8	1I	127	VAL
8	1I	140	LEU
8	1I	142	VAL
9	1N	1	MET
9	1N	9	VAL
9	1N	14	VAL
9	1N	28	THR
9	1N	48	MET

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Mol	Chain	Res	Type
9	1N	62	VAL
9	1N	65	LYS
9	1N	73	THR
9	1N	96	GLU
9	1N	131	GLN
10	1O	20	MET
10	1O	26	LYS
10	1O	28	SER
10	1O	92	GLU
10	1O	106	LEU
11	1P	40	SER
11	1P	45	LEU
11	1P	75	ILE
11	1P	95	VAL
11	1P	124	LYS
11	1P	126	VAL
11	1P	133	SER
11	1P	147	LEU
11	1P	148	LEU
11	1P	149	GLU
12	1Q	8	LYS
12	1Q	63	LYS
12	1Q	133	ARG
13	1R	6	SER
13	1R	36	THR
13	1R	67	LEU
13	1R	79	LEU
13	1R	99	LYS
13	1R	102	GLU
13	1R	111	LEU
13	1R	114	VAL
14	1S	8	GLU
14	1S	14	VAL
14	1S	25	ARG
14	1S	36	TYR
14	1S	46	VAL
14	1S	68	GLN
14	1S	69	VAL
15	1T	23	ARG
15	1T	28	VAL
15	1T	36	GLU
15	1T	49	VAL

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Mol	Chain	Res	Type
15	1T	59	THR
15	1T	67	SER
15	1T	128	GLU
16	1U	17	ILE
16	1U	59	ARG
16	1U	74	LEU
16	1U	84	LYS
16	1U	95	LEU
17	1V	61	VAL
17	1V	79	VAL
17	1V	85	LYS
18	1W	4	LYS
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	24	ILE
18	1W	96	ILE
19	1X	35	THR
19	1X	72	LYS
20	1Y	7	VAL
20	1Y	31	LEU
20	1Y	40	GLU
20	1Y	72	VAL
20	1Y	98	VAL
21	1Z	56	VAL
21	1Z	66	SER
21	1Z	100	VAL
21	1Z	128	VAL
21	1Z	132	ASN
21	1Z	139	VAL
21	1Z	140	ASP
21	1Z	153	SER
21	1Z	170	THR
23	11	46	LEU
24	12	19	VAL
24	12	25	VAL
24	12	40	SER
24	12	55	ARG
25	13	7	LYS
25	13	18	ASP
25	13	23	LEU
25	13	34	GLU

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Mol	Chain	Res	Type
25	13	35	ARG
25	13	54	VAL
25	13	55	ARG
25	13	60	GLU
26	14	15	ILE
26	14	22	ILE
26	14	23	GLU
26	14	49	PHE
26	14	50	VAL
26	14	52	THR
26	14	59	PHE
26	14	60	GLN
26	14	63	TYR
26	14	67	TYR
26	14	69	LYS
27	15	6	VAL
27	15	40	LYS
27	15	55	ARG
27	15	60	VAL
28	16	6	ARG
28	16	19	ARG
29	17	24	THR
29	17	41	ARG
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
31	19	4	ARG
33	1b	7	VAL
33	1b	12	GLU
33	1b	39	ILE
33	1b	45	GLN
33	1b	54	THR
33	1b	60	ASP
33	1b	64	ARG
33	1b	67	THR
33	1b	80	ILE
33	1b	90	MET
33	1b	108	ILE
33	1b	112	VAL
33	1b	127	ILE
33	1b	138	LEU
33	1b	142	LEU

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Mol	Chain	Res	Type
33	1b	146	GLN
33	1b	172	ILE
33	1b	185	ILE
33	1b	200	ILE
33	1b	208	ILE
33	1b	212	GLN
33	1b	215	LEU
33	1b	217	ARG
33	1b	233	SER
34	1c	3	ASN
34	1c	15	THR
34	1c	17	ASP
34	1c	26	LYS
34	1c	64	VAL
34	1c	89	GLU
34	1c	105	GLU
34	1c	175	LEU
34	1c	178	LEU
34	1c	195	VAL
34	1c	198	VAL
35	1d	19	LEU
35	1d	31	CYS
35	1d	85	LYS
35	1d	88	VAL
35	1d	108	LEU
35	1d	127	THR
35	1d	135	LEU
35	1d	144	ASP
35	1d	157	LEU
35	1d	158	ILE
35	1d	170	VAL
35	1d	175	SER
35	1d	177	ASP
35	1d	178	VAL
35	1d	179	GLU
35	1d	188	LEU
35	1d	194	LEU
36	1e	12	LEU
36	1e	20	GLN
36	1e	41	VAL
36	1e	51	VAL
36	1e	68	GLU

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Mol	Chain	Res	Type
36	1e	79	GLU
36	1e	82	VAL
36	1e	91	LEU
36	1e	151	LEU
37	1f	45	LEU
37	1f	55	ASP
37	1f	72	VAL
37	1f	75	LEU
37	1f	78	GLU
37	1f	81	ILE
38	1g	8	GLU
38	1g	9	VAL
38	1g	12	LEU
38	1g	16	LEU
38	1g	36	LYS
38	1g	50	ILE
38	1g	61	VAL
38	1g	63	LYS
38	1g	73	MET
38	1g	78	ARG
38	1g	89	MET
38	1g	104	LEU
38	1g	113	GLU
38	1g	115	ARG
38	1g	140	ASP
38	1g	156	TRP
39	1h	39	LEU
39	1h	51	VAL
39	1h	59	LEU
39	1h	83	ILE
39	1h	99	GLU
39	1h	112	LEU
40	1i	9	ARG
40	1i	23	ASN
40	1i	25	LYS
40	1i	50	LEU
40	1i	53	VAL
40	1i	64	THR
40	1i	74	ILE
40	1i	81	ILE
40	1i	83	ARG
40	1i	92	TYR

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Mol	Chain	Res	Type
40	1i	96	LEU
40	1i	97	LYS
40	1i	108	VAL
40	1i	128	ARG
41	1j	8	LEU
41	1j	15	THR
41	1j	35	SER
41	1j	38	ILE
41	1j	43	ARG
41	1j	46	ARG
41	1j	49	VAL
41	1j	81	THR
41	1j	92	THR
41	1j	98	ILE
41	1j	100	THR
42	1k	14	VAL
42	1k	31	THR
42	1k	48	ILE
42	1k	63	LEU
42	1k	81	ASP
42	1k	87	THR
42	1k	109	VAL
42	1k	114	VAL
42	1k	117	ASN
43	1l	18	VAL
43	1l	36	VAL
44	1m	4	ILE
44	1m	12	ASN
44	1m	15	VAL
44	1m	19	LEU
44	1m	29	ARG
44	1m	39	ILE
44	1m	49	THR
44	1m	70	LEU
44	1m	86	CYS
44	1m	106	ASN
44	1m	109	THR
44	1m	121	LYS
45	1n	4	LYS
45	1n	6	LEU
45	1n	18	VAL
46	1o	5	LYS

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Mol	Chain	Res	Type
46	1o	26	GLU
46	1o	39	LEU
46	1o	40	SER
46	1o	76	GLU
46	1o	88	ARG
47	1p	5	ARG
47	1p	21	VAL
47	1p	45	THR
47	1p	60	LEU
47	1p	61	SER
47	1p	62	VAL
47	1p	76	GLN
48	1q	9	VAL
48	1q	14	LYS
48	1q	31	LEU
48	1q	39	SER
48	1q	52	LYS
48	1q	53	LEU
48	1q	63	ARG
48	1q	65	ILE
48	1q	75	ARG
49	1r	26	LEU
49	1r	65	ILE
50	1s	4	SER
50	1s	28	LYS
50	1s	37	ARG
50	1s	44	MET
50	1s	48	THR
50	1s	67	VAL
51	1t	10	LEU
51	1t	19	SER
51	1t	24	LEU
51	1t	42	GLN
51	1t	80	ARG
3	2D	3	VAL
3	2D	32	SER
3	2D	126	GLN
3	2D	141	VAL
3	2D	142	VAL
3	2D	155	LEU
3	2D	162	SER
3	2D	173	VAL

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Mol	Chain	Res	Type
3	2D	183	ARG
3	2D	200	ASP
3	2D	204	ILE
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	275	LYS
4	2E	9	VAL
4	2E	21	VAL
4	2E	38	THR
4	2E	90	THR
4	2E	116	VAL
4	2E	134	ILE
4	2E	152	LYS
4	2E	181	LEU
4	2E	195	LEU
5	2F	17	ARG
5	2F	24	LEU
5	2F	28	ILE
5	2F	33	LEU
5	2F	74	ARG
5	2F	107	LYS
5	2F	108	LYS
5	2F	133	ASN
5	2F	137	LYS
5	2F	149	ASP
5	2F	158	THR
5	2F	186	ILE
5	2F	192	LEU
5	2F	196	LEU
5	2F	201	VAL
6	2G	3	LEU
6	2G	5	VAL
6	2G	7	LEU
6	2G	60	LEU
6	2G	88	ILE
6	2G	91	ARG
6	2G	124	SER
6	2G	137	GLU
6	2G	140	ILE
6	2G	145	THR
6	2G	149	VAL

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Mol	Chain	Res	Type
6	2G	150	ASP
6	2G	156	ASP
6	2G	157	ILE
6	2G	159	VAL
6	2G	170	ARG
7	2H	4	ILE
7	2H	7	LEU
7	2H	15	VAL
7	2H	23	ARG
7	2H	45	VAL
7	2H	50	VAL
7	2H	62	LYS
7	2H	84	SER
7	2H	89	ILE
7	2H	103	LEU
7	2H	114	VAL
7	2H	127	GLU
7	2H	129	THR
7	2H	130	ARG
7	2H	136	ILE
7	2H	141	VAL
8	2I	14	ASP
8	2I	15	VAL
8	2I	20	ASP
8	2I	38	LEU
8	2I	61	ARG
8	2I	68	LEU
8	2I	77	LEU
8	2I	85	GLU
8	2I	96	ASP
8	2I	116	LEU
8	2I	117	GLU
8	2I	125	GLU
8	2I	127	VAL
8	2I	133	HIS
9	2N	1	MET
9	2N	8	GLN
9	2N	9	VAL
9	2N	14	VAL
9	2N	28	THR
9	2N	38	HIS
9	2N	43	THR

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Mol	Chain	Res	Type
9	2N	48	MET
9	2N	59	LYS
9	2N	62	VAL
9	2N	68	GLU
9	2N	96	GLU
10	2O	1	MET
10	2O	52	VAL
10	2O	78	ARG
11	2P	7	ARG
11	2P	45	LEU
11	2P	65	ARG
11	2P	70	GLN
11	2P	95	VAL
11	2P	126	VAL
11	2P	133	SER
11	2P	136	GLU
11	2P	149	GLU
12	2Q	7	MET
12	2Q	12	GLN
12	2Q	25	ASP
12	2Q	56	ARG
12	2Q	106	VAL
12	2Q	110	THR
13	2R	36	THR
13	2R	67	LEU
13	2R	73	VAL
13	2R	79	LEU
13	2R	95	THR
13	2R	102	GLU
13	2R	111	LEU
14	2S	27	SER
14	2S	28	VAL
14	2S	44	LYS
14	2S	50	SER
14	2S	53	SER
14	2S	58	LEU
14	2S	63	THR
14	2S	80	LEU
14	2S	82	ILE
14	2S	83	LYS
14	2S	85	VAL
15	2T	18	ASP

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Mol	Chain	Res	Type
15	2T	28	VAL
15	2T	39	ARG
15	2T	63	VAL
15	2T	64	ARG
15	2T	96	ARG
16	2U	5	LYS
16	2U	33	ARG
16	2U	74	LEU
16	2U	77	SER
16	2U	95	LEU
16	2U	100	VAL
17	2V	7	THR
17	2V	39	LEU
17	2V	56	SER
17	2V	61	VAL
17	2V	76	LYS
17	2V	79	VAL
18	2W	11	ARG
18	2W	17	VAL
18	2W	60	ASN
18	2W	92	ARG
19	2X	45	THR
19	2X	81	VAL
19	2X	92	LEU
20	2Y	3	VAL
20	2Y	5	MET
20	2Y	28	LYS
20	2Y	30	VAL
20	2Y	67	LEU
20	2Y	72	VAL
20	2Y	98	VAL
20	2Y	99	CYS
20	2Y	106	LEU
21	2Z	5	LEU
21	2Z	18	LEU
21	2Z	32	HIS
21	2Z	42	VAL
21	2Z	66	SER
21	2Z	91	LEU
21	2Z	93	ASP
21	2Z	94	GLU
21	2Z	100	VAL

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Mol	Chain	Res	Type
21	2Z	121	HIS
21	2Z	137	ILE
21	2Z	150	LEU
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	161	VAL
21	2Z	171	ILE
21	2Z	174	VAL
22	20	10	THR
22	20	67	VAL
23	21	46	LEU
23	21	51	VAL
23	21	76	ARG
24	22	4	SER
24	22	30	ARG
24	22	34	GLU
24	22	59	ARG
24	22	66	GLU
24	22	70	GLN
25	23	54	VAL
25	23	59	VAL
26	24	5	ILE
26	24	14	ILE
26	24	34	GLU
26	24	35	VAL
26	24	59	PHE
26	24	67	TYR
27	25	6	VAL
27	25	58	LEU
28	26	20	ASN
28	26	34	LEU
28	26	48	VAL
28	26	52	VAL
29	27	1	MET
29	27	14	LYS
29	27	24	THR
29	27	41	ARG
29	27	43	THR
29	27	46	VAL
30	28	14	VAL
31	29	7	VAL
31	29	17	ILE

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Mol	Chain	Res	Type
31	29	33	LYS
33	2b	7	VAL
33	2b	16	HIS
33	2b	44	LEU
33	2b	47	THR
33	2b	49	GLU
33	2b	71	VAL
33	2b	76	GLN
33	2b	80	ILE
33	2b	94	ASN
33	2b	95	GLN
33	2b	96	ARG
33	2b	107	THR
33	2b	112	VAL
33	2b	115	LEU
33	2b	127	ILE
33	2b	130	ARG
33	2b	164	VAL
33	2b	185	ILE
33	2b	189	ASP
33	2b	191	ASP
33	2b	215	LEU
33	2b	220	ASP
33	2b	223	ILE
33	2b	229	VAL
33	2b	236	TYR
34	2c	46	GLU
34	2c	47	LEU
34	2c	49	SER
34	2c	70	VAL
34	2c	101	LEU
34	2c	105	GLU
34	2c	120	VAL
34	2c	125	GLU
34	2c	153	VAL
34	2c	182	ILE
35	2d	8	VAL
35	2d	17	VAL
35	2d	28	SER
35	2d	34	GLU
35	2d	47	ARG
35	2d	52	SER

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Mol	Chain	Res	Type
35	2d	53	ASP
35	2d	58	LEU
35	2d	59	ARG
35	2d	78	LEU
35	2d	86	LYS
35	2d	96	LEU
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	153	ARG
35	2d	155	LEU
35	2d	156	GLU
35	2d	162	LEU
35	2d	163	GLU
35	2d	169	LYS
35	2d	170	VAL
35	2d	178	VAL
35	2d	188	LEU
36	2e	5	ASP
36	2e	13	ILE
36	2e	20	GLN
36	2e	41	VAL
36	2e	51	VAL
36	2e	55	VAL
36	2e	72	GLN
36	2e	81	GLU
36	2e	90	VAL
36	2e	148	VAL
36	2e	151	LEU
37	2f	63	TYR
37	2f	69	GLU
37	2f	72	VAL
37	2f	81	ILE
38	2g	6	ARG
38	2g	9	VAL
38	2g	13	GLN
38	2g	15	ASP
38	2g	22	LEU
38	2g	23	VAL
38	2g	59	LEU
38	2g	79	ARG
38	2g	111	ARG

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Mol	Chain	Res	Type
38	2g	115	ARG
38	2g	146	GLU
39	2h	22	GLU
39	2h	25	ASP
39	2h	39	LEU
39	2h	45	ILE
39	2h	51	VAL
39	2h	52	ASP
39	2h	61	VAL
39	2h	97	VAL
39	2h	112	LEU
39	2h	127	LEU
40	2i	27	THR
40	2i	29	ASN
40	2i	38	GLN
40	2i	50	LEU
40	2i	65	VAL
40	2i	66	ARG
40	2i	89	ASN
40	2i	99	LEU
40	2i	108	VAL
40	2i	109	VAL
40	2i	113	LYS
40	2i	125	TYR
40	2i	128	ARG
41	2j	6	ILE
41	2j	8	LEU
41	2j	21	GLN
41	2j	29	ARG
41	2j	38	ILE
41	2j	55	LYS
41	2j	61	GLU
41	2j	65	LEU
41	2j	66	ARG
41	2j	67	THR
41	2j	71	LEU
41	2j	73	ASP
41	2j	96	ILE
41	2j	97	GLU
41	2j	100	THR
42	2k	41	THR
42	2k	48	ILE

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Mol	Chain	Res	Type
42	2k	105	VAL
42	2k	107	SER
42	2k	109	VAL
42	2k	112	THR
42	2k	114	VAL
43	2l	18	VAL
43	2l	33	ARG
43	2l	34	ARG
43	2l	36	VAL
43	2l	40	VAL
43	2l	81	SER
43	2l	86	ARG
43	2l	116	SER
44	2m	4	ILE
44	2m	62	ASN
44	2m	69	GLU
44	2m	92	HIS
44	2m	93	ARG
44	2m	98	VAL
44	2m	103	THR
44	2m	106	ASN
44	2m	114	ARG
45	2n	4	LYS
45	2n	13	THR
45	2n	15	LYS
45	2n	18	VAL
45	2n	33	VAL
46	2o	5	LYS
46	2o	26	GLU
46	2o	39	LEU
46	2o	60	VAL
46	2o	87	ILE
46	2o	88	ARG
47	2p	2	VAL
47	2p	20	VAL
47	2p	21	VAL
47	2p	54	GLU
47	2p	67	THR
47	2p	73	LEU
47	2p	74	LEU
48	2q	5	VAL
48	2q	14	LYS

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Mol	Chain	Res	Type
48	2q	31	LEU
48	2q	52	LYS
48	2q	63	ARG
48	2q	79	SER
48	2q	99	SER
49	2r	25	THR
49	2r	26	LEU
49	2r	65	ILE
49	2r	82	THR
49	2r	84	LYS
50	2s	27	GLU
50	2s	33	THR
50	2s	37	ARG
50	2s	45	VAL
50	2s	49	ILE
50	2s	57	HIS
50	2s	63	THR
50	2s	65	ASN
51	2t	9	ASN
51	2t	41	ILE
51	2t	45	GLN
51	2t	46	GLU
51	2t	89	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (133) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	48	GLN
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
7	1H	74	ASN
9	1N	94	HIS
12	1Q	12	GLN
13	1R	31	HIS
13	1R	71	GLN
14	1S	38	GLN
16	1U	94	ASN
18	1W	111	HIS
19	1X	31	HIS
19	1X	82	GLN

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Mol	Chain	Res	Type
20	1Y	6	HIS
21	1Z	55	HIS
21	1Z	151	HIS
22	10	17	GLN
22	10	70	GLN
24	12	9	GLN
26	14	60	GLN
28	16	20	ASN
30	18	35	GLN
33	1b	94	ASN
33	1b	95	GLN
33	1b	212	GLN
34	1c	6	HIS
34	1c	69	HIS
34	1c	104	GLN
35	1d	43	HIS
35	1d	77	ASN
35	1d	116	GLN
35	1d	123	HIS
35	1d	160	GLN
36	1e	78	HIS
36	1e	141	GLN
37	1f	18	GLN
37	1f	73	ASN
37	1f	100	ASN
38	1g	28	ASN
38	1g	56	GLN
38	1g	110	GLN
39	1h	15	ASN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	87	GLN
40	1i	124	GLN
41	1j	56	HIS
41	1j	69	ASN
42	1k	78	GLN
42	1k	116	HIS
43	1l	99	HIS
44	1m	77	ASN
44	1m	106	ASN
46	1o	13	GLN

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Mol	Chain	Res	Type
46	1o	46	HIS
47	1p	16	HIS
49	1r	63	GLN
50	1s	23	ASN
50	1s	47	HIS
50	1s	69	HIS
50	1s	83	HIS
51	1t	90	GLN
3	2D	166	GLN
4	2E	48	GLN
5	2F	69	HIS
6	2G	26	GLN
6	2G	79	ASN
6	2G	132	ASN
8	2I	133	HIS
9	2N	94	HIS
11	2P	27	HIS
11	2P	35	HIS
11	2P	70	GLN
12	2Q	12	GLN
13	2R	50	HIS
14	2S	38	GLN
15	2T	58	ASN
15	2T	84	GLN
16	2U	81	HIS
16	2U	94	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	32	HIS
21	2Z	73	GLN
21	2Z	75	ASN
22	20	17	GLN
22	20	50	ASN
24	22	56	GLN
26	24	40	HIS
28	26	20	ASN
30	28	35	GLN
33	2b	76	GLN
33	2b	110	GLN
33	2b	135	GLN
33	2b	140	HIS
34	2c	110	ASN

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Mol	Chain	Res	Type
34	2c	123	GLN
34	2c	162	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	123	HIS
35	2d	125	HIS
37	2f	73	ASN
37	2f	94	GLN
38	2g	28	ASN
38	2g	68	ASN
38	2g	86	GLN
39	2h	15	ASN
40	2i	3	GLN
40	2i	23	ASN
40	2i	58	HIS
40	2i	89	ASN
41	2j	13	HIS
41	2j	21	GLN
41	2j	33	GLN
42	2k	22	HIS
42	2k	26	ASN
42	2k	116	HIS
42	2k	117	ASN
43	2l	49	ASN
43	2l	75	HIS
43	2l	99	HIS
44	2m	40	ASN
44	2m	77	ASN
46	2o	13	GLN
49	2r	63	GLN
50	2s	57	HIS
50	2s	69	HIS
50	2s	83	HIS
51	2t	75	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	421 (14%)	26 (0%)
1	2A	2791/2915 (95%)	461 (16%)	24 (0%)
2	1B	119/121 (98%)	6 (5%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2B	118/121 (97%)	28 (23%)	0
32	1a	1497/1521 (98%)	240 (16%)	0
32	2a	1501/1521 (98%)	277 (18%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	70/74 (94%)	24 (34%)	0
54	2w	68/74 (91%)	29 (42%)	0
55	1x	75/77 (97%)	7 (9%)	0
55	2x	75/77 (97%)	9 (12%)	0
56	1y	71/74 (95%)	27 (38%)	0
56	2y	71/74 (95%)	32 (45%)	0
All	All	9344/9612 (97%)	1567 (16%)	50 (0%)

All (1567) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	63	U
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	78	A
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	154	G
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	266	G

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Mol	Chain	Res	Type
1	1A	269	U
1	1A	271(C)	C
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	272(B)	G
1	1A	272(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	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	418	G
1	1A	421	U
1	1A	428	A
1	1A	443	A
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	494	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G

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Mol	Chain	Res	Type
1	1A	551	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	584	C
1	1A	586	A
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(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	774	A
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	880	G
1	1A	882	G

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Mol	Chain	Res	Type
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	890	A
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G
1	1A	1066	U
1	1A	1068	G
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C

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Mol	Chain	Res	Type
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1080	C
1	1A	1081	U
1	1A	1083	U
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1097	U
1	1A	1099	G
1	1A	1101	U
1	1A	1104	C
1	1A	1108	U
1	1A	1110	G
1	1A	1112	G
1	1A	1116	C
1	1A	1135	C
1	1A	1136	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1241	A
1	1A	1244	G
1	1A	1253	A
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	1321	A
1	1A	1345	C

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Mol	Chain	Res	Type
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1384	A
1	1A	1385	G
1	1A	1395	A
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	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1540	U
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	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1648	C
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	1739	U

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Mol	Chain	Res	Type
1	1A	1746	G
1	1A	1756	G
1	1A	1762	A
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	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A
1	1A	1929	G
1	1A	1930	G
1	1A	1931	U
1	1A	1934	C
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2033	A
1	1A	2039	C

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Mol	Chain	Res	Type
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	2097	C
1	1A	2102	U
1	1A	2107	C
1	1A	2108	C
1	1A	2110	G
1	1A	2112	G
1	1A	2113	U
1	1A	2114	A
1	1A	2120	G
1	1A	2121	G
1	1A	2122	U
1	1A	2123	G
1	1A	2126	A
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2145	C
1	1A	2146	C
1	1A	2149	G
1	1A	2150	U
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	2160	G

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Mol	Chain	Res	Type
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	2171	A
1	1A	2172	U
1	1A	2174	C
1	1A	2177	C
1	1A	2179	C
1	1A	2180	U
1	1A	2182	G
1	1A	2184	G
1	1A	2189	U
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2278	A
1	1A	2280	G
1	1A	2283	C
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2312	U
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
1	1A	2400	G

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Mol	Chain	Res	Type
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	2441	C
1	1A	2448	A
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	2535	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2574	G
1	1A	2585	U
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2689	U
1	1A	2691	C
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A

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Mol	Chain	Res	Type
1	1A	2752	C
1	1A	2765	A
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	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	15	A
2	1B	56	G
2	1B	65	C
2	1B	73	A
2	1B	84	C
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	52	G
32	1a	54	C
32	1a	61	G
32	1a	65	U
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	111	G
32	1a	116	A
32	1a	120	A
32	1a	121	C

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Mol	Chain	Res	Type
32	1a	131	C
32	1a	144	G
32	1a	145	G
32	1a	147	G
32	1a	153	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(G)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	200	G
32	1a	203	U
32	1a	204	U
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	341	C
32	1a	342	C
32	1a	344	A
32	1a	345	C
32	1a	347	G
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	383	A
32	1a	384	G
32	1a	392	G

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Mol	Chain	Res	Type
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	441	A
32	1a	442	C
32	1a	452	A
32	1a	457	C
32	1a	461	A
32	1a	471	G
32	1a	483	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	527	G7M
32	1a	531	U
32	1a	532	A
32	1a	533	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	607	A
32	1a	627	G
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	673	G

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Mol	Chain	Res	Type
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	703	G
32	1a	722	A
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	753	A
32	1a	755	G
32	1a	766	A
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	851	G
32	1a	870	U
32	1a	913	A
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	966	M2G
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

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Mol	Chain	Res	Type
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1037	C
32	1a	1043	C
32	1a	1044	A
32	1a	1046	A
32	1a	1053	G
32	1a	1068	G
32	1a	1081	G
32	1a	1086	U
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1111	A
32	1a	1124	G
32	1a	1125	U
32	1a	1127	G
32	1a	1132	C
32	1a	1133	G
32	1a	1134	G
32	1a	1137	C
32	1a	1139	G
32	1a	1146	A

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Mol	Chain	Res	Type
32	1a	1152	A
32	1a	1159	U
32	1a	1183	A
32	1a	1184	G
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1213	A
32	1a	1214	C
32	1a	1227	A
32	1a	1238	A
32	1a	1250	A
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
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
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1312	G
32	1a	1323	G
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1371	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

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Mol	Chain	Res	Type
32	1a	1464	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1519	MA6
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	7	G
54	1w	8	4SU
54	1w	14	A
54	1w	18	G
54	1w	19	U
54	1w	21	A
54	1w	22	G
54	1w	23	A
54	1w	24	A
54	1w	26	G
54	1w	45	U
54	1w	46	A
54	1w	48	C
54	1w	49	G
54	1w	51	G
54	1w	56	C
54	1w	59	U
54	1w	62	C
54	1w	68	C
54	1w	70	C
54	1w	71	G
54	1w	74	C
55	1x	2	G
55	1x	9	G
55	1x	18	G
55	1x	19	G

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Mol	Chain	Res	Type
55	1x	47	U
55	1x	61	C
55	1x	69	C
56	1y	4	G
56	1y	5	G
56	1y	9	A
56	1y	13	C
56	1y	14	A
56	1y	18	G
56	1y	19	U
56	1y	21	A
56	1y	22	G
56	1y	25	C
56	1y	29	A
56	1y	33	U
56	1y	35	C
56	1y	40	C
56	1y	41	U
56	1y	44	A
56	1y	45	U
56	1y	46	A
56	1y	48	C
56	1y	49	G
56	1y	50	A
56	1y	56	C
56	1y	58	A
56	1y	59	U
56	1y	61	C
56	1y	65	U
56	1y	70	C
1	2A	8	A
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	36	G
1	2A	45	C
1	2A	49	A
1	2A	51	G
1	2A	61	G
1	2A	64	A
1	2A	71	A

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Mol	Chain	Res	Type
1	2A	74	A
1	2A	75	G
1	2A	83	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	250	G
1	2A	264	C
1	2A	266	G
1	2A	271(A)	A
1	2A	271(J)	C
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	317	G
1	2A	327	G

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Mol	Chain	Res	Type
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	358	U
1	2A	363(B)	G
1	2A	386	G
1	2A	396	G
1	2A	399	G
1	2A	403	U
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	422	A
1	2A	443	A
1	2A	444	C
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	494	G
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	529	A
1	2A	531	C
1	2A	532	A
1	2A	542	C
1	2A	545	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	605	C
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	620	G

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Mol	Chain	Res	Type
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	726	G
1	2A	730	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
1	2A	827	U
1	2A	828	U
1	2A	832	G
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	874	G
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	882	G
1	2A	883	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	899	A

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Mol	Chain	Res	Type
1	2A	900	A
1	2A	901	A
1	2A	907	U
1	2A	910	A
1	2A	917	A
1	2A	924	C
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	961	C
1	2A	963	U
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	999	U
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1043	C
1	2A	1114	G
1	2A	1116	C
1	2A	1128	A
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1169	G
1	2A	1171	G

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Mol	Chain	Res	Type
1	2A	1210	A
1	2A	1211	U
1	2A	1218	C
1	2A	1220	A
1	2A	1230	C
1	2A	1237	A
1	2A	1244	G
1	2A	1248	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1306	C
1	2A	1314	C
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1373	A
1	2A	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1420	U
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	1460	A
1	2A	1461	G
1	2A	1463	C
1	2A	1467	C
1	2A	1471	A

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Mol	Chain	Res	Type
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1542	A
1	2A	1543	C
1	2A	1545	A
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
1	2A	1610	A
1	2A	1647	G
1	2A	1648	C
1	2A	1653	G
1	2A	1654	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A

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Mol	Chain	Res	Type
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	1847	A
1	2A	1848	A
1	2A	1861	G
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1895	C
1	2A	1900	A
1	2A	1906	G
1	2A	1910	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1931	U
1	2A	1936	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2036	C
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G

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Mol	Chain	Res	Type
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2099	U
1	2A	2109	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	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	2139	C
1	2A	2145	C
1	2A	2146	C
1	2A	2149	G
1	2A	2150	U
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	2171	A
1	2A	2172	U
1	2A	2176	A
1	2A	2178	C

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Mol	Chain	Res	Type
1	2A	2183	C
1	2A	2185	C
1	2A	2186	G
1	2A	2188	C
1	2A	2189	U
1	2A	2190	G
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	2239	G
1	2A	2269	A
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2294	C
1	2A	2298	A
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2316	C
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2396	G
1	2A	2402	C
1	2A	2403	C
1	2A	2406	U
1	2A	2407	G

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Mol	Chain	Res	Type
1	2A	2422	A
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2465	C
1	2A	2468	G
1	2A	2469	A
1	2A	2476	A
1	2A	2484	G
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2549	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2569	G
1	2A	2573	C
1	2A	2578	G
1	2A	2585	U
1	2A	2602	A
1	2A	2609	U
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	2669	G
1	2A	2689	U
1	2A	2690	C

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Mol	Chain	Res	Type
1	2A	2691	C
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2758	A
1	2A	2760	C
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	2807	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2872	G
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	5	C
2	2B	8	U
2	2B	13	A
2	2B	17	C
2	2B	19	G
2	2B	20	C
2	2B	25	A
2	2B	30	C
2	2B	33	G
2	2B	34	U
2	2B	41	U
2	2B	42	C

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Mol	Chain	Res	Type
2	2B	45	A
2	2B	53	A
2	2B	56	G
2	2B	63	G
2	2B	67	G
2	2B	69	G
2	2B	73	A
2	2B	75	G
2	2B	85	G
2	2B	89	G
2	2B	108	U
2	2B	110	G
2	2B	111	G
2	2B	119	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	66	G
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	127	G
32	2a	131	C
32	2a	142	G
32	2a	143	A
32	2a	144	G
32	2a	163	C
32	2a	182	U
32	2a	189(D)	C
32	2a	189(F)	U
32	2a	189(J)	G
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U

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Mol	Chain	Res	Type
32	2a	204	U
32	2a	216	G
32	2a	217	C
32	2a	220	G
32	2a	247	G
32	2a	250	A
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	281	G
32	2a	289	G
32	2a	306	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	355	C
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	414	A
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	458	C
32	2a	470	C
32	2a	471	G

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Mol	Chain	Res	Type
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	517	G
32	2a	518	C
32	2a	521	G
32	2a	531	U
32	2a	532	A
32	2a	547	A
32	2a	559	A
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	575	G
32	2a	576	G
32	2a	596	C
32	2a	597	G
32	2a	630	G
32	2a	653	A
32	2a	665	A
32	2a	666	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	720	C
32	2a	723	U
32	2a	731	G
32	2a	733	A
32	2a	749	C
32	2a	755	G
32	2a	764	C
32	2a	773	G
32	2a	774	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	815	A

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Mol	Chain	Res	Type
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	836	G
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	857	C
32	2a	859	A
32	2a	880	C
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	933	G
32	2a	934	C
32	2a	935	A
32	2a	942	G
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	963	G
32	2a	966	M2G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	984	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	995	C
32	2a	997	U
32	2a	998	G
32	2a	999	C
32	2a	1001	A
32	2a	1004	A
32	2a	1005	A

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Mol	Chain	Res	Type
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1035	A
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1045	C
32	2a	1051	C
32	2a	1053	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1079	G
32	2a	1081	G
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1097	C
32	2a	1101	A
32	2a	1105	A
32	2a	1108	G
32	2a	1109	C
32	2a	1113	C
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C

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Mol	Chain	Res	Type
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	1146	A
32	2a	1147	C
32	2a	1149	C
32	2a	1152	A
32	2a	1154	G
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1172	C
32	2a	1182	G
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1211	U
32	2a	1213	A
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1255	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1264	C
32	2a	1267	C
32	2a	1268	A
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1283	G

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Mol	Chain	Res	Type
32	2a	1287	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1306	A
32	2a	1323	G
32	2a	1339	A
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1358	U
32	2a	1359	C
32	2a	1363	C
32	2a	1364	U
32	2a	1368	G
32	2a	1379	G
32	2a	1398	A
32	2a	1402	4OC
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	1457	G
32	2a	1487	G
32	2a	1492	A
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1519	MA6
32	2a	1520	G
32	2a	1523	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

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Mol	Chain	Res	Type
53	2v	15	A
54	2w	2	C
54	2w	5	G
54	2w	8	4SU
54	2w	9	A
54	2w	10	G
54	2w	11	U
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	27	A
54	2w	46	A
54	2w	49	G
54	2w	56	C
54	2w	61	C
54	2w	62	C
54	2w	64	U
54	2w	68	C
54	2w	69	C
54	2w	70	C
54	2w	71	G
54	2w	72	C
54	2w	73	U
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	21	A
55	2x	22	G
55	2x	47	U
55	2x	52	G
55	2x	63	G
55	2x	69	C
56	2y	5	G
56	2y	7	G
56	2y	8	4SU

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Mol	Chain	Res	Type
56	2y	9	A
56	2y	15	A
56	2y	18	G
56	2y	19	U
56	2y	21	A
56	2y	22	G
56	2y	25	C
56	2y	26	G
56	2y	27	A
56	2y	29	A
56	2y	33	U
56	2y	34	C
56	2y	37	A
56	2y	40	C
56	2y	41	U
56	2y	45	U
56	2y	46	A
56	2y	48	C
56	2y	49	G
56	2y	50	A
56	2y	52	G
56	2y	53	G
56	2y	58	A
56	2y	59	U
56	2y	61	C
56	2y	62	C
56	2y	69	C
56	2y	70	C
56	2y	73	U

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
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	827	U
1	1A	974	G

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Mol	Chain	Res	Type
1	1A	1067	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	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	774	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2156	G
1	2A	2406	U
1	2A	2689	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	1A	2605	57,1	18,21,22	1.41	3 (16%)	21,30,33	1.95	5 (23%)
1	OMG	1A	2251	57,55,1	23,26,27	1.31	3 (13%)	32,38,41	1.97	6 (18%)
54	L3X	1w	76	1,54	24,28,29	1.42	3 (12%)	27,40,43	2.10	9 (33%)
1	5MU	1A	1915	1	19,22,23	1.38	5 (26%)	27,32,35	2.09	5 (18%)
32	MA6	2a	1518	32	23,26,27	0.42	0	33,38,41	2.04	9 (27%)
32	G7M	1a	527	57,32	23,26,27	1.47	4 (17%)	34,39,42	1.68	5 (14%)
56	4SU	2y	8	56	18,21,22	1.79	5 (27%)	25,30,33	1.93	5 (20%)
1	OMU	1A	2552	1	19,22,23	1.21	2 (10%)	25,31,34	1.93	5 (20%)
55	31H	1x	76	55,57	31,34,35	1.18	3 (9%)	35,47,50	2.09	11 (31%)
55	4SU	1x	8	55	18,21,22	2.14	6 (33%)	25,30,33	1.65	7 (28%)
32	MA6	1a	1519	32	23,26,27	0.46	0	33,38,41	2.09	9 (27%)
1	5MU	2A	1915	1	19,22,23	1.41	5 (26%)	27,32,35	2.15	6 (22%)
55	5MC	2x	32	55	19,22,23	1.74	3 (15%)	26,32,35	1.28	3 (11%)
1	5MU	1A	1939	57,1	19,22,23	1.41	5 (26%)	27,32,35	2.30	6 (22%)
55	5MU	2x	54	55	19,22,23	1.38	4 (21%)	27,32,35	2.07	6 (22%)
43	0TD	1l	92	43	8,9,10	4.56	1 (12%)	6,11,13	2.89	2 (33%)
1	5MC	1A	1942	1	19,22,23	1.68	3 (15%)	26,32,35	1.15	2 (7%)
1	PSU	1A	1917	1	18,21,22	1.34	2 (11%)	21,30,33	2.01	4 (19%)
54	L3X	2w	76	1,54	24,28,29	1.40	3 (12%)	27,40,43	2.14	9 (33%)
54	5MU	1w	54	54	19,22,23	1.38	4 (21%)	27,32,35	1.90	6 (22%)
1	2MA	2A	2503	57,1	22,25,26	1.47	4 (18%)	32,37,40	2.30	8 (25%)
32	UR3	2a	1498	32	19,22,23	1.01	1 (5%)	26,32,35	1.76	3 (11%)
54	4SU	2w	8	54	18,21,22	1.77	4 (22%)	25,30,33	3.15	6 (24%)
55	5MU	1x	54	55	19,22,23	1.45	5 (26%)	27,32,35	1.99	5 (18%)
1	5MC	2A	1942	1	19,22,23	1.64	2 (10%)	26,32,35	1.16	3 (11%)
32	5MC	2a	1400	32	19,22,23	1.67	3 (15%)	26,32,35	1.18	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	2MA	1A	2503	57,1	22,25,26	1.42	5 (22%)	32,37,40	2.30	10 (31%)
54	PSU	2w	55	57,54	18,21,22	1.36	2 (11%)	21,30,33	2.03	4 (19%)
32	5MC	2a	1404	32	19,22,23	1.62	3 (15%)	26,32,35	1.23	3 (11%)
56	5MU	1y	54	56	19,22,23	1.42	5 (26%)	27,32,35	1.96	7 (25%)
1	PSU	2A	2605	1	18,21,22	1.29	2 (11%)	21,30,33	2.06	4 (19%)
56	5MU	2y	54	56	19,22,23	1.48	4 (21%)	27,32,35	1.91	8 (29%)
32	G7M	2a	527	57,32	23,26,27	1.49	3 (13%)	34,39,42	1.67	5 (14%)
32	MA6	1a	1518	32	23,26,27	0.42	0	33,38,41	2.00	9 (27%)
1	PSU	2A	1917	1	18,21,22	1.39	2 (11%)	21,30,33	2.01	4 (19%)
55	PSU	2x	55	55	18,21,22	1.38	2 (11%)	21,30,33	2.08	4 (19%)
32	2MG	2a	1207	32	23,26,27	1.27	3 (13%)	33,38,41	2.11	6 (18%)
55	31H	2x	76	55,57	31,34,35	1.20	3 (9%)	35,47,50	2.11	13 (37%)
56	4SU	1y	8	56	18,21,22	1.88	6 (33%)	25,30,33	1.69	5 (20%)
1	5MC	1A	1962	57,1	19,22,23	1.74	3 (15%)	26,32,35	1.17	3 (11%)
1	OMU	2A	2552	1	19,22,23	1.26	2 (10%)	25,31,34	1.76	6 (24%)
32	M2G	2a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.90	6 (18%)
1	PSU	1A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	2.12	4 (19%)
56	PSU	1y	55	56	18,21,22	1.40	2 (11%)	21,30,33	2.12	4 (19%)
32	5MC	2a	1407	32	19,22,23	1.67	3 (15%)	26,32,35	1.24	3 (11%)
54	4SU	1w	8	54	18,21,22	1.90	5 (27%)	25,30,33	1.95	5 (20%)
55	5MC	1x	32	55	19,22,23	1.48	3 (15%)	26,32,35	1.24	2 (7%)
1	5MU	2A	1939	1	19,22,23	1.34	5 (26%)	27,32,35	2.37	6 (22%)
43	0TD	2l	92	43	8,9,10	4.63	2 (25%)	6,11,13	4.99	2 (33%)
32	5MC	1a	1400	32	19,22,23	1.70	3 (15%)	26,32,35	1.17	4 (15%)
32	PSU	2a	516	32	18,21,22	1.36	2 (11%)	21,30,33	1.95	3 (14%)
54	PSU	1w	55	57,54	18,21,22	1.40	2 (11%)	21,30,33	2.04	3 (14%)
32	UR3	1a	1498	32	19,22,23	1.02	1 (5%)	26,32,35	1.83	4 (15%)
32	MA6	2a	1519	32	23,26,27	0.44	0	33,38,41	2.09	10 (30%)
32	4OC	1a	1402	32	20,23,24	0.76	0	25,32,35	0.96	1 (4%)
55	PSU	1x	55	55	18,21,22	1.37	2 (11%)	21,30,33	2.03	3 (14%)
32	5MC	1a	967	32	19,22,23	1.54	3 (15%)	26,32,35	1.07	2 (7%)
54	5MU	2w	54	54	19,22,23	1.38	4 (21%)	27,32,35	1.73	6 (22%)
32	PSU	1a	516	32	18,21,22	1.44	2 (11%)	21,30,33	2.03	3 (14%)
32	5MC	1a	1407	32	19,22,23	1.79	3 (15%)	26,32,35	1.18	4 (15%)
32	4OC	2a	1402	57,32	20,23,24	0.75	0	25,32,35	1.09	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
56	PSU	2y	55	56	18,21,22	1.42	2 (11%)	21,30,33	1.98	3 (14%)
1	OMC	1A	1920	1	19,22,23	0.77	0	25,31,34	0.93	1 (4%)
1	5MC	2A	1962	57,1	19,22,23	1.65	3 (15%)	26,32,35	1.14	3 (11%)
55	4SU	2x	8	55	18,21,22	2.00	7 (38%)	25,30,33	1.32	3 (12%)
1	PSU	2A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	1.93	3 (14%)
32	5MC	2a	967	32	19,22,23	1.64	2 (10%)	26,32,35	1.07	2 (7%)
1	OMG	2A	2251	55,1	23,26,27	1.23	3 (13%)	32,38,41	1.97	7 (21%)
32	5MC	1a	1404	32	19,22,23	1.65	3 (15%)	26,32,35	1.10	2 (7%)
1	OMC	2A	1920	1	19,22,23	0.78	0	25,31,34	0.96	1 (4%)
32	2MG	1a	1207	32	23,26,27	1.24	3 (13%)	33,38,41	2.25	10 (30%)
32	M2G	1a	966	32	24,27,28	1.30	4 (16%)	33,40,43	1.87	6 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	57,55,1	-	0/9/27/28	0/3/3/3
54	L3X	1w	76	1,54	-	1/13/31/32	0/3/3/3
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	G7M	1a	527	57,32	-	3/7/25/26	0/3/3/3
56	4SU	2y	8	56	-	3/7/25/26	0/2/2/2
1	OMU	1A	2552	1	-	0/9/27/28	0/2/2/2
55	31H	1x	76	55,57	-	5/22/40/41	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	57,1	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
54	L3X	2w	76	1,54	-	2/13/31/32	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	57,1	-	1/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	57,1	-	1/7/25/26	0/3/3/3
54	PSU	2w	55	57,54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
56	5MU	2y	54	56	-	3/7/25/26	0/2/2/2
32	G7M	2a	527	57,32	-	2/7/25/26	0/3/3/3
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	1/9/27/28	0/3/3/3
55	31H	2x	76	55,57	-	4/22/40/41	0/3/3/3
56	4SU	1y	8	56	-	1/7/25/26	0/2/2/2
1	5MC	1A	1962	57,1	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1	-	0/9/27/28	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	57,54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
55	PSU	1x	55	55	-	2/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	57,32	-	3/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PSU	2y	55	56	-	2/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
1	5MC	2A	1962	57,1	-	2/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,1	-	0/9/27/28	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	2MG	1a	1207	32	-	2/9/27/28	0/3/3/3
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3

All (205) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.51	1.69	1.82
43	1l	92	0TD	CB-SB	-12.39	1.69	1.82
32	1a	1407	5MC	C5-C4	6.88	1.49	1.44
1	1A	1962	5MC	C5-C4	6.37	1.48	1.44
55	2x	32	5MC	C5-C4	6.34	1.48	1.44
32	1a	1400	5MC	C5-C4	6.29	1.48	1.44
1	1A	1942	5MC	C5-C4	6.17	1.48	1.44
32	2a	1400	5MC	C5-C4	6.07	1.48	1.44
32	2a	967	5MC	C5-C4	6.02	1.48	1.44
1	2A	1962	5MC	C5-C4	5.94	1.48	1.44
32	2a	1407	5MC	C5-C4	5.93	1.48	1.44
32	1a	1404	5MC	C5-C4	5.93	1.48	1.44
1	2A	1942	5MC	C5-C4	5.84	1.48	1.44
32	2a	1404	5MC	C5-C4	5.77	1.48	1.44
32	1a	967	5MC	C5-C4	5.37	1.48	1.44
55	1x	32	5MC	C5-C4	5.11	1.48	1.44
55	1x	8	4SU	C4-N3	-4.96	1.32	1.37
54	1w	8	4SU	C4-S4	-4.95	1.59	1.68
54	2w	8	4SU	C4-S4	-4.92	1.60	1.68
56	2y	8	4SU	C4-S4	-4.78	1.60	1.68
56	1y	8	4SU	C4-S4	-4.61	1.60	1.68
32	2a	527	G7M	C5-N7	-4.49	1.34	1.39
55	2x	8	4SU	C4-S4	-4.44	1.60	1.68
55	2x	8	4SU	C4-N3	-4.41	1.33	1.37
1	2A	2503	2MA	C5-C4	4.36	1.46	1.39
55	1x	8	4SU	C4-S4	-4.35	1.61	1.68
32	1a	527	G7M	C5-N7	-4.34	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2503	2MA	C5-C4	4.20	1.46	1.39
56	2y	55	PSU	C6-C5	4.03	1.39	1.35
54	2w	76	L3X	C5-N7	-3.97	1.31	1.39
54	1w	76	L3X	C5-N7	-3.97	1.31	1.39
56	1y	55	PSU	C6-C5	3.96	1.39	1.35
55	2x	76	31H	C5-N7	-3.93	1.31	1.39
55	1x	76	31H	C5-N7	-3.91	1.31	1.39
54	1w	55	PSU	C6-C5	3.84	1.39	1.35
1	2A	1917	PSU	C6-C5	3.82	1.39	1.35
55	1x	8	4SU	C2-N3	-3.77	1.31	1.38
54	2w	55	PSU	C6-C5	3.75	1.39	1.35
56	1y	8	4SU	C4-N3	-3.73	1.33	1.37
32	1a	516	PSU	C6-C5	3.70	1.39	1.35
32	2a	516	PSU	C6-C5	3.65	1.39	1.35
1	1A	1917	PSU	C6-C5	3.61	1.39	1.35
55	2x	55	PSU	C6-C5	3.50	1.39	1.35
54	1w	8	4SU	C4-N3	-3.48	1.34	1.37
55	1x	8	4SU	C5-C4	-3.47	1.38	1.42
55	1x	55	PSU	C6-C5	3.37	1.39	1.35
1	1A	1911	PSU	C6-C5	3.37	1.39	1.35
32	2a	1207	2MG	C5-C4	3.32	1.47	1.38
32	2a	966	M2G	C5-C4	3.31	1.47	1.38
1	2A	2605	PSU	C6-C5	3.30	1.38	1.35
32	1a	527	G7M	C5-C4	3.28	1.46	1.38
56	2y	54	5MU	C2-N1	3.27	1.43	1.38
1	1A	2251	OMG	C5-C4	3.26	1.47	1.38
1	2A	1911	PSU	C6-C5	3.25	1.38	1.35
32	2a	527	G7M	C5-C4	3.23	1.46	1.38
1	1A	2605	PSU	C4-N3	-3.22	1.32	1.38
54	1w	76	L3X	C5-C4	-3.15	1.33	1.39
1	2A	1942	5MC	C6-C5	3.11	1.39	1.34
55	2x	76	31H	C5-C4	-3.11	1.33	1.39
1	2A	2251	OMG	C5-C4	3.11	1.47	1.38
56	2y	8	4SU	C4-N3	-3.11	1.34	1.37
32	1a	1207	2MG	C5-C4	3.08	1.47	1.38
32	1a	966	M2G	C5-C4	3.07	1.47	1.38
32	1a	966	M2G	C2-N2	3.06	1.40	1.35
54	1w	8	4SU	C5-C4	-3.03	1.38	1.42
54	2w	8	4SU	C2-N1	3.01	1.43	1.38
55	1x	76	31H	C5-C4	-3.00	1.33	1.39
32	2a	1404	5MC	C6-C5	3.00	1.39	1.34
55	1x	54	5MU	C6-C5	2.98	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	76	L3X	C5-C4	-2.91	1.33	1.39
1	2A	1939	5MU	C6-C5	2.91	1.39	1.34
54	1w	54	5MU	C6-C5	2.88	1.39	1.34
1	1A	1942	5MC	C6-C5	2.88	1.39	1.34
32	2a	1407	5MC	C6-C5	2.86	1.39	1.34
55	2x	8	4SU	C5-C4	-2.86	1.39	1.42
56	2y	54	5MU	C6-C5	2.85	1.39	1.34
55	2x	54	5MU	C6-C5	2.84	1.39	1.34
54	2w	8	4SU	O2-C2	2.82	1.28	1.23
32	1a	1404	5MC	C6-C5	2.81	1.39	1.34
1	1A	1939	5MU	C6-N1	-2.81	1.33	1.38
32	1a	967	5MC	C6-C5	2.80	1.39	1.34
56	1y	54	5MU	C6-C5	2.79	1.39	1.34
55	2x	8	4SU	C2-N3	-2.78	1.33	1.38
32	2a	1400	5MC	C6-C5	2.78	1.39	1.34
55	2x	32	5MC	C6-C5	2.76	1.39	1.34
1	1A	1911	PSU	C4-N3	-2.74	1.33	1.38
1	2A	1915	5MU	C6-C5	2.73	1.39	1.34
54	2w	54	5MU	C6-C5	2.73	1.39	1.34
1	1A	1939	5MU	C4-N3	-2.73	1.33	1.38
55	1x	54	5MU	C4-N3	-2.72	1.33	1.38
55	2x	76	31H	C5-C6	-2.71	1.33	1.41
1	1A	1915	5MU	C2-N1	2.70	1.42	1.38
32	1a	516	PSU	C4-N3	-2.69	1.33	1.38
1	1A	2251	OMG	C6-N1	-2.69	1.33	1.38
1	1A	2552	OMU	C4-N3	-2.69	1.34	1.38
1	2A	2552	OMU	C4-N3	-2.67	1.34	1.38
32	2a	967	5MC	C6-C5	2.65	1.38	1.34
32	1a	1400	5MC	C6-C5	2.64	1.38	1.34
56	1y	8	4SU	C2-N1	2.63	1.42	1.38
55	1x	76	31H	C5-C6	-2.62	1.33	1.41
32	2a	966	M2G	C2-N2	2.62	1.39	1.35
54	1w	54	5MU	C2-N1	2.60	1.42	1.38
1	2A	1911	PSU	C4-N3	-2.60	1.34	1.38
32	1a	1407	5MC	C6-C5	2.59	1.38	1.34
54	2w	8	4SU	C5-C4	-2.58	1.39	1.42
1	1A	1962	5MC	C6-C5	2.57	1.38	1.34
56	1y	54	5MU	C4-C5	2.57	1.49	1.44
1	2A	1962	5MC	C6-C5	2.57	1.38	1.34
56	1y	8	4SU	C5-C4	-2.56	1.39	1.42
55	1x	54	5MU	C2-N1	2.55	1.42	1.38
1	1A	1962	5MC	C6-N1	-2.54	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	76	L3X	C5-C6	-2.54	1.33	1.41
43	2l	92	0TD	CB-CA	2.53	1.55	1.54
56	2y	54	5MU	C4-N3	-2.52	1.34	1.38
1	2A	2251	OMG	C6-N1	-2.52	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.52	1.33	1.38
56	2y	8	4SU	C5-C4	-2.52	1.39	1.42
1	2A	1915	5MU	C4-N3	-2.51	1.34	1.38
1	2A	1939	5MU	C4-N3	-2.51	1.34	1.38
1	1A	2503	2MA	C5-N7	-2.50	1.34	1.39
1	2A	1917	PSU	C4-N3	-2.49	1.34	1.38
55	2x	55	PSU	C4-N3	-2.49	1.34	1.38
54	1w	55	PSU	C4-N3	-2.49	1.34	1.38
1	2A	1915	5MU	C4-C5	2.49	1.48	1.44
1	1A	1939	5MU	C2-N3	-2.49	1.33	1.38
55	2x	8	4SU	O2-C2	2.48	1.27	1.23
1	1A	1939	5MU	C6-C5	2.48	1.38	1.34
54	2w	76	L3X	C5-C6	-2.47	1.34	1.41
1	2A	2503	2MA	C5-N7	-2.47	1.34	1.39
55	2x	54	5MU	C2-N1	2.46	1.42	1.38
55	1x	32	5MC	C6-N1	-2.46	1.33	1.38
32	1a	1207	2MG	C6-N1	-2.45	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.45	1.34	1.38
56	1y	54	5MU	C4-N3	-2.45	1.34	1.38
1	1A	2605	PSU	C2-N3	-2.44	1.33	1.37
1	1A	1915	5MU	C6-C5	2.44	1.38	1.34
55	2x	54	5MU	C4-N3	-2.44	1.34	1.38
1	2A	2503	2MA	C5-C6	2.44	1.47	1.41
54	2w	54	5MU	C4-N3	-2.44	1.34	1.38
1	2A	1939	5MU	C4-C5	2.43	1.48	1.44
54	2w	54	5MU	C2-N1	2.42	1.42	1.38
1	1A	2251	OMG	C5-N7	-2.42	1.34	1.39
32	2a	966	M2G	C6-N1	-2.41	1.34	1.38
32	1a	527	G7M	C6-N1	-2.41	1.34	1.38
1	1A	1917	PSU	C4-N3	-2.40	1.34	1.38
54	2w	55	PSU	C4-N3	-2.40	1.34	1.38
55	1x	32	5MC	C6-C5	2.39	1.38	1.34
54	1w	8	4SU	C2-N1	2.38	1.42	1.38
32	2a	516	PSU	C4-N3	-2.38	1.34	1.38
1	1A	1915	5MU	C4-N3	-2.38	1.34	1.38
1	2A	2251	OMG	C5-N7	-2.35	1.34	1.39
55	1x	55	PSU	C4-N3	-2.35	1.34	1.38
56	2y	8	4SU	C2-N1	2.35	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	54	5MU	C4-C5	2.34	1.48	1.44
1	1A	1915	5MU	C4-C5	2.34	1.48	1.44
32	1a	1498	UR3	C2-N1	2.33	1.41	1.38
1	2A	1915	5MU	C2-N1	2.33	1.42	1.38
56	1y	55	PSU	C4-N3	-2.33	1.34	1.38
1	1A	2605	PSU	C6-C5	2.33	1.37	1.35
32	1a	1400	5MC	C6-N1	-2.30	1.34	1.38
32	2a	1207	2MG	C2-N3	2.30	1.36	1.32
1	2A	2605	PSU	C4-N3	-2.30	1.34	1.38
32	2a	527	G7M	C6-N1	-2.29	1.34	1.38
1	2A	2552	OMU	C5-C4	2.29	1.48	1.43
55	2x	54	5MU	C4-C5	2.29	1.48	1.44
32	1a	966	M2G	C6-N1	-2.28	1.34	1.38
56	1y	54	5MU	C2-N1	2.28	1.42	1.38
32	1a	1404	5MC	C6-N1	-2.26	1.34	1.38
1	1A	2503	2MA	C5-C6	2.25	1.47	1.41
56	2y	55	PSU	C4-N3	-2.25	1.34	1.38
1	1A	1939	5MU	C4-C5	2.24	1.48	1.44
56	2y	54	5MU	C4-C5	2.24	1.48	1.44
55	2x	32	5MC	C6-N1	-2.23	1.34	1.38
55	1x	8	4SU	O2-C2	2.23	1.27	1.23
32	1a	967	5MC	C6-N1	-2.21	1.34	1.38
54	1w	54	5MU	C4-N3	-2.21	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.19	1.34	1.38
1	2A	2503	2MA	C8-N7	2.18	1.35	1.31
55	1x	54	5MU	C4-C5	2.18	1.48	1.44
1	1A	2552	OMU	C5-C4	2.18	1.48	1.43
1	2A	1915	5MU	C6-N1	-2.17	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.16	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.15	1.34	1.38
54	2w	54	5MU	C4-C5	2.15	1.48	1.44
56	2y	8	4SU	C2-N3	-2.15	1.34	1.38
32	2a	966	M2G	C5-N7	-2.14	1.34	1.39
32	2a	1400	5MC	C6-N1	-2.14	1.34	1.38
56	1y	54	5MU	C6-N1	-2.13	1.34	1.38
1	1A	2503	2MA	C4-N9	-2.12	1.33	1.37
32	1a	966	M2G	C5-N7	-2.12	1.34	1.39
1	1A	1942	5MC	C6-N1	-2.09	1.34	1.38
55	2x	8	4SU	C2-N1	2.09	1.41	1.38
1	1A	2503	2MA	C8-N7	2.08	1.35	1.31
54	1w	8	4SU	C2-N3	-2.08	1.34	1.38
32	1a	527	G7M	C4-N9	-2.07	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1915	5MU	C6-N1	-2.07	1.34	1.38
55	1x	8	4SU	C6-C5	2.06	1.39	1.35
32	2a	1498	UR3	C6-C5	2.06	1.39	1.35
55	1x	54	5MU	C2-N3	-2.05	1.34	1.38
32	1a	1407	5MC	C6-N1	-2.05	1.34	1.38
56	1y	8	4SU	C2-N3	-2.04	1.34	1.38
55	2x	8	4SU	C6-C5	2.04	1.39	1.35
32	1a	1207	2MG	C2-N3	2.02	1.35	1.32
1	2A	1939	5MU	C6-N1	-2.01	1.34	1.38
56	1y	8	4SU	O2-C2	2.00	1.26	1.23

All (357) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	2l	92	0TD	CSB-SB-CB	-11.56	81.58	102.36
54	2w	8	4SU	C4-N3-C2	-9.28	118.42	127.31
1	2A	2503	2MA	C5-C4-N3	-8.13	118.62	127.18
54	2w	8	4SU	C5-C4-S4	-7.47	115.78	124.31
1	1A	2503	2MA	C5-C4-N3	-7.38	119.40	127.18
54	2w	8	4SU	C5-C4-N3	7.26	121.50	114.75
32	2a	1498	UR3	C4-N3-C2	-7.19	118.80	124.58
32	1a	1498	UR3	C4-N3-C2	-7.07	118.89	124.58
32	1a	1207	2MG	C2-N3-C4	6.85	120.57	112.00
32	2a	1207	2MG	C2-N3-C4	6.67	120.35	112.00
55	2x	55	PSU	N1-C2-N3	6.58	122.11	115.17
1	2A	2503	2MA	N3-C4-N9	6.54	135.29	126.99
56	1y	55	PSU	N1-C2-N3	6.52	122.05	115.17
32	2a	966	M2G	C5-C4-N3	-6.42	118.17	128.39
1	2A	1917	PSU	N1-C2-N3	6.41	121.93	115.17
1	1A	1911	PSU	N1-C2-N3	6.40	121.92	115.17
55	1x	55	PSU	N1-C2-N3	6.35	121.87	115.17
32	1a	516	PSU	N1-C2-N3	6.35	121.87	115.17
54	1w	55	PSU	N1-C2-N3	6.31	121.83	115.17
1	1A	2605	PSU	N1-C2-N3	6.20	121.71	115.17
1	2A	2605	PSU	N1-C2-N3	6.14	121.65	115.17
56	2y	55	PSU	N1-C2-N3	6.13	121.63	115.17
32	1a	966	M2G	C5-C4-N3	-6.13	118.64	128.39
32	2a	1207	2MG	C5-C4-N3	-6.11	118.67	128.39
43	1l	92	0TD	CSB-SB-CB	-6.09	91.42	102.36
1	2A	1911	PSU	N1-C2-N3	6.09	121.59	115.17
32	2a	516	PSU	N1-C2-N3	6.08	121.58	115.17
54	2w	55	PSU	N1-C2-N3	6.05	121.56	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1917	PSU	N1-C2-N3	6.05	121.55	115.17
1	1A	2251	OMG	C5-C4-N3	-6.05	118.76	128.39
1	2A	2251	OMG	C5-C4-N3	-6.04	118.77	128.39
32	1a	1207	2MG	C5-C4-N3	-5.94	118.94	128.39
1	1A	2503	2MA	N3-C4-N9	5.93	134.52	126.99
1	1A	2552	OMU	N3-C2-N1	5.90	122.57	114.89
1	2A	1939	5MU	C4-N3-C2	-5.88	119.64	127.34
55	1x	76	31H	N1-C2-N3	-5.77	119.85	128.58
54	2w	76	L3X	N1-C2-N3	-5.76	119.87	128.58
55	2x	76	31H	N1-C2-N3	-5.59	120.11	128.58
54	1w	76	L3X	N1-C2-N3	-5.59	120.12	128.58
54	1w	8	4SU	C5-C4-N3	5.59	119.95	114.75
1	1A	1939	5MU	C4-N3-C2	-5.58	120.02	127.34
1	2A	1939	5MU	N3-C2-N1	5.52	122.07	114.89
32	1a	527	G7M	N9-C4-N3	5.32	136.59	125.95
1	2A	1915	5MU	C4-N3-C2	-5.31	120.38	127.34
56	2y	8	4SU	C4-N3-C2	-5.30	122.23	127.31
32	2a	527	G7M	N9-C4-N3	5.20	136.36	125.95
32	2a	527	G7M	C5-C4-N3	-5.19	118.34	128.15
54	1w	8	4SU	C4-N3-C2	-5.15	122.38	127.31
32	2a	1518	MA6	N1-C2-N3	-5.06	120.92	128.58
55	1x	76	31H	C5-C4-N3	-5.05	119.76	126.72
55	1x	54	5MU	N3-C2-N1	5.04	121.45	114.89
54	2w	76	L3X	C5-C4-N3	-5.03	119.79	126.72
32	1a	1518	MA6	N1-C2-N3	-5.03	120.97	128.58
1	2A	1939	5MU	C5-C4-N3	5.01	119.68	115.32
32	2a	1519	MA6	N1-C2-N3	-5.01	121.00	128.58
56	2y	8	4SU	C5-C4-N3	5.01	119.41	114.75
1	1A	1915	5MU	C4-N3-C2	-5.00	120.79	127.34
55	2x	76	31H	C5-C4-N3	-4.99	119.84	126.72
1	2A	2251	OMG	N9-C4-N3	4.98	135.91	125.95
1	2A	2552	OMU	N3-C2-N1	4.98	121.37	114.89
1	2A	1915	5MU	N3-C2-N1	4.98	121.37	114.89
55	2x	54	5MU	N3-C2-N1	4.95	121.34	114.89
32	1a	527	G7M	C5-C4-N3	-4.95	118.80	128.15
1	1A	1939	5MU	C5-C4-N3	4.94	119.62	115.32
54	1w	76	L3X	C5-C4-N3	-4.92	119.95	126.72
1	1A	2251	OMG	N9-C4-N3	4.91	135.76	125.95
55	2x	54	5MU	C4-N3-C2	-4.86	120.96	127.34
1	1A	1915	5MU	N3-C2-N1	4.86	121.22	114.89
32	2a	966	M2G	N9-C4-N3	4.86	135.67	125.95
32	1a	1519	MA6	N1-C2-N3	-4.85	121.24	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1519	MA6	C5-C4-N3	-4.84	120.05	126.72
1	1A	1939	5MU	N3-C2-N1	4.84	121.19	114.89
1	2A	1915	5MU	C5-C4-N3	4.78	119.48	115.32
1	2A	2251	OMG	C2-N3-C4	4.72	120.43	112.30
55	1x	54	5MU	C4-N3-C2	-4.72	121.16	127.34
32	1a	966	M2G	N9-C4-N3	4.68	135.32	125.95
1	1A	2251	OMG	C2-N3-C4	4.67	120.34	112.30
1	2A	1939	5MU	O4-C4-C5	-4.66	119.59	124.92
1	1A	1939	5MU	O4-C4-C5	-4.65	119.59	124.92
32	2a	1518	MA6	C5-C4-N3	-4.65	120.32	126.72
54	2w	8	4SU	O2-C2-N1	-4.64	116.75	122.80
32	2a	527	G7M	C2-N3-C4	4.63	120.27	112.30
56	1y	54	5MU	C4-N3-C2	-4.61	121.29	127.34
32	1a	966	M2G	C2-N3-C4	4.60	121.02	112.51
1	1A	2552	OMU	C4-N3-C2	-4.60	120.90	126.61
32	2a	1519	MA6	C5-C4-N3	-4.60	120.39	126.72
56	1y	8	4SU	C5-C4-N3	4.52	118.95	114.75
55	2x	54	5MU	O4-C4-C5	-4.48	119.79	124.92
1	1A	1911	PSU	C4-N3-C2	-4.48	120.20	126.37
32	1a	527	G7M	C2-N3-C4	4.46	119.99	112.30
56	1y	54	5MU	N3-C2-N1	4.46	120.69	114.89
1	2A	2605	PSU	C4-N3-C2	-4.45	120.25	126.37
1	2A	1939	5MU	C5-C6-N1	-4.44	118.49	123.31
54	1w	54	5MU	N3-C2-N1	4.42	120.64	114.89
56	1y	55	PSU	O2-C2-N1	-4.41	118.24	122.79
1	1A	1939	5MU	C5-C6-N1	-4.41	118.53	123.31
1	1A	1915	5MU	O4-C4-C5	-4.40	119.88	124.92
32	2a	1207	2MG	N9-C4-N3	4.40	134.75	125.95
54	1w	54	5MU	O4-C4-C5	-4.36	119.93	124.92
1	1A	1915	5MU	C5-C4-N3	4.36	119.11	115.32
32	2a	966	M2G	C2-N3-C4	4.36	120.57	112.51
55	2x	54	5MU	C5-C4-N3	4.31	119.07	115.32
54	1w	54	5MU	C4-N3-C2	-4.31	121.69	127.34
1	2A	1915	5MU	O4-C4-C5	-4.30	119.99	124.92
56	2y	55	PSU	O2-C2-N1	-4.27	118.38	122.79
56	1y	54	5MU	C5-C4-N3	4.23	119.00	115.32
55	1x	8	4SU	C6-C5-C4	-4.20	116.31	119.95
1	2A	2552	OMU	C4-N3-C2	-4.20	121.40	126.61
55	2x	55	PSU	C4-N3-C2	-4.19	120.60	126.37
54	2w	55	PSU	O2-C2-N1	-4.18	118.47	122.79
56	1y	8	4SU	C4-N3-C2	-4.17	123.32	127.31
32	1a	1207	2MG	N9-C4-N3	4.16	134.26	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1518	MA6	C2-N1-C6	4.12	121.91	111.83
56	2y	54	5MU	N3-C2-N1	4.10	120.23	114.89
1	1A	1917	PSU	C4-N3-C2	-4.10	120.73	126.37
1	1A	2605	PSU	C4-N3-C2	-4.05	120.79	126.37
55	1x	54	5MU	C5-C4-N3	4.04	118.83	115.32
1	1A	1911	PSU	O2-C2-N1	-4.00	118.66	122.79
32	1a	516	PSU	C4-N3-C2	-4.00	120.86	126.37
1	2A	1917	PSU	C4-N3-C2	-3.99	120.87	126.37
32	2a	1518	MA6	C2-N1-C6	3.99	121.58	111.83
54	2w	54	5MU	O4-C4-C5	-3.98	120.36	124.92
32	2a	1519	MA6	C4-C5-N7	-3.98	106.03	110.58
55	1x	54	5MU	O4-C4-C5	-3.97	120.38	124.92
54	2w	8	4SU	N3-C2-N1	3.97	120.06	114.89
1	2A	1911	PSU	C4-N3-C2	-3.95	120.93	126.37
56	1y	55	PSU	C4-N3-C2	-3.92	120.97	126.37
32	1a	1519	MA6	C4-C5-N7	-3.91	106.11	110.58
56	2y	54	5MU	C5-C4-N3	3.90	118.71	115.32
32	1a	1519	MA6	C2-N1-C6	3.88	121.32	111.83
54	1w	55	PSU	C4-N3-C2	-3.88	121.03	126.37
32	2a	1519	MA6	C2-N1-C6	3.87	121.29	111.83
54	1w	54	5MU	C5-C4-N3	3.87	118.69	115.32
56	2y	54	5MU	O4-C4-C5	-3.86	120.50	124.92
32	2a	516	PSU	C4-N3-C2	-3.85	121.06	126.37
55	1x	8	4SU	O2-C2-N1	3.85	127.80	122.80
32	1a	1518	MA6	C5-C4-N3	-3.84	121.42	126.72
1	1A	2503	2MA	N6-C6-N1	3.83	122.20	117.03
32	2a	1519	MA6	C5-N7-C8	3.81	109.43	103.45
55	1x	55	PSU	O2-C2-N1	-3.80	118.87	122.79
56	2y	54	5MU	C4-N3-C2	-3.79	122.38	127.34
56	2y	8	4SU	N3-C2-N1	3.78	119.81	114.89
32	1a	1518	MA6	C5-N7-C8	3.78	109.39	103.45
32	1a	1207	2MG	C6-C5-N7	3.77	137.16	130.29
32	1a	1519	MA6	C5-N7-C8	3.76	109.37	103.45
54	2w	54	5MU	N3-C2-N1	3.76	119.79	114.89
55	1x	55	PSU	C4-N3-C2	-3.76	121.19	126.37
55	1x	32	5MC	C5-C6-N1	-3.76	119.23	123.31
1	2A	1939	5MU	O2-C2-N1	-3.71	117.96	122.80
54	1w	55	PSU	O2-C2-N1	-3.70	118.97	122.79
55	2x	76	31H	O4'-C1'-N9	-3.68	101.03	108.09
54	2w	55	PSU	C4-N3-C2	-3.66	121.33	126.37
32	2a	1518	MA6	C4-C5-N7	-3.65	106.40	110.58
32	1a	1518	MA6	N9-C8-N7	-3.63	108.78	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	55	PSU	O2-C2-N1	-3.63	119.04	122.79
32	2a	1518	MA6	C5-N7-C8	3.63	109.15	103.45
54	2w	54	5MU	C4-N3-C2	-3.62	122.59	127.34
32	2a	1519	MA6	C2-N3-C4	3.62	120.67	111.83
54	2w	54	5MU	C5-C4-N3	3.61	118.46	115.32
54	1w	8	4SU	C5-C4-S4	-3.61	120.18	124.31
32	2a	1518	MA6	C2-N3-C4	3.60	120.61	111.83
32	1a	1519	MA6	C2-N3-C4	3.57	120.56	111.83
55	2x	32	5MC	C5-C6-N1	-3.56	119.45	123.31
1	1A	2552	OMU	O2-C2-N1	-3.54	118.19	122.80
56	2y	55	PSU	C4-N3-C2	-3.53	121.50	126.37
1	1A	1917	PSU	O2-C2-N1	-3.53	119.15	122.79
1	2A	1962	5MC	C5-C6-N1	-3.53	119.48	123.31
55	2x	8	4SU	C5-C4-N3	3.52	118.02	114.75
32	2a	516	PSU	O2-C2-N1	-3.50	119.18	122.79
54	2w	76	L3X	N9-C8-N7	-3.50	108.97	113.94
1	2A	1915	5MU	C5-C6-N1	-3.49	119.52	123.31
56	1y	54	5MU	O4-C4-C5	-3.49	120.92	124.92
55	1x	76	31H	N9-C8-N7	-3.48	109.00	113.94
1	1A	1942	5MC	C5-C6-N1	-3.48	119.54	123.31
55	2x	76	31H	N9-C8-N7	-3.46	109.03	113.94
32	2a	1400	5MC	C5-C6-N1	-3.45	119.56	123.31
32	2a	1404	5MC	C5-C6-N1	-3.45	119.56	123.31
54	2w	76	L3X	C2-N3-C4	3.44	120.24	111.83
55	1x	76	31H	C2-N3-C4	3.41	120.16	111.83
54	1w	76	L3X	N9-C8-N7	-3.41	109.10	113.94
1	2A	1917	PSU	O2-C2-N1	-3.39	119.29	122.79
55	1x	54	5MU	C5-C6-N1	-3.39	119.63	123.31
32	1a	516	PSU	O2-C2-N1	-3.37	119.32	122.79
32	1a	1518	MA6	C4-C5-N7	-3.35	106.75	110.58
32	2a	1407	5MC	C5-C6-N1	-3.34	119.69	123.31
1	1A	2503	2MA	C4-C5-N7	-3.34	106.77	110.58
56	2y	54	5MU	C1'-N1-C2	3.32	123.55	117.59
55	2x	76	31H	C2-N3-C4	3.31	119.93	111.83
32	2a	1207	2MG	C6-C5-N7	3.30	136.30	130.29
32	1a	1407	5MC	C5-C6-N1	-3.30	119.73	123.31
1	2A	2503	2MA	N6-C6-N1	3.30	121.48	117.03
32	2a	1407	5MC	C5-C4-N3	-3.29	118.38	121.75
1	2A	2605	PSU	O2-C2-N1	-3.29	119.39	122.79
54	1w	76	L3X	C2-N3-C4	3.29	119.86	111.83
1	2A	2503	2MA	C4-C5-N7	-3.28	106.83	110.58
32	1a	1518	MA6	C2-N3-C4	3.28	119.83	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1498	UR3	C5-C4-N3	3.26	119.33	115.04
1	1A	1939	5MU	O2-C2-N1	-3.24	118.57	122.80
56	2y	8	4SU	C5-C4-S4	-3.24	120.60	124.31
32	2a	967	5MC	C5-C6-N1	-3.24	119.79	123.31
1	2A	1942	5MC	C5-C6-N1	-3.22	119.81	123.31
32	1a	1400	5MC	C5-C6-N1	-3.20	119.83	123.31
32	2a	1519	MA6	N9-C8-N7	-3.18	109.42	113.94
1	2A	1911	PSU	O2-C2-N1	-3.14	119.55	122.79
32	1a	967	5MC	C5-C6-N1	-3.14	119.91	123.31
55	2x	76	31H	C5-N7-C8	3.12	108.36	103.45
32	1a	1519	MA6	N9-C8-N7	-3.12	109.51	113.94
32	2a	1498	UR3	C5-C4-N3	3.11	119.14	115.04
32	2a	1518	MA6	N9-C8-N7	-3.11	109.52	113.94
56	1y	54	5MU	C5-C6-N1	-3.11	119.94	123.31
32	1a	1207	2MG	C4-C5-N7	-3.11	105.75	110.67
54	2w	76	L3X	C5-N7-C8	3.10	108.32	103.45
55	1x	76	31H	C5-N7-C8	3.09	108.31	103.45
54	1w	76	L3X	C5-N7-C8	3.08	108.29	103.45
1	1A	2503	2MA	C4-N9-C8	3.04	108.93	105.74
32	1a	1404	5MC	C5-C4-N3	-3.02	118.66	121.75
43	2l	92	0TD	OD2-CG-CB	3.02	119.67	113.15
55	2x	54	5MU	C5-C6-N1	-3.02	120.04	123.31
54	1w	8	4SU	N3-C2-N1	3.01	118.81	114.89
1	1A	2251	OMG	C6-C5-N7	3.00	135.76	130.29
55	1x	76	31H	C4'-O4'-C1'	-2.98	102.88	109.47
1	1A	1915	5MU	C5-C6-N1	-2.91	120.15	123.31
1	2A	1942	5MC	C5-C4-N3	-2.90	118.78	121.75
32	1a	966	M2G	C6-C5-N7	2.90	135.57	130.29
55	2x	76	31H	C4'-O4'-C1'	-2.90	103.07	109.47
56	1y	8	4SU	N3-C2-N1	2.89	118.66	114.89
1	1A	2503	2MA	C2-N1-C6	2.89	122.54	118.10
55	2x	8	4SU	C6-C5-C4	-2.89	117.45	119.95
1	1A	1962	5MC	C5-C4-N3	-2.88	118.80	121.75
55	2x	76	31H	C5-C4-N9	2.85	108.92	105.81
32	1a	1404	5MC	C5-C6-N1	-2.85	120.22	123.31
56	1y	8	4SU	C1'-N1-C2	2.84	122.69	117.59
32	1a	1519	MA6	N3-C4-N9	2.84	131.99	127.17
32	2a	1207	2MG	C4-C5-N7	-2.83	106.19	110.67
32	2a	1518	MA6	N3-C4-N9	2.83	131.97	127.17
32	2a	1404	5MC	C5-C4-N3	-2.82	118.86	121.75
32	1a	1400	5MC	C5-C4-N3	-2.81	118.87	121.75
1	2A	2503	2MA	C4-N9-C8	2.81	108.69	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1962	5MC	CM5-C5-C6	-2.78	119.09	122.85
55	1x	32	5MC	C5-C4-N3	-2.78	118.91	121.75
1	1A	1962	5MC	C5-C6-N1	-2.78	120.30	123.31
54	1w	76	L3X	C5-C4-N9	2.77	108.83	105.81
1	2A	2251	OMG	C6-C5-N7	2.77	135.32	130.29
43	1l	92	0TD	OD2-CG-CB	2.77	119.12	113.15
32	2a	966	M2G	C6-C5-N7	2.74	135.27	130.29
55	1x	8	4SU	C5-C4-N3	2.73	117.29	114.75
1	1A	1942	5MC	C5-C4-N3	-2.72	118.97	121.75
55	2x	32	5MC	C5-C4-N3	-2.71	118.98	121.75
1	2A	2552	OMU	C5-C4-N3	2.70	118.58	114.80
56	2y	54	5MU	C1'-N1-C6	-2.67	116.75	121.15
54	2w	76	L3X	N3-C4-N9	2.67	131.71	127.17
32	1a	1519	MA6	C4-C5-C6	2.63	118.63	115.91
32	1a	1518	MA6	N3-C4-N9	2.63	131.64	127.17
1	2A	2251	OMG	O6-C6-C5	-2.62	119.62	126.53
1	1A	2503	2MA	C5-N7-C8	2.62	107.57	103.45
55	1x	76	31H	N3-C4-N9	2.61	131.60	127.17
1	2A	1962	5MC	C5-C4-N3	-2.60	119.09	121.75
55	1x	76	31H	C5-C4-N9	2.59	108.63	105.81
32	2a	1519	MA6	N3-C4-N9	2.59	131.57	127.17
55	2x	32	5MC	O2-C2-N3	-2.57	118.28	122.33
32	1a	1402	4OC	C6-C5-C4	2.55	120.07	117.00
55	2x	8	4SU	C1'-N1-C2	2.55	122.17	117.59
32	1a	1407	5MC	C5-C4-N3	-2.54	119.15	121.75
32	2a	1400	5MC	C5-C4-N3	-2.53	119.17	121.75
55	1x	8	4SU	C1'-N1-C2	2.52	122.13	117.59
1	1A	2605	PSU	C5-C6-N1	-2.52	118.64	122.14
1	2A	2503	2MA	C5-N7-C8	2.52	107.41	103.45
32	2a	966	M2G	C4-C5-N7	-2.52	106.67	110.67
1	2A	2552	OMU	C2'-C1'-N1	-2.52	109.47	114.24
32	1a	527	G7M	O6-C6-C5	-2.50	122.44	128.01
32	2a	967	5MC	C5-C4-N3	-2.50	119.20	121.75
56	1y	54	5MU	C5M-C5-C4	2.47	121.42	118.78
56	2y	54	5MU	O2-C2-N3	-2.47	116.94	121.49
54	2w	76	L3X	C5-C4-N9	2.46	108.50	105.81
1	1A	2251	OMG	C4-C5-N7	-2.46	106.77	110.67
32	1a	1207	2MG	N1-C2-N2	2.45	119.06	116.56
1	2A	1915	5MU	O2-C2-N1	-2.45	119.60	122.80
54	1w	8	4SU	C1'-N1-C2	2.43	121.96	117.59
32	1a	1207	2MG	CM2-N2-C2	-2.42	118.45	123.65
1	2A	2503	2MA	C2-N1-C6	2.41	121.81	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	966	M2G	O6-C6-C5	-2.41	120.17	126.53
32	2a	1407	5MC	O2-C2-N3	-2.41	118.53	122.33
32	1a	967	5MC	C5-C4-N3	-2.41	119.29	121.75
54	2w	8	4SU	S4-C4-N3	2.41	122.72	120.20
54	1w	54	5MU	C5-C6-N1	-2.39	120.71	123.31
55	2x	76	31H	N3-C4-N9	2.39	131.23	127.17
1	2A	2552	OMU	O2-C2-N1	-2.39	119.69	122.80
1	1A	2605	PSU	O2-C2-N1	-2.38	120.33	122.79
54	1w	76	L3X	N3-C4-N9	2.38	131.22	127.17
54	2w	55	PSU	C6-C5-C4	-2.38	116.57	118.17
55	2x	54	5MU	O2-C2-N1	-2.37	119.70	122.80
1	2A	1920	OMC	O2-C2-N3	-2.37	118.59	122.33
32	1a	1207	2MG	N2-C2-N3	-2.37	117.49	120.51
32	2a	1498	UR3	C3U-N3-C4	2.36	121.15	117.87
1	1A	2552	OMU	C5-C4-N3	2.36	118.10	114.80
55	2x	76	31H	C4-C5-N7	-2.35	107.89	110.58
1	1A	2552	OMU	O4-C4-C5	-2.35	121.11	125.16
32	1a	1400	5MC	O2-C2-N3	-2.34	118.64	122.33
1	1A	1911	PSU	C5-C6-N1	-2.34	118.89	122.14
1	1A	1920	OMC	O2-C2-N3	-2.34	118.64	122.33
1	1A	2251	OMG	O6-C6-C5	-2.32	120.40	126.53
1	1A	2503	2MA	N9-C8-N7	-2.31	110.65	113.94
32	1a	1407	5MC	CM5-C5-C6	-2.31	119.73	122.85
32	2a	1518	MA6	C4-C5-C6	2.31	118.29	115.91
32	1a	1518	MA6	C4-N9-C8	2.30	108.15	105.74
32	2a	1400	5MC	O2-C2-N3	-2.29	118.72	122.33
55	1x	8	4SU	C4-N3-C2	2.29	129.51	127.31
54	2w	54	5MU	C5-C6-N1	-2.29	120.83	123.31
32	2a	1402	4OC	C6-C5-C4	2.28	119.75	117.00
1	1A	2503	2MA	C6-C5-N7	2.27	136.47	132.09
32	1a	966	M2G	C4-C5-N7	-2.26	107.08	110.67
56	1y	8	4SU	C5-C4-S4	-2.26	121.72	124.31
32	2a	527	G7M	O6-C6-C5	-2.26	122.96	128.01
55	1x	76	31H	C4-C5-N7	-2.26	108.00	110.58
32	1a	1207	2MG	C8-N7-C5	2.26	108.28	104.26
1	2A	1942	5MC	O2-C2-N3	-2.23	118.82	122.33
1	2A	2552	OMU	O4-C4-C5	-2.23	121.33	125.16
55	2x	55	PSU	C5-C6-N1	-2.22	119.06	122.14
55	1x	8	4SU	S4-C4-N3	-2.21	117.89	120.20
54	1w	76	L3X	C4-C5-N7	-2.20	108.07	110.58
1	1A	2605	PSU	O2-C2-N3	-2.19	117.96	121.86
56	2y	54	5MU	C5-C6-N1	-2.17	120.95	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	76	31H	C6-C5-C4	2.17	120.14	117.18
55	1x	76	31H	O4'-C1'-C2'	-2.17	101.97	106.62
32	1a	1498	UR3	C6-N1-C2	-2.17	120.03	121.80
1	2A	2251	OMG	C4-C5-N7	-2.17	107.23	110.67
55	1x	76	31H	C6-C5-C4	2.16	120.13	117.18
54	1w	76	L3X	C6-C5-C4	2.16	120.12	117.18
54	2w	76	L3X	C4-C5-N7	-2.14	108.14	110.58
54	1w	54	5MU	O2-C2-N1	-2.12	120.03	122.80
56	1y	54	5MU	O2-C2-N1	-2.12	120.04	122.80
32	2a	1404	5MC	O2-C2-N3	-2.12	118.99	122.33
1	2A	2605	PSU	C5-C6-N1	-2.11	119.21	122.14
55	2x	76	31H	O4'-C1'-C2'	-2.11	102.11	106.62
55	1x	8	4SU	O2-C2-N3	-2.10	117.61	121.49
1	2A	2503	2MA	N9-C8-N7	-2.09	110.97	113.94
54	2w	76	L3X	C6-C5-C4	2.09	120.03	117.18
32	1a	1498	UR3	C1'-N1-C2	2.08	120.45	117.04
32	2a	1519	MA6	C4-C5-C6	2.08	118.06	115.91
32	2a	966	M2G	O6-C6-C5	-2.07	121.08	126.53
1	2A	1962	5MC	CM5-C5-C6	-2.06	120.06	122.85
55	2x	76	31H	O2'-C2'-C3'	2.06	116.20	111.16
32	2a	527	G7M	C5-C6-N1	2.06	116.09	111.84
32	1a	1400	5MC	CM5-C5-C6	-2.05	120.07	122.85
32	2a	1519	MA6	C5-C4-N9	2.05	108.04	105.81
56	2y	8	4SU	C6-N1-C2	-2.04	118.51	121.00
1	2A	1917	PSU	C5-C6-N1	-2.04	119.30	122.14
32	1a	1207	2MG	C2-N1-C6	-2.04	122.08	124.55
1	1A	1917	PSU	C5-C6-N1	-2.04	119.31	122.14
56	1y	55	PSU	O4'-C1'-C2'	2.04	107.97	105.15
1	1A	2503	2MA	CM2-C2-N1	2.03	120.17	117.13
32	2a	1402	4OC	O2-C2-N3	-2.02	119.14	122.33
32	1a	1407	5MC	O2-C2-N3	-2.02	119.15	122.33
32	2a	1207	2MG	C2-N1-C6	-2.02	122.11	124.55
32	1a	527	G7M	C5-C6-N1	2.02	116.00	111.84
54	2w	54	5MU	C1'-N1-C2	2.01	121.21	117.59
1	2A	2251	OMG	C5-C6-N1	2.00	118.35	113.25

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2

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Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1207	2MG	N3-C2-N2-CM2
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
43	2l	92	0TD	CA-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
54	2w	76	L3X	C3'-C4'-C5'-O5'
54	2w	76	L3X	O4'-C4'-C5'-O5'
55	1x	76	31H	C3'-C4'-C5'-O5'
55	1x	76	31H	C-CA-CB-CG
55	1x	76	31H	N-CA-CB-CG
56	2y	8	4SU	C3'-C4'-C5'-O5'
56	2y	8	4SU	O4'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
55	2x	76	31H	O4'-C4'-C5'-O5'
56	2y	55	PSU	C3'-C4'-C5'-O5'
56	2y	55	PSU	O4'-C4'-C5'-O5'
55	2x	76	31H	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
1	2A	1962	5MC	O4'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
55	1x	55	PSU	O4'-C4'-C5'-O5'
55	1x	76	31H	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
1	2A	1962	5MC	C3'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
55	1x	55	PSU	C3'-C4'-C5'-O5'
55	1x	76	31H	C4'-C5'-O5'-P
55	2x	76	31H	C4'-C5'-O5'-P
56	1y	55	PSU	O4'-C1'-C5-C4
32	1a	1400	5MC	C3'-C4'-C5'-O5'
55	2x	76	31H	CB-CG-SD-CE
1	2A	2503	2MA	O4'-C4'-C5'-O5'
1	1A	2503	2MA	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
32	1a	527	G7M	C4'-C5'-O5'-P
32	1a	1519	MA6	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
56	2y	8	4SU	C4'-C5'-O5'-P
32	1a	967	5MC	O4'-C4'-C5'-O5'
54	1w	76	L3X	O4'-C4'-C5'-O5'
56	2y	54	5MU	C2'-C1'-N1-C6
56	2y	54	5MU	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
56	1y	8	4SU	C2'-C1'-N1-C2
32	2a	1402	4OC	C2'-C1'-N1-C2
56	2y	54	5MU	C2'-C1'-N1-C2

There are no ring outliers.

29 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	1w	76	L3X	1	0
1	1A	1915	5MU	2	0
32	2a	1518	MA6	3	0
56	2y	8	4SU	2	0
1	1A	2552	OMU	2	0
55	1x	76	31H	2	0
55	1x	8	4SU	2	0
32	1a	1519	MA6	1	0
1	2A	1915	5MU	1	0
1	1A	1939	5MU	1	0
54	2w	76	L3X	2	0
54	1w	54	5MU	1	0
1	2A	2503	2MA	1	0
54	2w	8	4SU	7	0
32	2a	1404	5MC	2	0
56	2y	54	5MU	1	0
32	1a	1518	MA6	2	0
55	2x	76	31H	2	0
56	1y	8	4SU	2	0
1	2A	2552	OMU	1	0
54	1w	8	4SU	1	0
43	2l	92	0TD	1	0
54	1w	55	PSU	3	0
32	2a	1519	MA6	3	0
32	1a	1402	4OC	2	0
54	2w	54	5MU	2	0
32	2a	1402	4OC	2	0
1	2A	2251	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	966	M2G	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2761 ligands modelled in this entry, 2757 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	CLM	1A	4097	-	20,20,20	0.97	2 (10%)	23,27,27	1.22	2 (8%)
61	SF4	1d	501	35	0,12,12	-	-	-		
61	SF4	2d	303	35	0,12,12	-	-	-		
59	CLM	2A	3863	-	20,20,20	1.01	1 (5%)	23,27,27	1.02	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	CLM	1A	4097	-	-	2/20/22/22	0/1/1/1
61	SF4	1d	501	35	-	-	0/6/5/5
61	SF4	2d	303	35	-	-	0/6/5/5
59	CLM	2A	3863	-	-	0/20/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1A	4097	CLM	C6-C5	-2.43	1.48	1.51
59	2A	3863	CLM	C6-C5	-2.37	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1A	4097	CLM	C9-N9	-2.34	1.39	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	1A	4097	CLM	O5-C5-C6	-3.43	103.76	111.20
59	2A	3863	CLM	C6-C5-C3	2.65	116.48	111.72
59	1A	4097	CLM	C6-C5-C3	2.54	116.27	111.72
59	2A	3863	CLM	O5-C5-C6	-2.02	106.82	111.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1A	4097	CLM	N2-C3-C4-O4
59	1A	4097	CLM	C5-C3-C4-O4

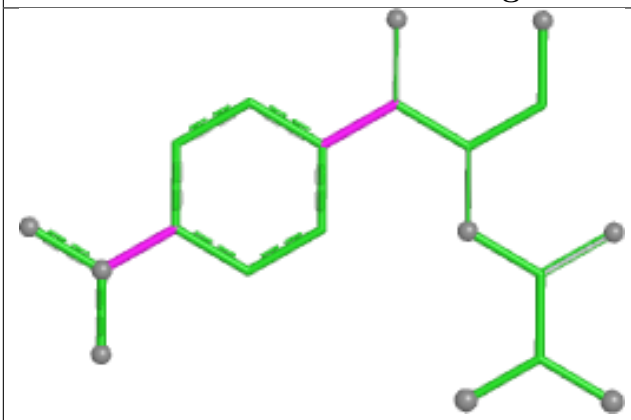
There are no ring outliers.

2 monomers are involved in 2 short contacts:

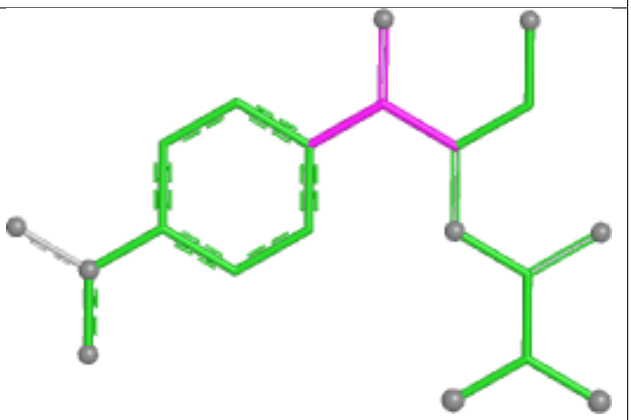
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	1A	4097	CLM	1	0
61	2d	303	SF4	1	0

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

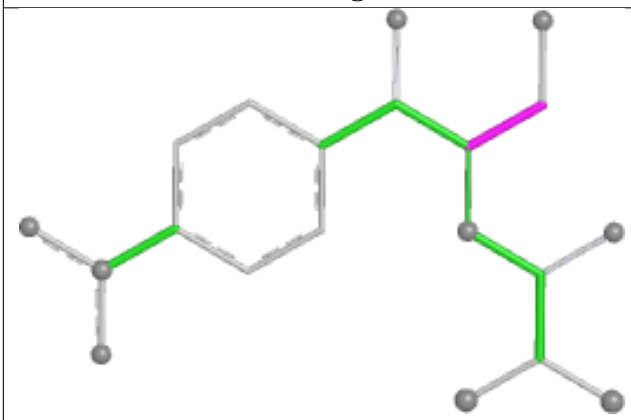
Ligand CLM 1A 4097



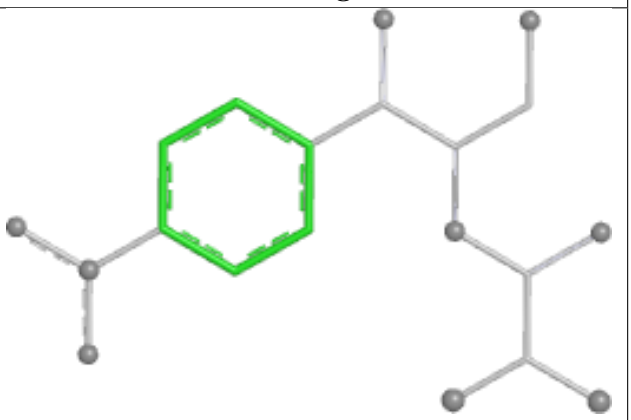
Bond lengths



Bond angles

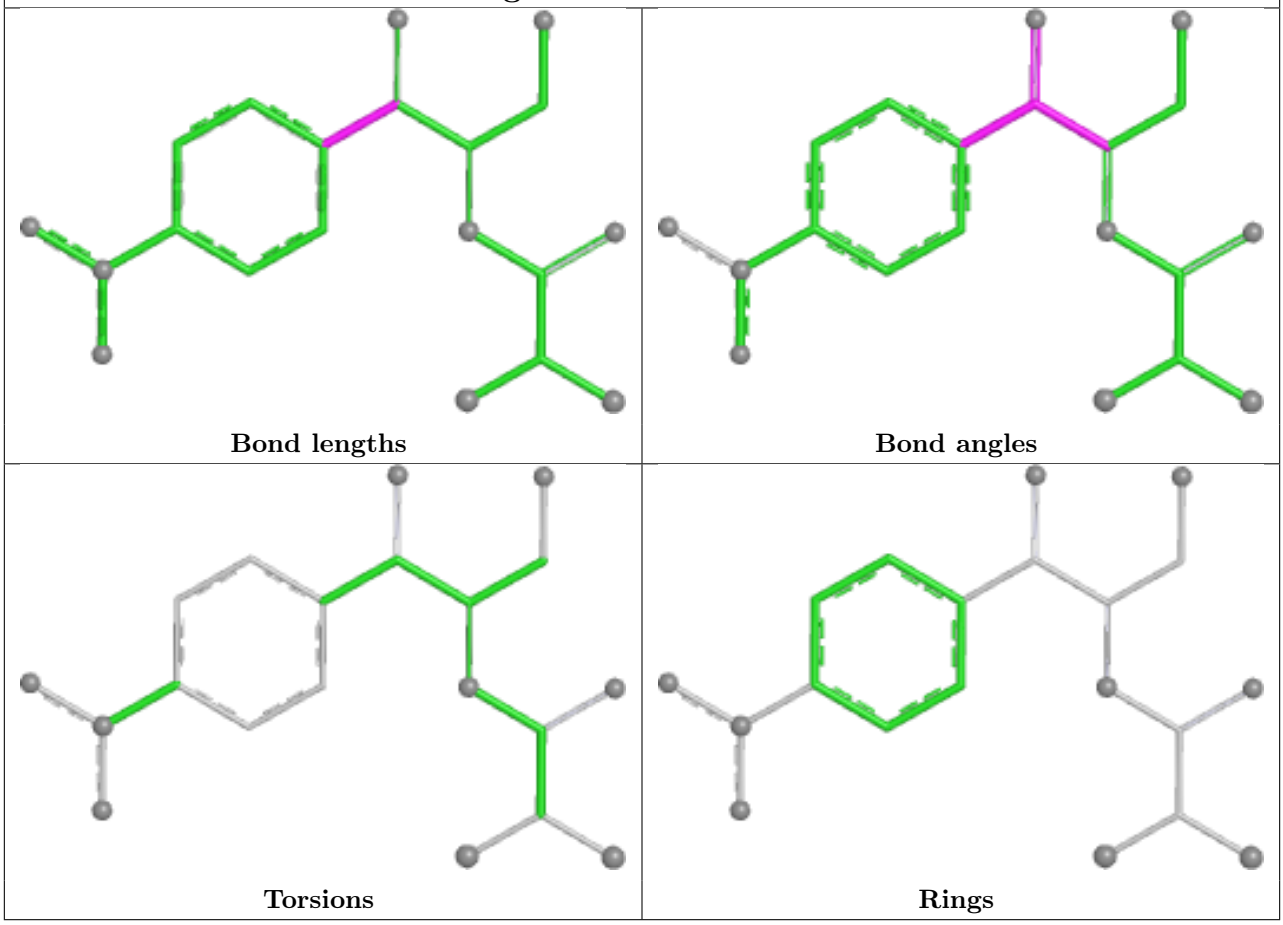


Torsions



Rings

Ligand CLM 2A 3863



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, 95^{th} 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%)	-0.45	125 (4%) 39 39	23, 38, 94, 106	0
1	2A	2789/2915 (95%)	0.08	116 (4%) 40 41	34, 60, 92, 105	0
2	1B	120/121 (99%)	-0.33	0 100 100	31, 52, 67, 87	0
2	2B	120/121 (99%)	0.81	0 100 100	65, 79, 87, 91	0
3	1D	275/276 (99%)	0.05	4 (1%) 72 73	24, 40, 54, 72	0
3	2D	275/276 (99%)	0.48	8 (2%) 53 55	33, 53, 66, 81	0
4	1E	204/206 (99%)	-0.05	1 (0%) 87 89	20, 42, 61, 73	0
4	2E	204/206 (99%)	0.53	4 (1%) 65 65	36, 60, 71, 83	0
5	1F	202/210 (96%)	0.10	1 (0%) 87 89	21, 45, 68, 80	0
5	2F	202/210 (96%)	0.61	3 (1%) 72 73	39, 70, 80, 86	0
6	1G	181/182 (99%)	0.75	13 (7%) 21 20	43, 61, 75, 86	0
6	2G	181/182 (99%)	1.39	33 (18%) 3 3	70, 79, 85, 91	0
7	1H	174/180 (96%)	0.38	3 (1%) 69 69	40, 54, 66, 72	0
7	2H	174/180 (96%)	1.44	39 (22%) 2 2	70, 81, 88, 95	0
8	1I	146/148 (98%)	0.85	6 (4%) 41 42	43, 73, 81, 84	0
8	2I	146/148 (98%)	1.37	28 (19%) 3 2	59, 74, 81, 84	0
9	1N	140/140 (100%)	0.06	2 (1%) 73 74	27, 40, 60, 72	0
9	2N	140/140 (100%)	0.95	10 (7%) 22 21	47, 66, 77, 84	0
10	1O	122/122 (100%)	0.16	1 (0%) 82 84	32, 42, 60, 66	0
10	2O	122/122 (100%)	0.53	0 100 100	45, 59, 71, 75	0
11	1P	149/150 (99%)	0.20	2 (1%) 75 75	23, 48, 67, 74	0
11	2P	149/150 (99%)	0.80	7 (4%) 36 36	41, 69, 82, 87	0
12	1Q	141/141 (100%)	0.03	1 (0%) 84 86	26, 43, 58, 72	0
12	2Q	141/141 (100%)	1.02	11 (7%) 19 18	48, 67, 76, 83	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	27, 37, 50, 60	0
13	2R	118/118 (100%)	0.57	2 (1%) 69 69	42, 55, 64, 71	0
14	1S	110/112 (98%)	0.29	1 (0%) 81 83	41, 52, 63, 67	0
14	2S	110/112 (98%)	1.54	31 (28%) 1 1	64, 74, 80, 83	0
15	1T	131/146 (89%)	0.26	4 (3%) 51 52	32, 47, 68, 79	0
15	2T	131/146 (89%)	0.70	4 (3%) 51 52	51, 61, 76, 80	0
16	1U	116/118 (98%)	-0.23	1 (0%) 81 83	23, 33, 49, 61	0
16	2U	116/118 (98%)	0.80	2 (1%) 69 69	48, 62, 75, 79	0
17	1V	101/101 (100%)	0.03	2 (1%) 65 65	26, 42, 58, 70	0
17	2V	101/101 (100%)	1.04	8 (7%) 18 18	47, 70, 76, 87	0
18	1W	112/113 (99%)	-0.10	2 (1%) 67 68	27, 35, 53, 75	0
18	2W	112/113 (99%)	0.48	3 (2%) 56 57	41, 51, 69, 90	0
19	1X	95/96 (98%)	0.14	3 (3%) 50 51	29, 40, 64, 81	0
19	2X	95/96 (98%)	0.90	7 (7%) 20 19	48, 62, 77, 86	0
20	1Y	107/110 (97%)	0.33	1 (0%) 81 83	38, 51, 68, 79	0
20	2Y	107/110 (97%)	1.15	16 (14%) 5 5	63, 71, 80, 86	0
21	1Z	154/206 (74%)	0.84	14 (9%) 15 14	42, 64, 85, 88	0
21	2Z	160/206 (77%)	1.51	43 (26%) 1 1	64, 80, 89, 93	0
22	10	83/85 (97%)	0.17	3 (3%) 46 47	29, 40, 57, 64	0
22	20	83/85 (97%)	1.29	12 (14%) 6 5	46, 65, 74, 80	0
23	11	97/98 (98%)	0.33	1 (1%) 79 80	28, 47, 71, 74	0
23	21	97/98 (98%)	0.96	6 (6%) 26 26	40, 59, 74, 78	0
24	12	70/72 (97%)	0.37	1 (1%) 73 74	38, 50, 62, 73	0
24	22	70/72 (97%)	0.91	3 (4%) 40 40	61, 71, 77, 79	0
25	13	59/60 (98%)	-0.01	0 100 100	28, 39, 58, 70	0
25	23	59/60 (98%)	0.93	4 (6%) 23 22	58, 67, 75, 79	0
26	14	69/71 (97%)	1.28	14 (20%) 3 2	53, 76, 86, 88	0
26	24	69/71 (97%)	1.76	24 (34%) 1 0	78, 85, 90, 94	0
27	15	59/60 (98%)	-0.15	0 100 100	21, 35, 51, 59	0
27	25	59/60 (98%)	0.56	0 100 100	39, 53, 68, 75	0
28	16	53/54 (98%)	-0.04	0 100 100	33, 45, 59, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.78	5 (9%) 14 13	55, 64, 70, 71	0
29	17	48/49 (97%)	-0.10	4 (8%) 17 17	24, 31, 53, 64	0
29	27	48/49 (97%)	0.36	3 (6%) 26 25	34, 44, 64, 76	0
30	18	64/65 (98%)	-0.11	0 100 100	27, 37, 45, 57	0
30	28	64/65 (98%)	0.75	1 (1%) 70 71	45, 58, 64, 68	0
31	19	37/37 (100%)	-0.13	0 100 100	33, 42, 56, 63	0
31	29	37/37 (100%)	1.08	4 (10%) 11 10	61, 68, 74, 80	0
32	1a	1488/1521 (97%)	0.26	27 (1%) 67 68	38, 69, 92, 102	0
32	2a	1491/1521 (98%)	0.69	89 (5%) 27 27	52, 79, 94, 104	0
33	1b	231/256 (90%)	1.36	49 (21%) 2 2	66, 78, 85, 90	0
33	2b	231/256 (90%)	1.66	73 (31%) 1 0	73, 84, 89, 94	0
34	1c	206/239 (86%)	1.06	22 (10%) 11 10	59, 73, 82, 88	0
34	2c	206/239 (86%)	1.93	88 (42%) 0 0	76, 84, 88, 92	0
35	1d	208/209 (99%)	1.31	39 (18%) 3 2	59, 70, 78, 81	0
35	2d	208/209 (99%)	1.21	29 (13%) 6 5	63, 74, 81, 85	0
36	1e	148/162 (91%)	0.80	5 (3%) 48 49	49, 66, 74, 77	0
36	2e	148/162 (91%)	1.35	25 (16%) 4 3	67, 77, 83, 86	0
37	1f	100/101 (99%)	0.86	2 (2%) 65 65	60, 70, 77, 80	0
37	2f	100/101 (99%)	1.02	6 (6%) 27 27	62, 73, 79, 80	0
38	1g	155/156 (99%)	0.98	16 (10%) 12 11	63, 73, 83, 89	0
38	2g	155/156 (99%)	1.63	44 (28%) 1 1	73, 80, 86, 91	0
39	1h	137/138 (99%)	0.87	5 (3%) 46 47	59, 67, 74, 77	0
39	2h	137/138 (99%)	1.30	19 (13%) 6 5	69, 77, 82, 86	0
40	1i	127/128 (99%)	1.32	20 (15%) 5 4	56, 77, 83, 85	0
40	2i	127/128 (99%)	2.40	77 (60%) 0 0	73, 84, 89, 92	0
41	1j	97/105 (92%)	1.68	33 (34%) 1 0	62, 78, 84, 86	0
41	2j	96/105 (91%)	2.26	53 (55%) 0 0	72, 84, 89, 93	0
42	1k	114/129 (88%)	0.86	7 (6%) 27 26	45, 68, 77, 86	0
42	2k	114/129 (88%)	1.27	15 (13%) 7 6	57, 74, 82, 84	0
43	1l	121/132 (91%)	0.86	6 (4%) 34 33	50, 60, 69, 81	0
43	2l	121/132 (91%)	1.41	28 (23%) 2 1	61, 72, 78, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	1.23	12 (9%) 13 12	60, 72, 80, 91	0
44	2m	122/126 (96%)	1.77	33 (27%) 1 1	73, 82, 88, 93	0
45	1n	60/61 (98%)	1.19	7 (11%) 9 8	60, 70, 76, 78	0
45	2n	60/61 (98%)	2.59	37 (61%) 0 0	77, 84, 89, 90	0
46	1o	88/89 (98%)	0.94	6 (6%) 23 22	51, 66, 76, 78	0
46	2o	88/89 (98%)	0.93	8 (9%) 15 14	64, 74, 81, 84	0
47	1p	82/88 (93%)	1.46	16 (19%) 3 2	56, 72, 78, 81	0
47	2p	82/88 (93%)	1.09	7 (8%) 16 16	62, 71, 78, 83	0
48	1q	99/105 (94%)	1.29	16 (16%) 4 3	54, 69, 77, 80	0
48	2q	99/105 (94%)	1.05	7 (7%) 22 21	64, 74, 80, 87	0
49	1r	68/88 (77%)	0.69	1 (1%) 72 73	57, 68, 75, 78	0
49	2r	68/88 (77%)	1.14	6 (8%) 15 15	68, 75, 80, 82	0
50	1s	83/93 (89%)	1.34	11 (13%) 7 6	67, 75, 82, 84	0
50	2s	83/93 (89%)	2.36	54 (65%) 0 0	78, 86, 91, 94	0
51	1t	96/106 (90%)	1.32	17 (17%) 4 3	64, 72, 79, 82	0
51	2t	96/106 (90%)	0.94	6 (6%) 26 25	60, 72, 82, 84	0
52	1u	23/27 (85%)	1.27	4 (17%) 4 3	65, 71, 76, 79	0
52	2u	23/27 (85%)	2.08	11 (47%) 0 0	76, 81, 85, 86	0
53	1v	13/24 (54%)	1.15	5 (38%) 1 0	50, 71, 91, 94	0
53	2v	13/24 (54%)	2.06	5 (38%) 1 0	72, 85, 99, 101	0
54	1w	69/74 (93%)	1.25	12 (17%) 4 3	49, 93, 100, 101	0
54	2w	68/74 (91%)	1.56	10 (14%) 6 5	66, 96, 100, 101	0
55	1x	72/77 (93%)	0.42	1 (1%) 73 74	30, 68, 84, 88	0
55	2x	72/77 (93%)	0.86	3 (4%) 40 41	50, 82, 91, 97	0
56	1y	70/74 (94%)	2.19	41 (58%) 0 0	60, 98, 103, 105	0
56	2y	70/74 (94%)	2.15	42 (60%) 0 0	70, 99, 104, 104	0
All	All	20885/21740 (96%)	0.54	1802 (8%) 16 15	20, 66, 89, 106	0

All (1802) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	10.4
44	1m	124	PRO	9.7

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Mol	Chain	Res	Type	RSRZ
44	1m	123	ALA	8.4
1	2A	2111	C	7.2
44	2m	123	ALA	6.7
40	2i	102	LEU	6.5
1	1A	2115	G	6.5
1	2A	2147	G	6.5
45	2n	2	ALA	6.5
45	1n	2	ALA	6.4
38	2g	80	VAL	6.4
1	1A	2112	G	6.2
1	1A	2145	C	6.2
1	2A	2112	G	6.1
44	2m	102	ARG	6.1
1	2A	2145	C	6.1
1	2A	2115	G	6.0
33	2b	237	ALA	5.9
41	2j	65	LEU	5.8
23	11	2	SER	5.7
38	1g	80	VAL	5.7
1	2A	2117	A	5.5
7	1H	2	SER	5.4
1	2A	2113	U	5.3
45	2n	34	TYR	5.2
21	1Z	146	ILE	5.2
40	2i	66	ARG	5.1
1	1A	2113	U	5.1
44	2m	122	LYS	5.1
40	2i	5	TYR	5.1
40	2i	9	ARG	5.0
45	2n	25	VAL	5.0
1	2A	2146	C	5.0
33	2b	165	VAL	5.0
41	2j	75	ILE	4.9
3	2D	276	LYS	4.9
44	1m	122	LYS	4.9
1	1A	2803	C	4.9
45	2n	39	LEU	4.9
12	2Q	121	ALA	4.9
21	1Z	104	PHE	4.8
3	2D	2	ALA	4.8
38	2g	83	ALA	4.8
40	2i	14	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
19	1X	94	GLY	4.7
50	2s	82	GLY	4.7
26	24	56	VAL	4.7
1	2A	2127	G	4.7
40	2i	99	LEU	4.7
41	2j	47	PHE	4.6
26	24	51	ASP	4.6
1	2A	2110	G	4.6
1	2A	2167	U	4.6
22	20	3	HIS	4.6
1	1A	2146	C	4.5
41	2j	32	ALA	4.5
1	2A	2133	G	4.5
1	1A	2114	A	4.5
1	1A	2121	G	4.5
1	2A	2114	A	4.5
6	2G	3	LEU	4.5
1	2A	2160	G	4.4
1	2A	2128	C	4.4
11	2P	78	PRO	4.4
33	1b	237	ALA	4.4
1	1A	1078	U	4.4
40	1i	2	GLU	4.4
22	20	69	PHE	4.4
50	2s	22	LEU	4.4
42	2k	124	LYS	4.4
18	2W	112	GLY	4.3
33	2b	71	VAL	4.3
33	2b	236	TYR	4.3
45	2n	4	LYS	4.3
1	2A	2174	C	4.3
21	1Z	141	VAL	4.3
38	2g	85	TYR	4.3
1	1A	2120	G	4.2
34	2c	152	ILE	4.2
33	2b	230	VAL	4.2
34	2c	149	ALA	4.2
40	2i	36	TYR	4.2
34	2c	78	GLY	4.2
23	21	28	GLY	4.2
34	2c	159	GLY	4.2
44	2m	6	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
53	2v	13	A	4.2
34	2c	77	ILE	4.2
39	2h	2	LEU	4.2
51	1t	103	GLY	4.1
26	24	65	ASP	4.1
34	2c	155	GLY	4.1
26	14	56	VAL	4.1
1	2A	2170	A	4.1
1	2A	2144	U	4.1
34	1c	182	ILE	4.1
41	2j	76	ASN	4.0
1	1A	2130	U	4.0
40	2i	27	THR	4.0
40	2i	56	LEU	4.0
40	2i	109	VAL	4.0
1	2A	2143	C	4.0
22	10	6	GLY	4.0
33	2b	122	PHE	4.0
41	2j	79	ARG	4.0
40	2i	11	LYS	4.0
1	2A	2123	G	4.0
23	21	2	SER	4.0
52	2u	14	TRP	4.0
56	2y	33	U	4.0
40	2i	19	LEU	4.0
41	2j	67	THR	4.0
1	2A	2155	G	3.9
1	2A	2159	G	3.9
53	2v	12	A	3.9
44	1m	121	LYS	3.9
41	1j	98	ILE	3.9
45	2n	7	ILE	3.9
1	2A	2169	A	3.9
32	2a	1033	G	3.9
56	1y	75	C	3.9
8	2I	20	ASP	3.9
50	2s	13	ASP	3.9
1	1A	2129	C	3.9
26	24	59	PHE	3.9
20	2Y	1	MET	3.9
34	2c	163	ALA	3.9
45	2n	53	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
41	2j	42	THR	3.9
1	1A	2133	G	3.8
1	2A	2166	G	3.8
43	1l	64	TYR	3.8
44	1m	2	ALA	3.8
38	2g	16	LEU	3.8
34	2c	73	PRO	3.8
33	1b	97	TRP	3.8
34	2c	186	PHE	3.8
1	1A	2110	G	3.8
1	1A	2141	G	3.8
1	2A	2116	G	3.8
38	2g	5	ARG	3.8
56	1y	35	C	3.8
36	2e	101	ILE	3.8
34	2c	129	ALA	3.8
34	2c	2	GLY	3.8
45	2n	38	GLY	3.8
1	1A	2174	C	3.8
1	2A	2803	C	3.8
1	2A	2104	G	3.8
50	2s	30	LEU	3.8
40	2i	49	PRO	3.8
38	1g	4	ARG	3.8
1	1A	2144	U	3.8
15	1T	131	ALA	3.8
1	1A	2119	A	3.8
52	2u	11	GLY	3.8
22	20	84	LEU	3.8
1	2A	2138	C	3.8
15	1T	130	ALA	3.7
45	2n	16	PHE	3.7
1	2A	2109	U	3.7
32	2a	1532	U	3.7
1	1A	2143	C	3.7
7	2H	165	ALA	3.7
26	14	59	PHE	3.7
38	1g	82	GLY	3.7
50	2s	71	LEU	3.7
50	2s	2	PRO	3.7
56	2y	13	C	3.7
34	2c	207	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
38	2g	12	LEU	3.7
40	2i	63	ILE	3.7
35	2d	154	ASN	3.7
34	2c	190	ARG	3.7
45	2n	33	VAL	3.7
54	2w	72	C	3.7
1	1A	2116	G	3.7
1	1A	2159	G	3.7
50	1s	13	ASP	3.7
40	2i	62	TYR	3.7
53	2v	14	A	3.6
1	1A	2178	C	3.6
1	2A	2142	C	3.6
38	2g	65	ALA	3.6
38	1g	81	GLY	3.6
3	1D	276	LYS	3.6
40	2i	96	LEU	3.6
34	2c	62	ASP	3.6
1	1A	2167	U	3.6
40	2i	7	THR	3.6
3	2D	38	LYS	3.6
19	2X	95	LEU	3.6
41	2j	93	GLY	3.6
45	2n	14	PRO	3.6
1	2A	2793	G	3.6
45	2n	21	TYR	3.6
36	2e	115	VAL	3.6
38	2g	156	TRP	3.6
1	1A	2117	A	3.6
40	1i	126	SER	3.6
56	1y	15	A	3.6
33	2b	187	LEU	3.6
34	2c	157	ILE	3.6
46	2o	3	ILE	3.6
1	2A	2804	C	3.6
18	2W	60	ASN	3.6
1	1A	2792	G	3.6
1	2A	882	G	3.6
1	2A	2802	G	3.6
43	1l	126	LYS	3.6
50	2s	16	LEU	3.6
48	1q	36	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
45	2n	3	ARG	3.5
6	2G	77	ILE	3.5
32	2a	1030(B)	C	3.5
40	1i	41	VAL	3.5
50	2s	11	VAL	3.5
50	2s	79	THR	3.5
44	2m	87	TYR	3.5
21	2Z	150	LEU	3.5
46	1o	57	LEU	3.5
50	1s	71	LEU	3.5
1	1A	2123	G	3.5
1	2A	2181	G	3.5
14	2S	49	VAL	3.5
41	2j	44	VAL	3.5
50	2s	63	THR	3.5
21	1Z	149	SER	3.5
41	1j	4	ILE	3.5
6	1G	48	GLU	3.5
40	2i	17	VAL	3.5
33	2b	121	LEU	3.5
37	2f	21	LEU	3.5
33	2b	123	ALA	3.5
35	1d	195	ALA	3.5
52	2u	2	GLY	3.5
33	2b	185	ILE	3.5
35	1d	150	GLU	3.4
1	1A	2134	A	3.4
49	1r	86	VAL	3.4
19	1X	95	LEU	3.4
38	2g	2	ALA	3.4
40	2i	92	TYR	3.4
33	1b	17	PHE	3.4
40	2i	10	ARG	3.4
38	2g	84	ASN	3.4
1	1A	2135	A	3.4
1	2A	2135	A	3.4
1	1A	2147	G	3.4
38	2g	21	VAL	3.4
34	2c	87	LEU	3.4
50	2s	15	LEU	3.4
1	1A	2794	C	3.4
26	24	63	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
50	2s	4	SER	3.4
56	2y	34	C	3.4
33	2b	48	MET	3.4
1	1A	2158	A	3.4
49	2r	86	VAL	3.4
33	1b	10	LEU	3.4
1	2A	2805	G	3.4
32	2a	1202	G	3.4
1	1A	1094	U	3.4
40	2i	4	TYR	3.4
1	1A	2177	C	3.4
21	2Z	141	VAL	3.4
21	2Z	174	VAL	3.4
56	2y	38	A	3.4
35	1d	2	GLY	3.4
38	2g	82	GLY	3.4
34	2c	53	ALA	3.4
1	1A	2181	G	3.3
1	2A	2125	G	3.3
1	2A	2154	G	3.3
1	2A	2318	G	3.3
32	2a	1034	G	3.3
40	2i	33	PHE	3.3
1	2A	2175	C	3.3
56	2y	36	C	3.3
29	27	48	LYS	3.3
17	2V	20	LEU	3.3
43	1l	94	PRO	3.3
26	14	64	GLY	3.3
38	2g	76	ARG	3.3
40	2i	67	GLY	3.3
47	2p	19	ILE	3.3
44	1m	59	TYR	3.3
1	1A	2132	U	3.3
1	2A	2148	G	3.3
1	2A	2129	C	3.3
36	2e	119	LEU	3.3
40	2i	79	LEU	3.3
44	2m	90	LEU	3.3
51	1t	10	LEU	3.3
7	2H	52	VAL	3.3
52	2u	16	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
3	2D	275	LYS	3.3
33	2b	152	PHE	3.3
26	14	63	TYR	3.3
34	2c	184	TYR	3.3
32	2a	1036	G	3.3
14	2S	20	ARG	3.3
45	2n	54	PRO	3.3
56	2y	35	C	3.3
33	1b	165	VAL	3.3
36	2e	90	VAL	3.3
41	2j	34	VAL	3.3
35	1d	173	TRP	3.3
34	2c	14	ILE	3.3
41	2j	74	ILE	3.3
32	2a	1035	A	3.3
53	2v	24	A	3.3
32	2a	1257	U	3.3
14	2S	58	LEU	3.3
41	2j	88	LEU	3.3
1	1A	2165	G	3.3
40	2i	26	VAL	3.3
42	1k	14	VAL	3.3
1	1A	2164	C	3.3
34	2c	158	GLY	3.3
54	1w	70	C	3.3
56	1y	36	C	3.3
6	2G	20	ILE	3.3
33	1b	200	ILE	3.3
41	2j	38	ILE	3.3
42	2k	29	ILE	3.3
50	2s	38	SER	3.2
1	1A	1096	A	3.2
40	2i	101	PHE	3.2
53	1v	13	A	3.2
8	2I	68	LEU	3.2
38	2g	124	LEU	3.2
22	10	3	HIS	3.2
7	2H	125	VAL	3.2
45	2n	17	LYS	3.2
1	1A	2131	G	3.2
1	1A	2175	C	3.2
33	1b	188	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
11	2P	79	ARG	3.2
32	2a	1531	A	3.2
41	1j	85	LEU	3.2
4	2E	204	ALA	3.2
1	1A	2108	C	3.2
1	1A	2136	C	3.2
1	1A	2140	C	3.2
8	2I	128	LEU	3.2
36	2e	123	LEU	3.2
35	1d	138	TYR	3.2
34	2c	13	GLY	3.2
43	1l	18	VAL	3.2
50	1s	84	GLY	3.2
50	2s	33	THR	3.2
45	2n	57	ARG	3.2
1	1A	2138	C	3.2
56	2y	6	C	3.2
56	2y	26	G	3.2
14	2S	54	LEU	3.2
9	2N	9	VAL	3.2
18	1W	112	GLY	3.2
1	1A	2180	U	3.2
33	2b	214	ILE	3.2
22	20	2	ALA	3.1
40	2i	106	ALA	3.1
43	2l	51	ALA	3.1
33	2b	97	TRP	3.1
41	1j	58	ASP	3.1
43	1l	28	LYS	3.1
7	2H	128	PRO	3.1
41	2j	62	HIS	3.1
56	2y	69	C	3.1
14	2S	48	LEU	3.1
21	1Z	150	LEU	3.1
1	2A	2149	G	3.1
1	2A	2319	G	3.1
34	2c	75	VAL	3.1
34	2c	192	THR	3.1
1	2A	2189	U	3.1
34	2c	200	ALA	3.1
34	2c	10	PHE	3.1
34	2c	128	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
41	2j	53	PRO	3.1
50	2s	12	ASP	3.1
19	1X	66	LEU	3.1
33	1b	11	LEU	3.1
48	1q	31	LEU	3.1
1	1A	889	C	3.1
54	2w	2	C	3.1
34	2c	68	VAL	3.1
47	1p	2	VAL	3.1
50	2s	46	GLY	3.1
1	1A	2166	G	3.1
33	2b	201	ILE	3.1
50	2s	77	THR	3.1
1	1A	2122	U	3.1
33	2b	120	ALA	3.1
33	2b	161	ALA	3.1
21	2Z	149	SER	3.1
34	1c	2	GLY	3.1
6	2G	28	VAL	3.1
34	2c	124	ILE	3.1
1	1A	1068	G	3.1
1	1A	2160	G	3.1
1	1A	2170	A	3.1
54	2w	1	G	3.1
54	2w	15	A	3.1
56	1y	12	U	3.1
50	2s	14	HIS	3.1
52	1u	23	PRO	3.1
8	2I	38	LEU	3.1
14	2S	3	ARG	3.1
34	2c	185	GLY	3.1
8	2I	15	VAL	3.1
1	2A	888	C	3.1
35	1d	126	ILE	3.1
52	2u	13	ILE	3.1
8	2I	55	ALA	3.0
32	2a	1251	A	3.0
56	1y	27	A	3.0
56	1y	59	U	3.0
1	2A	2162	G	3.0
1	2A	2165	G	3.0
32	1a	1030(A)	G	3.0

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Mol	Chain	Res	Type	RSRZ
54	1w	71	G	3.0
14	2S	32	LEU	3.0
19	2X	94	GLY	3.0
9	2N	73	THR	3.0
1	1A	885	C	3.0
8	2I	146	ALA	3.0
32	2a	980	C	3.0
32	2a	1030	C	3.0
38	2g	147	ALA	3.0
40	2i	61	ALA	3.0
50	2s	24	ALA	3.0
56	1y	13	C	3.0
56	1y	34	C	3.0
32	2a	1030(A)	G	3.0
44	2m	100	GLY	3.0
26	14	50	VAL	3.0
33	2b	197	VAL	3.0
34	2c	195	VAL	3.0
41	2j	6	ILE	3.0
47	1p	21	VAL	3.0
40	2i	103	THR	3.0
6	1G	73	ALA	3.0
44	2m	72	ALA	3.0
1	1A	2188	C	3.0
7	2H	94	TYR	3.0
34	2c	48	TYR	3.0
41	2j	37	PRO	3.0
8	2I	44	LEU	3.0
12	2Q	10	ARG	3.0
32	1a	1257	U	3.0
52	2u	24	ARG	3.0
26	14	51	ASP	3.0
23	21	81	LYS	3.0
1	1A	2156	G	3.0
1	2A	2124	G	3.0
1	2A	2182	G	3.0
41	2j	23	ILE	3.0
42	1k	13	GLN	3.0
14	2S	98	VAL	3.0
34	1c	207	VAL	3.0
45	2n	13	THR	3.0
41	1j	62	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
35	2d	4	TYR	3.0
34	2c	52	LEU	3.0
38	2g	32	ARG	3.0
1	1A	2128	C	3.0
1	2A	886	C	3.0
39	2h	10	LEU	3.0
34	2c	199	LYS	3.0
40	2i	91	ASP	3.0
40	2i	118	LYS	3.0
47	1p	35	LYS	3.0
34	2c	198	VAL	2.9
1	2A	2120	G	2.9
56	1y	17	G	2.9
35	1d	149	ALA	2.9
36	2e	94	ALA	2.9
41	1j	32	ALA	2.9
26	24	58	ARG	2.9
34	1c	193	TYR	2.9
40	2i	95	LYS	2.9
50	2s	80	TYR	2.9
1	1A	2118	U	2.9
1	2A	2122	U	2.9
1	2A	2130	U	2.9
35	2d	2	GLY	2.9
6	2G	52	ILE	2.9
7	2H	44	VAL	2.9
34	2c	55	VAL	2.9
38	1g	9	VAL	2.9
42	1k	92	GLU	2.9
50	2s	45	VAL	2.9
41	1j	79	ARG	2.9
41	2j	43	ARG	2.9
43	2l	56	ALA	2.9
39	2h	112	LEU	2.9
42	2k	25	TYR	2.9
1	2A	2188	C	2.9
56	1y	11	U	2.9
35	2d	23	GLY	2.9
45	2n	55	GLY	2.9
1	2A	2126	A	2.9
17	2V	22	VAL	2.9
33	2b	112	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
34	2c	130	VAL	2.9
48	2q	21	VAL	2.9
33	2b	21	ARG	2.9
45	1n	3	ARG	2.9
33	1b	34	ALA	2.9
38	1g	83	ALA	2.9
45	2n	20	ALA	2.9
46	1o	19	PRO	2.9
47	1p	43	LYS	2.9
36	2e	20	GLN	2.9
20	1Y	92	ASN	2.9
21	1Z	166	SER	2.9
35	1d	152	SER	2.9
38	1g	84	ASN	2.9
39	1h	115	SER	2.9
1	2A	893	C	2.9
1	2A	2103	C	2.9
14	2S	35	ILE	2.9
33	1b	127	ILE	2.9
41	1j	74	ILE	2.9
42	2k	48	ILE	2.9
6	2G	15	VAL	2.9
6	2G	70	VAL	2.9
32	1a	1531	A	2.9
32	2a	1250	A	2.9
41	2j	46	ARG	2.9
45	2n	40	CYS	2.9
50	1s	29	ARG	2.9
35	1d	169	LYS	2.9
56	2y	46	A	2.9
21	2Z	159	PRO	2.9
40	2i	64	THR	2.9
35	2d	48	ALA	2.9
21	2Z	144	LEU	2.9
41	2j	8	LEU	2.9
1	1A	2168	G	2.9
32	2a	1002	G	2.9
39	2h	9	MET	2.9
36	2e	74	GLY	2.9
43	1l	14	GLY	2.9
33	1b	201	ILE	2.8
36	2e	130	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
38	1g	79	ARG	2.8
1	2A	2132	U	2.8
6	1G	182	LYS	2.8
48	1q	17	LYS	2.8
9	1N	9	VAL	2.8
33	2b	136	VAL	2.8
7	2H	12	PRO	2.8
34	2c	187	ALA	2.8
50	2s	5	LEU	2.8
20	2Y	5	MET	2.8
21	2Z	87	ASP	2.8
41	2j	63	PHE	2.8
26	24	67	TYR	2.8
43	2l	64	TYR	2.8
23	21	29	GLY	2.8
38	2g	81	GLY	2.8
46	1o	89	GLY	2.8
6	1G	76	SER	2.8
32	1a	1001(A)	G	2.8
32	2a	1026	G	2.8
50	2s	35	SER	2.8
1	1A	2172	U	2.8
7	2H	17	VAL	2.8
55	2x	47	U	2.8
41	2j	41	PRO	2.8
1	1A	1064	C	2.8
1	1A	2179	C	2.8
1	2A	2896	C	2.8
50	2s	75	ALA	2.8
22	10	7	LEU	2.8
34	2c	33	LEU	2.8
38	1g	12	LEU	2.8
8	2I	82	ARG	2.8
38	2g	62	PHE	2.8
40	2i	20	ARG	2.8
34	1c	81	GLY	2.8
35	2d	68	TYR	2.8
48	2q	95	TYR	2.8
35	1d	77	ASN	2.8
38	2g	42	ILE	2.8
40	2i	28	VAL	2.8
42	2k	30	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	1A	2101	G	2.8
1	2A	883	G	2.8
1	2A	2168	G	2.8
32	1a	1036	G	2.8
54	1w	4	G	2.8
56	1y	1	G	2.8
56	2y	1	G	2.8
9	2N	112	LEU	2.8
40	2i	43	ALA	2.8
56	2y	75	C	2.8
1	2A	2173	A	2.8
24	22	1	MET	2.8
41	1j	86	MET	2.8
47	1p	82	GLN	2.8
25	23	29	ARG	2.8
50	2s	18	LYS	2.8
21	2Z	171	ILE	2.8
26	14	67	TYR	2.8
33	2b	80	ILE	2.8
45	2n	42	ILE	2.8
14	2S	85	VAL	2.8
40	2i	108	VAL	2.8
41	2j	91	PRO	2.8
43	2l	43	VAL	2.8
50	1s	9	VAL	2.8
9	2N	43	THR	2.8
21	2Z	172	ALA	2.8
33	2b	73	THR	2.8
32	1a	204	U	2.8
33	2b	77	ALA	2.8
39	1h	2	LEU	2.8
41	2j	27	ALA	2.8
56	1y	45	U	2.8
1	1A	2149	G	2.8
1	2A	2121	G	2.8
32	2a	1032	G	2.8
1	1A	2804	C	2.8
40	2i	2	GLU	2.8
41	1j	84	GLN	2.8
41	2j	60	ARG	2.8
41	2j	54	PHE	2.8
50	2s	72	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
34	2c	84	ILE	2.7
34	2c	134	ILE	2.7
41	2j	82	ILE	2.7
33	2b	91	PRO	2.7
41	2j	59	SER	2.7
3	2D	205	VAL	2.7
33	2b	215	LEU	2.7
51	2t	99	LEU	2.7
36	1e	138	ALA	2.7
40	1i	13	ALA	2.7
47	1p	1	MET	2.7
18	2W	92	ARG	2.7
54	1w	1	G	2.7
1	1A	888	C	2.7
1	1A	2173	A	2.7
1	2A	2105	C	2.7
1	2A	2119	A	2.7
53	1v	12	A	2.7
56	1y	74	C	2.7
26	14	49	PHE	2.7
31	29	37	GLY	2.7
34	2c	205	GLY	2.7
47	1p	80	PHE	2.7
34	2c	182	ILE	2.7
43	2l	8	ASN	2.7
7	2H	134	SER	2.7
14	2S	46	VAL	2.7
33	1b	229	VAL	2.7
37	1f	88	VAL	2.7
40	1i	114	TYR	2.7
45	2n	18	VAL	2.7
50	2s	67	VAL	2.7
21	2Z	157	LEU	2.7
35	1d	188	LEU	2.7
34	2c	168	ALA	2.7
35	2d	165	MET	2.7
50	2s	66	MET	2.7
38	2g	4	ARG	2.7
43	2l	41	ARG	2.7
41	1j	64	GLU	2.7
1	1A	1081	U	2.7
47	2p	82	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	1A	2157	G	2.7
20	2Y	80	GLY	2.7
32	2a	976	G	2.7
32	2a	1031	G	2.7
32	2a	1048	G	2.7
35	1d	23	GLY	2.7
50	2s	84	GLY	2.7
56	2y	5	G	2.7
1	1A	548	A	2.7
1	1A	2142	C	2.7
1	2A	2134	A	2.7
32	2a	1254	C	2.7
56	2y	70	C	2.7
41	1j	78	ASN	2.7
7	2H	19	VAL	2.7
33	1b	230	VAL	2.7
33	2b	184	VAL	2.7
34	2c	86	VAL	2.7
34	2c	135	LYS	2.7
52	1u	21	TYR	2.7
40	1i	66	ARG	2.7
40	1i	106	ALA	2.7
40	2i	46	ALA	2.7
41	1j	100	THR	2.7
44	2m	105	THR	2.7
45	2n	29	ARG	2.7
1	2A	2897	U	2.7
32	2a	1150	U	2.7
34	2c	41	GLY	2.7
6	2G	141	PHE	2.7
21	2Z	146	ILE	2.7
26	24	49	PHE	2.7
43	2l	32	PHE	2.7
1	2A	2139	C	2.7
1	2A	2183	C	2.7
32	2a	1357	A	2.7
44	2m	121	LYS	2.7
56	2y	48	C	2.7
35	2d	133	VAL	2.7
39	2h	97	VAL	2.7
40	2i	16	ARG	2.7
40	2i	42	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
6	1G	146	TYR	2.7
6	2G	146	TYR	2.7
14	2S	79	ALA	2.7
40	2i	13	ALA	2.7
40	2i	76	ALA	2.7
44	1m	105	THR	2.7
50	2s	48	THR	2.7
33	1b	19	HIS	2.7
34	2c	6	HIS	2.7
1	2A	2118	U	2.7
56	2y	19	U	2.7
17	2V	50	PRO	2.6
33	2b	17	PHE	2.6
35	2d	206	PHE	2.6
41	2j	86	MET	2.6
42	2k	126	ARG	2.6
1	2A	899	A	2.6
32	2a	1001	A	2.6
41	1j	34	VAL	2.6
56	2y	37	A	2.6
1	1A	1059	G	2.6
1	1A	2207	G	2.6
32	2a	1038	C	2.6
32	2a	1109	C	2.6
41	1j	83	GLU	2.6
54	2w	71	G	2.6
56	1y	22	G	2.6
26	14	32	TYR	2.6
33	1b	236	TYR	2.6
40	2i	114	TYR	2.6
47	2p	38	TYR	2.6
50	2s	52	TYR	2.6
50	2s	34	TRP	2.6
1	1A	2897	U	2.6
33	2b	14	GLY	2.6
40	2i	100	GLY	2.6
40	2i	18	PHE	2.6
40	2i	59	PHE	2.6
6	1G	82	LEU	2.6
11	1P	105	LEU	2.6
17	2V	94	LEU	2.6
1	2A	885	C	2.6

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Mol	Chain	Res	Type	RSRZ
32	2a	1149	C	2.6
34	2c	60	ALA	2.6
34	2c	160	ALA	2.6
40	2i	45	ALA	2.6
54	1w	72	C	2.6
19	2X	69	TYR	2.6
34	2c	193	TYR	2.6
38	2g	154	TYR	2.6
46	1o	69	TYR	2.6
56	2y	52	G	2.6
41	2j	55	LYS	2.6
51	1t	47	GLY	2.6
35	1d	191	ARG	2.6
40	2i	128	ARG	2.6
51	2t	98	PRO	2.6
51	1t	63	ILE	2.6
20	2Y	89	PHE	2.6
33	2b	70	PHE	2.6
8	1I	38	LEU	2.6
14	2S	80	LEU	2.6
33	1b	187	LEU	2.6
38	1g	59	LEU	2.6
46	1o	66	LEU	2.6
36	2e	55	VAL	2.6
44	2m	117	VAL	2.6
40	2i	126	SER	2.6
3	1D	2	ALA	2.6
21	2Z	173	ALA	2.6
33	2b	34	ALA	2.6
51	1t	95	ALA	2.6
48	1q	45	HIS	2.6
1	1A	2185	C	2.6
32	2a	1116	C	2.6
32	2a	1260	C	2.6
38	1g	85	TYR	2.6
41	1j	57	LYS	2.6
1	1A	2793	G	2.6
1	2A	2106	G	2.6
33	2b	131	PRO	2.6
34	2c	109	PRO	2.6
50	2s	68	GLY	2.6
52	2u	6	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
8	2I	88	ILE	2.6
26	24	31	ILE	2.6
45	2n	36	PHE	2.6
8	2I	12	LEU	2.6
21	2Z	91	LEU	2.6
22	20	75	LEU	2.6
35	1d	192	GLU	2.6
37	2f	61	LEU	2.6
38	1g	124	LEU	2.6
6	2G	160	VAL	2.6
19	2X	81	VAL	2.6
33	1b	136	VAL	2.6
39	2h	15	ASN	2.6
6	2G	158	ALA	2.6
22	20	43	THR	2.6
1	1A	899	A	2.6
1	1A	2176	A	2.6
1	2A	2801(A)	A	2.6
33	2b	199	TYR	2.6
38	2g	41	ARG	2.5
45	2n	31	ARG	2.5
1	1A	2104	G	2.5
1	1A	2127	G	2.5
1	1A	2162	G	2.5
1	2A	2893	G	2.5
7	2H	136	ILE	2.5
32	1a	346	G	2.5
41	1j	75	ILE	2.5
44	2m	78	ILE	2.5
54	2w	26	G	2.5
14	2S	12	PHE	2.5
33	1b	129	GLU	2.5
33	2b	57	PHE	2.5
34	2c	90	GLU	2.5
40	2i	110	GLU	2.5
48	1q	71	PHE	2.5
28	26	11	LEU	2.5
32	2a	1358	U	2.5
33	2b	221	LEU	2.5
56	2y	12	U	2.5
39	2h	79	VAL	2.5
40	2i	73	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
42	2k	117	ASN	2.5
8	1I	146	ALA	2.5
20	2Y	105	ALA	2.5
34	2c	4	LYS	2.5
34	2c	24	ALA	2.5
40	2i	94	ALA	2.5
41	2j	26	ALA	2.5
44	1m	120	LYS	2.5
44	2m	76	ALA	2.5
41	2j	48	THR	2.5
1	1A	1095	A	2.5
21	1Z	1	MET	2.5
32	1a	1001	A	2.5
33	2b	92	TYR	2.5
53	2v	15	A	2.5
6	2G	2	PRO	2.5
20	2Y	53	PRO	2.5
40	1i	90	PRO	2.5
48	1q	28	PRO	2.5
1	1A	898	C	2.5
1	2A	2136	C	2.5
32	2a	972	C	2.5
34	2c	167	TRP	2.5
38	1g	156	TRP	2.5
40	2i	105	ASP	2.5
42	1k	36	ASP	2.5
50	1s	26	GLY	2.5
6	1G	77	ILE	2.5
21	2Z	53	ILE	2.5
33	2b	127	ILE	2.5
33	2b	211	ILE	2.5
33	2b	163	PHE	2.5
1	2A	171	G	2.5
1	2A	1171	G	2.5
32	2a	630	G	2.5
34	1c	33	LEU	2.5
36	2e	12	LEU	2.5
41	2j	71	LEU	2.5
43	2l	60	LEU	2.5
45	2n	6	LEU	2.5
56	2y	45	U	2.5
21	2Z	86	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
33	1b	15	VAL	2.5
41	2j	49	VAL	2.5
42	2k	105	VAL	2.5
45	2n	49	HIS	2.5
50	2s	25	LYS	2.5
51	2t	9	ASN	2.5
8	2I	46	ALA	2.5
29	27	45	ALA	2.5
45	2n	30	ALA	2.5
44	2m	86	CYS	2.5
45	2n	35	ARG	2.5
1	2A	1847	A	2.5
8	2I	16	GLY	2.5
21	1Z	160	GLY	2.5
32	2a	1256	A	2.5
34	2c	9	GLY	2.5
44	1m	68	GLY	2.5
51	1t	69	GLY	2.5
53	1v	14	A	2.5
33	1b	9	GLU	2.5
1	2A	894	C	2.5
47	2p	48	TRP	2.5
54	2w	25	C	2.5
56	2y	56	C	2.5
4	2E	195	LEU	2.5
8	2I	75	LEU	2.5
33	2b	11	LEU	2.5
38	1g	26	PHE	2.5
40	2i	37	PHE	2.5
50	1s	15	LEU	2.5
1	1A	1066	U	2.5
1	1A	1082	U	2.5
50	2s	9	VAL	2.5
1	1A	2182	G	2.5
1	2A	2141	G	2.5
32	2a	1001(A)	G	2.5
32	2a	1024	G	2.5
56	1y	5	G	2.5
56	1y	39	G	2.5
7	2H	156	ALA	2.5
47	1p	81	ARG	2.5
6	2G	76	SER	2.5

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Mol	Chain	Res	Type	RSRZ
36	2e	16	THR	2.5
35	1d	33	MET	2.5
33	2b	234	PRO	2.5
36	2e	22	GLY	2.5
36	2e	99	GLY	2.5
20	2Y	55	TYR	2.5
26	24	25	TYR	2.5
42	1k	25	TYR	2.5
7	2H	9	ILE	2.5
1	1A	1057	A	2.5
54	1w	15	A	2.5
56	1y	21	A	2.5
56	1y	24	A	2.5
6	2G	53	LEU	2.5
21	2Z	33	LEU	2.5
12	2Q	104	PHE	2.5
1	1A	652(S)	C	2.5
1	1A	2111	C	2.5
1	2A	2137	C	2.5
1	2A	2179	C	2.5
41	2j	68	HIS	2.5
6	2G	92	VAL	2.5
7	2H	114	VAL	2.5
9	1N	140	VAL	2.5
1	2A	2102	U	2.5
6	2G	163	ALA	2.5
14	2S	55	ALA	2.5
21	2Z	7	ALA	2.5
34	2c	189	ALA	2.5
35	2d	164	ALA	2.5
44	2m	118	ALA	2.5
21	2Z	170	THR	2.5
1	1A	2805	G	2.5
1	2A	11	G	2.5
26	24	66	SER	2.5
33	2b	67	THR	2.5
34	2c	154	SER	2.5
41	1j	42	THR	2.5
41	2j	15	THR	2.5
33	1b	232	PRO	2.4
7	2H	124	GLU	2.4
26	24	64	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
33	1b	14	GLY	2.4
34	2c	194	GLY	2.4
41	1j	93	GLY	2.4
44	2m	68	GLY	2.4
50	2s	8	GLY	2.4
6	1G	114	ILE	2.4
7	1H	175	LYS	2.4
13	2R	69	ASP	2.4
21	1Z	120	ILE	2.4
22	20	5	LYS	2.4
34	1c	14	ILE	2.4
40	2i	125	TYR	2.4
46	2o	87	ILE	2.4
51	1t	55	ILE	2.4
8	2I	140	LEU	2.4
33	2b	196	LEU	2.4
34	2c	47	LEU	2.4
35	2d	196	LEU	2.4
38	2g	38	LEU	2.4
40	2i	40	LEU	2.4
1	1A	2169	A	2.4
45	2n	37	PHE	2.4
56	1y	14	A	2.4
15	1T	115	ARG	2.4
35	2d	122	ARG	2.4
1	1A	2161	C	2.4
7	2H	79	VAL	2.4
1	1A	2150	U	2.4
6	2G	50	ALA	2.4
9	2N	57	ALA	2.4
38	2g	89	MET	2.4
49	2r	20	ALA	2.4
54	2w	73	U	2.4
56	1y	19	U	2.4
47	1p	45	THR	2.4
41	2j	35	SER	2.4
24	12	11	GLU	2.4
1	2A	1533	G	2.4
1	2A	2807	G	2.4
3	2D	5	LYS	2.4
32	2a	1220	G	2.4
35	2d	167	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
40	2i	68	GLY	2.4
45	2n	9	LYS	2.4
56	2y	4	G	2.4
34	2c	5	ILE	2.4
7	2H	88	LEU	2.4
21	2Z	9	TYR	2.4
24	22	70	GLN	2.4
33	2b	154	LEU	2.4
34	2c	12	LEU	2.4
35	1d	19	LEU	2.4
35	2d	155	LEU	2.4
39	1h	59	LEU	2.4
47	1p	6	LEU	2.4
40	2i	104	ARG	2.4
46	2o	64	ARG	2.4
1	1A	229	A	2.4
1	1A	887	A	2.4
32	2a	1447	A	2.4
8	2I	19	VAL	2.4
21	2Z	71	VAL	2.4
29	17	46	VAL	2.4
1	2A	884	C	2.4
32	2a	1362	C	2.4
45	1n	20	ALA	2.4
41	2j	87	THR	2.4
40	2i	98	PRO	2.4
26	14	69	LYS	2.4
33	1b	223	ILE	2.4
1	2A	271(M)	G	2.4
6	2G	172	LEU	2.4
16	1U	117	GLN	2.4
21	2Z	5	LEU	2.4
33	1b	221	LEU	2.4
35	2d	162	LEU	2.4
41	1j	88	LEU	2.4
41	2j	40	LEU	2.4
44	2m	66	LEU	2.4
50	2s	20	LEU	2.4
26	24	61	ARG	2.4
50	2s	29	ARG	2.4
26	14	43	TYR	2.4
34	2c	29	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
42	2k	75	TYR	2.4
38	2g	26	PHE	2.4
5	2F	6	VAL	2.4
40	1i	109	VAL	2.4
44	2m	54	VAL	2.4
48	2q	85	VAL	2.4
32	1a	1447	A	2.4
38	2g	37	ASN	2.4
34	1c	113	ALA	2.4
44	2m	64	TRP	2.4
44	2m	75	ALA	2.4
51	1t	59	ALA	2.4
33	2b	231	GLU	2.4
41	1j	81	THR	2.4
1	1A	1075	C	2.4
1	1A	2102	U	2.4
1	2A	1026	U	2.4
1	2A	2108	C	2.4
7	2H	84	SER	2.4
8	1I	91	SER	2.4
32	2a	950	U	2.4
32	2a	1000	U	2.4
32	2a	1114	C	2.4
50	2s	42	PRO	2.4
45	1n	32	SER	2.4
56	1y	69	C	2.4
4	2E	10	GLY	2.4
12	1Q	15	GLY	2.4
12	2Q	61	GLY	2.4
43	2l	29	GLY	2.4
41	1j	82	ILE	2.4
41	1j	96	ILE	2.4
50	2s	31	ILE	2.4
50	2s	62	ILE	2.4
5	2F	148	LEU	2.4
8	2I	116	LEU	2.4
33	1b	21	ARG	2.4
38	2g	13	GLN	2.4
38	2g	99	LEU	2.4
1	1A	1176	G	2.4
1	1A	2802	G	2.4
33	1b	33	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
34	1c	48	TYR	2.4
8	2I	37	VAL	2.4
22	20	30	VAL	2.4
25	23	9	VAL	2.4
33	1b	7	VAL	2.4
33	2b	229	VAL	2.4
44	2m	7	VAL	2.4
42	1k	117	ASN	2.4
8	2I	53	ALA	2.4
12	2Q	28	ALA	2.4
32	2a	1503	A	2.4
33	1b	134	GLU	2.4
33	2b	170	GLU	2.4
54	1w	23	A	2.4
33	1b	125	PRO	2.3
35	1d	40	PRO	2.3
45	2n	22	THR	2.3
34	2c	144	SER	2.3
1	2A	2180	U	2.3
32	1a	1532	U	2.3
31	29	21	GLY	2.3
32	1a	1028	C	2.3
32	2a	1045	C	2.3
51	1t	102	GLY	2.3
51	2t	103	GLY	2.3
56	1y	48	C	2.3
6	1G	51	ARG	2.3
14	1S	3	ARG	2.3
14	2S	97	ARG	2.3
26	14	55	ARG	2.3
26	24	5	ILE	2.3
38	1g	5	ARG	2.3
43	2l	100	ILE	2.3
44	2m	84	ILE	2.3
50	2s	78	ARG	2.3
34	1c	12	LEU	2.3
34	2c	94	LEU	2.3
48	2q	98	LEU	2.3
38	2g	151	TYR	2.3
47	1p	38	TYR	2.3
6	2G	37	VAL	2.3
7	2H	45	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
34	2c	153	VAL	2.3
39	2h	61	VAL	2.3
40	1i	113	LYS	2.3
45	1n	4	LYS	2.3
1	1A	1058	G	2.3
32	1a	630	G	2.3
32	2a	1283	G	2.3
35	1d	154	ASN	2.3
56	1y	18	G	2.3
6	1G	151	ALA	2.3
35	1d	163	GLU	2.3
38	2g	40	ALA	2.3
45	1n	30	ALA	2.3
56	1y	23	A	2.3
56	1y	46	A	2.3
56	2y	29	A	2.3
56	2y	44	A	2.3
41	2j	30	SER	2.3
45	2n	19	ARG	2.3
48	2q	97	SER	2.3
15	2T	69	GLY	2.3
50	2s	81	ARG	2.3
51	1t	101	GLY	2.3
9	2N	69	GLN	2.3
32	2a	1211	U	2.3
14	2S	110	LEU	2.3
34	2c	8	ILE	2.3
34	2c	178	LEU	2.3
34	2c	188	LEU	2.3
35	1d	5	ILE	2.3
40	2i	50	LEU	2.3
1	2A	1536	C	2.3
38	2g	33	ASP	2.3
40	1i	91	ASP	2.3
54	1w	66	C	2.3
33	1b	48	MET	2.3
3	1D	38	LYS	2.3
21	2Z	136	PHE	2.3
33	1b	133	LYS	2.3
7	2H	157	TYR	2.3
33	2b	93	VAL	2.3
36	2e	51	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
37	2f	59	TYR	2.3
43	2l	82	VAL	2.3
48	1q	85	VAL	2.3
48	2q	35	VAL	2.3
21	1Z	51	ALA	2.3
33	1b	167	PRO	2.3
38	2g	117	ALA	2.3
40	2i	52	ALA	2.3
44	1m	30	ALA	2.3
1	2A	2101	G	2.3
1	2A	2156	G	2.3
41	1j	87	THR	2.3
43	2l	44	THR	2.3
41	2j	45	ARG	2.3
51	1t	8	ARG	2.3
56	1y	7	G	2.3
56	2y	18	G	2.3
56	2y	57	G	2.3
28	26	42	TRP	2.3
32	1a	1030(D)	A	2.3
33	1b	227	GLY	2.3
40	2i	72	GLY	2.3
41	2j	31	GLY	2.3
18	1W	111	HIS	2.3
21	2Z	121	HIS	2.3
34	2c	31	HIS	2.3
6	2G	175	LEU	2.3
7	2H	7	LEU	2.3
24	22	10	LEU	2.3
35	1d	120	LEU	2.3
35	1d	194	LEU	2.3
40	1i	19	LEU	2.3
41	2j	50	ILE	2.3
43	2l	10	LEU	2.3
49	2r	65	ILE	2.3
50	1s	20	LEU	2.3
1	1A	1060	U	2.3
1	1A	1065	U	2.3
32	2a	992	U	2.3
56	1y	43	U	2.3
19	2X	1	MET	2.3
1	1A	1076	C	2.3

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Mol	Chain	Res	Type	RSRZ
32	2a	999	C	2.3
32	2a	1019	C	2.3
32	2a	1054	C	2.3
33	2b	169	LYS	2.3
56	1y	72	C	2.3
6	2G	38	VAL	2.3
8	1I	142	VAL	2.3
20	2Y	42	VAL	2.3
21	1Z	139	VAL	2.3
35	1d	128	VAL	2.3
44	2m	58	GLU	2.3
34	1c	23	TYR	2.3
6	2G	46	ALA	2.3
34	1c	60	ALA	2.3
34	2c	137	ALA	2.3
38	2g	93	PRO	2.3
51	2t	94	ALA	2.3
44	2m	104	ARG	2.3
52	1u	24	ARG	2.3
20	2Y	57	GLN	2.3
35	1d	171	GLY	2.3
43	2l	63	GLY	2.3
44	2m	101	GLN	2.3
47	1p	78	GLY	2.3
50	2s	47	HIS	2.3
52	2u	4	GLY	2.3
1	2A	892	G	2.3
1	2A	2206	G	2.3
32	2a	1053	G	2.3
32	2a	1117	G	2.3
32	2a	1224	G	2.3
32	2a	1356	G	2.3
1	2A	528	A	2.3
6	2G	29	TRP	2.3
7	2H	98	LEU	2.3
8	2I	9	LEU	2.3
34	2c	196	LEU	2.3
35	1d	157	LEU	2.3
35	2d	135	LEU	2.3
37	2f	45	LEU	2.3
41	2j	90	LEU	2.3
54	1w	7	G	2.3

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Mol	Chain	Res	Type	RSRZ
56	1y	10	G	2.3
56	2y	30	G	2.3
54	2w	24	A	2.3
7	2H	175	LYS	2.3
12	2Q	22	LYS	2.3
14	2S	33	LYS	2.3
20	2Y	54	LYS	2.3
34	2c	45	LYS	2.3
1	1A	2189	U	2.3
32	1a	163	C	2.3
32	1a	999	C	2.3
38	2g	43	PHE	2.3
48	1q	27	PHE	2.3
55	2x	1	C	2.3
8	2I	107	VAL	2.3
17	2V	33	VAL	2.3
34	2c	151	VAL	2.3
34	2c	173	VAL	2.3
35	1d	148	VAL	2.3
21	2Z	15	PRO	2.3
21	2Z	95	PRO	2.3
9	2N	45	ASN	2.2
11	1P	15	ARG	2.3
25	23	35	ARG	2.3
29	17	47	ARG	2.3
40	1i	9	ARG	2.3
43	2l	94	PRO	2.3
50	2s	50	ALA	2.2
52	2u	17	THR	2.2
4	2E	161	GLY	2.2
20	2Y	25	GLY	2.2
26	24	45	GLY	2.2
26	24	54	GLY	2.2
3	1D	275	LYS	2.2
11	2P	135	LEU	2.2
16	2U	62	ILE	2.2
22	20	49	LYS	2.2
35	1d	83	SER	2.2
37	2f	89	MET	2.2
38	2g	77	SER	2.2
41	1j	30	SER	2.2
42	2k	16	SER	2.2

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Mol	Chain	Res	Type	RSRZ
43	2l	54	LYS	2.2
48	1q	98	LEU	2.2
51	1t	53	LEU	2.2
51	1t	84	LEU	2.2
1	1A	1098	A	2.2
1	1A	2126	A	2.2
1	2A	2158	A	2.2
32	2a	965	A	2.2
32	2a	983	A	2.2
32	2a	1248	A	2.2
42	2k	36	ASP	2.2
32	2a	1030(C)	G	2.2
32	2a	1127	G	2.2
56	2y	39	G	2.2
32	1a	1000	U	2.2
32	2a	1196	U	2.2
26	24	57	GLU	2.2
6	1G	83	ARG	2.2
7	2H	21	PRO	2.2
7	2H	107	VAL	2.2
11	2P	15	ARG	2.2
34	1c	106	VAL	2.2
35	1d	170	VAL	2.2
38	2g	105	VAL	2.2
40	2i	21	PRO	2.2
41	2j	28	ARG	2.2
44	1m	102	ARG	2.2
50	2s	51	VAL	2.2
55	2x	16	C	2.2
56	2y	74	C	2.2
7	2H	102	ALA	2.2
15	2T	130	ALA	2.2
41	1j	76	ASN	2.2
8	2I	29	TYR	2.2
14	2S	92	TYR	2.2
33	2b	31	TYR	2.2
35	1d	54	TYR	2.2
40	2i	117	HIS	2.2
7	2H	14	GLY	2.2
14	2S	45	GLY	2.2
21	2Z	147	GLY	2.2
40	2i	127	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
14	2S	4	LEU	2.2
26	24	9	LEU	2.2
35	1d	135	LEU	2.2
35	2d	78	LEU	2.2
49	2r	76	LEU	2.2
6	2G	157	ILE	2.2
21	2Z	153	SER	2.2
34	2c	39	ILE	2.2
36	2e	118	ILE	2.2
50	2s	49	ILE	2.2
6	1G	49	ASP	2.2
21	2Z	148	ASP	2.2
10	1O	108	GLU	2.2
32	2a	994	A	2.2
45	2n	46	GLU	2.2
53	1v	24	A	2.2
56	2y	9	A	2.2
32	2a	1020	U	2.2
32	2a	1049	U	2.2
1	1A	2125	G	2.2
1	1A	2154	G	2.2
9	2N	74	ARG	2.2
32	2a	1190	G	2.2
54	1w	3	G	2.2
14	2S	29	PHE	2.2
40	1i	18	PHE	2.2
34	2c	138	VAL	2.2
38	2g	112	PRO	2.2
40	2i	41	VAL	2.2
1	2A	2161	C	2.2
17	2V	31	ALA	2.2
19	2X	46	ALA	2.2
32	1a	1008	C	2.2
40	2i	119	ALA	2.2
44	2m	42	ALA	2.2
56	2y	68	C	2.2
14	2S	57	LYS	2.2
20	2Y	88	LYS	2.2
33	1b	16	HIS	2.2
33	2b	140	HIS	2.2
11	2P	6	LEU	2.2
21	1Z	102	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
21	2Z	41	LEU	2.2
33	2b	98	LEU	2.2
36	2e	53	LEU	2.2
37	2f	14	LEU	2.2
39	1h	133	LEU	2.2
40	2i	22	GLY	2.2
42	2k	118	GLY	2.2
46	1o	61	GLY	2.2
33	1b	80	ILE	2.2
35	2d	5	ILE	2.2
48	2q	60	ILE	2.2
51	1t	11	SER	2.2
13	2R	68	ARG	2.2
34	2c	83	ARG	2.2
35	2d	49	ARG	2.2
41	2j	66	ARG	2.2
50	2s	3	ARG	2.2
1	1A	1045	A	2.2
1	2A	2310	A	2.2
32	2a	532	A	2.2
32	2a	1213	A	2.2
32	2a	1235	U	2.2
53	1v	15	A	2.2
6	2G	80	PHE	2.2
46	2o	75	PRO	2.2
7	2H	35	VAL	2.2
7	2H	169	VAL	2.2
8	2I	3	VAL	2.2
12	2Q	106	VAL	2.2
20	2Y	45	VAL	2.2
31	29	16	VAL	2.2
41	1j	44	VAL	2.2
43	2l	24	VAL	2.2
43	2l	39	VAL	2.2
1	1A	2124	G	2.2
1	2A	2321	G	2.2
1	2A	2894	G	2.2
17	2V	85	LYS	2.2
32	1a	1034	G	2.2
33	1b	22	LYS	2.2
33	1b	40	HIS	2.2
33	1b	120	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
33	2b	186	ALA	2.2
34	2c	65	ALA	2.2
34	2c	71	ALA	2.2
34	2c	92	ALA	2.2
52	2u	3	LYS	2.2
43	2l	80	HIS	2.2
6	2G	135	LEU	2.2
12	2Q	32	TYR	2.2
23	21	98	LEU	2.2
32	2a	979	C	2.2
39	1h	62	TYR	2.2
42	2k	31	THR	2.2
40	2i	24	GLY	2.2
41	1j	90	LEU	2.2
56	1y	42	C	2.2
26	24	39	CYS	2.2
21	2Z	57	ILE	2.2
33	2b	162	ILE	2.2
33	2b	182	ILE	2.2
33	2b	200	ILE	2.2
45	1n	7	ILE	2.2
33	2b	86	GLU	2.2
47	1p	34	GLU	2.2
8	2I	27	ARG	2.2
29	27	47	ARG	2.2
48	1q	91	ARG	2.2
19	2X	85	PRO	2.2
33	1b	26	PRO	2.2
1	1A	1073	A	2.1
1	2A	12	U	2.2
14	2S	93	LYS	2.2
8	2I	92	VAL	2.1
21	2Z	105	VAL	2.1
32	1a	160	A	2.1
32	2a	975	A	2.1
34	1c	135	LYS	2.2
36	2e	45	PHE	2.2
50	2s	74	PHE	2.2
34	1c	68	VAL	2.1
36	1e	148	VAL	2.1
43	2l	18	VAL	2.1
43	2l	40	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
44	2m	98	VAL	2.1
3	2D	203	ASN	2.1
8	2I	36	ALA	2.1
26	14	60	GLN	2.1
29	17	45	ALA	2.1
33	2b	101	MET	2.1
33	2b	188	ALA	2.1
1	1A	545	G	2.1
7	1H	174	GLY	2.1
32	1a	1024	G	2.1
32	1a	1032	G	2.1
32	2a	951	G	2.1
32	2a	1042	G	2.1
32	2a	1222	G	2.1
36	1e	85	GLY	2.1
38	2g	59	LEU	2.1
45	2n	44	LEU	2.1
47	2p	6	LEU	2.1
7	2H	121	ILE	2.1
14	2S	7	TYR	2.1
35	1d	207	TYR	2.1
36	2e	109	ILE	2.1
41	1j	6	ILE	2.1
42	2k	32	ILE	2.1
50	1s	40	ILE	2.1
32	2a	1027	C	2.1
32	2a	1137	C	2.1
32	2a	1249	C	2.1
32	2a	1259	C	2.1
42	2k	119	CYS	2.1
56	2y	25	C	2.1
9	2N	83	LYS	2.1
39	2h	67	PRO	2.1
44	2m	97	PRO	2.1
50	2s	28	LYS	2.1
22	20	45	PHE	2.1
33	1b	24	TRP	2.1
33	1b	163	PHE	2.1
21	2Z	128	VAL	2.1
35	1d	92	VAL	2.1
38	2g	9	VAL	2.1
40	1i	28	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
40	1i	108	VAL	2.1
40	2i	44	VAL	2.1
40	2i	65	VAL	2.1
45	2n	56	VAL	2.1
1	1A	12	U	2.1
1	1A	1086	A	2.1
1	2A	2171	A	2.1
14	2S	38	GLN	2.1
36	2e	10	MET	2.1
48	1q	26	GLN	2.1
54	1w	73	U	2.1
56	2y	32	U	2.1
33	2b	88	ALA	2.1
35	1d	111	ALA	2.1
36	1e	21	ALA	2.1
39	2h	110	ALA	2.1
40	1i	15	ALA	2.1
51	2t	95	ALA	2.1
56	1y	44	A	2.1
56	2y	27	A	2.1
6	2G	139	LEU	2.1
20	2Y	106	LEU	2.1
26	14	54	GLY	2.1
34	2c	15	THR	2.1
36	2e	114	GLY	2.1
40	2i	39	GLY	2.1
41	2j	36	GLY	2.1
41	2j	100	THR	2.1
43	2l	88	GLY	2.1
44	2m	81	LEU	2.1
51	1t	72	LEU	2.1
8	1I	79	ILE	2.1
33	1b	42	ILE	2.1
33	1b	222	ILE	2.1
33	2b	39	ILE	2.1
33	2b	42	ILE	2.1
33	2b	208	ILE	2.1
36	1e	11	ILE	2.1
39	2h	80	ILE	2.1
47	1p	33	ILE	2.1
26	24	55	ARG	2.1
38	2g	113	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
44	2m	21	TYR	2.1
49	2r	87	ARG	2.1
1	1A	2152	G	2.1
1	1A	2155	G	2.1
1	2A	2100	G	2.1
1	2A	2153	G	2.1
1	2A	2207	G	2.1
32	2a	1003	G	2.1
56	1y	49	G	2.1
39	2h	135	CYS	2.1
1	1A	2103	C	2.1
32	1a	1027	C	2.1
39	2h	4	ASP	2.1
55	1x	1	C	2.1
56	1y	56	C	2.1
6	2G	74	LYS	2.1
15	1T	35	LYS	2.1
21	2Z	127	LYS	2.1
40	1i	21	PRO	2.1
41	1j	77	PRO	2.1
14	2S	87	PHE	2.1
35	2d	79	PHE	2.1
35	2d	110	PHE	2.1
33	1b	164	VAL	2.1
34	1c	107	GLN	2.1
35	2d	112	VAL	2.1
35	2d	119	GLN	2.1
39	2h	70	GLN	2.1
40	2i	53	VAL	2.1
43	2l	104	VAL	2.1
48	1q	21	VAL	2.1
6	2G	169	ALA	2.1
49	2r	60	ALA	2.1
28	26	20	ASN	2.1
56	2y	11	U	2.1
6	2G	120	LEU	2.1
32	2a	996	A	2.1
7	2H	48	GLY	2.1
8	1I	9	LEU	2.1
21	2Z	160	GLY	2.1
33	2b	61	LEU	2.1
35	1d	155	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
38	1g	22	LEU	2.1
51	1t	24	LEU	2.1
56	1y	58	A	2.1
56	2y	23	A	2.1
34	1c	96	GLY	2.1
35	1d	127	THR	2.1
50	1s	39	THR	2.1
7	2H	51	ARG	2.1
33	2b	130	ARG	2.1
46	2o	17	ARG	2.1
33	1b	39	ILE	2.1
33	2b	108	ILE	2.1
51	1t	100	ILE	2.1
21	2Z	29	TYR	2.1
34	1c	184	TYR	2.1
29	17	48	LYS	2.1
35	1d	84	LYS	2.1
41	2j	17	ASP	2.1
48	1q	87	LYS	2.1
17	1V	73	SER	2.1
1	1A	2153	G	2.1
32	2a	973	G	2.1
54	2w	18	G	2.1
56	2y	7	G	2.1
56	2y	51	G	2.1
25	23	2	PRO	2.1
32	1a	1030(B)	C	2.1
39	2h	89	PRO	2.1
12	2Q	35	VAL	2.1
21	1Z	136	PHE	2.1
21	2Z	88	PHE	2.1
28	26	52	VAL	2.1
34	1c	76	VAL	2.1
15	2T	116	ALA	2.1
21	2Z	21	ALA	2.1
3	2D	268	ARG	2.1
6	2G	118	ARG	2.1
32	2a	997	U	2.1
32	2a	1040	U	2.1
34	2c	127	ARG	2.1
35	2d	47	ARG	2.1
41	1j	65	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
43	2l	49	ASN	2.1
50	1s	22	LEU	2.1
21	2Z	22	GLY	2.1
40	2i	69	GLY	2.1
46	2o	86	GLY	2.1
46	2o	89	GLY	2.1
52	2u	15	ARG	2.1
6	2G	161	THR	2.1
33	1b	54	THR	2.1
47	2p	45	THR	2.1
1	1A	890	A	2.1
1	1A	1069	A	2.1
1	1A	2892	A	2.1
20	2Y	44	ILE	2.1
34	1c	77	ILE	2.1
41	1j	50	ILE	2.1
47	1p	19	ILE	2.1
44	2m	120	LYS	2.1
44	1m	23	TYR	2.1
23	21	38	SER	2.1
40	2i	90	PRO	2.1
1	1A	886	C	2.1
47	2p	16	HIS	2.1
1	1A	1056	G	2.0
1	1A	2186	G	2.0
1	2A	1042	G	2.0
32	1a	216	G	2.0
32	2a	517	G	2.0
32	2a	1047	G	2.0
32	2a	1365	G	2.0
56	1y	2	C	2.1
56	1y	67	G	2.0
56	2y	17	G	2.0
7	2H	37	VAL	2.0
21	2Z	74	VAL	2.0
21	2Z	139	VAL	2.0
34	2c	203	PHE	2.0
35	2d	121	VAL	2.0
36	2e	33	VAL	2.0
36	2e	67	VAL	2.0
41	2j	94	VAL	2.0
50	2s	10	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
7	2H	96	ALA	2.0
12	2Q	20	ALA	2.0
34	1c	61	ALA	2.0
34	2c	156	ARG	2.0
35	1d	132	ARG	2.0
35	1d	153	ARG	2.0
39	2h	84	ARG	2.0
44	2m	33	ALA	2.0
45	2n	59	ALA	2.0
5	2F	176	LEU	2.0
14	2S	61	ASN	2.0
20	2Y	90	LEU	2.0
21	2Z	67	LEU	2.0
33	2b	138	LEU	2.0
33	2b	158	LEU	2.0
33	2b	180	LEU	2.0
34	2c	91	LEU	2.0
41	2j	85	LEU	2.0
48	1q	53	LEU	2.0
6	1G	44	GLY	2.0
11	2P	34	GLY	2.0
12	2Q	33	GLY	2.0
17	1V	101	GLY	2.0
17	2V	53	GLU	2.0
22	20	76	GLY	2.0
41	1j	36	GLY	2.0
42	1k	42	TRP	2.0
47	1p	48	TRP	2.0
48	1q	8	GLY	2.0
16	2U	51	LYS	2.0
26	24	14	ILE	2.0
26	24	27	THR	2.0
36	2e	129	ILE	2.0
38	2g	27	ILE	2.0
38	2g	49	ILE	2.0
43	2l	7	ILE	2.0
1	2A	896	A	2.0
32	2a	1363(A)	A	2.0
56	2y	24	A	2.0
35	1d	102	ASP	2.0
7	2H	2	SER	2.0
7	2H	10	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
7	2H	36	PRO	2.0
8	2I	1	MET	2.0
9	2N	1	MET	2.0
21	2Z	16	SER	2.0
30	28	63	PRO	2.0
50	2s	59	PRO	2.0
50	2s	76	PRO	2.0
33	2b	16	HIS	2.0
38	2g	153	HIS	2.0
1	2A	2789	C	2.0
6	2G	128	ARG	2.0
7	2H	6	ARG	2.0
8	2I	18	VAL	2.0
32	1a	1029	C	2.0
34	2c	66	VAL	2.0
35	2d	132	ARG	2.0
35	2d	178	VAL	2.0
35	2d	198	VAL	2.0
38	2g	78	ARG	2.0
39	2h	12	ARG	2.0
39	2h	30	ARG	2.0
40	1i	14	VAL	2.0
40	1i	37	PHE	2.0
40	2i	107	ARG	2.0
43	2l	59	ARG	2.0
50	2s	19	VAL	2.0
56	2y	31	C	2.0
56	2y	72	C	2.0
1	1A	880	G	2.0
1	2A	1170	G	2.0
32	1a	1021	G	2.0
32	2a	993	G	2.0
32	2a	1124	G	2.0
32	2a	1273	G	2.0
7	2H	103	LEU	2.0
21	1Z	168	GLU	2.0
28	26	10	LEU	2.0
33	2b	13	ALA	2.0
33	2b	118	LEU	2.0
33	2b	177	ALA	2.0
54	1w	67	G	2.0
56	1y	30	G	2.0

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Mol	Chain	Res	Type	RSRZ
56	1y	57	G	2.0
36	2e	31	LEU	2.0
43	2l	52	LEU	2.0
5	1F	207	GLY	2.0
11	2P	26	GLY	2.0
14	2S	59	LYS	2.0
15	2T	55	ASN	2.0
21	2Z	143	GLY	2.0
22	20	12	ASN	2.0
26	24	28	LYS	2.0
33	1b	203	GLY	2.0
34	2c	181	ASN	2.0
4	1E	77	ILE	2.0
26	24	44	THR	2.0
33	1b	214	ILE	2.0
34	1c	57	ILE	2.0
37	1f	25	ILE	2.0
39	2h	3	THR	2.0
43	2l	85	ILE	2.0
52	1u	13	ILE	2.0
1	1A	2109	U	2.0
1	2A	405	U	2.0
1	2A	2150	U	2.0
1	1A	1460	A	2.0
31	29	30	PRO	2.0
32	1a	344	A	2.0
32	2a	974	A	2.0
32	2a	1319	A	2.0
33	1b	189	ASP	2.0
56	1y	29	A	2.0
56	1y	38	A	2.0
35	2d	181	MET	2.0
14	2S	34	HIS	2.0
14	2S	36	TYR	2.0
46	2o	69	TYR	2.0
48	1q	97	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	4SU	2y	8	20/21	0.44	0.18	93,99,108,115	0
56	4SU	1y	8	20/21	0.51	0.17	92,98,101,118	0
56	5MU	2y	54	21/22	0.52	0.17	96,99,105,120	0
56	PSU	2y	55	20/21	0.56	0.17	96,103,107,108	0
56	PSU	1y	55	20/21	0.62	0.15	94,98,104,112	0
54	4SU	2w	8	20/21	0.62	0.15	90,97,110,116	0
56	5MU	1y	54	21/22	0.63	0.13	90,94,100,113	0
54	5MU	2w	54	21/22	0.69	0.14	83,91,95,98	0
54	PSU	2w	55	20/21	0.70	0.13	88,94,103,103	0
54	4SU	1w	8	20/21	0.71	0.13	94,96,106,110	0
54	PSU	1w	55	20/21	0.78	0.13	81,90,98,98	0
32	2MG	2a	1207	24/25	0.78	0.16	82,88,96,101	0
54	5MU	1w	54	21/22	0.83	0.12	72,83,88,93	0
1	5MU	2A	1915	21/22	0.85	0.14	75,77,81,91	0
55	5MU	2x	54	21/22	0.86	0.14	79,86,90,97	0
32	PSU	2a	516	20/21	0.87	0.13	76,83,88,91	0
55	PSU	2x	55	20/21	0.87	0.12	77,82,88,96	0
32	M2G	2a	966	25/26	0.88	0.16	60,70,81,88	0
55	PSU	1x	55	20/21	0.88	0.12	60,65,77,78	0
55	4SU	2x	8	20/21	0.88	0.12	77,81,87,88	0
32	5MC	2a	967	21/22	0.89	0.13	68,74,80,83	0
43	0TD	1l	92	10/11	0.89	0.14	54,56,61,70	0
55	5MU	1x	54	21/22	0.90	0.12	65,74,76,83	0
1	PSU	2A	1917	20/21	0.90	0.12	67,75,84,85	0
55	5MC	2x	32	21/22	0.91	0.15	66,78,80,80	0
32	5MC	2a	1404	21/22	0.92	0.13	54,61,67,72	0
55	4SU	1x	8	20/21	0.92	0.11	58,64,79,80	0
32	G7M	2a	527	24/25	0.92	0.12	65,72,80,82	0
32	2MG	1a	1207	24/25	0.92	0.10	68,73,79,87	0
32	PSU	1a	516	20/21	0.92	0.10	62,66,72,72	0
1	PSU	2A	1911	20/21	0.92	0.11	64,69,77,81	0
32	5MC	2a	1400	21/22	0.92	0.15	68,76,80,86	0
32	4OC	2a	1402	22/23	0.93	0.12	56,64,68,72	0
54	L3X	2w	76	26/27	0.93	0.12	52,59,63,64	0
1	5MU	1A	1915	21/22	0.93	0.10	51,60,65,69	0
32	5MC	2a	1407	21/22	0.93	0.12	54,60,67,75	0
1	OMC	2A	1920	21/22	0.93	0.13	58,67,71,79	0
55	5MC	1x	32	21/22	0.94	0.12	51,57,64,66	0
43	0TD	2l	92	10/11	0.94	0.12	67,72,77,86	0
32	MA6	2a	1518	24/25	0.94	0.12	56,69,73,76	0
32	UR3	2a	1498	21/22	0.95	0.11	59,63,69,71	0
55	31H	2x	76	32/33	0.95	0.12	42,54,62,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	M2G	1a	966	25/26	0.95	0.12	55,60,70,72	0
32	MA6	2a	1519	24/25	0.95	0.13	56,65,71,72	0
32	5MC	1a	967	21/22	0.96	0.09	55,61,68,71	0
1	5MC	1A	1942	21/22	0.96	0.09	36,42,49,61	0
1	5MU	2A	1939	21/22	0.96	0.08	34,38,45,47	0
1	5MC	2A	1942	21/22	0.96	0.09	54,59,65,73	0
55	31H	1x	76	32/33	0.96	0.10	24,38,45,54	10
1	5MC	2A	1962	21/22	0.96	0.09	47,51,61,72	0
54	L3X	1w	76	26/27	0.96	0.08	37,42,48,51	0
1	2MA	2A	2503	23/24	0.96	0.10	34,42,44,45	0
32	5MC	1a	1404	21/22	0.96	0.09	39,44,47,47	0
1	PSU	1A	1911	20/21	0.96	0.09	44,49,58,58	0
32	G7M	1a	527	24/25	0.96	0.09	49,54,59,63	0
1	PSU	1A	1917	20/21	0.96	0.08	48,56,61,64	0
32	5MC	1a	1407	21/22	0.97	0.08	34,43,45,46	0
32	MA6	1a	1519	24/25	0.97	0.09	40,45,50,55	0
1	OMC	1A	1920	21/22	0.97	0.08	37,46,49,52	0
32	5MC	1a	1400	21/22	0.97	0.08	41,50,53,55	0
1	OMG	2A	2251	24/25	0.97	0.08	38,44,50,55	0
32	4OC	1a	1402	22/23	0.97	0.07	36,46,53,58	0
1	OMU	2A	2552	21/22	0.97	0.08	37,42,48,51	0
1	PSU	2A	2605	20/21	0.97	0.07	39,45,51,52	0
1	PSU	1A	2605	20/21	0.97	0.07	24,30,35,38	0
1	5MC	1A	1962	21/22	0.98	0.06	27,38,41,46	0
1	OMG	1A	2251	24/25	0.98	0.06	23,28,33,34	0
1	2MA	1A	2503	23/24	0.98	0.06	19,24,28,31	0
1	OMU	1A	2552	21/22	0.98	0.07	26,30,33,37	0
32	UR3	1a	1498	21/22	0.98	0.07	35,44,47,50	0
32	MA6	1a	1518	24/25	0.98	0.09	40,46,49,51	0
1	5MU	1A	1939	21/22	0.98	0.06	24,28,33,34	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2j	201	1/1	0.47	0.21	88,88,88,88	0
57	MG	2A	3669	1/1	0.49	0.27	83,83,83,83	0
57	MG	2A	3573	1/1	0.51	0.26	86,86,86,86	0
57	MG	2A	3752	1/1	0.54	0.17	80,80,80,80	0
57	MG	1A	3880	1/1	0.55	0.35	80,80,80,80	0
57	MG	1w	105	1/1	0.56	0.22	88,88,88,88	0
57	MG	1A	3798	1/1	0.58	0.16	61,61,61,61	0
57	MG	2w	101	1/1	0.60	0.21	83,83,83,83	0
57	MG	1B	229	1/1	0.61	0.29	86,86,86,86	0
57	MG	2A	3513	1/1	0.64	0.37	85,85,85,85	0
57	MG	2A	3681	1/1	0.65	0.19	70,70,70,70	0
57	MG	2B	201	1/1	0.66	0.26	82,82,82,82	0
57	MG	2A	3858	1/1	0.67	0.25	75,75,75,75	0
57	MG	2A	3424	1/1	0.68	0.48	88,88,88,88	0
57	MG	2A	3710	1/1	0.68	0.18	71,71,71,71	0
57	MG	2A	3278	1/1	0.68	0.15	75,75,75,75	0
57	MG	2A	3801	1/1	0.68	0.18	71,71,71,71	0
57	MG	2A	3325	1/1	0.68	0.41	79,79,79,79	0
57	MG	2A	3660	1/1	0.68	0.18	78,78,78,78	0
57	MG	2A	3364	1/1	0.68	0.23	77,77,77,77	0
57	MG	2A	3672	1/1	0.68	0.12	76,76,76,76	0
57	MG	2A	3691	1/1	0.69	0.26	74,74,74,74	0
57	MG	2A	3706	1/1	0.69	0.22	76,76,76,76	0
57	MG	1A	3997	1/1	0.69	0.15	64,64,64,64	0
57	MG	2a	1805	1/1	0.69	0.24	71,71,71,71	0
57	MG	2A	3106	1/1	0.69	0.25	71,71,71,71	0
57	MG	2A	3757	1/1	0.69	0.21	66,66,66,66	0
57	MG	2A	3662	1/1	0.70	0.27	70,70,70,70	0
57	MG	1A	3640	1/1	0.70	0.19	80,80,80,80	0
57	MG	2a	1747	1/1	0.70	0.33	77,77,77,77	0
57	MG	2A	3299	1/1	0.71	0.29	84,84,84,84	0
57	MG	1B	231	1/1	0.71	0.14	81,81,81,81	0
57	MG	2A	3539	1/1	0.71	0.19	62,62,62,62	0
57	MG	2A	3817	1/1	0.71	0.18	60,60,60,60	0
57	MG	1A	3360	1/1	0.71	0.24	77,77,77,77	0
57	MG	1A	4064	1/1	0.72	0.15	69,69,69,69	0
57	MG	1x	103	1/1	0.72	0.24	70,70,70,70	0
57	MG	2A	3099	1/1	0.72	0.16	76,76,76,76	0
57	MG	1A	3684	1/1	0.72	0.21	81,81,81,81	0
57	MG	1A	3999	1/1	0.72	0.15	63,63,63,63	0
57	MG	2a	1636	1/1	0.72	0.29	75,75,75,75	0
57	MG	2a	1739	1/1	0.72	0.32	72,72,72,72	0
57	MG	1a	1679	1/1	0.72	0.24	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3657	1/1	0.72	0.12	85,85,85,85	0
57	MG	2A	3730	1/1	0.72	0.14	73,73,73,73	0
57	MG	2A	3312	1/1	0.72	0.29	76,76,76,76	0
57	MG	2A	3606	1/1	0.73	0.26	68,68,68,68	0
57	MG	1w	101	1/1	0.73	0.16	81,81,81,81	0
57	MG	2A	3777	1/1	0.73	0.21	75,75,75,75	0
57	MG	1A	3877	1/1	0.73	0.23	72,72,72,72	0
57	MG	1R	207	1/1	0.73	0.20	45,45,45,45	0
57	MG	2A	3336	1/1	0.73	0.11	75,75,75,75	0
57	MG	10	108	1/1	0.73	0.27	74,74,74,74	0
57	MG	1A	3210	1/1	0.73	0.11	79,79,79,79	0
57	MG	2a	1642	1/1	0.73	0.32	83,83,83,83	0
57	MG	2A	3112	1/1	0.73	0.31	83,83,83,83	0
57	MG	2A	3200	1/1	0.73	0.22	74,74,74,74	0
57	MG	1a	1682	1/1	0.73	0.24	80,80,80,80	0
57	MG	2A	3585	1/1	0.73	0.28	75,75,75,75	0
57	MG	2A	3751	1/1	0.73	0.21	50,50,50,50	0
57	MG	2A	3349	1/1	0.74	0.20	59,59,59,59	0
57	MG	2A	3735	1/1	0.74	0.28	72,72,72,72	0
57	MG	2G	201	1/1	0.74	0.34	81,81,81,81	0
57	MG	2A	3255	1/1	0.74	0.20	74,74,74,74	0
57	MG	2a	1638	1/1	0.74	0.36	84,84,84,84	0
57	MG	2A	3371	1/1	0.74	0.29	74,74,74,74	0
57	MG	2a	1709	1/1	0.74	0.27	76,76,76,76	0
57	MG	2A	3686	1/1	0.74	0.14	67,67,67,67	0
57	MG	1A	3707	1/1	0.74	0.20	54,54,54,54	0
57	MG	2a	1787	1/1	0.74	0.26	76,76,76,76	0
57	MG	2A	3332	1/1	0.74	0.27	81,81,81,81	0
57	MG	1A	3520	1/1	0.74	0.28	75,75,75,75	0
57	MG	2A	3845	1/1	0.74	0.32	76,76,76,76	0
57	MG	2A	3294	1/1	0.75	0.17	58,58,58,58	0
57	MG	16	102	1/1	0.75	0.30	64,64,64,64	0
57	MG	2A	3069	1/1	0.75	0.23	70,70,70,70	0
57	MG	1A	3712	1/1	0.75	0.23	68,68,68,68	0
57	MG	2A	3644	1/1	0.75	0.18	47,47,47,47	0
57	MG	1B	210	1/1	0.75	0.21	71,71,71,71	0
57	MG	2a	1707	1/1	0.75	0.28	81,81,81,81	0
57	MG	1a	1703	1/1	0.75	0.26	73,73,73,73	0
57	MG	2A	3197	1/1	0.75	0.33	86,86,86,86	0
57	MG	1a	1722	1/1	0.75	0.45	75,75,75,75	0
57	MG	2A	3215	1/1	0.75	0.23	67,67,67,67	0
57	MG	2A	3810	1/1	0.75	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1U	210	1/1	0.75	0.43	66,66,66,66	0
57	MG	1A	3938	1/1	0.75	0.17	69,69,69,69	0
57	MG	1E	310	1/1	0.76	0.23	80,80,80,80	0
57	MG	2B	214	1/1	0.76	0.17	79,79,79,79	0
57	MG	1w	103	1/1	0.76	0.17	78,78,78,78	0
57	MG	2a	1608	1/1	0.76	0.26	75,75,75,75	0
57	MG	2A	3372	1/1	0.76	0.18	70,70,70,70	0
57	MG	2A	3195	1/1	0.76	0.19	69,69,69,69	0
57	MG	2A	3496	1/1	0.76	0.18	77,77,77,77	0
57	MG	2A	3258	1/1	0.76	0.18	74,74,74,74	0
57	MG	2A	3676	1/1	0.76	0.22	65,65,65,65	0
57	MG	2a	1712	1/1	0.76	0.31	78,78,78,78	0
57	MG	1a	1793	1/1	0.76	0.27	78,78,78,78	0
57	MG	2A	3199	1/1	0.76	0.35	70,70,70,70	0
57	MG	2A	3352	1/1	0.76	0.28	77,77,77,77	0
57	MG	2A	3705	1/1	0.76	0.20	79,79,79,79	0
57	MG	2a	1821	1/1	0.76	0.23	75,75,75,75	0
57	MG	2A	3850	1/1	0.76	0.21	65,65,65,65	0
57	MG	2v	103	1/1	0.76	0.43	79,79,79,79	0
57	MG	2A	3357	1/1	0.76	0.32	63,63,63,63	0
57	MG	2a	1622	1/1	0.77	0.26	81,81,81,81	0
57	MG	2A	3218	1/1	0.77	0.40	73,73,73,73	0
57	MG	2A	3485	1/1	0.77	0.24	69,69,69,69	0
57	MG	1A	3851	1/1	0.77	0.16	83,83,83,83	0
57	MG	2a	1699	1/1	0.77	0.15	71,71,71,71	0
57	MG	1A	3806	1/1	0.77	0.20	70,70,70,70	0
57	MG	1A	4010	1/1	0.77	0.11	77,77,77,77	0
57	MG	2A	3683	1/1	0.77	0.20	79,79,79,79	0
57	MG	2a	1714	1/1	0.77	0.38	71,71,71,71	0
57	MG	2A	3279	1/1	0.77	0.19	68,68,68,68	0
57	MG	2A	3062	1/1	0.77	0.13	78,78,78,78	0
57	MG	2A	3214	1/1	0.77	0.23	62,62,62,62	0
57	MG	2a	1804	1/1	0.77	0.22	76,76,76,76	0
57	MG	2A	3609	1/1	0.77	0.23	65,65,65,65	0
57	MG	2A	3166	1/1	0.77	0.12	74,74,74,74	0
57	MG	2i	201	1/1	0.77	0.11	77,77,77,77	0
57	MG	2A	3321	1/1	0.77	0.25	69,69,69,69	0
57	MG	2A	3388	1/1	0.77	0.22	71,71,71,71	0
57	MG	2A	3741	1/1	0.77	0.20	67,67,67,67	0
57	MG	2A	3770	1/1	0.78	0.18	50,50,50,50	0
57	MG	2A	3704	1/1	0.78	0.18	74,74,74,74	0
57	MG	1a	1720	1/1	0.78	0.31	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3858	1/1	0.78	0.21	62,62,62,62	0
57	MG	2A	3277	1/1	0.78	0.39	73,73,73,73	0
57	MG	2A	3711	1/1	0.78	0.21	73,73,73,73	0
57	MG	2A	3719	1/1	0.78	0.20	70,70,70,70	0
57	MG	2A	3857	1/1	0.78	0.17	66,66,66,66	0
57	MG	2A	3720	1/1	0.78	0.19	60,60,60,60	0
57	MG	1a	1784	1/1	0.78	0.13	81,81,81,81	0
57	MG	2A	3333	1/1	0.78	0.38	76,76,76,76	0
57	MG	2B	216	1/1	0.78	0.15	64,64,64,64	0
57	MG	2a	1817	1/1	0.78	0.21	74,74,74,74	0
57	MG	2a	1820	1/1	0.78	0.25	69,69,69,69	0
57	MG	2F	307	1/1	0.78	0.15	72,72,72,72	0
57	MG	1A	3678	1/1	0.78	0.14	63,63,63,63	0
57	MG	2A	3630	1/1	0.78	0.24	64,64,64,64	0
57	MG	2t	201	1/1	0.78	0.19	66,66,66,66	0
57	MG	2A	3175	1/1	0.78	0.19	58,58,58,58	0
57	MG	1a	1636	1/1	0.78	0.42	89,89,89,89	0
57	MG	2y	101	1/1	0.78	0.18	78,78,78,78	0
57	MG	2A	3687	1/1	0.79	0.33	78,78,78,78	0
57	MG	2A	3274	1/1	0.79	0.11	77,77,77,77	0
57	MG	2a	1808	1/1	0.79	0.20	77,77,77,77	0
57	MG	2a	1812	1/1	0.79	0.15	79,79,79,79	0
57	MG	2a	1671	1/1	0.79	0.16	71,71,71,71	0
57	MG	2A	3378	1/1	0.79	0.14	69,69,69,69	0
57	MG	2A	3675	1/1	0.79	0.19	64,64,64,64	0
57	MG	2A	3115	1/1	0.79	0.23	77,77,77,77	0
57	MG	20	101	1/1	0.79	0.27	74,74,74,74	0
57	MG	2q	202	1/1	0.79	0.12	81,81,81,81	0
57	MG	2A	3324	1/1	0.79	0.20	66,66,66,66	0
57	MG	2A	3481	1/1	0.79	0.31	76,76,76,76	0
57	MG	2a	1626	1/1	0.79	0.25	74,74,74,74	0
57	MG	1a	1799	1/1	0.79	0.12	72,72,72,72	0
57	MG	1A	3809	1/1	0.80	0.12	49,49,49,49	0
57	MG	2A	3209	1/1	0.80	0.17	72,72,72,72	0
57	MG	2A	3627	1/1	0.80	0.18	84,84,84,84	0
57	MG	2A	3342	1/1	0.80	0.31	81,81,81,81	0
57	MG	2a	1645	1/1	0.80	0.14	64,64,64,64	0
57	MG	2a	1656	1/1	0.80	0.34	76,76,76,76	0
57	MG	1A	4001	1/1	0.80	0.12	46,46,46,46	0
57	MG	1A	3831	1/1	0.80	0.21	73,73,73,73	0
57	MG	1x	101	1/1	0.80	0.31	71,71,71,71	0
57	MG	2A	3363	1/1	0.80	0.28	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3664	1/1	0.80	0.13	67,67,67,67	0
57	MG	1A	4026	1/1	0.80	0.12	71,71,71,71	0
57	MG	2a	1730	1/1	0.80	0.21	83,83,83,83	0
57	MG	1a	1677	1/1	0.80	0.28	78,78,78,78	0
57	MG	1A	3347	1/1	0.80	0.25	65,65,65,65	0
57	MG	2a	1769	1/1	0.80	0.19	83,83,83,83	0
57	MG	2A	3837	1/1	0.80	0.14	71,71,71,71	0
57	MG	2a	1789	1/1	0.80	0.24	86,86,86,86	0
57	MG	1A	3545	1/1	0.80	0.23	60,60,60,60	0
57	MG	1A	3607	1/1	0.80	0.16	38,38,38,38	0
57	MG	2A	3392	1/1	0.80	0.17	75,75,75,75	0
57	MG	1a	1707	1/1	0.80	0.18	80,80,80,80	0
57	MG	2a	1815	1/1	0.80	0.19	77,77,77,77	0
57	MG	2A	3436	1/1	0.80	0.28	64,64,64,64	0
57	MG	2B	211	1/1	0.80	0.31	83,83,83,83	0
57	MG	1B	230	1/1	0.80	0.20	73,73,73,73	0
57	MG	1A	3219	1/1	0.80	0.19	65,65,65,65	0
57	MG	2A	3167	1/1	0.80	0.22	78,78,78,78	0
57	MG	1a	1759	1/1	0.80	0.16	68,68,68,68	0
57	MG	2T	3502	1/1	0.80	0.22	76,76,76,76	0
57	MG	1A	3514	1/1	0.80	0.22	68,68,68,68	0
57	MG	1O	205	1/1	0.80	0.13	76,76,76,76	0
57	MG	1A	3807	1/1	0.80	0.22	51,51,51,51	0
57	MG	1A	4022	1/1	0.81	0.15	84,84,84,84	0
57	MG	2A	3446	1/1	0.81	0.28	75,75,75,75	0
57	MG	1A	3305	1/1	0.81	0.27	52,52,52,52	0
57	MG	2A	3168	1/1	0.81	0.19	76,76,76,76	0
57	MG	1A	4048	1/1	0.81	0.16	58,58,58,58	0
57	MG	2A	3190	1/1	0.81	0.36	77,77,77,77	0
57	MG	2a	1746	1/1	0.81	0.28	75,75,75,75	0
57	MG	1A	3314	1/1	0.81	0.16	54,54,54,54	0
57	MG	1t	201	1/1	0.81	0.26	69,69,69,69	0
57	MG	1a	1676	1/1	0.81	0.20	70,70,70,70	0
57	MG	2E	307	1/1	0.81	0.16	60,60,60,60	0
57	MG	2a	1795	1/1	0.81	0.16	64,64,64,64	0
57	MG	2A	3597	1/1	0.81	0.15	71,71,71,71	0
57	MG	1A	3532	1/1	0.81	0.24	79,79,79,79	0
57	MG	1A	3040	1/1	0.81	0.26	61,61,61,61	0
57	MG	1A	3976	1/1	0.81	0.20	69,69,69,69	0
57	MG	1a	1685	1/1	0.81	0.24	73,73,73,73	0
57	MG	2a	1610	1/1	0.81	0.26	69,69,69,69	0
57	MG	2A	3051	1/1	0.81	0.18	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3169	1/1	0.81	0.23	66,66,66,66	0
57	MG	1A	3382	1/1	0.81	0.18	57,57,57,57	0
57	MG	2A	3088	1/1	0.81	0.12	65,65,65,65	0
57	MG	1A	3425	1/1	0.81	0.19	73,73,73,73	0
57	MG	1A	3479	1/1	0.81	0.26	75,75,75,75	0
57	MG	1a	1728	1/1	0.81	0.26	59,59,59,59	0
57	MG	2A	3422	1/1	0.81	0.29	66,66,66,66	0
57	MG	2w	104	1/1	0.81	0.19	82,82,82,82	0
57	MG	1a	1734	1/1	0.81	0.22	80,80,80,80	0
57	MG	1A	3583	1/1	0.82	0.19	67,67,67,67	0
57	MG	1s	101	1/1	0.82	0.17	78,78,78,78	0
57	MG	2T	3503	1/1	0.82	0.19	52,52,52,52	0
57	MG	2W	201	1/1	0.82	0.14	72,72,72,72	0
57	MG	1A	3079	1/1	0.82	0.19	64,64,64,64	0
57	MG	1a	1631	1/1	0.82	0.43	75,75,75,75	0
57	MG	2A	3208	1/1	0.82	0.11	68,68,68,68	0
57	MG	1A	3502	1/1	0.82	0.20	66,66,66,66	0
57	MG	1A	3646	1/1	0.82	0.12	64,64,64,64	0
57	MG	2A	3384	1/1	0.82	0.32	65,65,65,65	0
57	MG	2A	3386	1/1	0.82	0.18	69,69,69,69	0
57	MG	1A	3510	1/1	0.82	0.16	65,65,65,65	0
57	MG	1A	3399	1/1	0.82	0.11	55,55,55,55	0
57	MG	2A	3231	1/1	0.82	0.43	56,56,56,56	0
57	MG	2a	1669	1/1	0.82	0.31	70,70,70,70	0
57	MG	2A	3709	1/1	0.82	0.13	43,43,43,43	0
57	MG	2A	3244	1/1	0.82	0.15	63,63,63,63	0
57	MG	2A	3426	1/1	0.82	0.26	62,62,62,62	0
57	MG	2A	3427	1/1	0.82	0.27	57,57,57,57	0
57	MG	1x	111	1/1	0.82	0.15	65,65,65,65	0
57	MG	1B	213	1/1	0.82	0.20	75,75,75,75	0
57	MG	2a	1721	1/1	0.82	0.27	80,80,80,80	0
57	MG	2A	3472	1/1	0.82	0.15	64,64,64,64	0
57	MG	2a	1738	1/1	0.82	0.32	65,65,65,65	0
57	MG	1B	225	1/1	0.82	0.13	62,62,62,62	0
57	MG	2A	3748	1/1	0.82	0.21	66,66,66,66	0
57	MG	1A	3933	1/1	0.82	0.13	58,58,58,58	0
57	MG	2a	1760	1/1	0.82	0.21	85,85,85,85	0
57	MG	1A	3405	1/1	0.82	0.15	74,74,74,74	0
57	MG	2A	3510	1/1	0.82	0.15	56,56,56,56	0
57	MG	1A	3246	1/1	0.82	0.36	73,73,73,73	0
57	MG	2a	1793	1/1	0.82	0.14	67,67,67,67	0
57	MG	2A	3289	1/1	0.82	0.29	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3559	1/1	0.82	0.20	48,48,48,48	0
57	MG	1A	3985	1/1	0.82	0.12	69,69,69,69	0
57	MG	1A	3430	1/1	0.82	0.18	65,65,65,65	0
57	MG	1A	3549	1/1	0.82	0.29	60,60,60,60	0
57	MG	2A	3152	1/1	0.82	0.27	73,73,73,73	0
57	MG	1a	1737	1/1	0.82	0.35	83,83,83,83	0
57	MG	2A	3617	1/1	0.82	0.25	77,77,77,77	0
57	MG	1A	3554	1/1	0.82	0.13	54,54,54,54	0
57	MG	2A	3861	1/1	0.82	0.23	76,76,76,76	0
57	MG	1V	207	1/1	0.82	0.20	63,63,63,63	0
57	MG	2B	206	1/1	0.82	0.21	83,83,83,83	0
57	MG	2A	3170	1/1	0.82	0.19	84,84,84,84	0
57	MG	1a	1792	1/1	0.82	0.18	70,70,70,70	0
57	MG	2A	3338	1/1	0.82	0.20	60,60,60,60	0
57	MG	2A	3187	1/1	0.82	0.19	72,72,72,72	0
57	MG	1Y	202	1/1	0.82	0.10	64,64,64,64	0
57	MG	1O	204	1/1	0.83	0.14	66,66,66,66	0
57	MG	2a	1612	1/1	0.83	0.27	72,72,72,72	0
57	MG	2A	3101	1/1	0.83	0.20	74,74,74,74	0
57	MG	2A	3102	1/1	0.83	0.18	80,80,80,80	0
57	MG	2a	1631	1/1	0.83	0.23	63,63,63,63	0
57	MG	1A	3835	1/1	0.83	0.13	71,71,71,71	0
57	MG	1A	3331	1/1	0.83	0.18	59,59,59,59	0
57	MG	1S	201	1/1	0.83	0.22	43,43,43,43	0
57	MG	2A	3453	1/1	0.83	0.32	79,79,79,79	0
57	MG	2A	3120	1/1	0.83	0.25	79,79,79,79	0
57	MG	2A	3290	1/1	0.83	0.18	73,73,73,73	0
57	MG	2A	3484	1/1	0.83	0.18	62,62,62,62	0
57	MG	2a	1680	1/1	0.83	0.23	77,77,77,77	0
57	MG	2a	1682	1/1	0.83	0.15	65,65,65,65	0
57	MG	2a	1688	1/1	0.83	0.32	74,74,74,74	0
57	MG	2a	1689	1/1	0.83	0.20	73,73,73,73	0
57	MG	2A	3123	1/1	0.83	0.16	81,81,81,81	0
57	MG	2A	3744	1/1	0.83	0.16	76,76,76,76	0
57	MG	2A	3297	1/1	0.83	0.22	74,74,74,74	0
57	MG	2A	3148	1/1	0.83	0.29	71,71,71,71	0
57	MG	1A	3381	1/1	0.83	0.19	60,60,60,60	0
57	MG	2a	1720	1/1	0.83	0.28	72,72,72,72	0
57	MG	1A	3874	1/1	0.83	0.24	52,52,52,52	0
57	MG	2A	3761	1/1	0.83	0.14	72,72,72,72	0
57	MG	2a	1736	1/1	0.83	0.23	75,75,75,75	0
57	MG	1a	1788	1/1	0.83	0.16	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3481	1/1	0.83	0.12	62,62,62,62	0
57	MG	2A	3790	1/1	0.83	0.16	74,74,74,74	0
57	MG	1A	3636	1/1	0.83	0.18	61,61,61,61	0
57	MG	2a	1750	1/1	0.83	0.20	87,87,87,87	0
57	MG	1A	3639	1/1	0.83	0.20	62,62,62,62	0
57	MG	2a	1761	1/1	0.83	0.14	70,70,70,70	0
57	MG	1a	1800	1/1	0.83	0.15	51,51,51,51	0
57	MG	2a	1786	1/1	0.83	0.11	85,85,85,85	0
57	MG	2A	3337	1/1	0.83	0.13	72,72,72,72	0
57	MG	1A	4070	1/1	0.83	0.11	70,70,70,70	0
57	MG	1B	202	1/1	0.83	0.18	59,59,59,59	0
57	MG	2A	3344	1/1	0.83	0.13	61,61,61,61	0
57	MG	1a	1659	1/1	0.83	0.27	78,78,78,78	0
57	MG	1B	207	1/1	0.83	0.14	75,75,75,75	0
57	MG	2A	3354	1/1	0.83	0.17	79,79,79,79	0
57	MG	1A	3489	1/1	0.83	0.14	71,71,71,71	0
57	MG	1A	3944	1/1	0.83	0.11	30,30,30,30	0
57	MG	1A	3950	1/1	0.83	0.18	83,83,83,83	0
57	MG	1A	3026	1/1	0.83	0.18	73,73,73,73	0
57	MG	1a	1692	1/1	0.83	0.17	86,86,86,86	0
57	MG	1A	3978	1/1	0.83	0.14	70,70,70,70	0
57	MG	2A	3221	1/1	0.83	0.21	63,63,63,63	0
57	MG	1A	3814	1/1	0.83	0.18	65,65,65,65	0
57	MG	1A	3508	1/1	0.83	0.21	71,71,71,71	0
57	MG	2A	3389	1/1	0.83	0.15	69,69,69,69	0
57	MG	2A	3253	1/1	0.83	0.12	78,78,78,78	0
57	MG	2w	102	1/1	0.83	0.21	71,71,71,71	0
57	MG	2a	1603	1/1	0.83	0.14	83,83,83,83	0
57	MG	2A	3693	1/1	0.83	0.19	58,58,58,58	0
57	MG	1A	3945	1/1	0.84	0.13	66,66,66,66	0
57	MG	2A	3796	1/1	0.84	0.20	56,56,56,56	0
57	MG	1A	3470	1/1	0.84	0.18	67,67,67,67	0
57	MG	1D	311	1/1	0.84	0.29	78,78,78,78	0
57	MG	2a	1700	1/1	0.84	0.39	80,80,80,80	0
57	MG	2a	1701	1/1	0.84	0.24	69,69,69,69	0
57	MG	1A	3255	1/1	0.84	0.28	57,57,57,57	0
57	MG	2a	1708	1/1	0.84	0.22	70,70,70,70	0
57	MG	2A	3405	1/1	0.84	0.27	60,60,60,60	0
57	MG	1w	107	1/1	0.84	0.09	69,69,69,69	0
57	MG	1A	3811	1/1	0.84	0.15	65,65,65,65	0
57	MG	2a	1719	1/1	0.84	0.21	74,74,74,74	0
57	MG	2A	3316	1/1	0.84	0.18	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4067	1/1	0.84	0.16	66,66,66,66	0
57	MG	1A	4069	1/1	0.84	0.10	50,50,50,50	0
57	MG	1A	3982	1/1	0.84	0.11	74,74,74,74	0
57	MG	2A	3204	1/1	0.84	0.16	64,64,64,64	0
57	MG	2A	3454	1/1	0.84	0.29	63,63,63,63	0
57	MG	1T	201	1/1	0.84	0.28	69,69,69,69	0
57	MG	2A	3334	1/1	0.84	0.22	73,73,73,73	0
57	MG	2B	219	1/1	0.84	0.25	78,78,78,78	0
57	MG	2A	3700	1/1	0.84	0.14	59,59,59,59	0
57	MG	2A	3702	1/1	0.84	0.10	65,65,65,65	0
57	MG	2a	1768	1/1	0.84	0.09	87,87,87,87	0
57	MG	1U	203	1/1	0.84	0.13	60,60,60,60	0
57	MG	1A	4075	1/1	0.84	0.22	58,58,58,58	0
57	MG	1A	3426	1/1	0.84	0.11	56,56,56,56	0
57	MG	2A	3498	1/1	0.84	0.28	77,77,77,77	0
57	MG	1A	3993	1/1	0.84	0.14	40,40,40,40	0
57	MG	1A	3930	1/1	0.84	0.12	47,47,47,47	0
57	MG	2a	1801	1/1	0.84	0.15	75,75,75,75	0
57	MG	2A	3535	1/1	0.84	0.16	74,74,74,74	0
57	MG	1a	1780	1/1	0.84	0.18	80,80,80,80	0
57	MG	2A	3724	1/1	0.84	0.15	68,68,68,68	0
57	MG	1A	3728	1/1	0.84	0.14	58,58,58,58	0
57	MG	1a	1624	1/1	0.84	0.14	59,59,59,59	0
57	MG	2a	1630	1/1	0.84	0.25	78,78,78,78	0
57	MG	1A	3423	1/1	0.84	0.18	67,67,67,67	0
57	MG	1B	228	1/1	0.84	0.13	74,74,74,74	0
57	MG	2a	1825	1/1	0.84	0.26	72,72,72,72	0
57	MG	2A	3273	1/1	0.84	0.25	75,75,75,75	0
57	MG	2A	3607	1/1	0.84	0.16	66,66,66,66	0
57	MG	1a	1647	1/1	0.84	0.14	62,62,62,62	0
57	MG	2a	1648	1/1	0.84	0.25	76,76,76,76	0
57	MG	1A	3464	1/1	0.84	0.14	63,63,63,63	0
57	MG	1a	1825	1/1	0.84	0.25	69,69,69,69	0
57	MG	1a	1662	1/1	0.84	0.12	74,74,74,74	0
57	MG	2a	1679	1/1	0.84	0.15	75,75,75,75	0
57	MG	2x	102	1/1	0.84	0.31	75,75,75,75	0
57	MG	2A	3637	1/1	0.84	0.18	47,47,47,47	0
57	MG	2A	3701	1/1	0.85	0.16	62,62,62,62	0
57	MG	1A	3359	1/1	0.85	0.13	62,62,62,62	0
57	MG	2A	3703	1/1	0.85	0.16	68,68,68,68	0
57	MG	2a	1644	1/1	0.85	0.14	77,77,77,77	0
57	MG	2A	3070	1/1	0.85	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3182	1/1	0.85	0.33	58,58,58,58	0
57	MG	2a	1650	1/1	0.85	0.19	80,80,80,80	0
57	MG	2A	3266	1/1	0.85	0.23	78,78,78,78	0
57	MG	2A	3094	1/1	0.85	0.10	74,74,74,74	0
57	MG	1A	3812	1/1	0.85	0.24	72,72,72,72	0
57	MG	1A	3695	1/1	0.85	0.10	31,31,31,31	0
57	MG	1a	1752	1/1	0.85	0.18	62,62,62,62	0
57	MG	1A	4077	1/1	0.85	0.12	60,60,60,60	0
57	MG	1a	1765	1/1	0.85	0.28	68,68,68,68	0
57	MG	1A	3962	1/1	0.85	0.09	24,24,24,24	0
57	MG	2a	1694	1/1	0.85	0.18	77,77,77,77	0
57	MG	1a	1783	1/1	0.85	0.11	75,75,75,75	0
57	MG	15	106	1/1	0.85	0.15	72,72,72,72	0
57	MG	1a	1787	1/1	0.85	0.19	77,77,77,77	0
57	MG	2a	1706	1/1	0.85	0.20	76,76,76,76	0
57	MG	1A	3972	1/1	0.85	0.19	64,64,64,64	0
57	MG	1a	1790	1/1	0.85	0.13	61,61,61,61	0
57	MG	2A	3318	1/1	0.85	0.26	72,72,72,72	0
57	MG	1A	3621	1/1	0.85	0.18	50,50,50,50	0
57	MG	1a	1629	1/1	0.85	0.33	77,77,77,77	0
57	MG	1A	3539	1/1	0.85	0.17	63,63,63,63	0
57	MG	2A	3775	1/1	0.85	0.18	69,69,69,69	0
57	MG	1B	221	1/1	0.85	0.21	64,64,64,64	0
57	MG	2A	3183	1/1	0.85	0.14	55,55,55,55	0
57	MG	1a	1823	1/1	0.85	0.17	63,63,63,63	0
57	MG	2A	3592	1/1	0.85	0.20	75,75,75,75	0
57	MG	1B	222	1/1	0.85	0.17	59,59,59,59	0
57	MG	1A	3716	1/1	0.85	0.15	62,62,62,62	0
57	MG	1A	3638	1/1	0.85	0.09	18,18,18,18	0
57	MG	1v	101	1/1	0.85	0.18	75,75,75,75	0
57	MG	1A	3862	1/1	0.85	0.15	61,61,61,61	0
57	MG	2A	3347	1/1	0.85	0.10	68,68,68,68	0
57	MG	2a	1767	1/1	0.85	0.11	75,75,75,75	0
57	MG	1A	3732	1/1	0.85	0.20	64,64,64,64	0
57	MG	2A	3634	1/1	0.85	0.12	62,62,62,62	0
57	MG	2a	1781	1/1	0.85	0.23	88,88,88,88	0
57	MG	1A	3788	1/1	0.85	0.15	89,89,89,89	0
57	MG	2A	3353	1/1	0.85	0.18	73,73,73,73	0
57	MG	2A	3652	1/1	0.85	0.11	49,49,49,49	0
57	MG	2a	1791	1/1	0.85	0.14	67,67,67,67	0
57	MG	2A	3654	1/1	0.85	0.31	74,74,74,74	0
57	MG	1A	3297	1/1	0.85	0.20	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3355	1/1	0.85	0.10	61,61,61,61	0
57	MG	2E	301	1/1	0.85	0.20	61,61,61,61	0
57	MG	2E	303	1/1	0.85	0.18	74,74,74,74	0
57	MG	2A	3213	1/1	0.85	0.26	54,54,54,54	0
57	MG	1A	3881	1/1	0.85	0.13	29,29,29,29	0
57	MG	1A	3893	1/1	0.85	0.22	79,79,79,79	0
57	MG	2Q	202	1/1	0.85	0.25	67,67,67,67	0
57	MG	2A	3366	1/1	0.85	0.30	77,77,77,77	0
57	MG	2A	3370	1/1	0.85	0.34	70,70,70,70	0
57	MG	1x	107	1/1	0.85	0.10	68,68,68,68	0
57	MG	1A	3899	1/1	0.85	0.21	73,73,73,73	0
57	MG	21	101	1/1	0.85	0.40	59,59,59,59	0
57	MG	2A	3682	1/1	0.85	0.17	78,78,78,78	0
57	MG	2A	3373	1/1	0.85	0.12	66,66,66,66	0
57	MG	2A	3685	1/1	0.85	0.12	64,64,64,64	0
57	MG	1A	3357	1/1	0.85	0.16	66,66,66,66	0
57	MG	2A	3240	1/1	0.85	0.33	65,65,65,65	0
57	MG	2A	3241	1/1	0.85	0.31	54,54,54,54	0
57	MG	1A	3397	1/1	0.85	0.24	32,32,32,32	0
57	MG	2A	3249	1/1	0.85	0.39	79,79,79,79	0
57	MG	23	101	1/1	0.86	0.30	78,78,78,78	0
57	MG	1a	1794	1/1	0.86	0.10	73,73,73,73	0
57	MG	1A	4089	1/1	0.86	0.18	42,42,42,42	0
57	MG	1A	3006	1/1	0.86	0.26	70,70,70,70	0
57	MG	1a	1804	1/1	0.86	0.12	51,51,51,51	0
57	MG	2a	1614	1/1	0.86	0.17	65,65,65,65	0
57	MG	1A	3376	1/1	0.86	0.17	54,54,54,54	0
57	MG	2A	3665	1/1	0.86	0.14	73,73,73,73	0
57	MG	1A	3350	1/1	0.86	0.18	59,59,59,59	0
57	MG	1l	201	1/1	0.86	0.28	73,73,73,73	0
57	MG	1B	211	1/1	0.86	0.13	54,54,54,54	0
57	MG	1A	3979	1/1	0.86	0.14	70,70,70,70	0
57	MG	2a	1641	1/1	0.86	0.17	80,80,80,80	0
57	MG	2A	3207	1/1	0.86	0.15	67,67,67,67	0
57	MG	1A	3499	1/1	0.86	0.28	58,58,58,58	0
57	MG	1a	1665	1/1	0.86	0.12	61,61,61,61	0
57	MG	2a	1647	1/1	0.86	0.14	73,73,73,73	0
57	MG	1w	102	1/1	0.86	0.21	74,74,74,74	0
57	MG	1A	3558	1/1	0.86	0.12	61,61,61,61	0
57	MG	2a	1651	1/1	0.86	0.15	62,62,62,62	0
57	MG	1w	104	1/1	0.86	0.13	74,74,74,74	0
57	MG	2a	1660	1/1	0.86	0.13	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1667	1/1	0.86	0.12	67,67,67,67	0
57	MG	1A	3329	1/1	0.86	0.20	56,56,56,56	0
57	MG	1A	3995	1/1	0.86	0.11	56,56,56,56	0
57	MG	2a	1672	1/1	0.86	0.22	65,65,65,65	0
57	MG	1A	3593	1/1	0.86	0.35	71,71,71,71	0
57	MG	2A	3379	1/1	0.86	0.15	67,67,67,67	0
57	MG	2A	3382	1/1	0.86	0.13	76,76,76,76	0
57	MG	1A	3358	1/1	0.86	0.07	43,43,43,43	0
57	MG	1A	3745	1/1	0.86	0.11	55,55,55,55	0
57	MG	2A	3242	1/1	0.86	0.14	67,67,67,67	0
57	MG	1a	1695	1/1	0.86	0.26	63,63,63,63	0
57	MG	2A	3020	1/1	0.86	0.16	68,68,68,68	0
57	MG	2A	3040	1/1	0.86	0.21	65,65,65,65	0
57	MG	2A	3411	1/1	0.86	0.12	56,56,56,56	0
57	MG	1a	1697	1/1	0.86	0.11	63,63,63,63	0
57	MG	1A	4004	1/1	0.86	0.11	33,33,33,33	0
57	MG	2A	3261	1/1	0.86	0.12	53,53,53,53	0
57	MG	1A	4009	1/1	0.86	0.14	66,66,66,66	0
57	MG	2A	3435	1/1	0.86	0.34	65,65,65,65	0
57	MG	1A	3197	1/1	0.86	0.29	58,58,58,58	0
57	MG	1A	3623	1/1	0.86	0.20	64,64,64,64	0
57	MG	1A	3469	1/1	0.86	0.10	64,64,64,64	0
57	MG	2a	1722	1/1	0.86	0.25	70,70,70,70	0
57	MG	2a	1727	1/1	0.86	0.29	74,74,74,74	0
57	MG	2a	1728	1/1	0.86	0.11	63,63,63,63	0
57	MG	2A	3098	1/1	0.86	0.27	77,77,77,77	0
57	MG	2A	3465	1/1	0.86	0.23	60,60,60,60	0
57	MG	2A	3467	1/1	0.86	0.20	57,57,57,57	0
57	MG	1A	3404	1/1	0.86	0.28	69,69,69,69	0
57	MG	2A	3475	1/1	0.86	0.30	68,68,68,68	0
57	MG	2A	3281	1/1	0.86	0.15	65,65,65,65	0
57	MG	2A	3283	1/1	0.86	0.16	61,61,61,61	0
57	MG	1A	3529	1/1	0.86	0.15	62,62,62,62	0
57	MG	2A	3486	1/1	0.86	0.25	52,52,52,52	0
57	MG	2A	3798	1/1	0.86	0.10	80,80,80,80	0
57	MG	2A	3489	1/1	0.86	0.33	64,64,64,64	0
57	MG	1A	4066	1/1	0.86	0.07	19,19,19,19	0
57	MG	2A	3105	1/1	0.86	0.17	62,62,62,62	0
57	MG	1a	1753	1/1	0.86	0.13	60,60,60,60	0
57	MG	1A	3531	1/1	0.86	0.24	75,75,75,75	0
57	MG	2A	3534	1/1	0.86	0.20	60,60,60,60	0
57	MG	2A	3301	1/1	0.86	0.26	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3305	1/1	0.86	0.15	60,60,60,60	0
57	MG	2A	3549	1/1	0.86	0.15	53,53,53,53	0
57	MG	2A	3307	1/1	0.86	0.15	63,63,63,63	0
57	MG	2B	203	1/1	0.86	0.26	79,79,79,79	0
57	MG	2A	3569	1/1	0.86	0.11	38,38,38,38	0
57	MG	1A	3476	1/1	0.86	0.21	59,59,59,59	0
57	MG	2A	3315	1/1	0.86	0.15	62,62,62,62	0
57	MG	1A	3664	1/1	0.86	0.10	33,33,33,33	0
57	MG	1A	3957	1/1	0.86	0.10	56,56,56,56	0
57	MG	2a	1818	1/1	0.86	0.13	87,87,87,87	0
57	MG	2A	3604	1/1	0.86	0.15	74,74,74,74	0
57	MG	2A	3319	1/1	0.86	0.12	57,57,57,57	0
57	MG	1A	3825	1/1	0.86	0.14	55,55,55,55	0
57	MG	2A	3323	1/1	0.86	0.20	64,64,64,64	0
57	MG	1A	4088	1/1	0.86	0.15	44,44,44,44	0
57	MG	2A	3159	1/1	0.86	0.19	64,64,64,64	0
57	MG	2R	202	1/1	0.86	0.16	64,64,64,64	0
57	MG	2T	3501	1/1	0.86	0.20	71,71,71,71	0
57	MG	1a	1601	1/1	0.86	0.27	72,72,72,72	0
57	MG	1a	1613	1/1	0.86	0.28	68,68,68,68	0
57	MG	1a	1614	1/1	0.86	0.10	63,63,63,63	0
57	MG	1a	1619	1/1	0.86	0.13	46,46,46,46	0
57	MG	2A	3171	1/1	0.86	0.18	61,61,61,61	0
57	MG	2a	1606	1/1	0.87	0.35	79,79,79,79	0
57	MG	2A	3653	1/1	0.87	0.22	70,70,70,70	0
57	MG	1A	3581	1/1	0.87	0.17	50,50,50,50	0
57	MG	2a	1611	1/1	0.87	0.18	66,66,66,66	0
57	MG	1A	3800	1/1	0.87	0.12	56,56,56,56	0
57	MG	1a	1669	1/1	0.87	0.10	54,54,54,54	0
57	MG	1a	1673	1/1	0.87	0.24	68,68,68,68	0
57	MG	1A	3472	1/1	0.87	0.11	67,67,67,67	0
57	MG	2a	1627	1/1	0.87	0.32	71,71,71,71	0
57	MG	1A	3344	1/1	0.87	0.19	63,63,63,63	0
57	MG	2A	3668	1/1	0.87	0.14	50,50,50,50	0
57	MG	1A	3082	1/1	0.87	0.20	44,44,44,44	0
57	MG	2A	3232	1/1	0.87	0.22	46,46,46,46	0
57	MG	2A	3236	1/1	0.87	0.20	68,68,68,68	0
57	MG	1a	1680	1/1	0.87	0.25	74,74,74,74	0
57	MG	1A	3290	1/1	0.87	0.28	48,48,48,48	0
57	MG	1A	3102	1/1	0.87	0.18	60,60,60,60	0
57	MG	2A	3008	1/1	0.87	0.14	57,57,57,57	0
57	MG	2A	3247	1/1	0.87	0.19	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1649	1/1	0.87	0.18	73,73,73,73	0
57	MG	1A	3148	1/1	0.87	0.33	42,42,42,42	0
57	MG	2A	3391	1/1	0.87	0.15	78,78,78,78	0
57	MG	2A	3252	1/1	0.87	0.24	71,71,71,71	0
57	MG	2a	1657	1/1	0.87	0.18	86,86,86,86	0
57	MG	2A	3395	1/1	0.87	0.14	71,71,71,71	0
57	MG	2A	3404	1/1	0.87	0.23	48,48,48,48	0
57	MG	1A	3312	1/1	0.87	0.21	56,56,56,56	0
57	MG	1A	3830	1/1	0.87	0.15	61,61,61,61	0
57	MG	2A	3414	1/1	0.87	0.26	68,68,68,68	0
57	MG	2A	3419	1/1	0.87	0.21	65,65,65,65	0
57	MG	1A	3157	1/1	0.87	0.16	33,33,33,33	0
57	MG	1F	310	1/1	0.87	0.13	55,55,55,55	0
57	MG	1a	1710	1/1	0.87	0.17	69,69,69,69	0
57	MG	2A	3086	1/1	0.87	0.28	73,73,73,73	0
57	MG	2A	3433	1/1	0.87	0.13	69,69,69,69	0
57	MG	2A	3087	1/1	0.87	0.19	59,59,59,59	0
57	MG	2A	3275	1/1	0.87	0.28	77,77,77,77	0
57	MG	1A	3361	1/1	0.87	0.12	74,74,74,74	0
57	MG	1A	3845	1/1	0.87	0.09	62,62,62,62	0
57	MG	1a	1725	1/1	0.87	0.10	58,58,58,58	0
57	MG	1R	205	1/1	0.87	0.21	54,54,54,54	0
57	MG	1A	3364	1/1	0.87	0.16	58,58,58,58	0
57	MG	2A	3285	1/1	0.87	0.15	62,62,62,62	0
57	MG	1A	3657	1/1	0.87	0.08	32,32,32,32	0
57	MG	2a	1715	1/1	0.87	0.28	77,77,77,77	0
57	MG	2A	3480	1/1	0.87	0.27	68,68,68,68	0
57	MG	1a	1746	1/1	0.87	0.13	73,73,73,73	0
57	MG	1A	3433	1/1	0.87	0.13	58,58,58,58	0
57	MG	2A	3766	1/1	0.87	0.20	77,77,77,77	0
57	MG	1A	3866	1/1	0.87	0.18	46,46,46,46	0
57	MG	1A	4032	1/1	0.87	0.12	61,61,61,61	0
57	MG	2A	3117	1/1	0.87	0.16	52,52,52,52	0
57	MG	2a	1733	1/1	0.87	0.12	64,64,64,64	0
57	MG	2A	3778	1/1	0.87	0.23	79,79,79,79	0
57	MG	1A	3441	1/1	0.87	0.14	56,56,56,56	0
57	MG	1A	4049	1/1	0.87	0.14	52,52,52,52	0
57	MG	2A	3506	1/1	0.87	0.16	74,74,74,74	0
57	MG	1A	3445	1/1	0.87	0.11	53,53,53,53	0
57	MG	2A	3511	1/1	0.87	0.15	42,42,42,42	0
57	MG	2A	3149	1/1	0.87	0.23	68,68,68,68	0
57	MG	1A	3446	1/1	0.87	0.20	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3698	1/1	0.87	0.14	64,64,64,64	0
57	MG	2A	3536	1/1	0.87	0.23	63,63,63,63	0
57	MG	1A	3459	1/1	0.87	0.10	58,58,58,58	0
57	MG	2A	3543	1/1	0.87	0.14	71,71,71,71	0
57	MG	1a	1605	1/1	0.87	0.09	71,71,71,71	0
57	MG	2A	3556	1/1	0.87	0.10	69,69,69,69	0
57	MG	1a	1611	1/1	0.87	0.13	70,70,70,70	0
57	MG	2B	205	1/1	0.87	0.12	68,68,68,68	0
57	MG	1A	3541	1/1	0.87	0.17	47,47,47,47	0
57	MG	1A	3462	1/1	0.87	0.29	69,69,69,69	0
57	MG	2A	3582	1/1	0.87	0.23	69,69,69,69	0
57	MG	2A	3584	1/1	0.87	0.12	67,67,67,67	0
57	MG	1A	3225	1/1	0.87	0.17	51,51,51,51	0
57	MG	1A	3380	1/1	0.87	0.33	69,69,69,69	0
57	MG	1a	1628	1/1	0.87	0.11	58,58,58,58	0
57	MG	2A	3189	1/1	0.87	0.14	62,62,62,62	0
57	MG	1a	1815	1/1	0.87	0.15	74,74,74,74	0
57	MG	1A	3734	1/1	0.87	0.12	65,65,65,65	0
57	MG	1a	1824	1/1	0.87	0.21	68,68,68,68	0
57	MG	2A	3198	1/1	0.87	0.13	60,60,60,60	0
57	MG	1A	4093	1/1	0.87	0.17	52,52,52,52	0
57	MG	1a	1635	1/1	0.87	0.26	79,79,79,79	0
57	MG	2A	3632	1/1	0.87	0.18	65,65,65,65	0
57	MG	1A	3557	1/1	0.87	0.12	66,66,66,66	0
57	MG	2A	3205	1/1	0.87	0.14	63,63,63,63	0
57	MG	1A	3052	1/1	0.87	0.10	50,50,50,50	0
57	MG	2A	3650	1/1	0.87	0.18	81,81,81,81	0
57	MG	25	105	1/1	0.87	0.15	63,63,63,63	0
57	MG	2w	103	1/1	0.87	0.19	75,75,75,75	0
57	MG	26	101	1/1	0.87	0.27	78,78,78,78	0
57	MG	27	102	1/1	0.87	0.14	53,53,53,53	0
57	MG	1A	3795	1/1	0.87	0.11	28,28,28,28	0
57	MG	1A	3440	1/1	0.88	0.20	65,65,65,65	0
57	MG	1h	201	1/1	0.88	0.10	66,66,66,66	0
57	MG	1A	3546	1/1	0.88	0.22	61,61,61,61	0
57	MG	1n	102	1/1	0.88	0.21	62,62,62,62	0
57	MG	1a	1643	1/1	0.88	0.11	73,73,73,73	0
57	MG	2A	3645	1/1	0.88	0.14	52,52,52,52	0
57	MG	1A	3296	1/1	0.88	0.15	51,51,51,51	0
57	MG	2A	3210	1/1	0.88	0.22	74,74,74,74	0
57	MG	2A	3212	1/1	0.88	0.28	73,73,73,73	0
57	MG	1a	1655	1/1	0.88	0.24	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3656	1/1	0.88	0.14	64,64,64,64	0
57	MG	2a	1618	1/1	0.88	0.11	64,64,64,64	0
57	MG	1B	220	1/1	0.88	0.21	72,72,72,72	0
57	MG	1A	3823	1/1	0.88	0.08	38,38,38,38	0
57	MG	2A	3661	1/1	0.88	0.19	72,72,72,72	0
57	MG	2a	1628	1/1	0.88	0.20	68,68,68,68	0
57	MG	1A	3682	1/1	0.88	0.10	44,44,44,44	0
57	MG	2A	3381	1/1	0.88	0.20	64,64,64,64	0
57	MG	1a	1666	1/1	0.88	0.19	71,71,71,71	0
57	MG	1A	3984	1/1	0.88	0.12	66,66,66,66	0
57	MG	2A	3385	1/1	0.88	0.23	74,74,74,74	0
57	MG	1A	3551	1/1	0.88	0.21	66,66,66,66	0
57	MG	1A	3493	1/1	0.88	0.20	47,47,47,47	0
57	MG	1A	3089	1/1	0.88	0.10	37,37,37,37	0
57	MG	1x	105	1/1	0.88	0.20	71,71,71,71	0
57	MG	1A	3837	1/1	0.88	0.12	52,52,52,52	0
57	MG	1A	3998	1/1	0.88	0.11	64,64,64,64	0
57	MG	2A	3403	1/1	0.88	0.28	55,55,55,55	0
57	MG	1E	307	1/1	0.88	0.14	59,59,59,59	0
57	MG	1A	3095	1/1	0.88	0.14	61,61,61,61	0
57	MG	2A	3027	1/1	0.88	0.14	63,63,63,63	0
57	MG	1F	303	1/1	0.88	0.11	59,59,59,59	0
57	MG	2A	3694	1/1	0.88	0.14	59,59,59,59	0
57	MG	2A	3416	1/1	0.88	0.18	60,60,60,60	0
57	MG	1A	3709	1/1	0.88	0.10	58,58,58,58	0
57	MG	2A	3256	1/1	0.88	0.24	57,57,57,57	0
57	MG	2A	3056	1/1	0.88	0.32	74,74,74,74	0
57	MG	1O	202	1/1	0.88	0.17	66,66,66,66	0
57	MG	2A	3263	1/1	0.88	0.17	65,65,65,65	0
57	MG	2A	3264	1/1	0.88	0.27	65,65,65,65	0
57	MG	2A	3708	1/1	0.88	0.15	71,71,71,71	0
57	MG	2a	1693	1/1	0.88	0.19	67,67,67,67	0
57	MG	2A	3265	1/1	0.88	0.18	65,65,65,65	0
57	MG	2a	1697	1/1	0.88	0.22	68,68,68,68	0
57	MG	1A	3226	1/1	0.88	0.16	46,46,46,46	0
57	MG	2A	3443	1/1	0.88	0.17	50,50,50,50	0
57	MG	1A	3065	1/1	0.88	0.11	56,56,56,56	0
57	MG	2A	3083	1/1	0.88	0.13	62,62,62,62	0
57	MG	1A	3721	1/1	0.88	0.20	73,73,73,73	0
57	MG	2A	3457	1/1	0.88	0.12	72,72,72,72	0
57	MG	2A	3733	1/1	0.88	0.16	72,72,72,72	0
57	MG	1a	1711	1/1	0.88	0.27	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1R	206	1/1	0.88	0.11	32,32,32,32	0
57	MG	1A	3418	1/1	0.88	0.35	69,69,69,69	0
57	MG	1A	4023	1/1	0.88	0.12	53,53,53,53	0
57	MG	2A	3476	1/1	0.88	0.27	68,68,68,68	0
57	MG	1A	3466	1/1	0.88	0.19	58,58,58,58	0
57	MG	2A	3754	1/1	0.88	0.08	44,44,44,44	0
57	MG	2a	1723	1/1	0.88	0.30	66,66,66,66	0
57	MG	2a	1725	1/1	0.88	0.45	75,75,75,75	0
57	MG	1a	1733	1/1	0.88	0.40	79,79,79,79	0
57	MG	1T	203	1/1	0.88	0.18	54,54,54,54	0
57	MG	1a	1735	1/1	0.88	0.30	53,53,53,53	0
57	MG	1A	3614	1/1	0.88	0.09	15,15,15,15	0
57	MG	1A	4036	1/1	0.88	0.09	52,52,52,52	0
57	MG	1A	3737	1/1	0.88	0.09	65,65,65,65	0
57	MG	2A	3497	1/1	0.88	0.25	49,49,49,49	0
57	MG	1A	3739	1/1	0.88	0.11	22,22,22,22	0
57	MG	2A	3302	1/1	0.88	0.33	64,64,64,64	0
57	MG	1a	1757	1/1	0.88	0.20	50,50,50,50	0
57	MG	2A	3121	1/1	0.88	0.14	60,60,60,60	0
57	MG	1A	3129	1/1	0.88	0.18	53,53,53,53	0
57	MG	2A	3523	1/1	0.88	0.14	63,63,63,63	0
57	MG	2A	3527	1/1	0.88	0.13	70,70,70,70	0
57	MG	2A	3842	1/1	0.88	0.13	76,76,76,76	0
57	MG	2a	1775	1/1	0.88	0.14	67,67,67,67	0
57	MG	2a	1777	1/1	0.88	0.13	75,75,75,75	0
57	MG	2A	3530	1/1	0.88	0.08	43,43,43,43	0
57	MG	2a	1785	1/1	0.88	0.15	80,80,80,80	0
57	MG	2A	3136	1/1	0.88	0.13	68,68,68,68	0
57	MG	1A	3915	1/1	0.88	0.15	38,38,38,38	0
57	MG	2a	1788	1/1	0.88	0.27	77,77,77,77	0
57	MG	1a	1776	1/1	0.88	0.21	70,70,70,70	0
57	MG	1A	3926	1/1	0.88	0.11	32,32,32,32	0
57	MG	18	105	1/1	0.88	0.14	52,52,52,52	0
57	MG	1A	3768	1/1	0.88	0.09	23,23,23,23	0
57	MG	1a	1603	1/1	0.88	0.11	67,67,67,67	0
57	MG	1a	1604	1/1	0.88	0.11	59,59,59,59	0
57	MG	2A	3566	1/1	0.88	0.16	64,64,64,64	0
57	MG	2A	3328	1/1	0.88	0.20	68,68,68,68	0
57	MG	2B	215	1/1	0.88	0.16	73,73,73,73	0
57	MG	1A	3530	1/1	0.88	0.16	45,45,45,45	0
57	MG	1A	3258	1/1	0.88	0.11	79,79,79,79	0
57	MG	1A	3334	1/1	0.88	0.14	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3178	1/1	0.88	0.14	60,60,60,60	0
57	MG	2A	3586	1/1	0.88	0.14	69,69,69,69	0
57	MG	1A	3272	1/1	0.88	0.16	52,52,52,52	0
57	MG	2e	201	1/1	0.88	0.12	72,72,72,72	0
57	MG	2A	3594	1/1	0.88	0.24	69,69,69,69	0
57	MG	2O	201	1/1	0.88	0.20	57,57,57,57	0
57	MG	2l	201	1/1	0.88	0.16	64,64,64,64	0
57	MG	1A	3946	1/1	0.88	0.13	72,72,72,72	0
57	MG	1A	3087	1/1	0.88	0.19	34,34,34,34	0
57	MG	1a	1627	1/1	0.88	0.28	59,59,59,59	0
57	MG	1a	1805	1/1	0.88	0.08	58,58,58,58	0
57	MG	1A	4094	1/1	0.88	0.11	52,52,52,52	0
57	MG	2A	3616	1/1	0.88	0.10	36,36,36,36	0
57	MG	2Z	301	1/1	0.88	0.10	82,82,82,82	0
57	MG	1A	3542	1/1	0.88	0.23	59,59,59,59	0
57	MG	2x	103	1/1	0.88	0.15	81,81,81,81	0
57	MG	1A	3654	1/1	0.88	0.16	52,52,52,52	0
57	MG	1A	3383	1/1	0.89	0.20	44,44,44,44	0
57	MG	1A	4082	1/1	0.89	0.11	23,23,23,23	0
57	MG	1a	1779	1/1	0.89	0.17	65,65,65,65	0
57	MG	1A	3535	1/1	0.89	0.27	58,58,58,58	0
57	MG	25	103	1/1	0.89	0.24	61,61,61,61	0
57	MG	1A	3661	1/1	0.89	0.10	57,57,57,57	0
57	MG	2A	3621	1/1	0.89	0.15	53,53,53,53	0
57	MG	2A	3623	1/1	0.89	0.10	60,60,60,60	0
57	MG	2a	1602	1/1	0.89	0.10	70,70,70,70	0
57	MG	1A	3299	1/1	0.89	0.16	56,56,56,56	0
57	MG	2a	1605	1/1	0.89	0.34	77,77,77,77	0
57	MG	1A	3960	1/1	0.89	0.09	38,38,38,38	0
57	MG	2a	1607	1/1	0.89	0.12	58,58,58,58	0
57	MG	1a	1615	1/1	0.89	0.19	68,68,68,68	0
57	MG	1a	1789	1/1	0.89	0.11	71,71,71,71	0
57	MG	1A	3467	1/1	0.89	0.17	34,34,34,34	0
57	MG	1A	3968	1/1	0.89	0.12	57,57,57,57	0
57	MG	1a	1625	1/1	0.89	0.21	62,62,62,62	0
57	MG	2a	1616	1/1	0.89	0.16	72,72,72,72	0
57	MG	2a	1617	1/1	0.89	0.31	73,73,73,73	0
57	MG	1A	3680	1/1	0.89	0.12	63,63,63,63	0
57	MG	1A	3260	1/1	0.89	0.06	30,30,30,30	0
57	MG	2A	3194	1/1	0.89	0.19	58,58,58,58	0
57	MG	1A	3269	1/1	0.89	0.20	63,63,63,63	0
57	MG	2A	3367	1/1	0.89	0.11	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3196	1/1	0.89	0.32	58,58,58,58	0
57	MG	1A	3248	1/1	0.89	0.22	68,68,68,68	0
57	MG	1A	3834	1/1	0.89	0.09	55,55,55,55	0
57	MG	1A	3319	1/1	0.89	0.17	53,53,53,53	0
57	MG	1a	1637	1/1	0.89	0.12	52,52,52,52	0
57	MG	2A	3203	1/1	0.89	0.08	66,66,66,66	0
57	MG	2a	1643	1/1	0.89	0.12	60,60,60,60	0
57	MG	1a	1639	1/1	0.89	0.30	65,65,65,65	0
57	MG	1A	3320	1/1	0.89	0.08	46,46,46,46	0
57	MG	1a	1646	1/1	0.89	0.10	66,66,66,66	0
57	MG	1A	3252	1/1	0.89	0.12	76,76,76,76	0
57	MG	1l	202	1/1	0.89	0.16	68,68,68,68	0
57	MG	1A	3994	1/1	0.89	0.17	65,65,65,65	0
57	MG	1A	3484	1/1	0.89	0.12	46,46,46,46	0
57	MG	2a	1652	1/1	0.89	0.13	64,64,64,64	0
57	MG	2a	1653	1/1	0.89	0.26	65,65,65,65	0
57	MG	2a	1655	1/1	0.89	0.12	81,81,81,81	0
57	MG	1A	3857	1/1	0.89	0.32	42,42,42,42	0
57	MG	1a	1663	1/1	0.89	0.14	64,64,64,64	0
57	MG	2a	1658	1/1	0.89	0.16	68,68,68,68	0
57	MG	1A	3121	1/1	0.89	0.10	46,46,46,46	0
57	MG	2a	1662	1/1	0.89	0.12	76,76,76,76	0
57	MG	2a	1664	1/1	0.89	0.24	69,69,69,69	0
57	MG	2A	3399	1/1	0.89	0.25	59,59,59,59	0
57	MG	2A	3216	1/1	0.89	0.20	64,64,64,64	0
57	MG	1A	3428	1/1	0.89	0.25	53,53,53,53	0
57	MG	1E	308	1/1	0.89	0.11	30,30,30,30	0
57	MG	2A	3695	1/1	0.89	0.14	52,52,52,52	0
57	MG	2A	3406	1/1	0.89	0.19	45,45,45,45	0
57	MG	1a	1670	1/1	0.89	0.25	72,72,72,72	0
57	MG	2a	1683	1/1	0.89	0.15	68,68,68,68	0
57	MG	1A	3863	1/1	0.89	0.09	34,34,34,34	0
57	MG	2A	3235	1/1	0.89	0.13	62,62,62,62	0
57	MG	1A	3723	1/1	0.89	0.15	60,60,60,60	0
57	MG	2A	3421	1/1	0.89	0.49	70,70,70,70	0
57	MG	2a	1695	1/1	0.89	0.23	80,80,80,80	0
57	MG	1A	3870	1/1	0.89	0.17	40,40,40,40	0
57	MG	1A	3496	1/1	0.89	0.14	50,50,50,50	0
57	MG	1x	104	1/1	0.89	0.17	69,69,69,69	0
57	MG	1A	3024	1/1	0.89	0.30	64,64,64,64	0
57	MG	2a	1703	1/1	0.89	0.16	75,75,75,75	0
57	MG	2A	3432	1/1	0.89	0.22	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3365	1/1	0.89	0.17	66,66,66,66	0
57	MG	1x	109	1/1	0.89	0.17	74,74,74,74	0
57	MG	1x	110	1/1	0.89	0.25	63,63,63,63	0
57	MG	2a	1711	1/1	0.89	0.13	68,68,68,68	0
57	MG	2A	3729	1/1	0.89	0.16	66,66,66,66	0
57	MG	2a	1713	1/1	0.89	0.25	80,80,80,80	0
57	MG	2A	3439	1/1	0.89	0.15	72,72,72,72	0
57	MG	1a	1683	1/1	0.89	0.12	57,57,57,57	0
57	MG	2a	1718	1/1	0.89	0.22	72,72,72,72	0
57	MG	2A	3001	1/1	0.89	0.35	62,62,62,62	0
57	MG	1A	4025	1/1	0.89	0.13	57,57,57,57	0
57	MG	1a	1691	1/1	0.89	0.22	78,78,78,78	0
57	MG	1A	3366	1/1	0.89	0.12	48,48,48,48	0
57	MG	1a	1693	1/1	0.89	0.14	68,68,68,68	0
57	MG	2A	3041	1/1	0.89	0.18	68,68,68,68	0
57	MG	2A	3468	1/1	0.89	0.15	62,62,62,62	0
57	MG	2A	3045	1/1	0.89	0.22	74,74,74,74	0
57	MG	2A	3048	1/1	0.89	0.23	67,67,67,67	0
57	MG	2A	3763	1/1	0.89	0.09	65,65,65,65	0
57	MG	2A	3267	1/1	0.89	0.12	59,59,59,59	0
57	MG	1A	3338	1/1	0.89	0.14	50,50,50,50	0
57	MG	1A	4033	1/1	0.89	0.09	61,61,61,61	0
57	MG	2a	1741	1/1	0.89	0.26	62,62,62,62	0
57	MG	2A	3060	1/1	0.89	0.13	65,65,65,65	0
57	MG	2A	3061	1/1	0.89	0.10	76,76,76,76	0
57	MG	1a	1699	1/1	0.89	0.18	53,53,53,53	0
57	MG	2A	3064	1/1	0.89	0.27	59,59,59,59	0
57	MG	1a	1700	1/1	0.89	0.31	59,59,59,59	0
57	MG	2a	1764	1/1	0.89	0.09	89,89,89,89	0
57	MG	2A	3282	1/1	0.89	0.14	64,64,64,64	0
57	MG	2A	3807	1/1	0.89	0.10	55,55,55,55	0
57	MG	1S	203	1/1	0.89	0.13	68,68,68,68	0
57	MG	2A	3816	1/1	0.89	0.08	54,54,54,54	0
57	MG	2A	3505	1/1	0.89	0.20	63,63,63,63	0
57	MG	2A	3818	1/1	0.89	0.11	43,43,43,43	0
57	MG	2A	3823	1/1	0.89	0.14	70,70,70,70	0
57	MG	2A	3829	1/1	0.89	0.14	45,45,45,45	0
57	MG	2A	3077	1/1	0.89	0.10	53,53,53,53	0
57	MG	2A	3287	1/1	0.89	0.12	65,65,65,65	0
57	MG	1A	3895	1/1	0.89	0.23	39,39,39,39	0
57	MG	2a	1790	1/1	0.89	0.20	67,67,67,67	0
57	MG	1T	202	1/1	0.89	0.26	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1792	1/1	0.89	0.25	66,66,66,66	0
57	MG	1A	3896	1/1	0.89	0.13	64,64,64,64	0
57	MG	1a	1712	1/1	0.89	0.10	85,85,85,85	0
57	MG	2a	1800	1/1	0.89	0.12	83,83,83,83	0
57	MG	1A	3512	1/1	0.89	0.17	58,58,58,58	0
57	MG	2a	1802	1/1	0.89	0.16	76,76,76,76	0
57	MG	2A	3097	1/1	0.89	0.20	63,63,63,63	0
57	MG	1A	4053	1/1	0.89	0.08	59,59,59,59	0
57	MG	1A	3633	1/1	0.89	0.08	21,21,21,21	0
57	MG	1A	3378	1/1	0.89	0.23	50,50,50,50	0
57	MG	2B	208	1/1	0.89	0.21	65,65,65,65	0
57	MG	2A	3310	1/1	0.89	0.12	61,61,61,61	0
57	MG	2A	3548	1/1	0.89	0.10	54,54,54,54	0
57	MG	2a	1819	1/1	0.89	0.25	74,74,74,74	0
57	MG	1Z	301	1/1	0.89	0.16	77,77,77,77	0
57	MG	10	105	1/1	0.89	0.28	65,65,65,65	0
57	MG	2a	1822	1/1	0.89	0.26	67,67,67,67	0
57	MG	1A	3339	1/1	0.89	0.09	36,36,36,36	0
57	MG	13	101	1/1	0.89	0.08	49,49,49,49	0
57	MG	2A	3114	1/1	0.89	0.18	63,63,63,63	0
57	MG	1a	1742	1/1	0.89	0.17	61,61,61,61	0
57	MG	2F	302	1/1	0.89	0.18	72,72,72,72	0
57	MG	2A	3575	1/1	0.89	0.11	43,43,43,43	0
57	MG	1A	3340	1/1	0.89	0.27	63,63,63,63	0
57	MG	1A	3460	1/1	0.89	0.11	57,57,57,57	0
57	MG	1A	4071	1/1	0.89	0.12	47,47,47,47	0
57	MG	2R	201	1/1	0.89	0.23	66,66,66,66	0
57	MG	2A	3327	1/1	0.89	0.12	71,71,71,71	0
57	MG	1a	1755	1/1	0.89	0.15	82,82,82,82	0
57	MG	2A	3331	1/1	0.89	0.13	60,60,60,60	0
57	MG	18	106	1/1	0.89	0.13	63,63,63,63	0
57	MG	1A	3342	1/1	0.89	0.12	71,71,71,71	0
57	MG	1A	3533	1/1	0.90	0.16	54,54,54,54	0
57	MG	1a	1701	1/1	0.90	0.29	68,68,68,68	0
57	MG	2A	3223	1/1	0.90	0.10	79,79,79,79	0
57	MG	2A	3227	1/1	0.90	0.13	50,50,50,50	0
57	MG	2A	3229	1/1	0.90	0.10	53,53,53,53	0
57	MG	1A	3477	1/1	0.90	0.08	66,66,66,66	0
57	MG	1Z	302	1/1	0.90	0.09	65,65,65,65	0
57	MG	2A	3037	1/1	0.90	0.27	71,71,71,71	0
57	MG	1a	1708	1/1	0.90	0.17	68,68,68,68	0
57	MG	2A	3390	1/1	0.90	0.09	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1620	1/1	0.90	0.11	73,73,73,73	0
57	MG	1A	3343	1/1	0.90	0.12	58,58,58,58	0
57	MG	2a	1623	1/1	0.90	0.32	73,73,73,73	0
57	MG	1A	3480	1/1	0.90	0.18	58,58,58,58	0
57	MG	2A	3393	1/1	0.90	0.25	67,67,67,67	0
57	MG	2A	3671	1/1	0.90	0.15	56,56,56,56	0
57	MG	11	103	1/1	0.90	0.09	67,67,67,67	0
57	MG	2A	3049	1/1	0.90	0.07	52,52,52,52	0
57	MG	2a	1633	1/1	0.90	0.24	62,62,62,62	0
57	MG	2a	1635	1/1	0.90	0.15	69,69,69,69	0
57	MG	1a	1714	1/1	0.90	0.16	64,64,64,64	0
57	MG	1A	3439	1/1	0.90	0.30	73,73,73,73	0
57	MG	2a	1640	1/1	0.90	0.18	72,72,72,72	0
57	MG	2A	3057	1/1	0.90	0.24	58,58,58,58	0
57	MG	1A	3313	1/1	0.90	0.26	54,54,54,54	0
57	MG	2A	3410	1/1	0.90	0.11	48,48,48,48	0
57	MG	1A	3285	1/1	0.90	0.10	42,42,42,42	0
57	MG	17	105	1/1	0.90	0.14	49,49,49,49	0
57	MG	2a	1646	1/1	0.90	0.11	63,63,63,63	0
57	MG	2A	3690	1/1	0.90	0.23	65,65,65,65	0
57	MG	1A	3158	1/1	0.90	0.10	56,56,56,56	0
57	MG	1A	4086	1/1	0.90	0.11	50,50,50,50	0
57	MG	1A	3817	1/1	0.90	0.13	49,49,49,49	0
57	MG	2A	3071	1/1	0.90	0.10	62,62,62,62	0
57	MG	2A	3696	1/1	0.90	0.07	70,70,70,70	0
57	MG	1A	3821	1/1	0.90	0.16	38,38,38,38	0
57	MG	2A	3425	1/1	0.90	0.14	55,55,55,55	0
57	MG	1A	4090	1/1	0.90	0.27	48,48,48,48	0
57	MG	1A	3356	1/1	0.90	0.21	43,43,43,43	0
57	MG	2A	3429	1/1	0.90	0.19	59,59,59,59	0
57	MG	2A	3268	1/1	0.90	0.22	68,68,68,68	0
57	MG	1A	3447	1/1	0.90	0.18	47,47,47,47	0
57	MG	1A	3964	1/1	0.90	0.11	53,53,53,53	0
57	MG	1B	206	1/1	0.90	0.21	49,49,49,49	0
57	MG	1A	3295	1/1	0.90	0.11	42,42,42,42	0
57	MG	1A	3689	1/1	0.90	0.09	26,26,26,26	0
57	MG	1A	3832	1/1	0.90	0.10	31,31,31,31	0
57	MG	2a	1677	1/1	0.90	0.14	67,67,67,67	0
57	MG	1a	1771	1/1	0.90	0.18	78,78,78,78	0
57	MG	1A	3506	1/1	0.90	0.11	58,58,58,58	0
57	MG	2a	1681	1/1	0.90	0.16	70,70,70,70	0
57	MG	1A	3567	1/1	0.90	0.06	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3462	1/1	0.90	0.08	61,61,61,61	0
57	MG	2a	1686	1/1	0.90	0.19	81,81,81,81	0
57	MG	1A	3981	1/1	0.90	0.09	75,75,75,75	0
57	MG	2A	3286	1/1	0.90	0.30	60,60,60,60	0
57	MG	2a	1690	1/1	0.90	0.14	70,70,70,70	0
57	MG	2A	3740	1/1	0.90	0.08	52,52,52,52	0
57	MG	2A	3107	1/1	0.90	0.29	73,73,73,73	0
57	MG	2A	3111	1/1	0.90	0.28	69,69,69,69	0
57	MG	2A	3473	1/1	0.90	0.18	71,71,71,71	0
57	MG	1a	1782	1/1	0.90	0.10	91,91,91,91	0
57	MG	2A	3292	1/1	0.90	0.10	59,59,59,59	0
57	MG	1A	3836	1/1	0.90	0.14	57,57,57,57	0
57	MG	2A	3296	1/1	0.90	0.30	64,64,64,64	0
57	MG	2a	1704	1/1	0.90	0.15	72,72,72,72	0
57	MG	2A	3759	1/1	0.90	0.11	67,67,67,67	0
57	MG	2A	3483	1/1	0.90	0.09	59,59,59,59	0
57	MG	1B	223	1/1	0.90	0.16	63,63,63,63	0
57	MG	1a	1632	1/1	0.90	0.19	61,61,61,61	0
57	MG	2a	1710	1/1	0.90	0.14	72,72,72,72	0
57	MG	1A	3702	1/1	0.90	0.13	47,47,47,47	0
57	MG	2A	3772	1/1	0.90	0.20	68,68,68,68	0
57	MG	2A	3774	1/1	0.90	0.14	76,76,76,76	0
57	MG	1A	3839	1/1	0.90	0.27	67,67,67,67	0
57	MG	2A	3490	1/1	0.90	0.23	63,63,63,63	0
57	MG	2A	3491	1/1	0.90	0.33	70,70,70,70	0
57	MG	2A	3492	1/1	0.90	0.17	62,62,62,62	0
57	MG	2A	3495	1/1	0.90	0.39	72,72,72,72	0
57	MG	2A	3797	1/1	0.90	0.19	65,65,65,65	0
57	MG	1A	3575	1/1	0.90	0.17	44,44,44,44	0
57	MG	1A	3204	1/1	0.90	0.09	48,48,48,48	0
57	MG	2A	3802	1/1	0.90	0.12	64,64,64,64	0
57	MG	2a	1726	1/1	0.90	0.39	76,76,76,76	0
57	MG	1a	1640	1/1	0.90	0.29	71,71,71,71	0
57	MG	2A	3311	1/1	0.90	0.19	78,78,78,78	0
57	MG	1A	3209	1/1	0.90	0.10	46,46,46,46	0
57	MG	2a	1731	1/1	0.90	0.26	63,63,63,63	0
57	MG	1a	1795	1/1	0.90	0.18	65,65,65,65	0
57	MG	2a	1734	1/1	0.90	0.31	67,67,67,67	0
57	MG	1B	233	1/1	0.90	0.10	57,57,57,57	0
57	MG	1B	234	1/1	0.90	0.13	72,72,72,72	0
57	MG	1a	1649	1/1	0.90	0.16	62,62,62,62	0
57	MG	2a	1740	1/1	0.90	0.28	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1650	1/1	0.90	0.24	77,77,77,77	0
57	MG	2A	3840	1/1	0.90	0.11	71,71,71,71	0
57	MG	1A	3588	1/1	0.90	0.11	53,53,53,53	0
57	MG	1A	3124	1/1	0.90	0.18	55,55,55,55	0
57	MG	1a	1660	1/1	0.90	0.19	66,66,66,66	0
57	MG	2A	3326	1/1	0.90	0.11	48,48,48,48	0
57	MG	2A	3537	1/1	0.90	0.17	54,54,54,54	0
57	MG	1A	3596	1/1	0.90	0.23	56,56,56,56	0
57	MG	2A	3862	1/1	0.90	0.25	65,65,65,65	0
57	MG	2A	3540	1/1	0.90	0.11	78,78,78,78	0
57	MG	2B	202	1/1	0.90	0.10	64,64,64,64	0
57	MG	1b	302	1/1	0.90	0.17	84,84,84,84	0
57	MG	1A	3336	1/1	0.90	0.09	49,49,49,49	0
57	MG	1A	3519	1/1	0.90	0.12	58,58,58,58	0
57	MG	2B	207	1/1	0.90	0.18	70,70,70,70	0
57	MG	1A	4005	1/1	0.90	0.11	23,23,23,23	0
57	MG	2A	3192	1/1	0.90	0.22	63,63,63,63	0
57	MG	1G	204	1/1	0.90	0.15	55,55,55,55	0
57	MG	1A	3617	1/1	0.90	0.12	70,70,70,70	0
57	MG	1a	1671	1/1	0.90	0.26	62,62,62,62	0
57	MG	2A	3339	1/1	0.90	0.11	61,61,61,61	0
57	MG	2B	220	1/1	0.90	0.30	73,73,73,73	0
57	MG	2A	3579	1/1	0.90	0.17	57,57,57,57	0
57	MG	1A	3876	1/1	0.90	0.14	37,37,37,37	0
57	MG	1A	3301	1/1	0.90	0.23	61,61,61,61	0
57	MG	1A	3303	1/1	0.90	0.25	36,36,36,36	0
57	MG	2a	1803	1/1	0.90	0.26	74,74,74,74	0
57	MG	1A	3626	1/1	0.90	0.07	32,32,32,32	0
57	MG	1A	3889	1/1	0.90	0.09	35,35,35,35	0
57	MG	2a	1807	1/1	0.90	0.29	67,67,67,67	0
57	MG	1A	3271	1/1	0.90	0.13	53,53,53,53	0
57	MG	2a	1810	1/1	0.90	0.14	63,63,63,63	0
57	MG	1A	3777	1/1	0.90	0.12	40,40,40,40	0
57	MG	2a	1814	1/1	0.90	0.16	70,70,70,70	0
57	MG	1A	3369	1/1	0.90	0.14	57,57,57,57	0
57	MG	2a	1816	1/1	0.90	0.12	74,74,74,74	0
57	MG	1a	1687	1/1	0.90	0.12	77,77,77,77	0
57	MG	2A	3358	1/1	0.90	0.10	62,62,62,62	0
57	MG	2A	3359	1/1	0.90	0.08	78,78,78,78	0
57	MG	2A	3610	1/1	0.90	0.16	72,72,72,72	0
57	MG	2U	202	1/1	0.90	0.19	51,51,51,51	0
57	MG	2V	201	1/1	0.90	0.10	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3360	1/1	0.90	0.15	47,47,47,47	0
57	MG	2X	101	1/1	0.90	0.14	73,73,73,73	0
57	MG	2A	3361	1/1	0.90	0.12	75,75,75,75	0
57	MG	1A	3898	1/1	0.90	0.09	45,45,45,45	0
57	MG	1A	3094	1/1	0.90	0.13	49,49,49,49	0
57	MG	1A	3900	1/1	0.90	0.11	49,49,49,49	0
57	MG	23	102	1/1	0.90	0.21	70,70,70,70	0
57	MG	2v	101	1/1	0.90	0.25	72,72,72,72	0
57	MG	1A	4055	1/1	0.90	0.10	31,31,31,31	0
57	MG	2v	104	1/1	0.90	0.15	70,70,70,70	0
57	MG	2A	3368	1/1	0.90	0.12	60,60,60,60	0
57	MG	1A	3902	1/1	0.90	0.24	40,40,40,40	0
57	MG	1X	106	1/1	0.90	0.12	83,83,83,83	0
57	MG	27	103	1/1	0.90	0.12	58,58,58,58	0
57	MG	2A	3641	1/1	0.90	0.10	44,44,44,44	0
57	MG	1x	112	1/1	0.90	0.17	66,66,66,66	0
57	MG	2A	3217	1/1	0.90	0.14	58,58,58,58	0
58	K	2A	3451	1/1	0.90	0.12	71,71,71,71	0
57	MG	1A	3386	1/1	0.91	0.09	52,52,52,52	0
57	MG	2a	1619	1/1	0.91	0.13	74,74,74,74	0
57	MG	2A	3380	1/1	0.91	0.26	58,58,58,58	0
57	MG	1a	1686	1/1	0.91	0.22	58,58,58,58	0
57	MG	1V	206	1/1	0.91	0.23	60,60,60,60	0
57	MG	1A	3020	1/1	0.91	0.11	44,44,44,44	0
57	MG	1W	202	1/1	0.91	0.17	50,50,50,50	0
57	MG	1x	106	1/1	0.91	0.19	60,60,60,60	0
57	MG	1A	3045	1/1	0.91	0.07	36,36,36,36	0
57	MG	1x	108	1/1	0.91	0.12	33,33,33,33	0
57	MG	1A	3916	1/1	0.91	0.19	37,37,37,37	0
57	MG	1A	3919	1/1	0.91	0.12	71,71,71,71	0
57	MG	1A	3401	1/1	0.91	0.16	54,54,54,54	0
57	MG	1A	3208	1/1	0.91	0.11	35,35,35,35	0
57	MG	1A	3140	1/1	0.91	0.18	47,47,47,47	0
57	MG	2A	3398	1/1	0.91	0.15	65,65,65,65	0
57	MG	2A	3230	1/1	0.91	0.10	50,50,50,50	0
57	MG	1A	4072	1/1	0.91	0.14	47,47,47,47	0
57	MG	2A	3016	1/1	0.91	0.11	70,70,70,70	0
57	MG	2A	3234	1/1	0.91	0.13	65,65,65,65	0
57	MG	1A	3414	1/1	0.91	0.16	62,62,62,62	0
57	MG	2A	3023	1/1	0.91	0.31	71,71,71,71	0
57	MG	13	104	1/1	0.91	0.15	52,52,52,52	0
57	MG	2A	3028	1/1	0.91	0.11	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3029	1/1	0.91	0.19	62,62,62,62	0
57	MG	2A	3243	1/1	0.91	0.12	62,62,62,62	0
57	MG	2A	3420	1/1	0.91	0.25	66,66,66,66	0
57	MG	13	105	1/1	0.91	0.14	62,62,62,62	0
57	MG	2A	3039	1/1	0.91	0.31	70,70,70,70	0
57	MG	1A	3943	1/1	0.91	0.10	28,28,28,28	0
57	MG	2A	3250	1/1	0.91	0.40	68,68,68,68	0
57	MG	1A	3068	1/1	0.91	0.26	48,48,48,48	0
57	MG	2a	1659	1/1	0.91	0.07	80,80,80,80	0
57	MG	2A	3042	1/1	0.91	0.17	56,56,56,56	0
57	MG	1a	1713	1/1	0.91	0.17	73,73,73,73	0
57	MG	1A	3420	1/1	0.91	0.27	67,67,67,67	0
57	MG	1A	3422	1/1	0.91	0.18	38,38,38,38	0
57	MG	1a	1721	1/1	0.91	0.18	68,68,68,68	0
57	MG	2A	3052	1/1	0.91	0.21	70,70,70,70	0
57	MG	2A	3054	1/1	0.91	0.18	68,68,68,68	0
57	MG	2a	1674	1/1	0.91	0.20	64,64,64,64	0
57	MG	1A	3151	1/1	0.91	0.17	43,43,43,43	0
57	MG	1a	1723	1/1	0.91	0.17	55,55,55,55	0
57	MG	2A	3450	1/1	0.91	0.15	67,67,67,67	0
57	MG	19	101	1/1	0.91	0.21	54,54,54,54	0
57	MG	1A	3955	1/1	0.91	0.18	56,56,56,56	0
57	MG	1A	4092	1/1	0.91	0.13	69,69,69,69	0
57	MG	2A	3063	1/1	0.91	0.22	68,68,68,68	0
57	MG	1A	3153	1/1	0.91	0.11	37,37,37,37	0
57	MG	2A	3276	1/1	0.91	0.10	61,61,61,61	0
57	MG	1A	3550	1/1	0.91	0.20	53,53,53,53	0
57	MG	2a	1692	1/1	0.91	0.36	67,67,67,67	0
57	MG	1A	3482	1/1	0.91	0.11	42,42,42,42	0
57	MG	1a	1612	1/1	0.91	0.14	77,77,77,77	0
57	MG	1A	3688	1/1	0.91	0.14	33,33,33,33	0
57	MG	2A	3764	1/1	0.91	0.14	64,64,64,64	0
57	MG	2A	3080	1/1	0.91	0.14	61,61,61,61	0
57	MG	2A	3767	1/1	0.91	0.14	61,61,61,61	0
57	MG	1A	3552	1/1	0.91	0.16	55,55,55,55	0
57	MG	1A	3362	1/1	0.91	0.08	54,54,54,54	0
57	MG	2A	3482	1/1	0.91	0.21	56,56,56,56	0
57	MG	1A	3291	1/1	0.91	0.16	54,54,54,54	0
57	MG	1A	3491	1/1	0.91	0.08	45,45,45,45	0
57	MG	2A	3288	1/1	0.91	0.11	66,66,66,66	0
57	MG	1A	3566	1/1	0.91	0.17	36,36,36,36	0
57	MG	1a	1763	1/1	0.91	0.09	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3291	1/1	0.91	0.36	75,75,75,75	0
57	MG	1A	3335	1/1	0.91	0.12	63,63,63,63	0
57	MG	1a	1769	1/1	0.91	0.08	55,55,55,55	0
57	MG	2A	3295	1/1	0.91	0.12	57,57,57,57	0
57	MG	1A	3847	1/1	0.91	0.14	62,62,62,62	0
57	MG	1a	1775	1/1	0.91	0.25	70,70,70,70	0
57	MG	1A	3983	1/1	0.91	0.10	51,51,51,51	0
57	MG	2A	3500	1/1	0.91	0.33	69,69,69,69	0
57	MG	1a	1630	1/1	0.91	0.23	70,70,70,70	0
57	MG	2A	3820	1/1	0.91	0.09	47,47,47,47	0
57	MG	1A	3568	1/1	0.91	0.18	61,61,61,61	0
57	MG	2a	1724	1/1	0.91	0.24	72,72,72,72	0
57	MG	2A	3828	1/1	0.91	0.10	66,66,66,66	0
57	MG	2A	3304	1/1	0.91	0.15	66,66,66,66	0
57	MG	2A	3109	1/1	0.91	0.11	60,60,60,60	0
57	MG	2A	3512	1/1	0.91	0.19	63,63,63,63	0
57	MG	1A	3292	1/1	0.91	0.13	59,59,59,59	0
57	MG	2A	3518	1/1	0.91	0.15	44,44,44,44	0
57	MG	2A	3308	1/1	0.91	0.15	68,68,68,68	0
57	MG	2A	3526	1/1	0.91	0.11	52,52,52,52	0
57	MG	2A	3309	1/1	0.91	0.11	63,63,63,63	0
57	MG	2a	1737	1/1	0.91	0.31	63,63,63,63	0
57	MG	1A	3986	1/1	0.91	0.11	76,76,76,76	0
57	MG	2A	3531	1/1	0.91	0.09	53,53,53,53	0
57	MG	1A	3717	1/1	0.91	0.29	60,60,60,60	0
57	MG	1A	3576	1/1	0.91	0.13	47,47,47,47	0
57	MG	2a	1745	1/1	0.91	0.18	70,70,70,70	0
57	MG	1A	3073	1/1	0.91	0.35	68,68,68,68	0
57	MG	2A	3119	1/1	0.91	0.20	61,61,61,61	0
57	MG	2a	1749	1/1	0.91	0.09	62,62,62,62	0
57	MG	1A	3864	1/1	0.91	0.12	50,50,50,50	0
57	MG	1a	1641	1/1	0.91	0.20	73,73,73,73	0
57	MG	1A	3865	1/1	0.91	0.10	45,45,45,45	0
57	MG	2A	3129	1/1	0.91	0.14	78,78,78,78	0
57	MG	2B	213	1/1	0.91	0.21	62,62,62,62	0
57	MG	2A	3133	1/1	0.91	0.21	57,57,57,57	0
57	MG	1D	313	1/1	0.91	0.10	36,36,36,36	0
57	MG	2A	3138	1/1	0.91	0.29	61,61,61,61	0
57	MG	2B	217	1/1	0.91	0.17	71,71,71,71	0
57	MG	2A	3562	1/1	0.91	0.13	45,45,45,45	0
57	MG	2a	1784	1/1	0.91	0.16	68,68,68,68	0
57	MG	2A	3142	1/1	0.91	0.15	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3144	1/1	0.91	0.18	45,45,45,45	0
57	MG	1A	3374	1/1	0.91	0.19	48,48,48,48	0
57	MG	2E	304	1/1	0.91	0.12	65,65,65,65	0
57	MG	1a	1648	1/1	0.91	0.21	63,63,63,63	0
57	MG	1A	3244	1/1	0.91	0.27	39,39,39,39	0
57	MG	2F	306	1/1	0.91	0.22	50,50,50,50	0
57	MG	2A	3157	1/1	0.91	0.17	64,64,64,64	0
57	MG	2A	3335	1/1	0.91	0.15	78,78,78,78	0
57	MG	1A	3100	1/1	0.91	0.20	72,72,72,72	0
57	MG	2a	1798	1/1	0.91	0.14	81,81,81,81	0
57	MG	1E	311	1/1	0.91	0.21	41,41,41,41	0
57	MG	2A	3590	1/1	0.91	0.14	67,67,67,67	0
57	MG	1a	1656	1/1	0.91	0.11	50,50,50,50	0
57	MG	1A	3509	1/1	0.91	0.09	50,50,50,50	0
57	MG	1A	4006	1/1	0.91	0.16	32,32,32,32	0
57	MG	2A	3603	1/1	0.91	0.10	46,46,46,46	0
57	MG	1A	3047	1/1	0.91	0.15	33,33,33,33	0
57	MG	2A	3345	1/1	0.91	0.09	67,67,67,67	0
57	MG	2a	1809	1/1	0.91	0.20	74,74,74,74	0
57	MG	2V	202	1/1	0.91	0.34	54,54,54,54	0
57	MG	2A	3346	1/1	0.91	0.08	65,65,65,65	0
57	MG	1A	3251	1/1	0.91	0.15	45,45,45,45	0
57	MG	2A	3176	1/1	0.91	0.20	69,69,69,69	0
57	MG	2A	3612	1/1	0.91	0.14	61,61,61,61	0
57	MG	1a	1826	1/1	0.91	0.14	62,62,62,62	0
57	MG	1b	301	1/1	0.91	0.09	82,82,82,82	0
57	MG	2A	3184	1/1	0.91	0.20	62,62,62,62	0
57	MG	23	103	1/1	0.91	0.11	56,56,56,56	0
57	MG	1a	1664	1/1	0.91	0.26	73,73,73,73	0
57	MG	1e	202	1/1	0.91	0.17	53,53,53,53	0
57	MG	1f	202	1/1	0.91	0.14	75,75,75,75	0
57	MG	1A	4020	1/1	0.91	0.07	44,44,44,44	0
57	MG	1A	3759	1/1	0.91	0.11	26,26,26,26	0
57	MG	2a	1601	1/1	0.91	0.16	75,75,75,75	0
57	MG	1A	3764	1/1	0.91	0.13	33,33,33,33	0
57	MG	1n	101	1/1	0.91	0.29	64,64,64,64	0
57	MG	2A	3642	1/1	0.91	0.14	57,57,57,57	0
57	MG	1A	3891	1/1	0.91	0.07	34,34,34,34	0
57	MG	1A	3892	1/1	0.91	0.13	24,24,24,24	0
57	MG	1A	3451	1/1	0.91	0.25	43,43,43,43	0
57	MG	2a	1609	1/1	0.91	0.09	78,78,78,78	0
57	MG	1A	3515	1/1	0.91	0.10	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3781	1/1	0.91	0.07	63,63,63,63	0
57	MG	1A	4038	1/1	0.91	0.12	55,55,55,55	0
57	MG	1A	3050	1/1	0.91	0.10	27,27,27,27	0
57	MG	2a	1615	1/1	0.91	0.18	64,64,64,64	0
57	MG	1A	3195	1/1	0.91	0.12	30,30,30,30	0
57	MG	1U	205	1/1	0.91	0.15	38,38,38,38	0
57	MG	1A	3501	1/1	0.92	0.16	61,61,61,61	0
57	MG	1A	3924	1/1	0.92	0.11	51,51,51,51	0
57	MG	1B	203	1/1	0.92	0.06	37,37,37,37	0
57	MG	2A	3180	1/1	0.92	0.14	54,54,54,54	0
57	MG	1A	3747	1/1	0.92	0.10	45,45,45,45	0
57	MG	28	102	1/1	0.92	0.16	54,54,54,54	0
57	MG	1A	3928	1/1	0.92	0.08	46,46,46,46	0
57	MG	2A	3356	1/1	0.92	0.24	56,56,56,56	0
57	MG	1B	208	1/1	0.92	0.20	62,62,62,62	0
57	MG	1A	3233	1/1	0.92	0.08	56,56,56,56	0
57	MG	1f	201	1/1	0.92	0.18	50,50,50,50	0
57	MG	1A	3004	1/1	0.92	0.08	28,28,28,28	0
57	MG	1A	3595	1/1	0.92	0.13	37,37,37,37	0
57	MG	1B	218	1/1	0.92	0.16	49,49,49,49	0
57	MG	1A	3245	1/1	0.92	0.11	51,51,51,51	0
57	MG	1A	3601	1/1	0.92	0.09	35,35,35,35	0
57	MG	1A	3207	1/1	0.92	0.10	51,51,51,51	0
57	MG	2A	3646	1/1	0.92	0.12	58,58,58,58	0
57	MG	1a	1651	1/1	0.92	0.13	71,71,71,71	0
57	MG	1A	3789	1/1	0.92	0.14	54,54,54,54	0
57	MG	2A	3201	1/1	0.92	0.13	69,69,69,69	0
57	MG	1A	3794	1/1	0.92	0.08	30,30,30,30	0
57	MG	2A	3655	1/1	0.92	0.19	63,63,63,63	0
57	MG	1a	1657	1/1	0.92	0.21	55,55,55,55	0
57	MG	2a	1621	1/1	0.92	0.19	68,68,68,68	0
57	MG	2A	3376	1/1	0.92	0.14	53,53,53,53	0
57	MG	2A	3377	1/1	0.92	0.15	67,67,67,67	0
57	MG	1A	3609	1/1	0.92	0.09	43,43,43,43	0
57	MG	1A	3610	1/1	0.92	0.09	43,43,43,43	0
57	MG	1A	3387	1/1	0.92	0.10	51,51,51,51	0
57	MG	2a	1629	1/1	0.92	0.07	81,81,81,81	0
57	MG	1A	3961	1/1	0.92	0.08	52,52,52,52	0
57	MG	1A	3616	1/1	0.92	0.08	35,35,35,35	0
57	MG	1A	3449	1/1	0.92	0.11	67,67,67,67	0
57	MG	2a	1634	1/1	0.92	0.26	70,70,70,70	0
57	MG	1D	305	1/1	0.92	0.16	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3967	1/1	0.92	0.12	42,42,42,42	0
57	MG	2A	3387	1/1	0.92	0.09	58,58,58,58	0
57	MG	2a	1639	1/1	0.92	0.14	67,67,67,67	0
57	MG	1A	3618	1/1	0.92	0.12	28,28,28,28	0
57	MG	1A	3970	1/1	0.92	0.11	54,54,54,54	0
57	MG	1A	3388	1/1	0.92	0.11	47,47,47,47	0
57	MG	1a	1675	1/1	0.92	0.20	71,71,71,71	0
57	MG	2A	3684	1/1	0.92	0.10	43,43,43,43	0
57	MG	1A	3973	1/1	0.92	0.09	64,64,64,64	0
57	MG	2A	3222	1/1	0.92	0.14	65,65,65,65	0
57	MG	1A	3452	1/1	0.92	0.25	55,55,55,55	0
57	MG	2A	3688	1/1	0.92	0.10	59,59,59,59	0
57	MG	2A	3689	1/1	0.92	0.16	61,61,61,61	0
57	MG	1A	3813	1/1	0.92	0.08	32,32,32,32	0
57	MG	1A	3392	1/1	0.92	0.10	46,46,46,46	0
57	MG	2A	3692	1/1	0.92	0.12	59,59,59,59	0
57	MG	2A	3401	1/1	0.92	0.21	53,53,53,53	0
57	MG	1F	314	1/1	0.92	0.11	55,55,55,55	0
57	MG	2A	3007	1/1	0.92	0.15	61,61,61,61	0
57	MG	1G	203	1/1	0.92	0.08	59,59,59,59	0
57	MG	2A	3014	1/1	0.92	0.11	46,46,46,46	0
57	MG	2A	3407	1/1	0.92	0.46	65,65,65,65	0
57	MG	2A	3409	1/1	0.92	0.16	43,43,43,43	0
57	MG	1A	3394	1/1	0.92	0.23	61,61,61,61	0
57	MG	1I	201	1/1	0.92	0.08	66,66,66,66	0
57	MG	2a	1666	1/1	0.92	0.14	59,59,59,59	0
57	MG	2A	3413	1/1	0.92	0.27	70,70,70,70	0
57	MG	2A	3238	1/1	0.92	0.11	61,61,61,61	0
57	MG	2A	3415	1/1	0.92	0.20	70,70,70,70	0
57	MG	1A	3525	1/1	0.92	0.15	58,58,58,58	0
57	MG	2A	3417	1/1	0.92	0.26	62,62,62,62	0
57	MG	2A	3418	1/1	0.92	0.30	60,60,60,60	0
57	MG	2A	3713	1/1	0.92	0.11	57,57,57,57	0
57	MG	2A	3718	1/1	0.92	0.20	66,66,66,66	0
57	MG	1A	3527	1/1	0.92	0.12	50,50,50,50	0
57	MG	1A	3171	1/1	0.92	0.26	43,43,43,43	0
57	MG	2A	3721	1/1	0.92	0.13	62,62,62,62	0
57	MG	1P	205	1/1	0.92	0.20	55,55,55,55	0
57	MG	2A	3725	1/1	0.92	0.10	58,58,58,58	0
57	MG	2A	3727	1/1	0.92	0.15	69,69,69,69	0
57	MG	1Q	205	1/1	0.92	0.09	55,55,55,55	0
57	MG	2A	3246	1/1	0.92	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3829	1/1	0.92	0.12	52,52,52,52	0
57	MG	1A	3463	1/1	0.92	0.10	53,53,53,53	0
57	MG	2A	3738	1/1	0.92	0.20	71,71,71,71	0
57	MG	1A	3321	1/1	0.92	0.14	61,61,61,61	0
57	MG	2A	3251	1/1	0.92	0.15	75,75,75,75	0
57	MG	2A	3742	1/1	0.92	0.21	65,65,65,65	0
57	MG	1A	3172	1/1	0.92	0.09	49,49,49,49	0
57	MG	2A	3043	1/1	0.92	0.21	70,70,70,70	0
57	MG	2A	3434	1/1	0.92	0.19	53,53,53,53	0
57	MG	2A	3254	1/1	0.92	0.08	81,81,81,81	0
57	MG	1A	3403	1/1	0.92	0.16	65,65,65,65	0
57	MG	2A	3756	1/1	0.92	0.23	51,51,51,51	0
57	MG	1a	1704	1/1	0.92	0.27	63,63,63,63	0
57	MG	2A	3758	1/1	0.92	0.12	57,57,57,57	0
57	MG	1A	3534	1/1	0.92	0.13	52,52,52,52	0
57	MG	2A	3260	1/1	0.92	0.15	63,63,63,63	0
57	MG	1A	3468	1/1	0.92	0.08	50,50,50,50	0
57	MG	1A	3672	1/1	0.92	0.05	23,23,23,23	0
57	MG	2A	3053	1/1	0.92	0.23	57,57,57,57	0
57	MG	2a	1717	1/1	0.92	0.17	63,63,63,63	0
57	MG	1A	3673	1/1	0.92	0.16	27,27,27,27	0
57	MG	1A	3841	1/1	0.92	0.09	71,71,71,71	0
57	MG	1A	3088	1/1	0.92	0.09	47,47,47,47	0
57	MG	1V	202	1/1	0.92	0.31	31,31,31,31	0
57	MG	2A	3270	1/1	0.92	0.13	73,73,73,73	0
57	MG	2A	3271	1/1	0.92	0.17	77,77,77,77	0
57	MG	1A	3332	1/1	0.92	0.18	51,51,51,51	0
57	MG	2A	3784	1/1	0.92	0.09	62,62,62,62	0
57	MG	2A	3787	1/1	0.92	0.09	51,51,51,51	0
57	MG	2A	3788	1/1	0.92	0.10	66,66,66,66	0
57	MG	1A	3406	1/1	0.92	0.33	37,37,37,37	0
57	MG	2A	3793	1/1	0.92	0.13	62,62,62,62	0
57	MG	1A	3852	1/1	0.92	0.13	76,76,76,76	0
57	MG	2a	1732	1/1	0.92	0.32	64,64,64,64	0
57	MG	2A	3477	1/1	0.92	0.25	68,68,68,68	0
57	MG	1A	4014	1/1	0.92	0.08	28,28,28,28	0
57	MG	2A	3065	1/1	0.92	0.36	75,75,75,75	0
57	MG	2A	3068	1/1	0.92	0.23	62,62,62,62	0
57	MG	1A	3475	1/1	0.92	0.09	56,56,56,56	0
57	MG	1a	1727	1/1	0.92	0.22	53,53,53,53	0
57	MG	2A	3813	1/1	0.92	0.10	61,61,61,61	0
57	MG	1Y	203	1/1	0.92	0.28	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3333	1/1	0.92	0.14	50,50,50,50	0
57	MG	1A	3415	1/1	0.92	0.13	45,45,45,45	0
57	MG	1A	3478	1/1	0.92	0.10	65,65,65,65	0
57	MG	1a	1736	1/1	0.92	0.21	60,60,60,60	0
57	MG	1A	3183	1/1	0.92	0.11	46,46,46,46	0
57	MG	1a	1739	1/1	0.92	0.10	65,65,65,65	0
57	MG	2A	3836	1/1	0.92	0.09	64,64,64,64	0
57	MG	2a	1762	1/1	0.92	0.10	62,62,62,62	0
57	MG	1A	3257	1/1	0.92	0.07	57,57,57,57	0
57	MG	1A	3706	1/1	0.92	0.10	39,39,39,39	0
57	MG	1A	3869	1/1	0.92	0.06	39,39,39,39	0
57	MG	1A	3081	1/1	0.92	0.13	46,46,46,46	0
57	MG	1A	3708	1/1	0.92	0.17	55,55,55,55	0
57	MG	2a	1776	1/1	0.92	0.15	60,60,60,60	0
57	MG	1A	3051	1/1	0.92	0.11	42,42,42,42	0
57	MG	1A	4051	1/1	0.92	0.06	31,31,31,31	0
57	MG	2a	1782	1/1	0.92	0.14	59,59,59,59	0
57	MG	1a	1760	1/1	0.92	0.09	63,63,63,63	0
57	MG	1A	3711	1/1	0.92	0.07	67,67,67,67	0
57	MG	1A	3878	1/1	0.92	0.10	40,40,40,40	0
57	MG	2A	3303	1/1	0.92	0.16	52,52,52,52	0
57	MG	2A	3521	1/1	0.92	0.15	60,60,60,60	0
57	MG	1A	4057	1/1	0.92	0.14	31,31,31,31	0
57	MG	1A	3371	1/1	0.92	0.11	57,57,57,57	0
57	MG	2A	3306	1/1	0.92	0.15	69,69,69,69	0
57	MG	1A	3564	1/1	0.92	0.18	35,35,35,35	0
57	MG	2B	209	1/1	0.92	0.20	65,65,65,65	0
57	MG	1A	3373	1/1	0.92	0.21	45,45,45,45	0
57	MG	2B	212	1/1	0.92	0.20	62,62,62,62	0
57	MG	1A	3302	1/1	0.92	0.34	70,70,70,70	0
57	MG	1a	1606	1/1	0.92	0.26	73,73,73,73	0
57	MG	1A	3722	1/1	0.92	0.10	40,40,40,40	0
57	MG	1A	3232	1/1	0.92	0.26	50,50,50,50	0
57	MG	1A	3724	1/1	0.92	0.19	76,76,76,76	0
57	MG	2B	218	1/1	0.92	0.24	81,81,81,81	0
57	MG	2A	3124	1/1	0.92	0.23	54,54,54,54	0
57	MG	2A	3317	1/1	0.92	0.11	51,51,51,51	0
57	MG	1a	1785	1/1	0.92	0.07	58,58,58,58	0
57	MG	2A	3130	1/1	0.92	0.10	47,47,47,47	0
57	MG	1A	3726	1/1	0.92	0.13	62,62,62,62	0
57	MG	2A	3134	1/1	0.92	0.23	53,53,53,53	0
57	MG	2E	308	1/1	0.92	0.15	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2F	301	1/1	0.92	0.16	49,49,49,49	0
57	MG	2A	3561	1/1	0.92	0.09	38,38,38,38	0
57	MG	2F	303	1/1	0.92	0.12	50,50,50,50	0
57	MG	1A	3569	1/1	0.92	0.25	58,58,58,58	0
57	MG	1a	1616	1/1	0.92	0.12	57,57,57,57	0
57	MG	1A	4081	1/1	0.92	0.19	54,54,54,54	0
57	MG	1a	1622	1/1	0.92	0.14	67,67,67,67	0
57	MG	2A	3146	1/1	0.92	0.12	57,57,57,57	0
57	MG	2Q	203	1/1	0.92	0.08	46,46,46,46	0
57	MG	2f	202	1/1	0.92	0.14	77,77,77,77	0
57	MG	1a	1623	1/1	0.92	0.15	64,64,64,64	0
57	MG	2A	3581	1/1	0.92	0.08	61,61,61,61	0
57	MG	1A	3571	1/1	0.92	0.13	41,41,41,41	0
57	MG	2l	202	1/1	0.92	0.10	77,77,77,77	0
57	MG	2l	203	1/1	0.92	0.07	72,72,72,72	0
57	MG	2A	3583	1/1	0.92	0.09	32,32,32,32	0
57	MG	1A	3733	1/1	0.92	0.12	48,48,48,48	0
57	MG	1a	1798	1/1	0.92	0.11	71,71,71,71	0
57	MG	2v	102	1/1	0.92	0.35	77,77,77,77	0
57	MG	1A	3494	1/1	0.92	0.17	56,56,56,56	0
57	MG	2A	3163	1/1	0.92	0.15	54,54,54,54	0
57	MG	2A	3164	1/1	0.92	0.11	46,46,46,46	0
57	MG	2A	3593	1/1	0.92	0.08	67,67,67,67	0
57	MG	1A	3907	1/1	0.92	0.09	41,41,41,41	0
57	MG	1A	3910	1/1	0.92	0.15	42,42,42,42	0
57	MG	1A	3270	1/1	0.92	0.24	53,53,53,53	0
57	MG	1a	1809	1/1	0.92	0.08	69,69,69,69	0
57	MG	1A	3307	1/1	0.92	0.06	30,30,30,30	0
58	K	1A	3570	1/1	0.92	0.12	58,58,58,58	0
57	MG	2A	3172	1/1	0.92	0.12	60,60,60,60	0
57	MG	1A	3247	1/1	0.93	0.13	62,62,62,62	0
57	MG	2A	3369	1/1	0.93	0.20	51,51,51,51	0
57	MG	27	101	1/1	0.93	0.25	66,66,66,66	0
57	MG	1A	3495	1/1	0.93	0.21	63,63,63,63	0
57	MG	2A	3643	1/1	0.93	0.19	68,68,68,68	0
57	MG	1A	3700	1/1	0.93	0.06	26,26,26,26	0
57	MG	1a	1661	1/1	0.93	0.09	67,67,67,67	0
57	MG	1A	3099	1/1	0.93	0.10	51,51,51,51	0
57	MG	2A	3647	1/1	0.93	0.10	45,45,45,45	0
57	MG	2a	1604	1/1	0.93	0.26	65,65,65,65	0
57	MG	1A	3989	1/1	0.93	0.08	38,38,38,38	0
57	MG	2A	3651	1/1	0.93	0.12	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1E	312	1/1	0.93	0.14	58,58,58,58	0
57	MG	2A	3202	1/1	0.93	0.16	61,61,61,61	0
57	MG	1A	3703	1/1	0.93	0.08	31,31,31,31	0
57	MG	1F	308	1/1	0.93	0.13	36,36,36,36	0
57	MG	1A	3437	1/1	0.93	0.12	50,50,50,50	0
57	MG	1A	3144	1/1	0.93	0.09	49,49,49,49	0
57	MG	2A	3383	1/1	0.93	0.18	63,63,63,63	0
57	MG	1A	3996	1/1	0.93	0.10	48,48,48,48	0
57	MG	1a	1672	1/1	0.93	0.09	66,66,66,66	0
57	MG	1A	3049	1/1	0.93	0.08	41,41,41,41	0
57	MG	1a	1674	1/1	0.93	0.27	75,75,75,75	0
57	MG	1A	3215	1/1	0.93	0.14	53,53,53,53	0
57	MG	1N	201	1/1	0.93	0.16	44,44,44,44	0
57	MG	1A	3585	1/1	0.93	0.20	66,66,66,66	0
57	MG	1A	3586	1/1	0.93	0.10	50,50,50,50	0
57	MG	1A	3443	1/1	0.93	0.11	55,55,55,55	0
57	MG	2a	1625	1/1	0.93	0.14	70,70,70,70	0
57	MG	1A	3590	1/1	0.93	0.11	42,42,42,42	0
57	MG	2A	3220	1/1	0.93	0.35	73,73,73,73	0
57	MG	1A	3868	1/1	0.93	0.22	34,34,34,34	0
57	MG	1A	3719	1/1	0.93	0.13	45,45,45,45	0
57	MG	2A	3006	1/1	0.93	0.19	68,68,68,68	0
57	MG	2A	3225	1/1	0.93	0.16	61,61,61,61	0
57	MG	1A	3027	1/1	0.93	0.12	77,77,77,77	0
57	MG	1A	4013	1/1	0.93	0.06	29,29,29,29	0
57	MG	2A	3010	1/1	0.93	0.08	66,66,66,66	0
57	MG	1A	3189	1/1	0.93	0.20	43,43,43,43	0
57	MG	2a	1637	1/1	0.93	0.25	73,73,73,73	0
57	MG	1A	3341	1/1	0.93	0.12	51,51,51,51	0
57	MG	2A	3018	1/1	0.93	0.18	64,64,64,64	0
57	MG	1A	3598	1/1	0.93	0.12	63,63,63,63	0
57	MG	1a	1694	1/1	0.93	0.14	55,55,55,55	0
57	MG	1A	3190	1/1	0.93	0.13	43,43,43,43	0
57	MG	1A	4024	1/1	0.93	0.07	47,47,47,47	0
57	MG	1A	3606	1/1	0.93	0.08	51,51,51,51	0
57	MG	2A	3034	1/1	0.93	0.10	61,61,61,61	0
57	MG	1A	3731	1/1	0.93	0.10	79,79,79,79	0
57	MG	1A	3885	1/1	0.93	0.09	46,46,46,46	0
57	MG	2A	3245	1/1	0.93	0.11	71,71,71,71	0
57	MG	1A	3888	1/1	0.93	0.11	32,32,32,32	0
57	MG	1V	205	1/1	0.93	0.19	55,55,55,55	0
57	MG	1a	1706	1/1	0.93	0.31	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4035	1/1	0.93	0.07	75,75,75,75	0
57	MG	1A	3265	1/1	0.93	0.09	65,65,65,65	0
57	MG	2a	1654	1/1	0.93	0.14	74,74,74,74	0
57	MG	1a	1709	1/1	0.93	0.44	77,77,77,77	0
57	MG	1A	3308	1/1	0.93	0.07	43,43,43,43	0
57	MG	1A	4045	1/1	0.93	0.12	64,64,64,64	0
57	MG	2A	3716	1/1	0.93	0.13	44,44,44,44	0
57	MG	1Y	201	1/1	0.93	0.16	50,50,50,50	0
57	MG	1A	3457	1/1	0.93	0.26	39,39,39,39	0
57	MG	1A	3458	1/1	0.93	0.20	39,39,39,39	0
57	MG	2A	3259	1/1	0.93	0.10	55,55,55,55	0
57	MG	2A	3722	1/1	0.93	0.11	70,70,70,70	0
57	MG	2A	3438	1/1	0.93	0.24	58,58,58,58	0
57	MG	2A	3055	1/1	0.93	0.21	66,66,66,66	0
57	MG	2A	3440	1/1	0.93	0.32	58,58,58,58	0
57	MG	2A	3441	1/1	0.93	0.26	64,64,64,64	0
57	MG	2a	1673	1/1	0.93	0.11	66,66,66,66	0
57	MG	2A	3442	1/1	0.93	0.10	57,57,57,57	0
57	MG	2a	1675	1/1	0.93	0.13	75,75,75,75	0
57	MG	2a	1676	1/1	0.93	0.11	74,74,74,74	0
57	MG	2A	3732	1/1	0.93	0.11	65,65,65,65	0
57	MG	1a	1715	1/1	0.93	0.08	51,51,51,51	0
57	MG	2A	3734	1/1	0.93	0.10	67,67,67,67	0
57	MG	1a	1717	1/1	0.93	0.30	71,71,71,71	0
57	MG	1a	1718	1/1	0.93	0.22	53,53,53,53	0
57	MG	1A	4050	1/1	0.93	0.13	38,38,38,38	0
57	MG	2a	1684	1/1	0.93	0.21	61,61,61,61	0
57	MG	1A	3894	1/1	0.93	0.07	39,39,39,39	0
57	MG	2A	3456	1/1	0.93	0.13	62,62,62,62	0
57	MG	1A	4052	1/1	0.93	0.12	50,50,50,50	0
57	MG	2A	3745	1/1	0.93	0.14	65,65,65,65	0
57	MG	10	106	1/1	0.93	0.10	56,56,56,56	0
57	MG	2A	3749	1/1	0.93	0.10	63,63,63,63	0
57	MG	2A	3463	1/1	0.93	0.15	61,61,61,61	0
57	MG	1A	3309	1/1	0.93	0.32	63,63,63,63	0
57	MG	2A	3066	1/1	0.93	0.15	59,59,59,59	0
57	MG	1A	3349	1/1	0.93	0.08	59,59,59,59	0
57	MG	2A	3470	1/1	0.93	0.09	64,64,64,64	0
57	MG	2A	3471	1/1	0.93	0.26	64,64,64,64	0
57	MG	2a	1702	1/1	0.93	0.14	80,80,80,80	0
57	MG	12	3702	1/1	0.93	0.10	45,45,45,45	0
57	MG	2A	3760	1/1	0.93	0.20	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3395	1/1	0.93	0.24	56,56,56,56	0
57	MG	1A	3266	1/1	0.93	0.26	68,68,68,68	0
57	MG	1A	3351	1/1	0.93	0.12	47,47,47,47	0
57	MG	15	105	1/1	0.93	0.21	46,46,46,46	0
57	MG	1A	3400	1/1	0.93	0.38	49,49,49,49	0
57	MG	2A	3769	1/1	0.93	0.11	43,43,43,43	0
57	MG	1A	3228	1/1	0.93	0.10	52,52,52,52	0
57	MG	2A	3771	1/1	0.93	0.12	67,67,67,67	0
57	MG	1a	1741	1/1	0.93	0.18	67,67,67,67	0
57	MG	1A	3113	1/1	0.93	0.17	31,31,31,31	0
57	MG	2a	1716	1/1	0.93	0.23	68,68,68,68	0
57	MG	2A	3089	1/1	0.93	0.10	47,47,47,47	0
57	MG	2A	3091	1/1	0.93	0.16	50,50,50,50	0
57	MG	1a	1744	1/1	0.93	0.15	56,56,56,56	0
57	MG	2A	3487	1/1	0.93	0.26	60,60,60,60	0
57	MG	18	101	1/1	0.93	0.27	60,60,60,60	0
57	MG	1a	1747	1/1	0.93	0.08	56,56,56,56	0
57	MG	1a	1751	1/1	0.93	0.07	57,57,57,57	0
57	MG	1A	3783	1/1	0.93	0.08	33,33,33,33	0
57	MG	2A	3794	1/1	0.93	0.11	68,68,68,68	0
57	MG	1A	3637	1/1	0.93	0.07	25,25,25,25	0
57	MG	1A	3918	1/1	0.93	0.08	34,34,34,34	0
57	MG	1A	3537	1/1	0.93	0.23	33,33,33,33	0
57	MG	1A	3791	1/1	0.93	0.10	51,51,51,51	0
57	MG	1A	3317	1/1	0.93	0.12	49,49,49,49	0
57	MG	2A	3298	1/1	0.93	0.08	63,63,63,63	0
57	MG	2A	3808	1/1	0.93	0.07	59,59,59,59	0
57	MG	2A	3809	1/1	0.93	0.17	64,64,64,64	0
57	MG	2a	1735	1/1	0.93	0.31	63,63,63,63	0
57	MG	1A	3927	1/1	0.93	0.08	42,42,42,42	0
57	MG	2A	3812	1/1	0.93	0.08	38,38,38,38	0
57	MG	1A	4087	1/1	0.93	0.08	51,51,51,51	0
57	MG	1a	1608	1/1	0.93	0.32	63,63,63,63	0
57	MG	1A	3061	1/1	0.93	0.12	45,45,45,45	0
57	MG	1A	3643	1/1	0.93	0.07	29,29,29,29	0
57	MG	2a	1744	1/1	0.93	0.20	69,69,69,69	0
57	MG	2A	3515	1/1	0.93	0.10	61,61,61,61	0
57	MG	2A	3118	1/1	0.93	0.21	76,76,76,76	0
57	MG	1A	3235	1/1	0.93	0.18	54,54,54,54	0
57	MG	1A	3649	1/1	0.93	0.08	43,43,43,43	0
57	MG	1A	3652	1/1	0.93	0.09	41,41,41,41	0
57	MG	2a	1754	1/1	0.93	0.10	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1757	1/1	0.93	0.08	50,50,50,50	0
57	MG	2A	3122	1/1	0.93	0.07	54,54,54,54	0
57	MG	2A	3528	1/1	0.93	0.08	47,47,47,47	0
57	MG	2A	3529	1/1	0.93	0.10	52,52,52,52	0
57	MG	1A	3653	1/1	0.93	0.12	48,48,48,48	0
57	MG	2a	1766	1/1	0.93	0.12	73,73,73,73	0
57	MG	2A	3848	1/1	0.93	0.08	52,52,52,52	0
57	MG	1A	4096	1/1	0.93	0.11	59,59,59,59	0
57	MG	2A	3851	1/1	0.93	0.12	56,56,56,56	0
57	MG	2A	3852	1/1	0.93	0.14	51,51,51,51	0
57	MG	2A	3853	1/1	0.93	0.14	48,48,48,48	0
57	MG	2A	3533	1/1	0.93	0.14	69,69,69,69	0
57	MG	2a	1778	1/1	0.93	0.19	74,74,74,74	0
57	MG	1a	1621	1/1	0.93	0.32	77,77,77,77	0
57	MG	2A	3313	1/1	0.93	0.23	68,68,68,68	0
57	MG	1B	201	1/1	0.93	0.17	63,63,63,63	0
57	MG	1A	3409	1/1	0.93	0.20	43,43,43,43	0
57	MG	1A	3413	1/1	0.93	0.08	49,49,49,49	0
57	MG	1A	3659	1/1	0.93	0.08	26,26,26,26	0
57	MG	1a	1626	1/1	0.93	0.26	64,64,64,64	0
57	MG	2A	3544	1/1	0.93	0.10	47,47,47,47	0
57	MG	1A	3239	1/1	0.93	0.12	47,47,47,47	0
57	MG	1A	3956	1/1	0.93	0.07	45,45,45,45	0
57	MG	2A	3551	1/1	0.93	0.08	52,52,52,52	0
57	MG	2B	210	1/1	0.93	0.14	75,75,75,75	0
57	MG	1A	3322	1/1	0.93	0.21	55,55,55,55	0
57	MG	2a	1797	1/1	0.93	0.18	70,70,70,70	0
57	MG	2A	3558	1/1	0.93	0.09	45,45,45,45	0
57	MG	2a	1799	1/1	0.93	0.16	79,79,79,79	0
57	MG	1A	3958	1/1	0.93	0.09	57,57,57,57	0
57	MG	1a	1796	1/1	0.93	0.12	73,73,73,73	0
57	MG	1A	3668	1/1	0.93	0.09	42,42,42,42	0
57	MG	2A	3153	1/1	0.93	0.16	43,43,43,43	0
57	MG	2A	3155	1/1	0.93	0.14	65,65,65,65	0
57	MG	2A	3570	1/1	0.93	0.13	53,53,53,53	0
57	MG	2a	1806	1/1	0.93	0.09	65,65,65,65	0
57	MG	1A	3670	1/1	0.93	0.06	22,22,22,22	0
57	MG	1A	3363	1/1	0.93	0.14	43,43,43,43	0
57	MG	2D	305	1/1	0.93	0.15	52,52,52,52	0
57	MG	2A	3576	1/1	0.93	0.11	50,50,50,50	0
57	MG	2a	1811	1/1	0.93	0.17	50,50,50,50	0
57	MG	2A	3161	1/1	0.93	0.12	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3580	1/1	0.93	0.14	54,54,54,54	0
57	MG	2A	3162	1/1	0.93	0.33	60,60,60,60	0
57	MG	1a	1802	1/1	0.93	0.13	70,70,70,70	0
57	MG	1a	1803	1/1	0.93	0.11	67,67,67,67	0
57	MG	2A	3165	1/1	0.93	0.18	64,64,64,64	0
57	MG	1A	3827	1/1	0.93	0.17	50,50,50,50	0
57	MG	2F	305	1/1	0.93	0.21	50,50,50,50	0
57	MG	1A	3828	1/1	0.93	0.12	56,56,56,56	0
57	MG	1a	1806	1/1	0.93	0.09	81,81,81,81	0
57	MG	1a	1638	1/1	0.93	0.19	60,60,60,60	0
57	MG	2d	301	1/1	0.93	0.33	63,63,63,63	0
57	MG	2N	201	1/1	0.93	0.07	62,62,62,62	0
57	MG	1A	3326	1/1	0.93	0.09	35,35,35,35	0
57	MG	1B	224	1/1	0.93	0.09	57,57,57,57	0
57	MG	2A	3173	1/1	0.93	0.09	61,61,61,61	0
57	MG	2k	201	1/1	0.93	0.12	73,73,73,73	0
57	MG	2A	3350	1/1	0.93	0.12	65,65,65,65	0
57	MG	1A	3328	1/1	0.93	0.17	62,62,62,62	0
57	MG	1a	1642	1/1	0.93	0.19	70,70,70,70	0
57	MG	1A	3971	1/1	0.93	0.11	65,65,65,65	0
57	MG	2r	101	1/1	0.93	0.18	84,84,84,84	0
57	MG	1A	3679	1/1	0.93	0.07	30,30,30,30	0
57	MG	2U	201	1/1	0.93	0.14	63,63,63,63	0
57	MG	1A	3199	1/1	0.93	0.42	39,39,39,39	0
57	MG	1A	3833	1/1	0.93	0.08	38,38,38,38	0
57	MG	2A	3613	1/1	0.93	0.15	68,68,68,68	0
57	MG	1A	3368	1/1	0.93	0.08	48,48,48,48	0
57	MG	2A	3188	1/1	0.93	0.22	74,74,74,74	0
57	MG	1A	3085	1/1	0.93	0.23	34,34,34,34	0
57	MG	1A	3427	1/1	0.93	0.16	59,59,59,59	0
57	MG	2A	3624	1/1	0.93	0.15	65,65,65,65	0
57	MG	2A	3191	1/1	0.93	0.09	68,68,68,68	0
57	MG	1D	310	1/1	0.93	0.17	28,28,28,28	0
57	MG	2A	3193	1/1	0.93	0.11	65,65,65,65	0
57	MG	1A	3086	1/1	0.93	0.21	30,30,30,30	0
57	MG	2A	3108	1/1	0.94	0.09	50,50,50,50	0
57	MG	2T	3504	1/1	0.94	0.16	59,59,59,59	0
57	MG	1A	3523	1/1	0.94	0.34	40,40,40,40	0
57	MG	1a	1730	1/1	0.94	0.20	54,54,54,54	0
57	MG	1A	3819	1/1	0.94	0.06	32,32,32,32	0
57	MG	1A	3083	1/1	0.94	0.25	46,46,46,46	0
57	MG	1U	208	1/1	0.94	0.19	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2W	202	1/1	0.94	0.09	43,43,43,43	0
57	MG	1A	3988	1/1	0.94	0.10	23,23,23,23	0
57	MG	1A	3318	1/1	0.94	0.12	53,53,53,53	0
57	MG	2A	3600	1/1	0.94	0.17	58,58,58,58	0
57	MG	20	102	1/1	0.94	0.13	68,68,68,68	0
57	MG	2A	3601	1/1	0.94	0.17	57,57,57,57	0
57	MG	1a	1738	1/1	0.94	0.29	62,62,62,62	0
57	MG	1A	3528	1/1	0.94	0.12	52,52,52,52	0
57	MG	1A	3250	1/1	0.94	0.16	69,69,69,69	0
57	MG	25	101	1/1	0.94	0.27	61,61,61,61	0
57	MG	1A	3647	1/1	0.94	0.09	53,53,53,53	0
57	MG	2A	3608	1/1	0.94	0.18	70,70,70,70	0
57	MG	1a	1743	1/1	0.94	0.14	65,65,65,65	0
57	MG	1A	3122	1/1	0.94	0.10	47,47,47,47	0
57	MG	2A	3127	1/1	0.94	0.14	53,53,53,53	0
57	MG	1X	105	1/1	0.94	0.07	51,51,51,51	0
57	MG	2A	3615	1/1	0.94	0.07	31,31,31,31	0
57	MG	1A	3377	1/1	0.94	0.22	40,40,40,40	0
57	MG	1A	3450	1/1	0.94	0.18	48,48,48,48	0
57	MG	2A	3618	1/1	0.94	0.11	54,54,54,54	0
57	MG	2A	3619	1/1	0.94	0.13	50,50,50,50	0
57	MG	1A	3018	1/1	0.94	0.11	33,33,33,33	0
57	MG	2A	3135	1/1	0.94	0.10	38,38,38,38	0
57	MG	1A	4000	1/1	0.94	0.11	46,46,46,46	0
57	MG	2A	3351	1/1	0.94	0.08	60,60,60,60	0
57	MG	1A	3655	1/1	0.94	0.14	59,59,59,59	0
57	MG	2A	3139	1/1	0.94	0.24	57,57,57,57	0
57	MG	2A	3141	1/1	0.94	0.14	59,59,59,59	0
57	MG	1A	4003	1/1	0.94	0.12	51,51,51,51	0
57	MG	1Z	303	1/1	0.94	0.18	57,57,57,57	0
57	MG	10	104	1/1	0.94	0.25	39,39,39,39	0
57	MG	1a	1761	1/1	0.94	0.13	68,68,68,68	0
57	MG	1A	3001	1/1	0.94	0.13	48,48,48,48	0
57	MG	2A	3150	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3198	1/1	0.94	0.07	45,45,45,45	0
57	MG	2A	3362	1/1	0.94	0.17	70,70,70,70	0
57	MG	2A	3649	1/1	0.94	0.08	59,59,59,59	0
57	MG	1A	3130	1/1	0.94	0.12	38,38,38,38	0
57	MG	11	101	1/1	0.94	0.54	48,48,48,48	0
57	MG	2A	3156	1/1	0.94	0.09	74,74,74,74	0
57	MG	1A	3538	1/1	0.94	0.22	54,54,54,54	0
57	MG	12	3701	1/1	0.94	0.07	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1777	1/1	0.94	0.10	55,55,55,55	0
57	MG	1a	1778	1/1	0.94	0.10	59,59,59,59	0
57	MG	1A	3200	1/1	0.94	0.10	49,49,49,49	0
57	MG	2A	3659	1/1	0.94	0.08	59,59,59,59	0
57	MG	1A	3540	1/1	0.94	0.25	46,46,46,46	0
57	MG	1A	3843	1/1	0.94	0.16	53,53,53,53	0
57	MG	1A	4016	1/1	0.94	0.08	30,30,30,30	0
57	MG	2A	3663	1/1	0.94	0.09	73,73,73,73	0
57	MG	1A	3844	1/1	0.94	0.09	52,52,52,52	0
57	MG	1A	3385	1/1	0.94	0.17	38,38,38,38	0
57	MG	2A	3666	1/1	0.94	0.12	69,69,69,69	0
57	MG	1a	1786	1/1	0.94	0.08	57,57,57,57	0
57	MG	1A	3330	1/1	0.94	0.12	48,48,48,48	0
57	MG	2A	3670	1/1	0.94	0.10	60,60,60,60	0
57	MG	1A	3850	1/1	0.94	0.15	42,42,42,42	0
57	MG	1A	3543	1/1	0.94	0.19	41,41,41,41	0
57	MG	1A	3261	1/1	0.94	0.06	33,33,33,33	0
57	MG	1A	4027	1/1	0.94	0.06	64,64,64,64	0
57	MG	2A	3679	1/1	0.94	0.11	57,57,57,57	0
57	MG	1A	4028	1/1	0.94	0.08	66,66,66,66	0
57	MG	2A	3179	1/1	0.94	0.20	59,59,59,59	0
57	MG	1A	4030	1/1	0.94	0.06	49,49,49,49	0
57	MG	2A	3182	1/1	0.94	0.23	66,66,66,66	0
57	MG	1a	1602	1/1	0.94	0.11	67,67,67,67	0
57	MG	1A	3264	1/1	0.94	0.23	67,67,67,67	0
57	MG	1A	3547	1/1	0.94	0.28	57,57,57,57	0
57	MG	1A	3859	1/1	0.94	0.14	52,52,52,52	0
57	MG	1A	3860	1/1	0.94	0.08	47,47,47,47	0
57	MG	1a	1801	1/1	0.94	0.10	63,63,63,63	0
57	MG	1A	4037	1/1	0.94	0.08	78,78,78,78	0
57	MG	1a	1609	1/1	0.94	0.10	73,73,73,73	0
57	MG	2A	3400	1/1	0.94	0.19	47,47,47,47	0
57	MG	1A	3465	1/1	0.94	0.16	52,52,52,52	0
57	MG	2A	3402	1/1	0.94	0.25	55,55,55,55	0
57	MG	1A	4040	1/1	0.94	0.08	58,58,58,58	0
57	MG	2A	3699	1/1	0.94	0.08	65,65,65,65	0
57	MG	1A	3138	1/1	0.94	0.28	39,39,39,39	0
57	MG	1A	4047	1/1	0.94	0.08	42,42,42,42	0
57	MG	1a	1811	1/1	0.94	0.13	76,76,76,76	0
57	MG	1A	3139	1/1	0.94	0.12	42,42,42,42	0
57	MG	1a	1817	1/1	0.94	0.07	64,64,64,64	0
57	MG	1A	3691	1/1	0.94	0.13	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3694	1/1	0.94	0.09	42,42,42,42	0
57	MG	1A	3059	1/1	0.94	0.13	54,54,54,54	0
57	MG	2a	1678	1/1	0.94	0.17	65,65,65,65	0
57	MG	1A	3041	1/1	0.94	0.07	32,32,32,32	0
57	MG	1A	3555	1/1	0.94	0.22	58,58,58,58	0
57	MG	1A	3872	1/1	0.94	0.14	31,31,31,31	0
57	MG	2A	3712	1/1	0.94	0.07	68,68,68,68	0
57	MG	1e	201	1/1	0.94	0.10	68,68,68,68	0
57	MG	1A	3022	1/1	0.94	0.06	46,46,46,46	0
57	MG	1A	3214	1/1	0.94	0.15	55,55,55,55	0
57	MG	2a	1687	1/1	0.94	0.15	68,68,68,68	0
57	MG	1A	3704	1/1	0.94	0.13	31,31,31,31	0
57	MG	1A	3275	1/1	0.94	0.12	46,46,46,46	0
57	MG	1A	3277	1/1	0.94	0.07	48,48,48,48	0
57	MG	2a	1691	1/1	0.94	0.12	44,44,44,44	0
57	MG	1A	3090	1/1	0.94	0.10	32,32,32,32	0
57	MG	1A	3882	1/1	0.94	0.08	32,32,32,32	0
57	MG	1A	3884	1/1	0.94	0.11	28,28,28,28	0
57	MG	1A	3289	1/1	0.94	0.26	47,47,47,47	0
57	MG	2A	3428	1/1	0.94	0.09	77,77,77,77	0
57	MG	1A	3886	1/1	0.94	0.10	52,52,52,52	0
57	MG	2A	3430	1/1	0.94	0.13	51,51,51,51	0
57	MG	1A	3710	1/1	0.94	0.12	59,59,59,59	0
57	MG	1A	3216	1/1	0.94	0.20	61,61,61,61	0
57	MG	1A	3046	1/1	0.94	0.05	40,40,40,40	0
57	MG	1A	3224	1/1	0.94	0.17	38,38,38,38	0
57	MG	2a	1705	1/1	0.94	0.09	74,74,74,74	0
57	MG	1A	3002	1/1	0.94	0.07	53,53,53,53	0
57	MG	2A	3226	1/1	0.94	0.12	56,56,56,56	0
57	MG	1A	3579	1/1	0.94	0.39	42,42,42,42	0
57	MG	1w	106	1/1	0.94	0.08	73,73,73,73	0
57	MG	1A	3483	1/1	0.94	0.16	57,57,57,57	0
57	MG	1a	1645	1/1	0.94	0.10	60,60,60,60	0
57	MG	1A	3078	1/1	0.94	0.08	26,26,26,26	0
57	MG	2A	3444	1/1	0.94	0.07	62,62,62,62	0
57	MG	1A	3897	1/1	0.94	0.07	31,31,31,31	0
57	MG	2A	3447	1/1	0.94	0.14	58,58,58,58	0
57	MG	1A	3488	1/1	0.94	0.14	41,41,41,41	0
57	MG	1A	3416	1/1	0.94	0.11	44,44,44,44	0
57	MG	1A	3490	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3417	1/1	0.94	0.15	41,41,41,41	0
57	MG	1A	3905	1/1	0.94	0.07	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3458	1/1	0.94	0.10	62,62,62,62	0
57	MG	2A	3459	1/1	0.94	0.20	45,45,45,45	0
57	MG	1A	3591	1/1	0.94	0.10	39,39,39,39	0
57	MG	1A	3592	1/1	0.94	0.16	35,35,35,35	0
57	MG	1A	3492	1/1	0.94	0.09	39,39,39,39	0
57	MG	2A	3466	1/1	0.94	0.10	39,39,39,39	0
57	MG	1B	209	1/1	0.94	0.14	37,37,37,37	0
57	MG	2A	3003	1/1	0.94	0.23	48,48,48,48	0
57	MG	2a	1729	1/1	0.94	0.41	73,73,73,73	0
57	MG	2A	3005	1/1	0.94	0.21	67,67,67,67	0
57	MG	1A	3594	1/1	0.94	0.24	59,59,59,59	0
57	MG	1A	3917	1/1	0.94	0.21	54,54,54,54	0
57	MG	1A	3735	1/1	0.94	0.06	52,52,52,52	0
57	MG	1A	3164	1/1	0.94	0.16	58,58,58,58	0
57	MG	2A	3011	1/1	0.94	0.12	58,58,58,58	0
57	MG	2A	3785	1/1	0.94	0.08	43,43,43,43	0
57	MG	2A	3013	1/1	0.94	0.11	50,50,50,50	0
57	MG	1A	3298	1/1	0.94	0.14	54,54,54,54	0
57	MG	2A	3789	1/1	0.94	0.07	48,48,48,48	0
57	MG	1A	3925	1/1	0.94	0.09	58,58,58,58	0
57	MG	1A	3743	1/1	0.94	0.19	61,61,61,61	0
57	MG	1A	3597	1/1	0.94	0.09	34,34,34,34	0
57	MG	1A	3421	1/1	0.94	0.13	57,57,57,57	0
57	MG	2A	3025	1/1	0.94	0.09	47,47,47,47	0
57	MG	1A	3757	1/1	0.94	0.12	45,45,45,45	0
57	MG	1A	3599	1/1	0.94	0.12	43,43,43,43	0
57	MG	2A	3488	1/1	0.94	0.29	72,72,72,72	0
57	MG	2a	1751	1/1	0.94	0.09	83,83,83,83	0
57	MG	2A	3805	1/1	0.94	0.08	56,56,56,56	0
57	MG	2a	1755	1/1	0.94	0.12	70,70,70,70	0
57	MG	2a	1756	1/1	0.94	0.11	75,75,75,75	0
57	MG	2A	3806	1/1	0.94	0.13	62,62,62,62	0
57	MG	1A	3761	1/1	0.94	0.06	29,29,29,29	0
57	MG	1A	3763	1/1	0.94	0.10	31,31,31,31	0
57	MG	1A	3167	1/1	0.94	0.10	39,39,39,39	0
57	MG	1A	3766	1/1	0.94	0.11	32,32,32,32	0
57	MG	1a	1678	1/1	0.94	0.29	65,65,65,65	0
57	MG	1A	3603	1/1	0.94	0.11	28,28,28,28	0
57	MG	2A	3272	1/1	0.94	0.08	72,72,72,72	0
57	MG	1B	235	1/1	0.94	0.08	48,48,48,48	0
57	MG	2a	1770	1/1	0.94	0.11	70,70,70,70	0
57	MG	2A	3499	1/1	0.94	0.37	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1681	1/1	0.94	0.13	64,64,64,64	0
57	MG	2A	3502	1/1	0.94	0.08	69,69,69,69	0
57	MG	2A	3825	1/1	0.94	0.08	60,60,60,60	0
57	MG	2a	1779	1/1	0.94	0.22	67,67,67,67	0
57	MG	1A	3605	1/1	0.94	0.07	28,28,28,28	0
57	MG	1D	309	1/1	0.94	0.11	41,41,41,41	0
57	MG	2A	3833	1/1	0.94	0.11	45,45,45,45	0
57	MG	2A	3507	1/1	0.94	0.05	39,39,39,39	0
57	MG	1A	3952	1/1	0.94	0.09	49,49,49,49	0
57	MG	2A	3838	1/1	0.94	0.09	59,59,59,59	0
57	MG	1A	3953	1/1	0.94	0.07	63,63,63,63	0
57	MG	1A	3048	1/1	0.94	0.11	24,24,24,24	0
57	MG	1a	1688	1/1	0.94	0.11	63,63,63,63	0
57	MG	2A	3847	1/1	0.94	0.06	47,47,47,47	0
57	MG	1a	1690	1/1	0.94	0.16	61,61,61,61	0
57	MG	2A	3516	1/1	0.94	0.12	28,28,28,28	0
57	MG	1A	3500	1/1	0.94	0.07	47,47,47,47	0
57	MG	2a	1796	1/1	0.94	0.20	71,71,71,71	0
57	MG	1A	3785	1/1	0.94	0.08	49,49,49,49	0
57	MG	2A	3522	1/1	0.94	0.10	52,52,52,52	0
57	MG	2A	3856	1/1	0.94	0.15	67,67,67,67	0
57	MG	1A	3786	1/1	0.94	0.06	42,42,42,42	0
57	MG	2A	3525	1/1	0.94	0.14	58,58,58,58	0
57	MG	2A	3860	1/1	0.94	0.11	66,66,66,66	0
57	MG	2A	3058	1/1	0.94	0.17	55,55,55,55	0
57	MG	1A	3959	1/1	0.94	0.09	43,43,43,43	0
57	MG	1A	3025	1/1	0.94	0.08	38,38,38,38	0
57	MG	1A	3236	1/1	0.94	0.12	63,63,63,63	0
57	MG	1A	3790	1/1	0.94	0.08	48,48,48,48	0
57	MG	2B	204	1/1	0.94	0.13	76,76,76,76	0
57	MG	1A	3237	1/1	0.94	0.26	35,35,35,35	0
57	MG	2A	3293	1/1	0.94	0.18	54,54,54,54	0
57	MG	1F	312	1/1	0.94	0.14	48,48,48,48	0
57	MG	1F	313	1/1	0.94	0.11	35,35,35,35	0
57	MG	1A	3965	1/1	0.94	0.06	45,45,45,45	0
57	MG	1A	3966	1/1	0.94	0.09	27,27,27,27	0
57	MG	1A	3111	1/1	0.94	0.09	46,46,46,46	0
57	MG	1A	3241	1/1	0.94	0.07	37,37,37,37	0
57	MG	2A	3541	1/1	0.94	0.14	51,51,51,51	0
57	MG	2A	3542	1/1	0.94	0.07	51,51,51,51	0
57	MG	1A	3969	1/1	0.94	0.23	52,52,52,52	0
57	MG	1A	3007	1/1	0.94	0.08	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3546	1/1	0.94	0.12	48,48,48,48	0
57	MG	2a	1823	1/1	0.94	0.13	70,70,70,70	0
57	MG	2A	3547	1/1	0.94	0.10	58,58,58,58	0
57	MG	1A	3436	1/1	0.94	0.10	53,53,53,53	0
57	MG	2d	302	1/1	0.94	0.09	70,70,70,70	0
57	MG	2A	3085	1/1	0.94	0.28	67,67,67,67	0
57	MG	1A	3802	1/1	0.94	0.07	22,22,22,22	0
57	MG	2A	3555	1/1	0.94	0.15	59,59,59,59	0
57	MG	1A	3116	1/1	0.94	0.19	42,42,42,42	0
57	MG	2A	3557	1/1	0.94	0.14	47,47,47,47	0
57	MG	2E	306	1/1	0.94	0.09	34,34,34,34	0
57	MG	1Q	201	1/1	0.94	0.34	42,42,42,42	0
57	MG	1A	3975	1/1	0.94	0.07	60,60,60,60	0
57	MG	2q	201	1/1	0.94	0.12	77,77,77,77	0
57	MG	1a	1716	1/1	0.94	0.14	56,56,56,56	0
57	MG	1Q	207	1/1	0.94	0.08	35,35,35,35	0
57	MG	2A	3563	1/1	0.94	0.16	64,64,64,64	0
57	MG	2A	3564	1/1	0.94	0.08	52,52,52,52	0
57	MG	2A	3096	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3186	1/1	0.94	0.06	39,39,39,39	0
57	MG	1a	1719	1/1	0.94	0.19	56,56,56,56	0
57	MG	2A	3314	1/1	0.94	0.29	65,65,65,65	0
57	MG	1A	3977	1/1	0.94	0.10	55,55,55,55	0
57	MG	2P	201	1/1	0.94	0.17	60,60,60,60	0
57	MG	1A	3628	1/1	0.94	0.06	21,21,21,21	0
57	MG	1A	3631	1/1	0.94	0.10	62,62,62,62	0
57	MG	2A	3103	1/1	0.94	0.10	59,59,59,59	0
57	MG	2x	104	1/1	0.94	0.11	69,69,69,69	0
57	MG	1A	3517	1/1	0.94	0.07	49,49,49,49	0
57	MG	1A	3187	1/1	0.94	0.08	50,50,50,50	0
57	MG	1A	3370	1/1	0.94	0.09	61,61,61,61	0
60	ZN	2n	501	1/1	0.94	0.07	106,106,106,106	0
57	MG	2A	3110	1/1	0.95	0.12	61,61,61,61	0
57	MG	2A	3602	1/1	0.95	0.13	51,51,51,51	0
57	MG	1A	3818	1/1	0.95	0.06	27,27,27,27	0
57	MG	2A	3340	1/1	0.95	0.11	61,61,61,61	0
57	MG	2A	3605	1/1	0.95	0.11	62,62,62,62	0
57	MG	2A	3341	1/1	0.95	0.18	64,64,64,64	0
57	MG	1U	202	1/1	0.95	0.25	42,42,42,42	0
57	MG	2Y	201	1/1	0.95	0.21	56,56,56,56	0
57	MG	2A	3343	1/1	0.95	0.18	64,64,64,64	0
57	MG	2A	3113	1/1	0.95	0.14	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3019	1/1	0.95	0.14	50,50,50,50	0
57	MG	1A	3990	1/1	0.95	0.12	40,40,40,40	0
57	MG	1U	206	1/1	0.95	0.17	37,37,37,37	0
57	MG	2A	3614	1/1	0.95	0.09	60,60,60,60	0
57	MG	1A	3010	1/1	0.95	0.05	34,34,34,34	0
57	MG	1U	209	1/1	0.95	0.29	36,36,36,36	0
57	MG	1A	3348	1/1	0.95	0.21	49,49,49,49	0
57	MG	25	104	1/1	0.95	0.11	51,51,51,51	0
57	MG	1V	201	1/1	0.95	0.19	30,30,30,30	0
57	MG	1A	3642	1/1	0.95	0.08	31,31,31,31	0
57	MG	2A	3620	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	3522	1/1	0.95	0.18	35,35,35,35	0
57	MG	2A	3622	1/1	0.95	0.17	66,66,66,66	0
57	MG	28	101	1/1	0.95	0.14	61,61,61,61	0
57	MG	1a	1748	1/1	0.95	0.05	35,35,35,35	0
57	MG	1A	3644	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3645	1/1	0.95	0.06	30,30,30,30	0
57	MG	2A	3629	1/1	0.95	0.06	38,38,38,38	0
57	MG	1A	3091	1/1	0.95	0.14	60,60,60,60	0
57	MG	2A	3131	1/1	0.95	0.12	49,49,49,49	0
57	MG	2A	3633	1/1	0.95	0.07	34,34,34,34	0
57	MG	2A	3132	1/1	0.95	0.06	49,49,49,49	0
57	MG	1a	1754	1/1	0.95	0.06	54,54,54,54	0
57	MG	1A	3274	1/1	0.95	0.20	36,36,36,36	0
57	MG	1A	3092	1/1	0.95	0.09	49,49,49,49	0
57	MG	1A	3431	1/1	0.95	0.08	44,44,44,44	0
57	MG	1A	3432	1/1	0.95	0.07	46,46,46,46	0
57	MG	2a	1613	1/1	0.95	0.10	73,73,73,73	0
57	MG	1A	3355	1/1	0.95	0.16	38,38,38,38	0
57	MG	1A	3435	1/1	0.95	0.10	35,35,35,35	0
57	MG	1a	1764	1/1	0.95	0.13	58,58,58,58	0
57	MG	2A	3648	1/1	0.95	0.09	55,55,55,55	0
57	MG	2A	3143	1/1	0.95	0.17	53,53,53,53	0
57	MG	1A	4007	1/1	0.95	0.08	21,21,21,21	0
57	MG	1a	1768	1/1	0.95	0.10	66,66,66,66	0
57	MG	1A	3029	1/1	0.95	0.07	38,38,38,38	0
57	MG	2A	3375	1/1	0.95	0.13	56,56,56,56	0
57	MG	1a	1770	1/1	0.95	0.20	75,75,75,75	0
57	MG	2a	1624	1/1	0.95	0.08	65,65,65,65	0
57	MG	10	103	1/1	0.95	0.08	51,51,51,51	0
57	MG	2A	3151	1/1	0.95	0.07	55,55,55,55	0
57	MG	1A	3658	1/1	0.95	0.08	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3150	1/1	0.95	0.23	42,42,42,42	0
57	MG	1A	3288	1/1	0.95	0.12	54,54,54,54	0
57	MG	10	107	1/1	0.95	0.16	61,61,61,61	0
57	MG	1A	3662	1/1	0.95	0.08	53,53,53,53	0
57	MG	10	109	1/1	0.95	0.08	46,46,46,46	0
57	MG	2A	3160	1/1	0.95	0.13	55,55,55,55	0
57	MG	1A	3217	1/1	0.95	0.12	34,34,34,34	0
57	MG	1A	3846	1/1	0.95	0.13	48,48,48,48	0
57	MG	1A	3536	1/1	0.95	0.10	38,38,38,38	0
57	MG	1A	3218	1/1	0.95	0.14	46,46,46,46	0
57	MG	1A	3074	1/1	0.95	0.09	27,27,27,27	0
57	MG	1A	3444	1/1	0.95	0.17	41,41,41,41	0
57	MG	1A	3853	1/1	0.95	0.06	26,26,26,26	0
57	MG	2A	3674	1/1	0.95	0.09	66,66,66,66	0
57	MG	1A	3220	1/1	0.95	0.20	47,47,47,47	0
57	MG	1A	3293	1/1	0.95	0.19	53,53,53,53	0
57	MG	2A	3677	1/1	0.95	0.10	65,65,65,65	0
57	MG	2A	3396	1/1	0.95	0.14	57,57,57,57	0
57	MG	2A	3397	1/1	0.95	0.13	44,44,44,44	0
57	MG	1A	3221	1/1	0.95	0.14	45,45,45,45	0
57	MG	17	104	1/1	0.95	0.15	58,58,58,58	0
57	MG	1A	3448	1/1	0.95	0.08	56,56,56,56	0
57	MG	1A	3861	1/1	0.95	0.07	47,47,47,47	0
57	MG	1A	3544	1/1	0.95	0.23	51,51,51,51	0
57	MG	1A	3222	1/1	0.95	0.06	38,38,38,38	0
57	MG	1A	3096	1/1	0.95	0.15	41,41,41,41	0
57	MG	1A	3367	1/1	0.95	0.25	64,64,64,64	0
57	MG	1A	3548	1/1	0.95	0.10	26,26,26,26	0
57	MG	1A	3867	1/1	0.95	0.09	42,42,42,42	0
57	MG	2A	3408	1/1	0.95	0.30	64,64,64,64	0
57	MG	1A	3075	1/1	0.95	0.06	32,32,32,32	0
57	MG	1A	3697	1/1	0.95	0.12	27,27,27,27	0
57	MG	1A	3456	1/1	0.95	0.21	39,39,39,39	0
57	MG	2A	3412	1/1	0.95	0.34	59,59,59,59	0
57	MG	2A	3698	1/1	0.95	0.08	64,64,64,64	0
57	MG	1A	3699	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	3873	1/1	0.95	0.28	42,42,42,42	0
57	MG	1a	1610	1/1	0.95	0.05	27,27,27,27	0
57	MG	1A	3076	1/1	0.95	0.27	50,50,50,50	0
57	MG	1A	4054	1/1	0.95	0.07	55,55,55,55	0
57	MG	1a	1818	1/1	0.95	0.06	52,52,52,52	0
57	MG	1a	1820	1/1	0.95	0.07	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1822	1/1	0.95	0.21	63,63,63,63	0
57	MG	1A	3227	1/1	0.95	0.10	43,43,43,43	0
57	MG	1A	4056	1/1	0.95	0.14	39,39,39,39	0
57	MG	1A	3553	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	4062	1/1	0.95	0.07	53,53,53,53	0
57	MG	1a	1618	1/1	0.95	0.06	60,60,60,60	0
57	MG	1A	3163	1/1	0.95	0.21	52,52,52,52	0
57	MG	1A	3230	1/1	0.95	0.21	32,32,32,32	0
57	MG	2A	3717	1/1	0.95	0.12	47,47,47,47	0
57	MG	2a	1685	1/1	0.95	0.21	57,57,57,57	0
57	MG	1A	3556	1/1	0.95	0.07	55,55,55,55	0
57	MG	1A	3101	1/1	0.95	0.08	41,41,41,41	0
57	MG	1A	3035	1/1	0.95	0.09	47,47,47,47	0
57	MG	1A	3108	1/1	0.95	0.17	39,39,39,39	0
57	MG	1A	3011	1/1	0.95	0.16	44,44,44,44	0
57	MG	1A	4074	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3379	1/1	0.95	0.12	55,55,55,55	0
57	MG	2A	3726	1/1	0.95	0.10	43,43,43,43	0
57	MG	1A	3715	1/1	0.95	0.06	35,35,35,35	0
57	MG	1A	3310	1/1	0.95	0.08	45,45,45,45	0
57	MG	1A	3017	1/1	0.95	0.09	52,52,52,52	0
57	MG	2a	1698	1/1	0.95	0.15	64,64,64,64	0
57	MG	1A	3173	1/1	0.95	0.12	41,41,41,41	0
57	MG	1A	3572	1/1	0.95	0.27	33,33,33,33	0
57	MG	1A	3175	1/1	0.95	0.24	33,33,33,33	0
57	MG	1A	3471	1/1	0.95	0.11	35,35,35,35	0
57	MG	2A	3445	1/1	0.95	0.11	42,42,42,42	0
57	MG	1A	3577	1/1	0.95	0.16	44,44,44,44	0
57	MG	1A	3578	1/1	0.95	0.10	39,39,39,39	0
57	MG	2A	3448	1/1	0.95	0.06	49,49,49,49	0
57	MG	2A	3743	1/1	0.95	0.08	40,40,40,40	0
57	MG	1A	3384	1/1	0.95	0.10	49,49,49,49	0
57	MG	1A	3474	1/1	0.95	0.09	40,40,40,40	0
57	MG	1A	3582	1/1	0.95	0.30	39,39,39,39	0
57	MG	1x	102	1/1	0.95	0.11	52,52,52,52	0
57	MG	2A	3228	1/1	0.95	0.19	46,46,46,46	0
57	MG	1A	3315	1/1	0.95	0.16	60,60,60,60	0
57	MG	1a	1644	1/1	0.95	0.10	67,67,67,67	0
57	MG	2A	3460	1/1	0.95	0.07	54,54,54,54	0
57	MG	2A	3461	1/1	0.95	0.07	70,70,70,70	0
57	MG	1A	3181	1/1	0.95	0.13	38,38,38,38	0
57	MG	1A	3042	1/1	0.95	0.14	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3911	1/1	0.95	0.26	37,37,37,37	0
57	MG	1A	3914	1/1	0.95	0.06	25,25,25,25	0
57	MG	1A	3120	1/1	0.95	0.17	44,44,44,44	0
57	MG	1A	3589	1/1	0.95	0.22	42,42,42,42	0
57	MG	2A	3765	1/1	0.95	0.09	58,58,58,58	0
57	MG	1A	3740	1/1	0.95	0.06	27,27,27,27	0
57	MG	1A	3742	1/1	0.95	0.07	20,20,20,20	0
57	MG	1B	212	1/1	0.95	0.08	42,42,42,42	0
57	MG	2A	3002	1/1	0.95	0.22	52,52,52,52	0
57	MG	2A	3474	1/1	0.95	0.50	66,66,66,66	0
57	MG	1A	3390	1/1	0.95	0.09	45,45,45,45	0
57	MG	2A	3004	1/1	0.95	0.32	61,61,61,61	0
57	MG	1a	1658	1/1	0.95	0.13	60,60,60,60	0
57	MG	2A	3478	1/1	0.95	0.28	68,68,68,68	0
57	MG	2A	3479	1/1	0.95	0.14	52,52,52,52	0
57	MG	2A	3783	1/1	0.95	0.07	58,58,58,58	0
57	MG	1B	214	1/1	0.95	0.06	55,55,55,55	0
57	MG	1B	216	1/1	0.95	0.10	53,53,53,53	0
57	MG	2A	3786	1/1	0.95	0.10	64,64,64,64	0
57	MG	1B	217	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3391	1/1	0.95	0.20	60,60,60,60	0
57	MG	1A	3746	1/1	0.95	0.11	42,42,42,42	0
57	MG	1A	3184	1/1	0.95	0.08	58,58,58,58	0
57	MG	2a	1743	1/1	0.95	0.16	68,68,68,68	0
57	MG	1A	3748	1/1	0.95	0.07	58,58,58,58	0
57	MG	1A	3754	1/1	0.95	0.11	52,52,52,52	0
57	MG	2A	3795	1/1	0.95	0.10	50,50,50,50	0
57	MG	1a	1667	1/1	0.95	0.15	58,58,58,58	0
57	MG	2a	1748	1/1	0.95	0.08	70,70,70,70	0
57	MG	2A	3257	1/1	0.95	0.10	67,67,67,67	0
57	MG	2A	3019	1/1	0.95	0.09	43,43,43,43	0
57	MG	2A	3800	1/1	0.95	0.07	76,76,76,76	0
57	MG	1a	1668	1/1	0.95	0.07	70,70,70,70	0
57	MG	1A	3756	1/1	0.95	0.07	18,18,18,18	0
57	MG	2A	3803	1/1	0.95	0.06	72,72,72,72	0
57	MG	2A	3493	1/1	0.95	0.33	64,64,64,64	0
57	MG	1A	3054	1/1	0.95	0.07	43,43,43,43	0
57	MG	2A	3262	1/1	0.95	0.09	63,63,63,63	0
57	MG	1B	226	1/1	0.95	0.10	67,67,67,67	0
57	MG	1A	3043	1/1	0.95	0.27	38,38,38,38	0
57	MG	1A	3323	1/1	0.95	0.16	36,36,36,36	0
57	MG	2A	3030	1/1	0.95	0.08	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3031	1/1	0.95	0.10	53,53,53,53	0
57	MG	2A	3032	1/1	0.95	0.07	50,50,50,50	0
57	MG	2A	3269	1/1	0.95	0.07	55,55,55,55	0
57	MG	2a	1772	1/1	0.95	0.18	65,65,65,65	0
57	MG	1A	3762	1/1	0.95	0.08	35,35,35,35	0
57	MG	2A	3508	1/1	0.95	0.10	76,76,76,76	0
57	MG	2A	3035	1/1	0.95	0.07	47,47,47,47	0
57	MG	1A	3485	1/1	0.95	0.13	42,42,42,42	0
57	MG	1B	232	1/1	0.95	0.08	60,60,60,60	0
57	MG	2a	1780	1/1	0.95	0.07	60,60,60,60	0
57	MG	1A	3060	1/1	0.95	0.07	38,38,38,38	0
57	MG	2A	3831	1/1	0.95	0.08	42,42,42,42	0
57	MG	2a	1783	1/1	0.95	0.16	57,57,57,57	0
57	MG	2A	3514	1/1	0.95	0.06	33,33,33,33	0
57	MG	1A	3947	1/1	0.95	0.06	55,55,55,55	0
57	MG	1A	3765	1/1	0.95	0.11	44,44,44,44	0
57	MG	1A	3327	1/1	0.95	0.07	44,44,44,44	0
57	MG	1D	308	1/1	0.95	0.12	52,52,52,52	0
57	MG	2A	3047	1/1	0.95	0.15	36,36,36,36	0
57	MG	1A	3125	1/1	0.95	0.18	38,38,38,38	0
57	MG	1A	3954	1/1	0.95	0.07	51,51,51,51	0
57	MG	1A	3769	1/1	0.95	0.06	65,65,65,65	0
57	MG	1A	3770	1/1	0.95	0.08	24,24,24,24	0
57	MG	1E	301	1/1	0.95	0.18	41,41,41,41	0
57	MG	1E	306	1/1	0.95	0.08	46,46,46,46	0
57	MG	1A	3775	1/1	0.95	0.05	29,29,29,29	0
57	MG	2A	3855	1/1	0.95	0.07	64,64,64,64	0
57	MG	1A	3402	1/1	0.95	0.09	71,71,71,71	0
57	MG	1A	3779	1/1	0.95	0.14	68,68,68,68	0
57	MG	1A	3192	1/1	0.95	0.17	38,38,38,38	0
57	MG	1A	3256	1/1	0.95	0.12	30,30,30,30	0
57	MG	1A	3193	1/1	0.95	0.07	42,42,42,42	0
57	MG	1F	307	1/1	0.95	0.07	46,46,46,46	0
57	MG	2A	3538	1/1	0.95	0.12	53,53,53,53	0
57	MG	1A	3963	1/1	0.95	0.05	46,46,46,46	0
57	MG	1A	3127	1/1	0.95	0.22	36,36,36,36	0
57	MG	1A	3608	1/1	0.95	0.10	43,43,43,43	0
57	MG	1A	3259	1/1	0.95	0.10	28,28,28,28	0
57	MG	2A	3067	1/1	0.95	0.13	43,43,43,43	0
57	MG	2A	3300	1/1	0.95	0.16	72,72,72,72	0
57	MG	1A	3412	1/1	0.95	0.09	45,45,45,45	0
57	MG	2a	1813	1/1	0.95	0.20	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1G	201	1/1	0.95	0.15	41,41,41,41	0
57	MG	1A	3611	1/1	0.95	0.11	60,60,60,60	0
57	MG	1A	3792	1/1	0.95	0.05	20,20,20,20	0
57	MG	2A	3072	1/1	0.95	0.18	67,67,67,67	0
57	MG	2A	3073	1/1	0.95	0.19	56,56,56,56	0
57	MG	2A	3074	1/1	0.95	0.12	47,47,47,47	0
57	MG	1A	3008	1/1	0.95	0.08	24,24,24,24	0
57	MG	1A	3063	1/1	0.95	0.21	50,50,50,50	0
57	MG	1N	202	1/1	0.95	0.09	45,45,45,45	0
57	MG	2A	3084	1/1	0.95	0.08	55,55,55,55	0
57	MG	1A	3796	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3262	1/1	0.95	0.09	56,56,56,56	0
57	MG	2D	301	1/1	0.95	0.12	52,52,52,52	0
57	MG	2D	302	1/1	0.95	0.10	53,53,53,53	0
57	MG	1A	3263	1/1	0.95	0.15	55,55,55,55	0
57	MG	2A	3565	1/1	0.95	0.08	38,38,38,38	0
57	MG	2E	302	1/1	0.95	0.14	61,61,61,61	0
57	MG	1P	204	1/1	0.95	0.05	42,42,42,42	0
57	MG	1A	3507	1/1	0.95	0.14	40,40,40,40	0
57	MG	2A	3090	1/1	0.95	0.17	57,57,57,57	0
57	MG	2A	3572	1/1	0.95	0.17	56,56,56,56	0
57	MG	1A	3131	1/1	0.95	0.08	70,70,70,70	0
57	MG	2A	3092	1/1	0.95	0.06	40,40,40,40	0
57	MG	2A	3320	1/1	0.95	0.06	64,64,64,64	0
57	MG	2A	3093	1/1	0.95	0.13	69,69,69,69	0
57	MG	1Q	204	1/1	0.95	0.09	62,62,62,62	0
57	MG	1A	3132	1/1	0.95	0.08	43,43,43,43	0
57	MG	1A	3419	1/1	0.95	0.46	78,78,78,78	0
57	MG	1R	201	1/1	0.95	0.10	37,37,37,37	0
57	MG	1R	202	1/1	0.95	0.08	46,46,46,46	0
57	MG	1A	3810	1/1	0.95	0.07	62,62,62,62	0
57	MG	1A	3511	1/1	0.95	0.07	60,60,60,60	0
57	MG	1A	3632	1/1	0.95	0.12	30,30,30,30	0
57	MG	2A	3591	1/1	0.95	0.16	65,65,65,65	0
57	MG	1A	3133	1/1	0.95	0.10	40,40,40,40	0
57	MG	1a	1729	1/1	0.95	0.24	61,61,61,61	0
57	MG	1A	3267	1/1	0.95	0.21	36,36,36,36	0
57	MG	1A	3136	1/1	0.95	0.08	49,49,49,49	0
57	MG	2A	3598	1/1	0.95	0.12	58,58,58,58	0
59	CLM	1A	4097	20/20	0.95	0.09	29,37,54,64	0
57	MG	1A	3987	1/1	0.95	0.08	52,52,52,52	0
57	MG	1A	3908	1/1	0.96	0.08	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3909	1/1	0.96	0.06	55,55,55,55	0
57	MG	1A	3784	1/1	0.96	0.05	40,40,40,40	0
57	MG	1A	3016	1/1	0.96	0.18	54,54,54,54	0
57	MG	1W	203	1/1	0.96	0.17	50,50,50,50	0
57	MG	1a	1724	1/1	0.96	0.09	56,56,56,56	0
57	MG	1W	207	1/1	0.96	0.13	33,33,33,33	0
57	MG	1X	101	1/1	0.96	0.38	33,33,33,33	0
57	MG	2A	3464	1/1	0.96	0.14	71,71,71,71	0
57	MG	1X	103	1/1	0.96	0.09	46,46,46,46	0
57	MG	1A	3434	1/1	0.96	0.13	38,38,38,38	0
57	MG	1A	3177	1/1	0.96	0.05	32,32,32,32	0
57	MG	1A	4058	1/1	0.96	0.05	60,60,60,60	0
57	MG	2A	3469	1/1	0.96	0.07	37,37,37,37	0
57	MG	1A	4061	1/1	0.96	0.08	49,49,49,49	0
57	MG	1A	3660	1/1	0.96	0.06	23,23,23,23	0
57	MG	2A	3075	1/1	0.96	0.07	45,45,45,45	0
57	MG	1A	3064	1/1	0.96	0.12	34,34,34,34	0
57	MG	2A	3079	1/1	0.96	0.16	54,54,54,54	0
57	MG	2a	1632	1/1	0.96	0.27	54,54,54,54	0
57	MG	1A	4065	1/1	0.96	0.07	62,62,62,62	0
57	MG	2A	3081	1/1	0.96	0.10	48,48,48,48	0
57	MG	1A	3143	1/1	0.96	0.10	51,51,51,51	0
57	MG	10	101	1/1	0.96	0.16	43,43,43,43	0
57	MG	1A	3438	1/1	0.96	0.09	45,45,45,45	0
57	MG	2A	3280	1/1	0.96	0.08	62,62,62,62	0
57	MG	1A	4068	1/1	0.96	0.15	58,58,58,58	0
57	MG	1A	3920	1/1	0.96	0.07	64,64,64,64	0
57	MG	1A	3665	1/1	0.96	0.06	35,35,35,35	0
57	MG	1A	3573	1/1	0.96	0.05	27,27,27,27	0
57	MG	1A	3574	1/1	0.96	0.10	60,60,60,60	0
57	MG	1A	4073	1/1	0.96	0.06	20,20,20,20	0
57	MG	1A	3797	1/1	0.96	0.05	45,45,45,45	0
57	MG	2A	3728	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	3498	1/1	0.96	0.14	47,47,47,47	0
57	MG	1A	4076	1/1	0.96	0.06	52,52,52,52	0
57	MG	1A	3337	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3677	1/1	0.96	0.15	46,46,46,46	0
57	MG	1A	3936	1/1	0.96	0.06	40,40,40,40	0
57	MG	1A	3804	1/1	0.96	0.05	25,25,25,25	0
57	MG	2A	3736	1/1	0.96	0.12	65,65,65,65	0
57	MG	2A	3737	1/1	0.96	0.07	66,66,66,66	0
57	MG	15	101	1/1	0.96	0.24	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	15	104	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3805	1/1	0.96	0.27	32,32,32,32	0
57	MG	2A	3104	1/1	0.96	0.24	54,54,54,54	0
57	MG	1A	3294	1/1	0.96	0.17	35,35,35,35	0
57	MG	16	101	1/1	0.96	0.09	57,57,57,57	0
57	MG	2a	1661	1/1	0.96	0.10	67,67,67,67	0
57	MG	2A	3501	1/1	0.96	0.35	69,69,69,69	0
57	MG	2a	1663	1/1	0.96	0.10	65,65,65,65	0
57	MG	2A	3747	1/1	0.96	0.06	66,66,66,66	0
57	MG	1A	3254	1/1	0.96	0.11	59,59,59,59	0
57	MG	17	101	1/1	0.96	0.05	34,34,34,34	0
57	MG	17	103	1/1	0.96	0.14	37,37,37,37	0
57	MG	1A	3442	1/1	0.96	0.12	46,46,46,46	0
57	MG	2A	3753	1/1	0.96	0.13	61,61,61,61	0
57	MG	1A	3580	1/1	0.96	0.06	37,37,37,37	0
57	MG	2A	3755	1/1	0.96	0.06	54,54,54,54	0
57	MG	2A	3509	1/1	0.96	0.08	53,53,53,53	0
57	MG	1A	3503	1/1	0.96	0.18	52,52,52,52	0
57	MG	18	103	1/1	0.96	0.10	40,40,40,40	0
57	MG	18	104	1/1	0.96	0.12	47,47,47,47	0
57	MG	1A	3951	1/1	0.96	0.06	63,63,63,63	0
57	MG	1A	4095	1/1	0.96	0.05	44,44,44,44	0
57	MG	1A	3687	1/1	0.96	0.08	39,39,39,39	0
57	MG	1A	3505	1/1	0.96	0.17	31,31,31,31	0
57	MG	2A	3517	1/1	0.96	0.07	69,69,69,69	0
57	MG	1A	3032	1/1	0.96	0.19	25,25,25,25	0
57	MG	2A	3520	1/1	0.96	0.13	62,62,62,62	0
57	MG	2A	3768	1/1	0.96	0.06	43,43,43,43	0
57	MG	1A	3055	1/1	0.96	0.13	41,41,41,41	0
57	MG	1B	204	1/1	0.96	0.23	62,62,62,62	0
57	MG	1A	3693	1/1	0.96	0.11	50,50,50,50	0
57	MG	2A	3524	1/1	0.96	0.07	45,45,45,45	0
57	MG	2A	3773	1/1	0.96	0.07	65,65,65,65	0
57	MG	1A	3389	1/1	0.96	0.19	28,28,28,28	0
57	MG	2A	3125	1/1	0.96	0.19	71,71,71,71	0
57	MG	2A	3776	1/1	0.96	0.06	52,52,52,52	0
57	MG	2A	3126	1/1	0.96	0.06	49,49,49,49	0
57	MG	2a	1696	1/1	0.96	0.09	56,56,56,56	0
57	MG	1A	3149	1/1	0.96	0.19	31,31,31,31	0
57	MG	2A	3128	1/1	0.96	0.05	61,61,61,61	0
57	MG	2A	3322	1/1	0.96	0.12	57,57,57,57	0
57	MG	1A	3104	1/1	0.96	0.10	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3126	1/1	0.96	0.20	38,38,38,38	0
57	MG	1A	3826	1/1	0.96	0.09	50,50,50,50	0
57	MG	1A	3345	1/1	0.96	0.07	66,66,66,66	0
57	MG	1A	3513	1/1	0.96	0.08	44,44,44,44	0
57	MG	1A	3346	1/1	0.96	0.15	36,36,36,36	0
57	MG	2A	3791	1/1	0.96	0.06	53,53,53,53	0
57	MG	1A	3152	1/1	0.96	0.16	44,44,44,44	0
57	MG	1A	3398	1/1	0.96	0.12	25,25,25,25	0
57	MG	1A	3518	1/1	0.96	0.17	49,49,49,49	0
57	MG	1A	3453	1/1	0.96	0.15	45,45,45,45	0
57	MG	2A	3140	1/1	0.96	0.13	41,41,41,41	0
57	MG	1a	1620	1/1	0.96	0.05	48,48,48,48	0
57	MG	2A	3799	1/1	0.96	0.07	79,79,79,79	0
57	MG	1A	3454	1/1	0.96	0.10	36,36,36,36	0
57	MG	1A	3455	1/1	0.96	0.12	46,46,46,46	0
57	MG	1A	3600	1/1	0.96	0.06	27,27,27,27	0
57	MG	1A	3106	1/1	0.96	0.08	38,38,38,38	0
57	MG	2A	3147	1/1	0.96	0.07	46,46,46,46	0
57	MG	2A	3550	1/1	0.96	0.06	56,56,56,56	0
57	MG	1A	3304	1/1	0.96	0.29	53,53,53,53	0
57	MG	1A	3128	1/1	0.96	0.24	40,40,40,40	0
57	MG	1A	3058	1/1	0.96	0.05	42,42,42,42	0
57	MG	1A	3109	1/1	0.96	0.16	38,38,38,38	0
57	MG	1A	3461	1/1	0.96	0.11	42,42,42,42	0
57	MG	1A	3034	1/1	0.96	0.20	34,34,34,34	0
57	MG	2A	3154	1/1	0.96	0.11	56,56,56,56	0
57	MG	1A	3165	1/1	0.96	0.06	33,33,33,33	0
57	MG	1A	3849	1/1	0.96	0.07	24,24,24,24	0
57	MG	1a	1634	1/1	0.96	0.10	63,63,63,63	0
57	MG	1A	3234	1/1	0.96	0.08	47,47,47,47	0
57	MG	1A	3612	1/1	0.96	0.05	24,24,24,24	0
57	MG	2A	3567	1/1	0.96	0.07	38,38,38,38	0
57	MG	1D	301	1/1	0.96	0.18	37,37,37,37	0
57	MG	1D	302	1/1	0.96	0.19	37,37,37,37	0
57	MG	2A	3832	1/1	0.96	0.05	55,55,55,55	0
57	MG	2A	3571	1/1	0.96	0.07	45,45,45,45	0
57	MG	2A	3835	1/1	0.96	0.06	56,56,56,56	0
57	MG	1A	3725	1/1	0.96	0.05	53,53,53,53	0
57	MG	1A	3613	1/1	0.96	0.05	34,34,34,34	0
57	MG	1A	3854	1/1	0.96	0.10	22,22,22,22	0
57	MG	1A	3408	1/1	0.96	0.20	32,32,32,32	0
57	MG	2a	1742	1/1	0.96	0.27	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3268	1/1	0.96	0.10	42,42,42,42	0
57	MG	1A	3411	1/1	0.96	0.10	37,37,37,37	0
57	MG	2A	3169	1/1	0.96	0.08	63,63,63,63	0
57	MG	1A	3991	1/1	0.96	0.07	26,26,26,26	0
57	MG	2A	3849	1/1	0.96	0.06	40,40,40,40	0
57	MG	2A	3365	1/1	0.96	0.07	47,47,47,47	0
57	MG	1E	304	1/1	0.96	0.09	33,33,33,33	0
57	MG	1A	3009	1/1	0.96	0.05	27,27,27,27	0
57	MG	1A	3203	1/1	0.96	0.15	35,35,35,35	0
57	MG	2a	1752	1/1	0.96	0.09	70,70,70,70	0
57	MG	2a	1753	1/1	0.96	0.09	68,68,68,68	0
57	MG	2A	3587	1/1	0.96	0.16	61,61,61,61	0
57	MG	1A	3622	1/1	0.96	0.11	60,60,60,60	0
57	MG	1E	309	1/1	0.96	0.10	33,33,33,33	0
57	MG	2A	3177	1/1	0.96	0.15	61,61,61,61	0
57	MG	2a	1758	1/1	0.96	0.15	61,61,61,61	0
57	MG	1A	3316	1/1	0.96	0.12	55,55,55,55	0
57	MG	1a	1652	1/1	0.96	0.08	54,54,54,54	0
57	MG	1A	3168	1/1	0.96	0.08	40,40,40,40	0
57	MG	2A	3181	1/1	0.96	0.08	46,46,46,46	0
57	MG	1A	3627	1/1	0.96	0.06	37,37,37,37	0
57	MG	1A	3741	1/1	0.96	0.07	37,37,37,37	0
57	MG	1F	305	1/1	0.96	0.19	33,33,33,33	0
57	MG	1F	306	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	3114	1/1	0.96	0.09	36,36,36,36	0
57	MG	1A	3629	1/1	0.96	0.06	32,32,32,32	0
57	MG	1A	4002	1/1	0.96	0.06	55,55,55,55	0
57	MG	1F	311	1/1	0.96	0.06	48,48,48,48	0
57	MG	1A	3744	1/1	0.96	0.07	56,56,56,56	0
57	MG	1A	3473	1/1	0.96	0.12	33,33,33,33	0
57	MG	1A	3871	1/1	0.96	0.21	39,39,39,39	0
57	MG	1F	315	1/1	0.96	0.19	54,54,54,54	0
57	MG	1A	3273	1/1	0.96	0.19	41,41,41,41	0
57	MG	1G	202	1/1	0.96	0.16	58,58,58,58	0
57	MG	1A	3028	1/1	0.96	0.19	29,29,29,29	0
57	MG	1A	3634	1/1	0.96	0.07	41,41,41,41	0
57	MG	1A	3875	1/1	0.96	0.07	32,32,32,32	0
57	MG	2A	3394	1/1	0.96	0.11	61,61,61,61	0
57	MG	1A	4012	1/1	0.96	0.06	53,53,53,53	0
57	MG	1A	3753	1/1	0.96	0.15	59,59,59,59	0
57	MG	1N	204	1/1	0.96	0.21	51,51,51,51	0
57	MG	1N	205	1/1	0.96	0.14	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1O	201	1/1	0.96	0.15	53,53,53,53	0
57	MG	2A	3206	1/1	0.96	0.07	58,58,58,58	0
57	MG	1A	3243	1/1	0.96	0.13	26,26,26,26	0
57	MG	2a	1794	1/1	0.96	0.14	66,66,66,66	0
57	MG	1O	203	1/1	0.96	0.20	66,66,66,66	0
57	MG	1A	3755	1/1	0.96	0.11	44,44,44,44	0
57	MG	2A	3631	1/1	0.96	0.15	46,46,46,46	0
57	MG	1A	3276	1/1	0.96	0.12	39,39,39,39	0
57	MG	2A	3211	1/1	0.96	0.15	72,72,72,72	0
57	MG	1P	202	1/1	0.96	0.25	36,36,36,36	0
57	MG	2A	3635	1/1	0.96	0.14	56,56,56,56	0
57	MG	2A	3636	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	3137	1/1	0.96	0.13	28,28,28,28	0
57	MG	2A	3639	1/1	0.96	0.05	46,46,46,46	0
57	MG	2A	3640	1/1	0.96	0.13	41,41,41,41	0
57	MG	1A	3324	1/1	0.96	0.13	30,30,30,30	0
57	MG	1A	3280	1/1	0.96	0.17	37,37,37,37	0
57	MG	1Q	202	1/1	0.96	0.07	36,36,36,36	0
57	MG	1A	3641	1/1	0.96	0.10	25,25,25,25	0
57	MG	1a	1689	1/1	0.96	0.16	66,66,66,66	0
57	MG	2A	3219	1/1	0.96	0.30	63,63,63,63	0
57	MG	2A	3024	1/1	0.96	0.08	53,53,53,53	0
57	MG	1A	3372	1/1	0.96	0.08	43,43,43,43	0
57	MG	2A	3026	1/1	0.96	0.21	54,54,54,54	0
57	MG	1A	3281	1/1	0.96	0.27	42,42,42,42	0
57	MG	1A	3284	1/1	0.96	0.25	34,34,34,34	0
57	MG	1A	4029	1/1	0.96	0.06	69,69,69,69	0
57	MG	1R	204	1/1	0.96	0.36	35,35,35,35	0
57	MG	1A	3118	1/1	0.96	0.22	28,28,28,28	0
57	MG	1a	1696	1/1	0.96	0.23	69,69,69,69	0
57	MG	2V	203	1/1	0.96	0.18	68,68,68,68	0
57	MG	2A	3423	1/1	0.96	0.19	58,58,58,58	0
57	MG	1A	4031	1/1	0.96	0.06	50,50,50,50	0
57	MG	2A	3658	1/1	0.96	0.15	44,44,44,44	0
57	MG	1a	1698	1/1	0.96	0.14	48,48,48,48	0
57	MG	1A	3767	1/1	0.96	0.06	30,30,30,30	0
57	MG	2A	3233	1/1	0.96	0.14	42,42,42,42	0
57	MG	2f	201	1/1	0.96	0.13	51,51,51,51	0
57	MG	2A	3038	1/1	0.96	0.14	61,61,61,61	0
57	MG	1A	3429	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	4034	1/1	0.96	0.08	45,45,45,45	0
57	MG	2A	3431	1/1	0.96	0.17	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1702	1/1	0.96	0.32	62,62,62,62	0
57	MG	2A	3239	1/1	0.96	0.23	44,44,44,44	0
57	MG	1A	3486	1/1	0.96	0.09	43,43,43,43	0
57	MG	1A	3487	1/1	0.96	0.08	50,50,50,50	0
57	MG	2A	3044	1/1	0.96	0.08	62,62,62,62	0
57	MG	1A	3771	1/1	0.96	0.07	28,28,28,28	0
57	MG	1A	3773	1/1	0.96	0.07	68,68,68,68	0
57	MG	1A	3287	1/1	0.96	0.14	37,37,37,37	0
57	MG	1U	204	1/1	0.96	0.08	38,38,38,38	0
57	MG	2A	3050	1/1	0.96	0.09	61,61,61,61	0
57	MG	2A	3678	1/1	0.96	0.10	39,39,39,39	0
57	MG	1A	4041	1/1	0.96	0.08	59,59,59,59	0
57	MG	2A	3680	1/1	0.96	0.07	67,67,67,67	0
57	MG	1A	3776	1/1	0.96	0.05	26,26,26,26	0
57	MG	1U	207	1/1	0.96	0.26	37,37,37,37	0
57	MG	1A	3212	1/1	0.96	0.27	54,54,54,54	0
57	MG	1A	3559	1/1	0.96	0.17	30,30,30,30	0
57	MG	1A	3904	1/1	0.96	0.13	53,53,53,53	0
57	MG	2A	3449	1/1	0.96	0.22	48,48,48,48	0
57	MG	1A	3174	1/1	0.96	0.07	35,35,35,35	0
57	MG	1A	3656	1/1	0.96	0.09	37,37,37,37	0
57	MG	1V	203	1/1	0.96	0.12	37,37,37,37	0
59	CLM	2A	3863	20/20	0.96	0.09	42,47,57,60	0
60	ZN	14	501	1/1	0.96	0.10	106,106,106,106	0
60	ZN	24	501	1/1	0.96	0.11	117,117,117,117	0
57	MG	2A	3455	1/1	0.96	0.07	52,52,52,52	0
57	MG	2A	3859	1/1	0.97	0.10	53,53,53,53	0
57	MG	1A	3206	1/1	0.97	0.08	37,37,37,37	0
57	MG	2A	3248	1/1	0.97	0.08	71,71,71,71	0
57	MG	2A	3116	1/1	0.97	0.08	37,37,37,37	0
57	MG	1A	3718	1/1	0.97	0.08	55,55,55,55	0
57	MG	1A	3147	1/1	0.97	0.07	42,42,42,42	0
57	MG	1A	3242	1/1	0.97	0.14	36,36,36,36	0
57	MG	1N	203	1/1	0.97	0.06	44,44,44,44	0
57	MG	1A	3424	1/1	0.97	0.13	40,40,40,40	0
57	MG	1A	3650	1/1	0.97	0.06	36,36,36,36	0
57	MG	1A	3974	1/1	0.97	0.04	51,51,51,51	0
57	MG	2A	3532	1/1	0.97	0.11	44,44,44,44	0
57	MG	1A	3651	1/1	0.97	0.06	64,64,64,64	0
57	MG	1A	3110	1/1	0.97	0.20	31,31,31,31	0
57	MG	1A	3062	1/1	0.97	0.28	61,61,61,61	0
57	MG	1A	3727	1/1	0.97	0.07	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3112	1/1	0.97	0.09	34,34,34,34	0
57	MG	1P	203	1/1	0.97	0.18	29,29,29,29	0
57	MG	2A	3697	1/1	0.97	0.14	40,40,40,40	0
57	MG	1A	3980	1/1	0.97	0.07	51,51,51,51	0
57	MG	1a	1726	1/1	0.97	0.12	47,47,47,47	0
57	MG	1A	3808	1/1	0.97	0.05	35,35,35,35	0
57	MG	1A	3178	1/1	0.97	0.10	29,29,29,29	0
57	MG	1A	3352	1/1	0.97	0.24	39,39,39,39	0
57	MG	1Q	203	1/1	0.97	0.05	47,47,47,47	0
57	MG	2A	3545	1/1	0.97	0.06	58,58,58,58	0
57	MG	2D	304	1/1	0.97	0.37	42,42,42,42	0
57	MG	1A	4083	1/1	0.97	0.07	45,45,45,45	0
57	MG	1A	4085	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3354	1/1	0.97	0.12	35,35,35,35	0
57	MG	1A	3890	1/1	0.97	0.06	22,22,22,22	0
57	MG	1A	3030	1/1	0.97	0.16	30,30,30,30	0
57	MG	2E	305	1/1	0.97	0.10	39,39,39,39	0
57	MG	1A	3602	1/1	0.97	0.07	54,54,54,54	0
57	MG	2A	3552	1/1	0.97	0.09	50,50,50,50	0
57	MG	2A	3553	1/1	0.97	0.07	35,35,35,35	0
57	MG	2A	3012	1/1	0.97	0.08	47,47,47,47	0
57	MG	1A	3736	1/1	0.97	0.06	44,44,44,44	0
57	MG	2A	3145	1/1	0.97	0.08	38,38,38,38	0
57	MG	2F	304	1/1	0.97	0.09	63,63,63,63	0
57	MG	1A	3815	1/1	0.97	0.28	33,33,33,33	0
57	MG	2A	3015	1/1	0.97	0.07	39,39,39,39	0
57	MG	1A	3816	1/1	0.97	0.06	37,37,37,37	0
57	MG	2A	3017	1/1	0.97	0.21	60,60,60,60	0
57	MG	1a	1633	1/1	0.97	0.06	31,31,31,31	0
57	MG	1A	3282	1/1	0.97	0.07	31,31,31,31	0
57	MG	1a	1745	1/1	0.97	0.09	52,52,52,52	0
57	MG	2P	202	1/1	0.97	0.10	66,66,66,66	0
57	MG	2Q	201	1/1	0.97	0.05	49,49,49,49	0
57	MG	1S	202	1/1	0.97	0.09	44,44,44,44	0
57	MG	1A	3992	1/1	0.97	0.06	32,32,32,32	0
57	MG	2A	3568	1/1	0.97	0.10	51,51,51,51	0
57	MG	1A	3604	1/1	0.97	0.07	42,42,42,42	0
57	MG	2A	3731	1/1	0.97	0.07	38,38,38,38	0
57	MG	1A	3393	1/1	0.97	0.08	55,55,55,55	0
57	MG	1A	3820	1/1	0.97	0.08	27,27,27,27	0
57	MG	1A	3056	1/1	0.97	0.20	46,46,46,46	0
57	MG	1A	3901	1/1	0.97	0.06	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3574	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3031	1/1	0.97	0.17	33,33,33,33	0
57	MG	1A	3666	1/1	0.97	0.06	24,24,24,24	0
57	MG	2A	3739	1/1	0.97	0.11	55,55,55,55	0
57	MG	2A	3577	1/1	0.97	0.07	37,37,37,37	0
57	MG	1A	3667	1/1	0.97	0.05	34,34,34,34	0
57	MG	1A	3286	1/1	0.97	0.17	46,46,46,46	0
57	MG	1A	3155	1/1	0.97	0.18	45,45,45,45	0
57	MG	2A	3036	1/1	0.97	0.08	31,31,31,31	0
57	MG	1A	3516	1/1	0.97	0.16	27,27,27,27	0
57	MG	2A	3746	1/1	0.97	0.14	39,39,39,39	0
57	MG	1A	3185	1/1	0.97	0.09	69,69,69,69	0
57	MG	1A	3752	1/1	0.97	0.05	38,38,38,38	0
57	MG	1a	1766	1/1	0.97	0.13	43,43,43,43	0
57	MG	2A	3437	1/1	0.97	0.24	60,60,60,60	0
57	MG	1A	3675	1/1	0.97	0.05	32,32,32,32	0
57	MG	1A	3561	1/1	0.97	0.09	51,51,51,51	0
57	MG	1A	3253	1/1	0.97	0.07	51,51,51,51	0
57	MG	1a	1653	1/1	0.97	0.10	49,49,49,49	0
57	MG	2a	1765	1/1	0.97	0.11	46,46,46,46	0
57	MG	1a	1654	1/1	0.97	0.07	56,56,56,56	0
57	MG	1A	3565	1/1	0.97	0.23	36,36,36,36	0
57	MG	1A	3067	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	3681	1/1	0.97	0.04	24,24,24,24	0
57	MG	1A	3838	1/1	0.97	0.04	39,39,39,39	0
57	MG	2a	1771	1/1	0.97	0.07	77,77,77,77	0
57	MG	1W	205	1/1	0.97	0.11	41,41,41,41	0
57	MG	1W	206	1/1	0.97	0.17	41,41,41,41	0
57	MG	1A	4015	1/1	0.97	0.05	33,33,33,33	0
57	MG	1A	3921	1/1	0.97	0.14	41,41,41,41	0
57	MG	2A	3452	1/1	0.97	0.10	22,22,22,22	0
57	MG	2A	3185	1/1	0.97	0.05	56,56,56,56	0
57	MG	2A	3186	1/1	0.97	0.06	63,63,63,63	0
57	MG	1A	4019	1/1	0.97	0.04	36,36,36,36	0
57	MG	1X	104	1/1	0.97	0.10	32,32,32,32	0
57	MG	2A	3611	1/1	0.97	0.10	46,46,46,46	0
57	MG	1A	3922	1/1	0.97	0.06	30,30,30,30	0
57	MG	1A	4021	1/1	0.97	0.07	35,35,35,35	0
57	MG	2A	3059	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	3119	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	3840	1/1	0.97	0.04	39,39,39,39	0
57	MG	1a	1791	1/1	0.97	0.10	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3521	1/1	0.97	0.15	35,35,35,35	0
57	MG	1A	3620	1/1	0.97	0.09	33,33,33,33	0
57	MG	1A	3188	1/1	0.97	0.09	44,44,44,44	0
57	MG	2A	3329	1/1	0.97	0.20	56,56,56,56	0
57	MG	2A	3330	1/1	0.97	0.09	58,58,58,58	0
57	MG	1A	3159	1/1	0.97	0.10	33,33,33,33	0
57	MG	1A	3524	1/1	0.97	0.21	33,33,33,33	0
57	MG	1A	3223	1/1	0.97	0.09	50,50,50,50	0
57	MG	1A	3937	1/1	0.97	0.04	30,30,30,30	0
57	MG	1A	3848	1/1	0.97	0.13	45,45,45,45	0
57	MG	1A	3940	1/1	0.97	0.04	46,46,46,46	0
57	MG	1A	3526	1/1	0.97	0.16	30,30,30,30	0
57	MG	1A	3103	1/1	0.97	0.08	37,37,37,37	0
57	MG	1A	3696	1/1	0.97	0.09	38,38,38,38	0
57	MG	1D	312	1/1	0.97	0.04	38,38,38,38	0
57	MG	2A	3076	1/1	0.97	0.06	26,26,26,26	0
57	MG	1A	3407	1/1	0.97	0.04	37,37,37,37	0
57	MG	2A	3638	1/1	0.97	0.14	46,46,46,46	0
57	MG	2A	3078	1/1	0.97	0.07	59,59,59,59	0
57	MG	1a	1807	1/1	0.97	0.05	64,64,64,64	0
57	MG	1A	3630	1/1	0.97	0.04	22,22,22,22	0
57	MG	2A	3804	1/1	0.97	0.12	48,48,48,48	0
57	MG	1a	1810	1/1	0.97	0.04	47,47,47,47	0
57	MG	1a	1684	1/1	0.97	0.18	55,55,55,55	0
57	MG	2A	3348	1/1	0.97	0.07	68,68,68,68	0
57	MG	1A	3036	1/1	0.97	0.06	39,39,39,39	0
57	MG	1a	1816	1/1	0.97	0.07	59,59,59,59	0
57	MG	1A	3855	1/1	0.97	0.08	32,32,32,32	0
57	MG	13	103	1/1	0.97	0.10	42,42,42,42	0
57	MG	1a	1819	1/1	0.97	0.05	59,59,59,59	0
57	MG	2A	3815	1/1	0.97	0.06	46,46,46,46	0
57	MG	1A	3856	1/1	0.97	0.06	52,52,52,52	0
57	MG	1A	4044	1/1	0.97	0.05	57,57,57,57	0
57	MG	1A	3053	1/1	0.97	0.07	53,53,53,53	0
57	MG	2a	1824	1/1	0.97	0.08	71,71,71,71	0
57	MG	2A	3819	1/1	0.97	0.06	58,58,58,58	0
57	MG	15	102	1/1	0.97	0.14	38,38,38,38	0
57	MG	2A	3224	1/1	0.97	0.17	42,42,42,42	0
57	MG	2A	3824	1/1	0.97	0.04	52,52,52,52	0
57	MG	15	103	1/1	0.97	0.21	26,26,26,26	0
57	MG	2A	3827	1/1	0.97	0.05	61,61,61,61	0
57	MG	1A	3166	1/1	0.97	0.17	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3196	1/1	0.97	0.17	38,38,38,38	0
57	MG	2A	3830	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3780	1/1	0.97	0.07	27,27,27,27	0
57	MG	1A	3635	1/1	0.97	0.07	32,32,32,32	0
57	MG	1A	3782	1/1	0.97	0.07	43,43,43,43	0
57	MG	2A	3503	1/1	0.97	0.10	57,57,57,57	0
57	MG	2A	3100	1/1	0.97	0.08	30,30,30,30	0
57	MG	1A	3107	1/1	0.97	0.06	30,30,30,30	0
57	MG	2a	1665	1/1	0.97	0.14	56,56,56,56	0
57	MG	1A	3084	1/1	0.97	0.20	30,30,30,30	0
57	MG	2A	3839	1/1	0.97	0.05	70,70,70,70	0
57	MG	1A	3023	1/1	0.97	0.07	16,16,16,16	0
57	MG	2a	1670	1/1	0.97	0.06	61,61,61,61	0
57	MG	1A	3584	1/1	0.97	0.13	40,40,40,40	0
57	MG	2A	3844	1/1	0.97	0.09	41,41,41,41	0
57	MG	2A	3667	1/1	0.97	0.06	33,33,33,33	0
57	MG	2A	3846	1/1	0.97	0.14	60,60,60,60	0
57	MG	2x	101	1/1	0.97	0.11	60,60,60,60	0
57	MG	1A	3170	1/1	0.97	0.05	28,28,28,28	0
57	MG	2A	3237	1/1	0.97	0.08	67,67,67,67	0
57	MG	1m	3001	1/1	0.97	0.09	67,67,67,67	0
57	MG	1A	3145	1/1	0.97	0.23	28,28,28,28	0
57	MG	1A	3146	1/1	0.97	0.06	31,31,31,31	0
57	MG	1a	1705	1/1	0.97	0.29	55,55,55,55	0
57	MG	1A	4059	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	4060	1/1	0.97	0.05	45,45,45,45	0
57	MG	1A	3205	1/1	0.97	0.12	19,19,19,19	0
60	ZN	2Y	202	1/1	0.97	0.06	89,89,89,89	0
57	MG	1A	3238	1/1	0.97	0.15	32,32,32,32	0
57	MG	1A	4063	1/1	0.97	0.06	29,29,29,29	0
57	MG	1A	3162	1/1	0.98	0.23	35,35,35,35	0
57	MG	2A	3158	1/1	0.98	0.15	43,43,43,43	0
57	MG	1A	3013	1/1	0.98	0.09	28,28,28,28	0
57	MG	2D	303	1/1	0.98	0.04	30,30,30,30	0
57	MG	1A	3913	1/1	0.98	0.03	29,29,29,29	0
57	MG	1A	3690	1/1	0.98	0.04	26,26,26,26	0
57	MG	1a	1756	1/1	0.98	0.10	50,50,50,50	0
57	MG	1B	205	1/1	0.98	0.05	40,40,40,40	0
57	MG	1A	3141	1/1	0.98	0.04	29,29,29,29	0
57	MG	2A	3033	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	3692	1/1	0.98	0.07	27,27,27,27	0
57	MG	1A	3410	1/1	0.98	0.06	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3578	1/1	0.98	0.07	45,45,45,45	0
57	MG	1A	3142	1/1	0.98	0.05	20,20,20,20	0
57	MG	1A	3191	1/1	0.98	0.17	32,32,32,32	0
57	MG	1A	3005	1/1	0.98	0.07	44,44,44,44	0
57	MG	1A	4011	1/1	0.98	0.04	71,71,71,71	0
57	MG	1A	3066	1/1	0.98	0.11	32,32,32,32	0
57	MG	1A	3497	1/1	0.98	0.11	45,45,45,45	0
57	MG	2A	3174	1/1	0.98	0.16	37,37,37,37	0
57	MG	1A	3923	1/1	0.98	0.05	63,63,63,63	0
57	MG	1A	3842	1/1	0.98	0.05	52,52,52,52	0
57	MG	2A	3588	1/1	0.98	0.08	58,58,58,58	0
57	MG	2A	3589	1/1	0.98	0.06	42,42,42,42	0
57	MG	1a	1772	1/1	0.98	0.05	60,60,60,60	0
57	MG	1a	1773	1/1	0.98	0.05	49,49,49,49	0
57	MG	2A	3046	1/1	0.98	0.12	50,50,50,50	0
57	MG	1a	1774	1/1	0.98	0.05	54,54,54,54	0
57	MG	1A	3194	1/1	0.98	0.11	33,33,33,33	0
57	MG	2A	3596	1/1	0.98	0.06	40,40,40,40	0
57	MG	1B	219	1/1	0.98	0.07	34,34,34,34	0
57	MG	1A	4017	1/1	0.98	0.06	28,28,28,28	0
57	MG	2A	3750	1/1	0.98	0.05	57,57,57,57	0
57	MG	2A	3599	1/1	0.98	0.11	54,54,54,54	0
57	MG	1A	3044	1/1	0.98	0.05	34,34,34,34	0
57	MG	1A	3375	1/1	0.98	0.19	41,41,41,41	0
57	MG	1A	3038	1/1	0.98	0.18	32,32,32,32	0
57	MG	1A	3929	1/1	0.98	0.04	41,41,41,41	0
57	MG	1W	201	1/1	0.98	0.05	45,45,45,45	0
57	MG	1A	3772	1/1	0.98	0.07	39,39,39,39	0
57	MG	1A	3932	1/1	0.98	0.03	19,19,19,19	0
57	MG	1W	204	1/1	0.98	0.23	40,40,40,40	0
57	MG	1A	3115	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	3774	1/1	0.98	0.05	47,47,47,47	0
57	MG	2A	3762	1/1	0.98	0.04	63,63,63,63	0
57	MG	1A	3072	1/1	0.98	0.03	12,12,12,12	0
57	MG	1A	3504	1/1	0.98	0.10	37,37,37,37	0
57	MG	1X	102	1/1	0.98	0.14	38,38,38,38	0
57	MG	1A	3117	1/1	0.98	0.10	41,41,41,41	0
57	MG	1A	3941	1/1	0.98	0.08	54,54,54,54	0
57	MG	1A	3942	1/1	0.98	0.04	43,43,43,43	0
57	MG	23	104	1/1	0.98	0.04	60,60,60,60	0
57	MG	1A	3778	1/1	0.98	0.06	50,50,50,50	0
57	MG	25	102	1/1	0.98	0.26	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1B	236	1/1	0.98	0.06	30,30,30,30	0
57	MG	1A	3300	1/1	0.98	0.07	34,34,34,34	0
57	MG	1A	3648	1/1	0.98	0.07	38,38,38,38	0
57	MG	1D	303	1/1	0.98	0.07	39,39,39,39	0
57	MG	1D	304	1/1	0.98	0.08	20,20,20,20	0
57	MG	1A	3231	1/1	0.98	0.17	32,32,32,32	0
57	MG	1D	306	1/1	0.98	0.21	31,31,31,31	0
57	MG	10	102	1/1	0.98	0.15	46,46,46,46	0
57	MG	2A	3625	1/1	0.98	0.11	43,43,43,43	0
57	MG	2A	3779	1/1	0.98	0.05	62,62,62,62	0
57	MG	2a	1763	1/1	0.98	0.04	74,74,74,74	0
57	MG	2A	3780	1/1	0.98	0.04	75,75,75,75	0
57	MG	1D	307	1/1	0.98	0.23	42,42,42,42	0
57	MG	2A	3628	1/1	0.98	0.06	50,50,50,50	0
57	MG	1A	3105	1/1	0.98	0.05	50,50,50,50	0
57	MG	1A	3949	1/1	0.98	0.05	57,57,57,57	0
57	MG	1a	1808	1/1	0.98	0.06	56,56,56,56	0
57	MG	1A	3713	1/1	0.98	0.03	15,15,15,15	0
57	MG	1A	3714	1/1	0.98	0.08	63,63,63,63	0
57	MG	2A	3082	1/1	0.98	0.07	49,49,49,49	0
57	MG	2a	1774	1/1	0.98	0.15	63,63,63,63	0
57	MG	1A	3201	1/1	0.98	0.17	26,26,26,26	0
57	MG	2A	3792	1/1	0.98	0.09	72,72,72,72	0
57	MG	1a	1812	1/1	0.98	0.03	47,47,47,47	0
57	MG	1A	3202	1/1	0.98	0.04	45,45,45,45	0
57	MG	1A	3787	1/1	0.98	0.08	24,24,24,24	0
57	MG	11	102	1/1	0.98	0.04	36,36,36,36	0
57	MG	1E	302	1/1	0.98	0.13	34,34,34,34	0
57	MG	1A	4046	1/1	0.98	0.04	52,52,52,52	0
57	MG	1E	305	1/1	0.98	0.13	36,36,36,36	0
57	MG	2A	3494	1/1	0.98	0.20	65,65,65,65	0
57	MG	1a	1821	1/1	0.98	0.05	60,60,60,60	0
57	MG	1A	3093	1/1	0.98	0.08	27,27,27,27	0
57	MG	13	102	1/1	0.98	0.03	30,30,30,30	0
57	MG	1A	3306	1/1	0.98	0.10	39,39,39,39	0
57	MG	2A	3095	1/1	0.98	0.14	48,48,48,48	0
57	MG	1A	3134	1/1	0.98	0.07	43,43,43,43	0
57	MG	1A	3720	1/1	0.98	0.08	27,27,27,27	0
57	MG	1A	3135	1/1	0.98	0.04	36,36,36,36	0
57	MG	1A	3793	1/1	0.98	0.05	20,20,20,20	0
57	MG	1A	3154	1/1	0.98	0.14	34,34,34,34	0
57	MG	1F	301	1/1	0.98	0.13	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1F	302	1/1	0.98	0.05	27,27,27,27	0
57	MG	2A	3814	1/1	0.98	0.11	51,51,51,51	0
57	MG	1A	3179	1/1	0.98	0.07	22,22,22,22	0
57	MG	1F	304	1/1	0.98	0.05	35,35,35,35	0
57	MG	1A	3560	1/1	0.98	0.08	26,26,26,26	0
57	MG	1A	3311	1/1	0.98	0.06	31,31,31,31	0
57	MG	2A	3374	1/1	0.98	0.09	67,67,67,67	0
57	MG	17	102	1/1	0.98	0.10	33,33,33,33	0
57	MG	2A	3821	1/1	0.98	0.04	40,40,40,40	0
57	MG	1A	3562	1/1	0.98	0.14	25,25,25,25	0
57	MG	1A	3563	1/1	0.98	0.28	34,34,34,34	0
57	MG	1A	3801	1/1	0.98	0.03	19,19,19,19	0
57	MG	1A	3663	1/1	0.98	0.09	38,38,38,38	0
57	MG	18	102	1/1	0.98	0.09	44,44,44,44	0
57	MG	1A	3803	1/1	0.98	0.05	47,47,47,47	0
57	MG	1A	3729	1/1	0.98	0.04	28,28,28,28	0
57	MG	1A	3879	1/1	0.98	0.05	43,43,43,43	0
57	MG	1A	3730	1/1	0.98	0.05	25,25,25,25	0
57	MG	1A	3240	1/1	0.98	0.12	29,29,29,29	0
57	MG	1A	3180	1/1	0.98	0.04	33,33,33,33	0
57	MG	1A	3039	1/1	0.98	0.21	37,37,37,37	0
57	MG	1A	3033	1/1	0.98	0.24	30,30,30,30	0
57	MG	1A	3211	1/1	0.98	0.06	38,38,38,38	0
57	MG	1A	3887	1/1	0.98	0.03	45,45,45,45	0
57	MG	1A	3278	1/1	0.98	0.16	40,40,40,40	0
57	MG	2A	3841	1/1	0.98	0.06	24,24,24,24	0
57	MG	1A	3671	1/1	0.98	0.07	30,30,30,30	0
57	MG	1A	3619	1/1	0.98	0.09	32,32,32,32	0
57	MG	1A	3279	1/1	0.98	0.12	29,29,29,29	0
57	MG	1A	3012	1/1	0.98	0.05	32,32,32,32	0
57	MG	1A	3676	1/1	0.98	0.05	31,31,31,31	0
57	MG	1A	3213	1/1	0.98	0.19	34,34,34,34	0
57	MG	1A	4078	1/1	0.98	0.07	15,15,15,15	0
57	MG	1A	3123	1/1	0.98	0.14	34,34,34,34	0
57	MG	1P	201	1/1	0.98	0.15	31,31,31,31	0
57	MG	1a	1617	1/1	0.98	0.07	41,41,41,41	0
57	MG	2a	1668	1/1	0.98	0.17	55,55,55,55	0
57	MG	1a	1731	1/1	0.98	0.09	55,55,55,55	0
57	MG	2A	3854	1/1	0.98	0.04	61,61,61,61	0
57	MG	1a	1732	1/1	0.98	0.08	49,49,49,49	0
57	MG	1A	3624	1/1	0.98	0.08	25,25,25,25	0
57	MG	2A	3137	1/1	0.98	0.13	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3625	1/1	0.98	0.06	54,54,54,54	0
57	MG	1A	4084	1/1	0.98	0.07	40,40,40,40	0
57	MG	1A	3160	1/1	0.98	0.09	30,30,30,30	0
57	MG	2A	3009	1/1	0.98	0.12	49,49,49,49	0
57	MG	1A	3822	1/1	0.98	0.04	29,29,29,29	0
57	MG	1A	3249	1/1	0.98	0.31	35,35,35,35	0
57	MG	1A	3824	1/1	0.98	0.14	40,40,40,40	0
57	MG	1A	3749	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	3903	1/1	0.98	0.21	22,22,22,22	0
57	MG	2A	3554	1/1	0.98	0.11	39,39,39,39	0
57	MG	1Q	206	1/1	0.98	0.20	40,40,40,40	0
57	MG	1A	3750	1/1	0.98	0.04	49,49,49,49	0
57	MG	1A	3751	1/1	0.98	0.06	23,23,23,23	0
57	MG	1A	3161	1/1	0.98	0.12	30,30,30,30	0
57	MG	2A	3707	1/1	0.98	0.06	64,64,64,64	0
57	MG	2A	3284	1/1	0.98	0.10	49,49,49,49	0
57	MG	2A	3560	1/1	0.98	0.08	44,44,44,44	0
57	MG	1R	203	1/1	0.98	0.28	38,38,38,38	0
57	MG	1A	3685	1/1	0.98	0.05	30,30,30,30	0
57	MG	2A	3021	1/1	0.98	0.06	29,29,29,29	0
57	MG	1a	1749	1/1	0.98	0.12	37,37,37,37	0
60	ZN	1n	103	1/1	0.98	0.04	71,71,71,71	0
57	MG	2A	3714	1/1	0.98	0.09	47,47,47,47	0
57	MG	1a	1750	1/1	0.98	0.07	43,43,43,43	0
60	ZN	26	102	1/1	0.98	0.04	60,60,60,60	0
57	MG	1A	3325	1/1	0.98	0.05	52,52,52,52	0
61	SF4	1d	501	8/8	0.98	0.05	62,70,75,80	0
61	SF4	2d	303	8/8	0.98	0.05	71,81,85,99	0
57	MG	1A	4008	1/1	0.99	0.03	32,32,32,32	0
57	MG	1A	4091	1/1	0.99	0.06	46,46,46,46	0
57	MG	1A	3705	1/1	0.99	0.04	33,33,33,33	0
57	MG	1A	3939	1/1	0.99	0.06	37,37,37,37	0
57	MG	1A	3760	1/1	0.99	0.03	37,37,37,37	0
57	MG	1A	3906	1/1	0.99	0.07	38,38,38,38	0
57	MG	1A	3615	1/1	0.99	0.07	31,31,31,31	0
57	MG	1A	3080	1/1	0.99	0.12	44,44,44,44	0
57	MG	1A	3070	1/1	0.99	0.06	20,20,20,20	0
57	MG	1a	1813	1/1	0.99	0.03	61,61,61,61	0
57	MG	1a	1814	1/1	0.99	0.03	69,69,69,69	0
57	MG	1A	3683	1/1	0.99	0.02	30,30,30,30	0
57	MG	1A	3071	1/1	0.99	0.18	30,30,30,30	0
57	MG	2A	3673	1/1	0.99	0.03	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4018	1/1	0.99	0.03	32,32,32,32	0
57	MG	1X	107	1/1	0.99	0.04	29,29,29,29	0
57	MG	1A	3912	1/1	0.99	0.05	28,28,28,28	0
57	MG	1a	1762	1/1	0.99	0.03	46,46,46,46	0
57	MG	1a	1607	1/1	0.99	0.06	51,51,51,51	0
57	MG	1E	303	1/1	0.99	0.18	31,31,31,31	0
57	MG	2A	3811	1/1	0.99	0.03	50,50,50,50	0
57	MG	1A	3948	1/1	0.99	0.03	40,40,40,40	0
57	MG	2A	3022	1/1	0.99	0.10	43,43,43,43	0
57	MG	1A	3283	1/1	0.99	0.15	31,31,31,31	0
57	MG	1a	1767	1/1	0.99	0.04	55,55,55,55	0
57	MG	1A	3686	1/1	0.99	0.07	26,26,26,26	0
57	MG	1A	3057	1/1	0.99	0.06	26,26,26,26	0
57	MG	1A	3353	1/1	0.99	0.09	36,36,36,36	0
57	MG	1A	3037	1/1	0.99	0.04	20,20,20,20	0
57	MG	1A	3799	1/1	0.99	0.03	46,46,46,46	0
57	MG	2A	3626	1/1	0.99	0.07	43,43,43,43	0
57	MG	1A	3176	1/1	0.99	0.10	31,31,31,31	0
57	MG	2A	3504	1/1	0.99	0.02	57,57,57,57	0
57	MG	1B	215	1/1	0.99	0.04	43,43,43,43	0
57	MG	2A	3826	1/1	0.99	0.07	46,46,46,46	0
57	MG	2a	1759	1/1	0.99	0.07	61,61,61,61	0
57	MG	1A	3021	1/1	0.99	0.12	27,27,27,27	0
57	MG	1A	3097	1/1	0.99	0.05	32,32,32,32	0
57	MG	1A	3098	1/1	0.99	0.12	20,20,20,20	0
57	MG	1A	3669	1/1	0.99	0.05	39,39,39,39	0
57	MG	1A	3015	1/1	0.99	0.05	36,36,36,36	0
57	MG	1A	3587	1/1	0.99	0.04	43,43,43,43	0
57	MG	1a	1781	1/1	0.99	0.05	46,46,46,46	0
57	MG	2A	3834	1/1	0.99	0.07	33,33,33,33	0
57	MG	1A	3396	1/1	0.99	0.29	34,34,34,34	0
57	MG	1A	3003	1/1	0.99	0.03	29,29,29,29	0
57	MG	1U	201	1/1	0.99	0.13	31,31,31,31	0
57	MG	1F	309	1/1	0.99	0.16	30,30,30,30	0
57	MG	1A	3077	1/1	0.99	0.06	31,31,31,31	0
57	MG	2a	1773	1/1	0.99	0.06	63,63,63,63	0
57	MG	1A	3014	1/1	0.99	0.09	28,28,28,28	0
57	MG	2A	3519	1/1	0.99	0.06	49,49,49,49	0
57	MG	1A	3701	1/1	0.99	0.03	17,17,17,17	0
57	MG	2A	3843	1/1	0.99	0.03	58,58,58,58	0
57	MG	1B	227	1/1	0.99	0.04	39,39,39,39	0
57	MG	1A	4079	1/1	0.99	0.06	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4080	1/1	0.99	0.08	31,31,31,31	0
57	MG	1A	4039	1/1	0.99	0.03	46,46,46,46	0
57	MG	1A	3931	1/1	0.99	0.02	45,45,45,45	0
57	MG	1A	3229	1/1	0.99	0.10	31,31,31,31	0
57	MG	1A	4042	1/1	0.99	0.05	43,43,43,43	0
57	MG	2A	3715	1/1	0.99	0.04	32,32,32,32	0
57	MG	2A	3782	1/1	0.99	0.04	55,55,55,55	0
60	ZN	1Y	204	1/1	0.99	0.02	60,60,60,60	0
57	MG	1a	1740	1/1	0.99	0.06	61,61,61,61	0
60	ZN	16	103	1/1	0.99	0.07	53,53,53,53	0
60	ZN	19	102	1/1	0.99	0.04	44,44,44,44	0
57	MG	1a	1797	1/1	0.99	0.06	54,54,54,54	0
57	MG	1A	4043	1/1	0.99	0.03	25,25,25,25	0
57	MG	1V	204	1/1	0.99	0.10	29,29,29,29	0
60	ZN	25	106	1/1	0.99	0.05	62,62,62,62	0
57	MG	1A	3069	1/1	0.99	0.11	25,25,25,25	0
60	ZN	29	501	1/1	0.99	0.04	68,68,68,68	0
57	MG	1A	3934	1/1	0.99	0.06	61,61,61,61	0
57	MG	1A	3156	1/1	0.99	0.13	26,26,26,26	0
57	MG	1A	3758	1/1	0.99	0.07	47,47,47,47	0
57	MG	1A	3883	1/1	1.00	0.06	33,33,33,33	0
57	MG	2A	3723	1/1	1.00	0.04	46,46,46,46	0
57	MG	1A	3935	1/1	1.00	0.05	28,28,28,28	0
57	MG	2A	3781	1/1	1.00	0.06	64,64,64,64	0
57	MG	2A	3822	1/1	1.00	0.06	41,41,41,41	0
57	MG	1A	3674	1/1	1.00	0.05	24,24,24,24	0
57	MG	1A	3738	1/1	1.00	0.05	49,49,49,49	0
57	MG	1a	1758	1/1	1.00	0.05	34,34,34,34	0
60	ZN	15	107	1/1	1.00	0.05	43,43,43,43	0
57	MG	2A	3595	1/1	1.00	0.04	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.