



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 05:54 am BST

PDB ID : 5V8I
Title : Thermus thermophilus 70S ribosome lacking ribosomal protein uS17
Authors : Gregory, S.T.; Jogl, G.
Deposited on : 2017-03-22
Resolution : 3.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

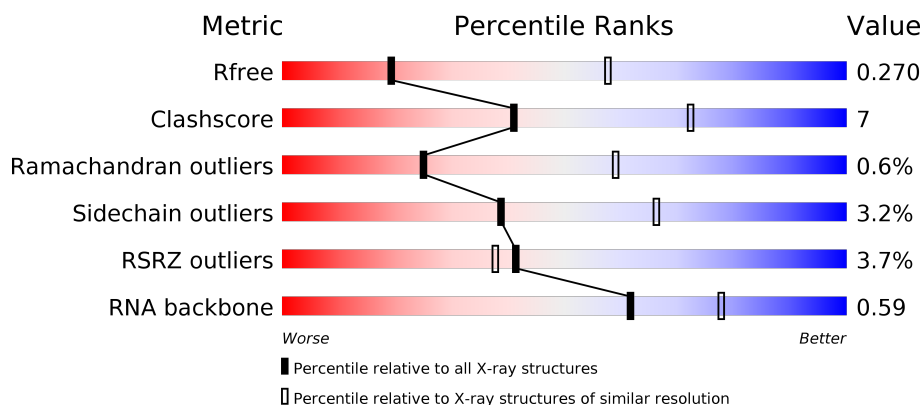
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

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

















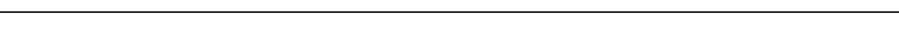

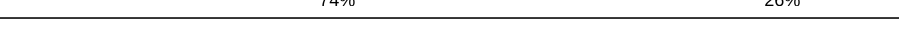

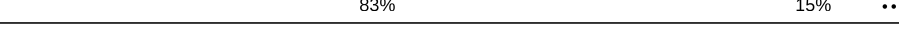






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)
RNA backbone	3102	1072 (3.62-2.90)

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

Mol	Chain	Length	Quality of chain
1	1A	2894	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>29%</div> <div>5%</div> </div> </div>
1	2A	2894	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>31%</div> <div>6%</div> </div> </div>
2	1B	120	<div> <div></div> <div> <div>81%</div> <div>16%</div> </div> </div>
2	2B	120	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>28%</div> </div> </div>


























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



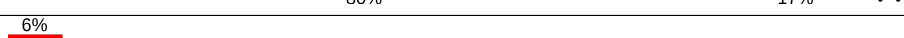



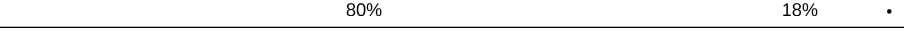


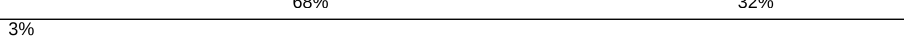


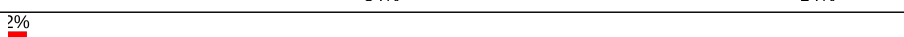



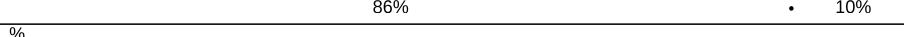



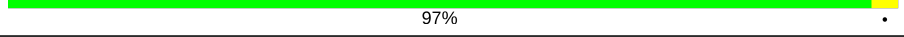
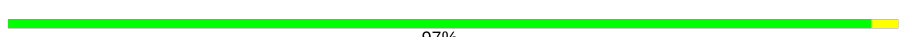



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Mol	Chain	Length	Quality of chain
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25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

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Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1522	
32	2a	1522	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

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Mol	Chain	Length	Quality of chain
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	135	
43	2l	135	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1r	88	
48	2r	88	
49	1s	93	
49	2s	93	
50	1t	106	
50	2t	106	
51	1u	27	
51	2u	27	
52	1y	113	
52	2y	113	

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
53	MPD	2A	3002	-	-	-	X
53	MPD	2B	201	-	-	-	X
54	MG	10	106	-	-	-	X
54	MG	19	103	-	-	-	X
54	MG	1A	3028	-	-	-	X
54	MG	1A	3030	-	-	-	X
54	MG	1A	3170	-	-	-	X
54	MG	1A	3211	-	-	-	X
54	MG	1A	3227	-	-	-	X
54	MG	1A	3260	-	-	-	X
54	MG	1A	3562	-	-	-	X
54	MG	1A	3600	-	-	-	X
54	MG	1A	3608	-	-	-	X
54	MG	1A	3637	-	-	-	X
54	MG	1A	3720	-	-	-	X
54	MG	1A	3732	-	-	-	X
54	MG	1A	3806	-	-	-	X
54	MG	1A	3834	-	-	-	X
54	MG	1A	3850	-	-	-	X
54	MG	1A	3879	-	-	-	X
54	MG	1B	1017	-	-	-	X
54	MG	1F	311	-	-	-	X
54	MG	1P	205	-	-	-	X
54	MG	1a	1650	-	-	-	X
54	MG	1a	1663	-	-	-	X
54	MG	1a	1665	-	-	-	X
54	MG	1a	1668	-	-	-	X
54	MG	1a	1694	-	-	-	X
54	MG	1a	1709	-	-	-	X
54	MG	1a	1734	-	-	-	X
54	MG	1a	1789	-	-	-	X
54	MG	1a	1821	-	-	-	X
54	MG	1a	1822	-	-	-	X
54	MG	1a	1839	-	-	-	X
54	MG	1a	1843	-	-	-	X
54	MG	1d	502	-	-	-	X
54	MG	1e	202	-	-	-	X
54	MG	1e	203	-	-	-	X
54	MG	1y	204	-	-	-	X
54	MG	23	101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	2A	3022	-	-	-	X
54	MG	2A	3045	-	-	-	X
54	MG	2A	3055	-	-	-	X
54	MG	2A	3058	-	-	-	X
54	MG	2A	3071	-	-	-	X
54	MG	2A	3075	-	-	-	X
54	MG	2A	3077	-	-	-	X
54	MG	2A	3086	-	-	-	X
54	MG	2A	3087	-	-	-	X
54	MG	2A	3105	-	-	-	X
54	MG	2A	3114	-	-	-	X
54	MG	2A	3138	-	-	-	X
54	MG	2A	3151	-	-	-	X
54	MG	2A	3183	-	-	-	X
54	MG	2A	3187	-	-	-	X
54	MG	2A	3202	-	-	-	X
54	MG	2A	3207	-	-	-	X
54	MG	2A	3209	-	-	-	X
54	MG	2A	3213	-	-	-	X
54	MG	2A	3230	-	-	-	X
54	MG	2A	3301	-	-	-	X
54	MG	2A	3317	-	-	-	X
54	MG	2A	3452	-	-	-	X
54	MG	2A	3488	-	-	-	X
54	MG	2A	3565	-	-	-	X
54	MG	2A	3615	-	-	-	X
54	MG	2A	3630	-	-	-	X
54	MG	2B	204	-	-	-	X
54	MG	2B	205	-	-	-	X
54	MG	2B	211	-	-	-	X
54	MG	2a	1608	-	-	-	X
54	MG	2a	1617	-	-	-	X
54	MG	2a	1655	-	-	-	X
54	MG	2a	1658	-	-	-	X
54	MG	2a	1659	-	-	-	X
54	MG	2a	1663	-	-	-	X
54	MG	2a	1664	-	-	-	X
54	MG	2a	1670	-	-	-	X
54	MG	2a	1675	-	-	-	X
54	MG	2a	1690	-	-	-	X
54	MG	2a	1701	-	-	-	X
54	MG	2i	201	-	-	-	X

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 290709 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	2862	Total	C	N	O	P	0	0	0
			61654	27444	11530	19819	2861			
1	2A	2858	Total	C	N	O	P	0	0	0
			61564	27404	11511	19793	2856			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	118	Total	C	N	O	P	0	0	0
			2536	1128	471	819	118			
2	2B	118	Total	C	N	O	P	0	0	0
			2536	1128	471	819	118			

- 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
			2131	1346	422	360	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	203	Total	C	N	O	S	0	0	1
			1586	1011	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1582	1009	297	274	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1427	917	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1425	913	259	249	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	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1095	700	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1077	688	186	202	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
			1121	722	208	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
			932	587	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
			932	587	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
			1121	715	212	187	7			
12	2Q	141	Total	C	N	O	S	0	0	0
			1121	715	212	187	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
			877	553	175	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	681	225	184	1			
15	2T	131	Total	C	N	O	S	0	0	0
			1083	676	224	182	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
			775	498	141	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
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			606	375	127	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			606	375	127	103	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
			756	475	150	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			761	478	151	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
			592	368	119	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
			546	346	96	99	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			536	342	98	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
			460	290	90	75	5			
27	25	59	Total	C	N	O	S	0	0	0
			456	287	89	75	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
			32249	14359	5977	10413	1500			
32	2a	1504	Total	C	N	O	P	0	0	0
			32334	14397	5992	10441	1504			

- 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
			1842	1175	330	332	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
			1558	979	305	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
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	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
			1133	716	214	199	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
			814	516	144	151	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
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	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
			1098	694	210	192	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
			987	625	194	168			
40	2i	126	Total	C	N	O	0	0	0
			967	613	187	167			

- 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
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	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
			834	520	156	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	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	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 S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	1r	68	Total	C	N	O	0	0	0
			555	355	108	92			
48	2r	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	1s	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
49	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1t	96	Total	C	N	O	S	0	0	0
			731	448	157	124	2			
50	2t	98	Total	C	N	O	S	0	0	0
			732	450	154	126	2			

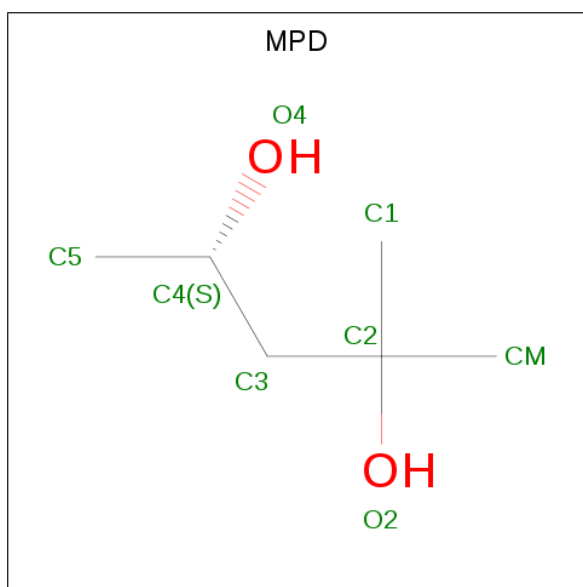
- Molecule 51 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
51	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 52 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	1y	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
52	2y	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			

- Molecule 53 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
53	1A	1	Total C O 8 6 2	0	0
53	1T	1	Total C O 8 6 2	0	0
53	18	1	Total C O 8 6 2	0	0
53	1a	1	Total C O 8 6 2	0	0
53	2A	1	Total C O 8 6 2	0	0
53	2A	1	Total C O 8 6 2	0	0
53	2B	1	Total C O 8 6 2	0	0

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	2E	2	Total Mg 2 2	0	0
54	17	3	Total Mg 3 3	0	0
54	1T	5	Total Mg 5 5	0	0
54	1N	3	Total Mg 3 3	0	0
54	20	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1o	1	Total 1	Mg 1	0	0
54	2W	2	Total 2	Mg 2	0	0
54	2I	1	Total 1	Mg 1	0	0
54	13	2	Total 2	Mg 2	0	0
54	1f	2	Total 2	Mg 2	0	0
54	1P	5	Total 5	Mg 5	0	0
54	2B	16	Total 16	Mg 16	0	0
54	2a	164	Total 164	Mg 164	0	0
54	1E	5	Total 5	Mg 5	0	0
54	1b	1	Total 1	Mg 1	0	0
54	2l	2	Total 2	Mg 2	0	0
54	2F	2	Total 2	Mg 2	0	0
54	16	1	Total 1	Mg 1	0	0
54	28	1	Total 1	Mg 1	0	0
54	2e	1	Total 1	Mg 1	0	0
54	1W	4	Total 4	Mg 4	0	0
54	1A	900	Total 900	Mg 900	0	0
54	1t	2	Total 2	Mg 2	0	0
54	2p	1	Total 1	Mg 1	0	0
54	1n	2	Total 2	Mg 2	0	0
54	2P	2	Total 2	Mg 2	0	0

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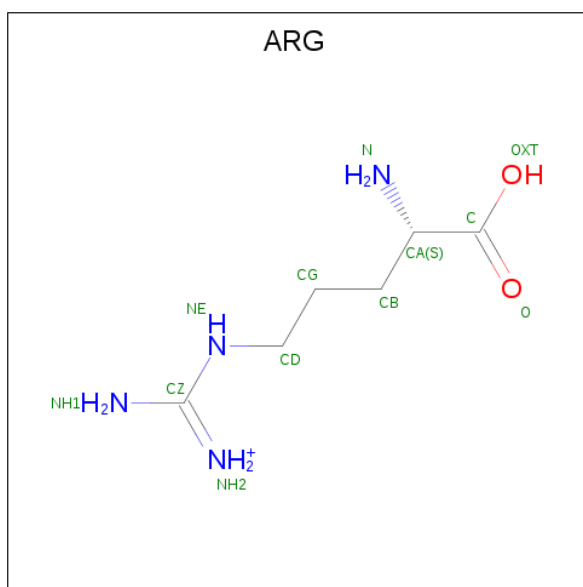
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1X	2	Total 2	Mg 2	0	0
54	1y	4	Total 4	Mg 4	0	0
54	2i	1	Total 1	Mg 1	0	0
54	2T	5	Total 5	Mg 5	0	0
54	1D	12	Total 12	Mg 12	0	0
54	1e	3	Total 3	Mg 3	0	0
54	2G	3	Total 3	Mg 3	0	0
54	2f	1	Total 1	Mg 1	0	0
54	1V	3	Total 3	Mg 3	0	0
54	2X	1	Total 1	Mg 1	0	0
54	1a	257	Total 257	Mg 257	0	0
54	2Q	2	Total 2	Mg 2	0	0
54	15	3	Total 3	Mg 3	0	0
54	2j	1	Total 1	Mg 1	0	0
54	1R	7	Total 7	Mg 7	0	0
54	1G	4	Total 4	Mg 4	0	0
54	2O	2	Total 2	Mg 2	0	0
54	11	4	Total 4	Mg 4	0	0
54	1d	6	Total 6	Mg 6	0	0
54	1H	2	Total 2	Mg 2	0	0
54	21	4	Total 4	Mg 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	2Y	1	Total 1	Mg 1	0	0
54	23	1	Total 1	Mg 1	0	0
54	2R	3	Total 3	Mg 3	0	0
54	1Z	1	Total 1	Mg 1	0	0
54	2D	6	Total 6	Mg 6	0	0
54	2k	1	Total 1	Mg 1	0	0
54	1U	3	Total 3	Mg 3	0	0
54	1O	1	Total 1	Mg 1	0	0
54	19	2	Total 2	Mg 2	0	0
54	1l	2	Total 2	Mg 2	0	0
54	2V	1	Total 1	Mg 1	0	0
54	1F	12	Total 12	Mg 12	0	0
54	10	6	Total 6	Mg 6	0	0
54	1g	3	Total 3	Mg 3	0	0
54	2t	1	Total 1	Mg 1	0	0
54	1Q	3	Total 3	Mg 3	0	0
54	2A	641	Total 641	Mg 641	0	0
54	1h	1	Total 1	Mg 1	0	0
54	1B	29	Total 29	Mg 29	0	0

- Molecule 55 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	1B	1	Total	C	N	O	0	0
			12	6	4	2		
55	1F	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

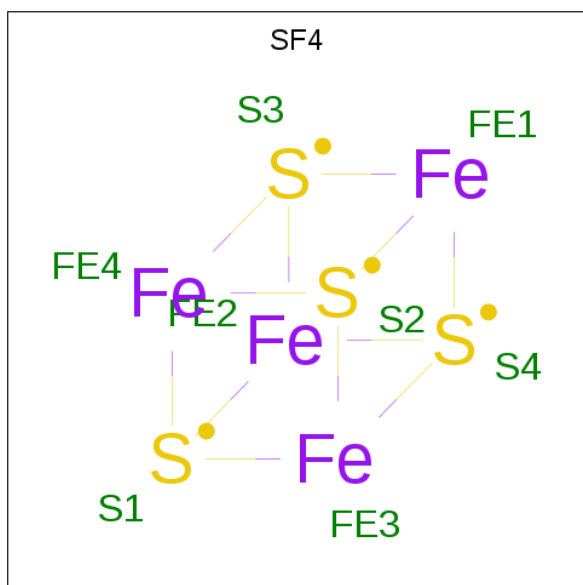
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1Y	1	Total	Zn	0	0
			1	1		
56	14	1	Total	Zn	0	0
			1	1		
56	1n	1	Total	Zn	0	0
			1	1		
56	15	1	Total	Zn	0	0
			1	1		
56	29	1	Total	Zn	0	0
			1	1		
56	19	1	Total	Zn	0	0
			1	1		
56	26	1	Total	Zn	0	0
			1	1		
56	25	1	Total	Zn	0	0
			1	1		
56	24	1	Total	Zn	0	0
			1	1		
56	2n	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2Y	1	Total	Zn	0	0
			1	1		
56	16	1	Total	Zn	0	0
			1	1		

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	1d	1	Total	Fe	S	0	0
			8	4	4		
57	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1A	1801	Total	O	0	0
			1801	1801		
58	1B	56	Total	O	0	0
			56	56		
58	1D	14	Total	O	0	0
			14	14		
58	1E	17	Total	O	0	0
			17	17		
58	1F	16	Total	O	0	0
			16	16		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1G	5	Total 5	O 5	0	0
58	1H	5	Total 5	O 5	0	0
58	1N	7	Total 7	O 7	0	0
58	1O	2	Total 2	O 2	0	0
58	1P	17	Total 17	O 17	0	0
58	1Q	5	Total 5	O 5	0	0
58	1R	5	Total 5	O 5	0	0
58	1T	8	Total 8	O 8	0	0
58	1U	6	Total 6	O 6	0	0
58	1V	5	Total 5	O 5	0	0
58	1W	2	Total 2	O 2	0	0
58	1X	6	Total 6	O 6	0	0
58	1Y	1	Total 1	O 1	0	0
58	1Z	1	Total 1	O 1	0	0
58	10	5	Total 5	O 5	0	0
58	11	3	Total 3	O 3	0	0
58	13	6	Total 6	O 6	0	0
58	15	3	Total 3	O 3	0	0
58	16	2	Total 2	O 2	0	0
58	17	1	Total 1	O 1	0	0
58	18	7	Total 7	O 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	19	3	Total 3	O 3	0	0
58	1a	424	Total 424	O 424	0	0
58	1c	1	Total 1	O 1	0	0
58	1d	8	Total 8	O 8	0	0
58	1e	4	Total 4	O 4	0	0
58	1f	1	Total 1	O 1	0	0
58	1h	1	Total 1	O 1	0	0
58	1j	1	Total 1	O 1	0	0
58	1l	3	Total 3	O 3	0	0
58	1m	1	Total 1	O 1	0	0
58	1o	3	Total 3	O 3	0	0
58	1p	1	Total 1	O 1	0	0
58	1t	2	Total 2	O 2	0	0
58	1y	3	Total 3	O 3	0	0
58	2A	1310	Total 1310	O 1310	0	0
58	2B	32	Total 32	O 32	0	0
58	2D	16	Total 16	O 16	0	0
58	2E	10	Total 10	O 10	0	0
58	2F	6	Total 6	O 6	0	0
58	2G	1	Total 1	O 1	0	0
58	2N	1	Total 1	O 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2O	3	Total 3	O 3	0	0
58	2P	14	Total 14	O 14	0	0
58	2Q	5	Total 5	O 5	0	0
58	2R	1	Total 1	O 1	0	0
58	2T	4	Total 4	O 4	0	0
58	2V	2	Total 2	O 2	0	0
58	2W	3	Total 3	O 3	0	0
58	2X	4	Total 4	O 4	0	0
58	2Y	1	Total 1	O 1	0	0
58	20	2	Total 2	O 2	0	0
58	21	1	Total 1	O 1	0	0
58	23	2	Total 2	O 2	0	0
58	25	1	Total 1	O 1	0	0
58	26	1	Total 1	O 1	0	0
58	27	2	Total 2	O 2	0	0
58	28	5	Total 5	O 5	0	0
58	2a	282	Total 282	O 282	0	0
58	2e	1	Total 1	O 1	0	0
58	2j	2	Total 2	O 2	0	0
58	2l	1	Total 1	O 1	0	0
58	2t	2	Total 2	O 2	0	0

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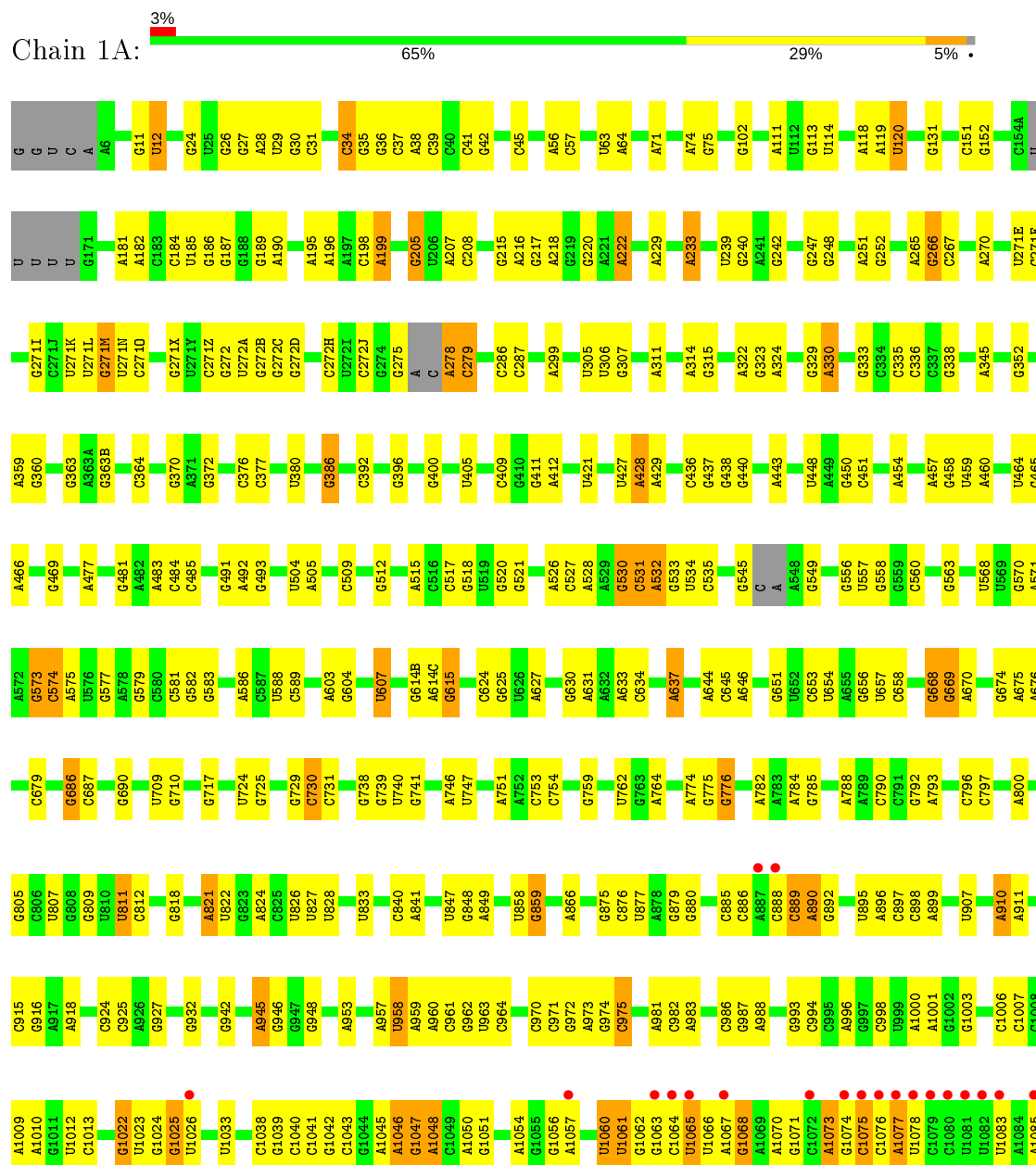
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2y	3	Total	O	0	0
			3	3		

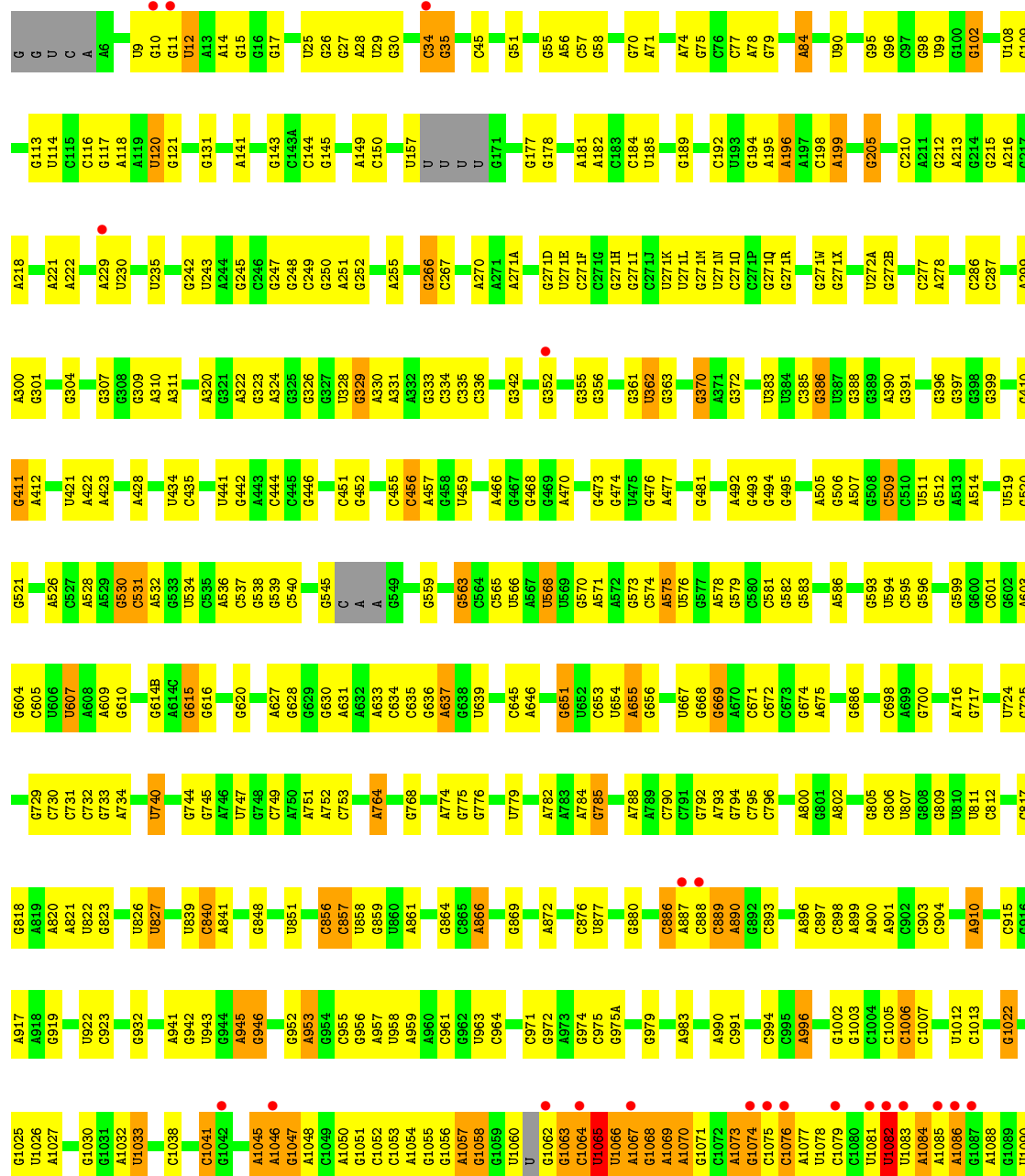
3 Residue-property plots

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

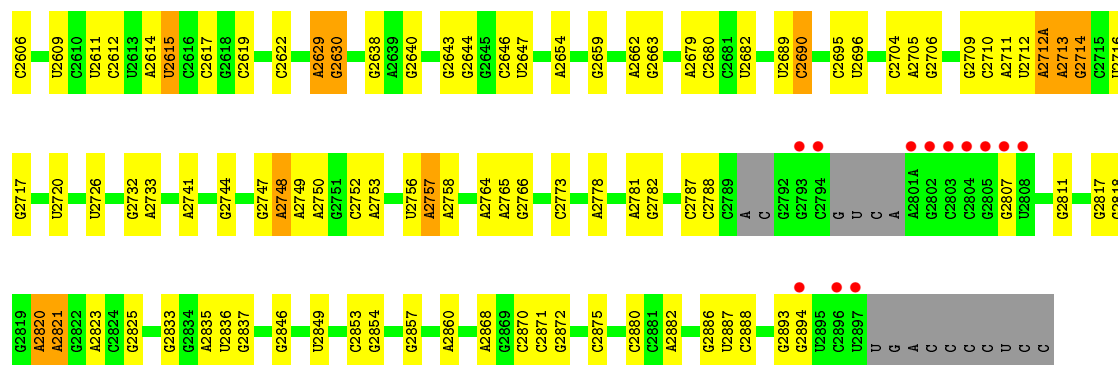
• Molecule 1: 23S Ribosomal RNA



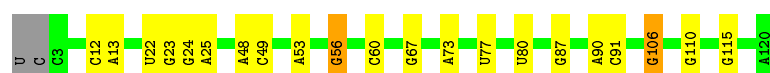
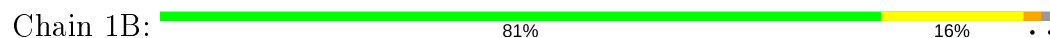
G2550	G2428	C2326	A2208	C2136	G1929	U1796	C1648	A1507	C1411	A1286	G1176	A1086
G2551	G2429	A2327	A2225	C2137	G1930	C1797	C1649	A1508	G1416	A1287	A1177	G1087
U2552	A2430	A2328	A2226	C2138	G1935	U1798	G1651	A1509	G1417	A1288	C1178	A1088
G2553	A2431	G2329	G2226	C2139	G1936	G1799	A1652	A1509A	C1417	U1292	C1179	G1089
U2554	A2432	G2330	A2227	G2140	A1936	G1800	G1653	U1512	U1420	C1293	G1185	U1090
A2564	A2435	G2337	G2228	G2141	A1937	G1801	A1654	C1513	G1421	G1299	G1186	G1091
A2565	A2436	U2333	G2229	C2142	A1938	A1802	A1655	U1517	G1422	U1300	G1187	C1092
A2566	A2437	G2234	A2230	C2143	A1939	A1803	C1662	G1517	G1423	A1301	U1188	U1093
G2567	A2438	G2235	G2231	U2144	U1940	G1804	C1663	C1530	G1424	A1309	A1189	U1094
A2572	A2439	C2343	G2232	C2145	A1952	U1805	A1664	C1531	G1425	G1309	A1096	A1095
A2573	A2440	G2344	G2233	C2146	A1953	G1816	A1665	C1532	U1428	U1199	U1097	A1096
A2574	A2441	G2345	G2234	G2147	U1955	G1817	U1671	U1532	G1429	C1200	U1401	U1401
A2575	A2442	G2346	G2235	G2148	U1956	A1824	G1674	G	U1430	G1203	A1102	A1102
G2583	A2443	U2348	G2236	U2150	U1963	A1825	U1672	U	C1431	G1206	A1103	A1103
U2584	A2444	G2349	G2237	G2151	G1964	G1826	G1673	A	G1432	A1321	C1104	U1105
U2585	A2445	C2350	U2244	G2152	A1972	G1827	C1683	C	G1433	A1322	U1106	G1106
C2586	A2446	G2351	G2245	G2153	G1973	G1828	C1684	G1537	A1434	G1332	A1210	C1109
A2595	A2447	U2356	G2246	G2154	U1974	A1829	U1686	U1540	A1435	G1333	U1211	G1110
A2596	A2448	U2357	U2247	G2155	A1975	A1830	G1687	G1541	A1436	U1334	A1212	G1111
U2597	A2449	G2358	G2248	G2156	A1976	A1831	G1688	U1542	A1437	U1335	A1213	G1112
U2598	A2450	C2359	U2249	G2157	A1977	A1832	U1689	A1543	A1438	A1336	U1113	U1113
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A2602	A2452	G2361	G2251	G2159	G1979	A1834	U1691	G1545	A1440	A1338	G1115	G1115
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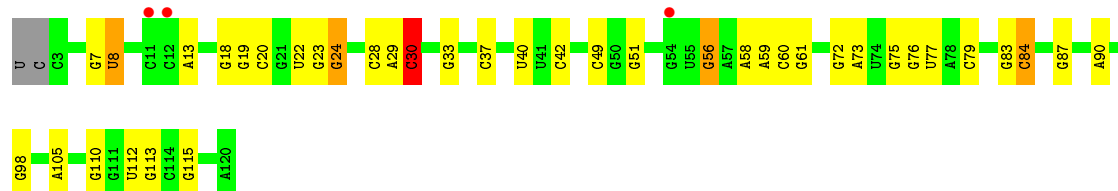
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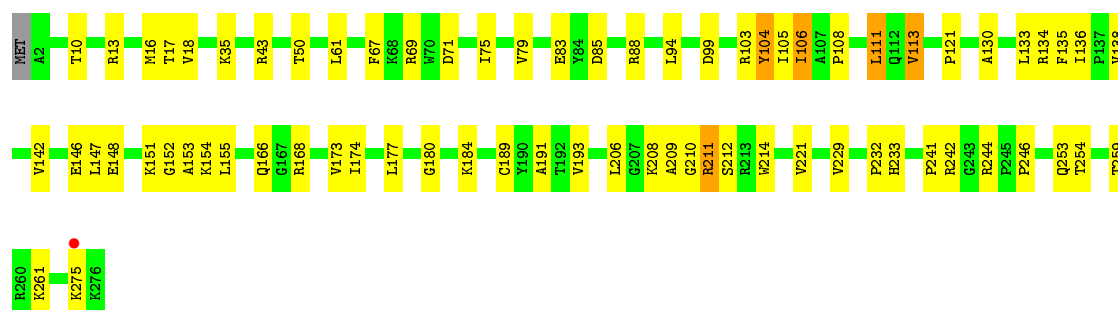
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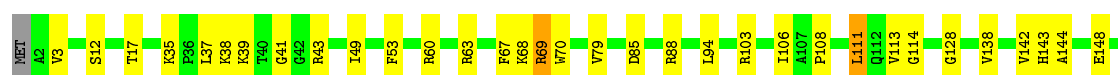
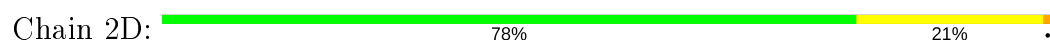
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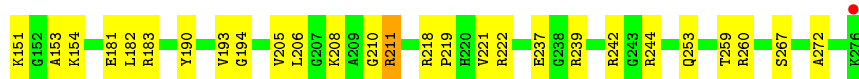


• Molecule 3: 50S ribosomal protein L2



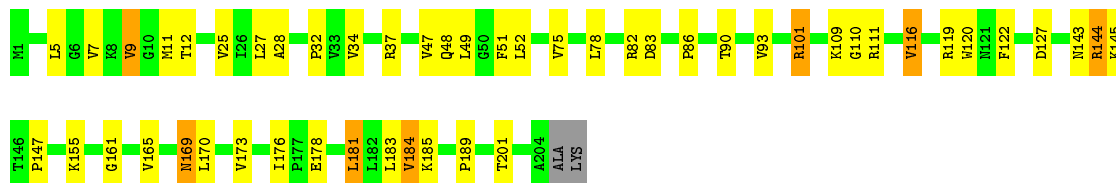
• Molecule 3: 50S ribosomal protein L2





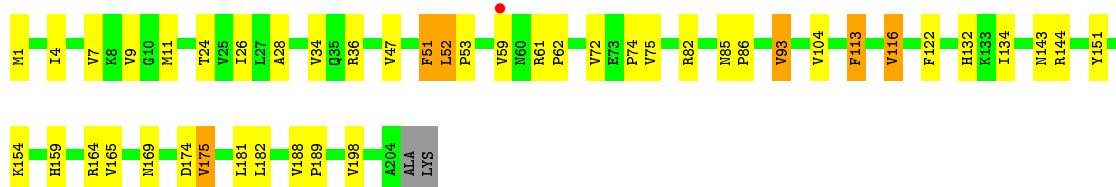
- Molecule 4: 50S ribosomal protein L3

Chain 1E: 75% 21% ..



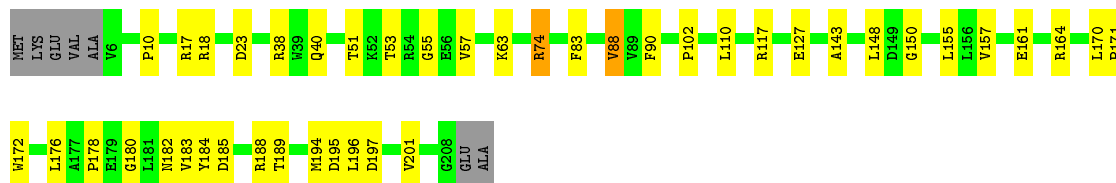
- Molecule 4: 50S ribosomal protein L3

Chain 2E: 77% 19% ..



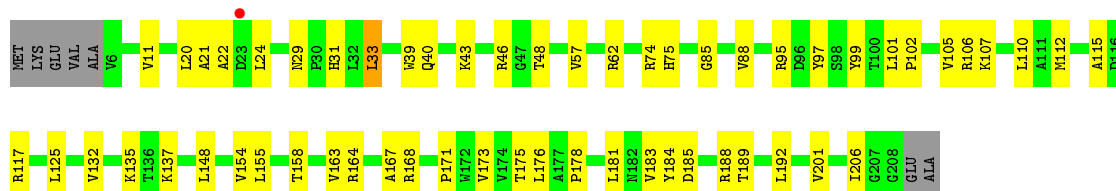
- Molecule 5: 50S ribosomal protein L4

Chain 1F: 76% 20% ..



- Molecule 5: 50S ribosomal protein L4

Chain 2F: 70% 27% .

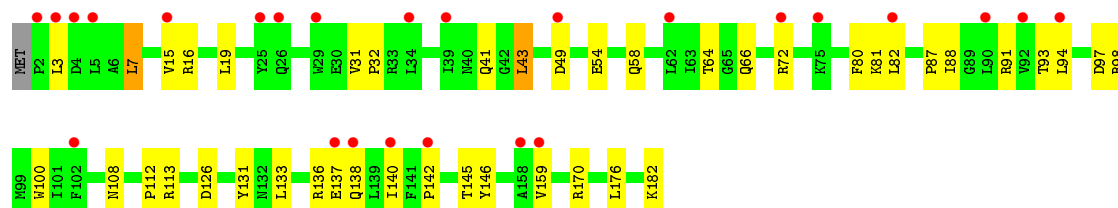
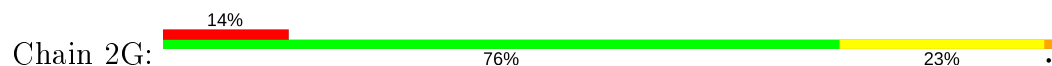


- Molecule 6: 50S ribosomal protein L5

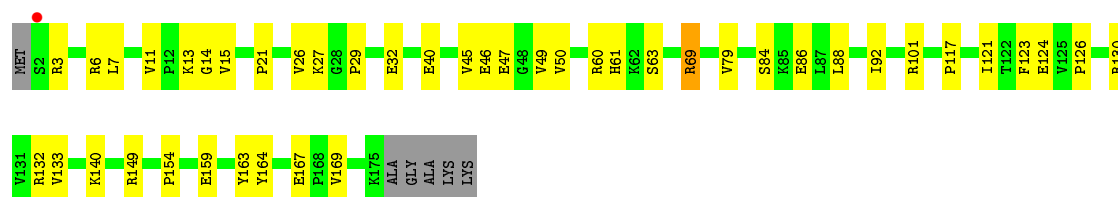
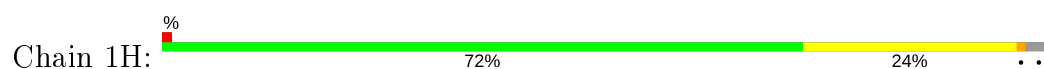
Chain 1G: 2% 76% 22% ..



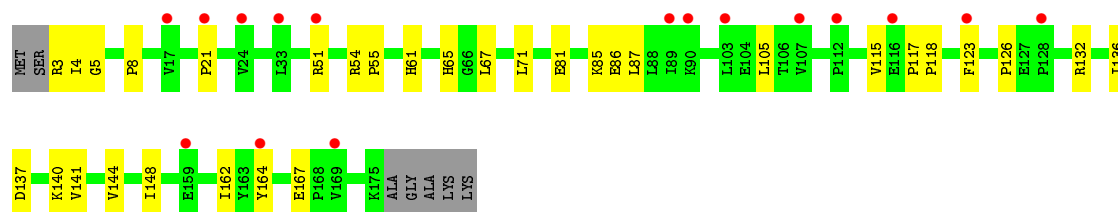
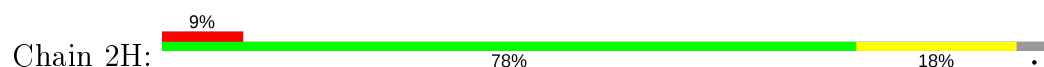
- Molecule 6: 50S ribosomal protein L5



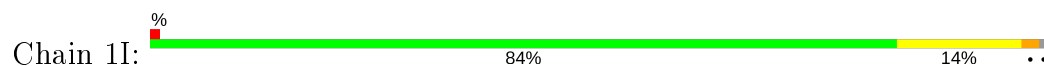
- Molecule 7: 50S ribosomal protein L6



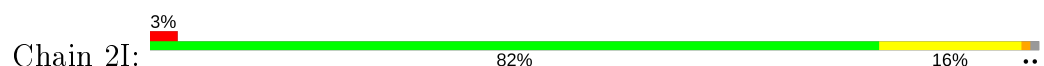
- Molecule 7: 50S ribosomal protein L6

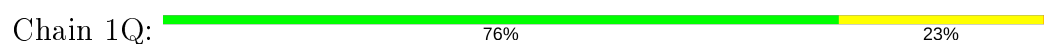


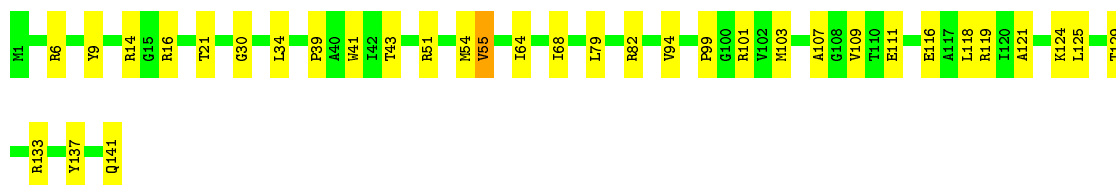
- Molecule 8: 50S ribosomal protein L9



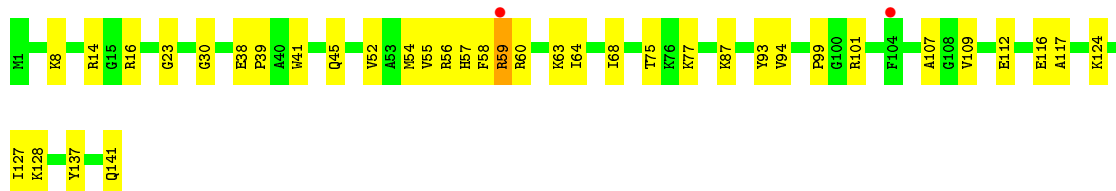
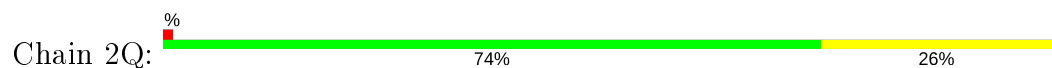
- Molecule 8: 50S ribosomal protein L9



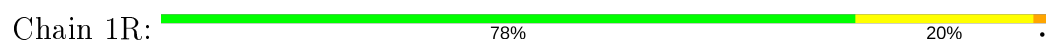




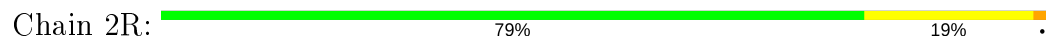
- Molecule 12: 50S ribosomal protein L16



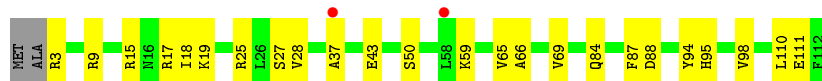
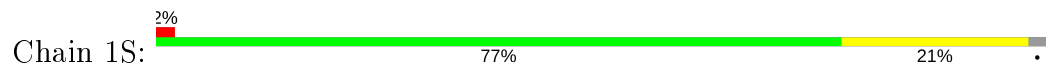
- Molecule 13: 50S ribosomal protein L17



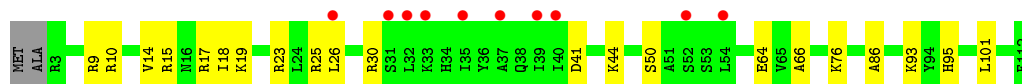
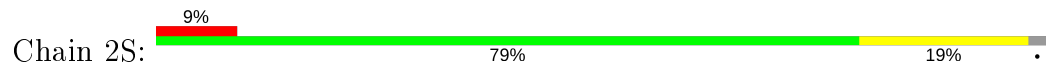
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18

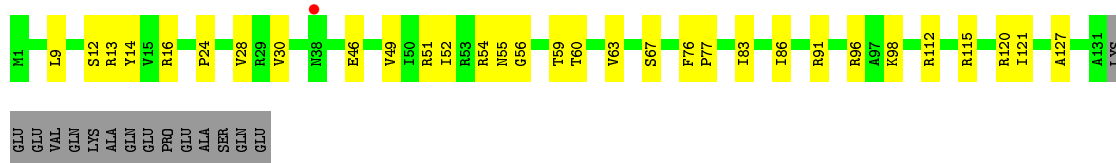


- Molecule 14: 50S ribosomal protein L18



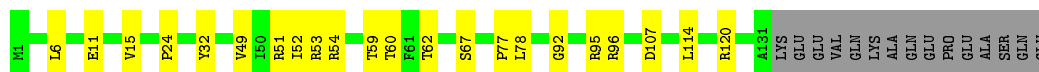
- Molecule 15: 50S ribosomal protein L19





- Molecule 15: 50S ribosomal protein L19

Chain 2T: 75% 15% 10%



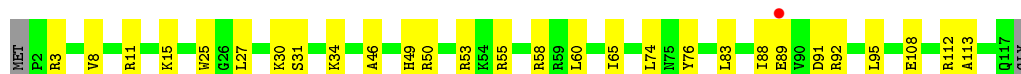
- Molecule 16: 50S ribosomal protein L20

Chain 1U: 80% 18% ..



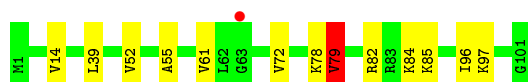
- Molecule 16: 50S ribosomal protein L20

Chain 2U: 75% 24% .



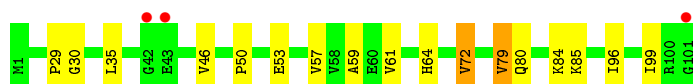
- Molecule 17: 50S ribosomal protein L21

Chain 1V: 87% 12% .



- Molecule 17: 50S ribosomal protein L21

Chain 2V: 83% 15% .

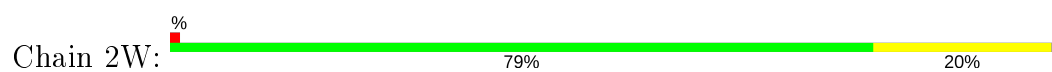


- Molecule 18: 50S ribosomal protein L22

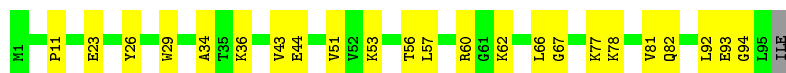
Chain 1W: 73% 24% ..



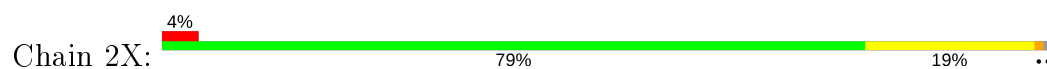
- Molecule 18: 50S ribosomal protein L22



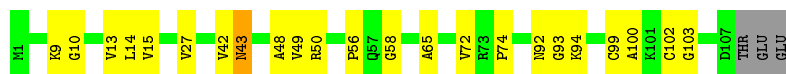
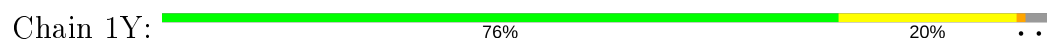
- Molecule 19: 50S ribosomal protein L23



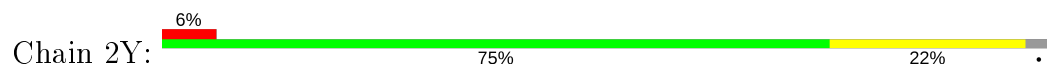
- Molecule 19: 50S ribosomal protein L23



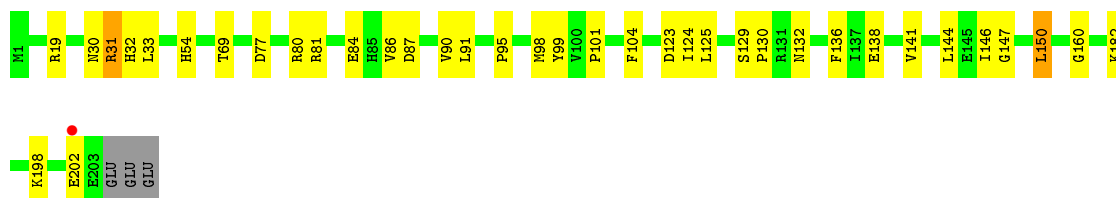
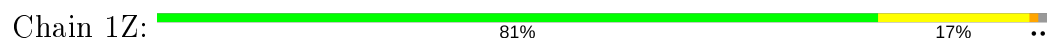
- Molecule 20: 50S ribosomal protein L24



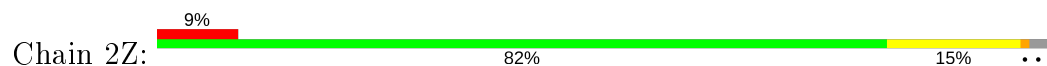
- Molecule 20: 50S ribosomal protein L24

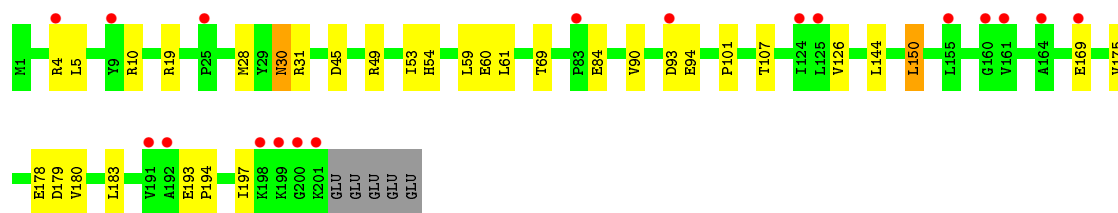


- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25





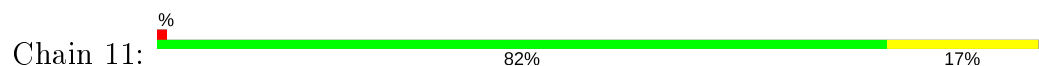
- Molecule 22: 50S ribosomal protein L27



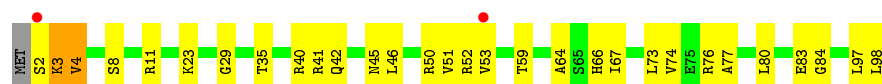
- Molecule 22: 50S ribosomal protein L27



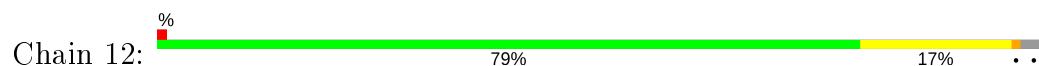
- Molecule 23: 50S ribosomal protein L28



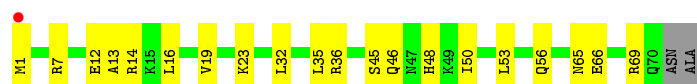
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29




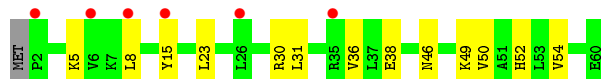
- Molecule 25: 50S ribosomal protein L30

Chain 13:  65% 32% ..



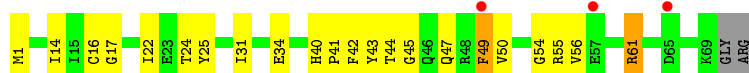
- Molecule 25: 50S ribosomal protein L30

Chain 23:  10% 77% 22% .



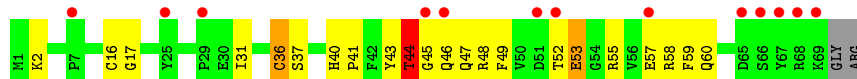
- Molecule 26: 50S ribosomal protein L31

Chain 14:  4% 66% 28% . .




- Molecule 26: 50S ribosomal protein L31

Chain 24:  18% 66% 27% . . .




- Molecule 27: 50S ribosomal protein L32

Chain 15:  77% 18% . .



- Molecule 27: 50S ribosomal protein L32

Chain 25:  80% 18% .

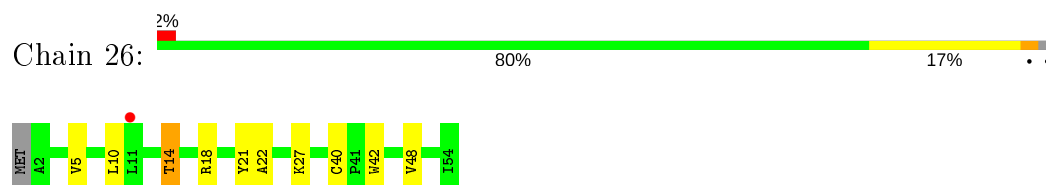


- Molecule 28: 50S ribosomal protein L33

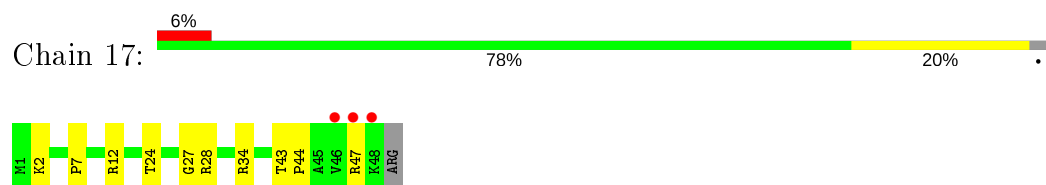
Chain 16:  72% 20% 6% .



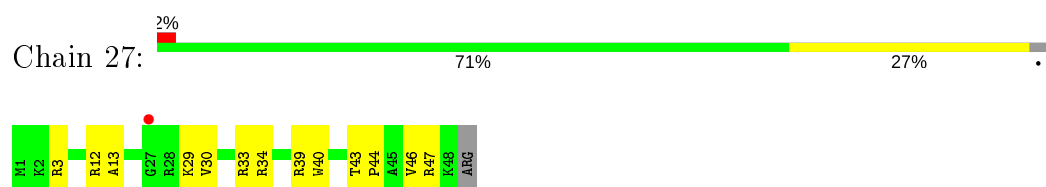
- Molecule 28: 50S ribosomal protein L33



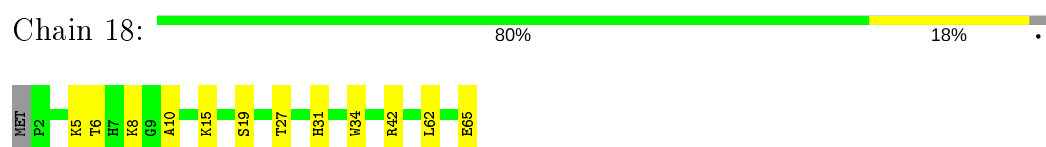
- Molecule 29: 50S ribosomal protein L34



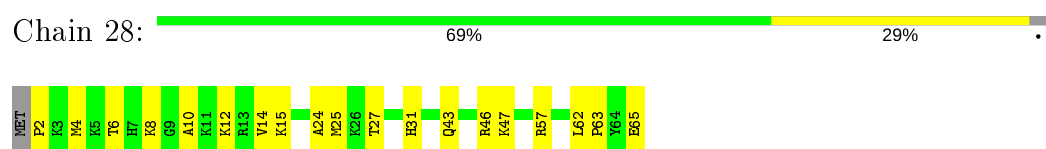
- Molecule 29: 50S ribosomal protein L34



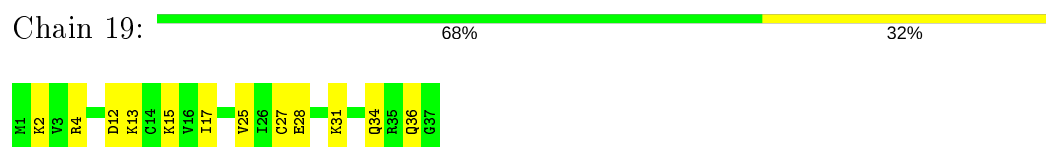
- Molecule 30: 50S ribosomal protein L35



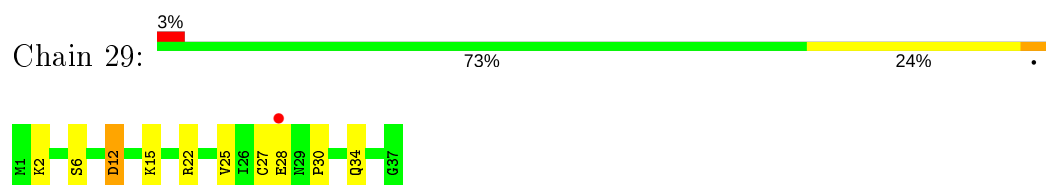
- Molecule 30: 50S ribosomal protein L35



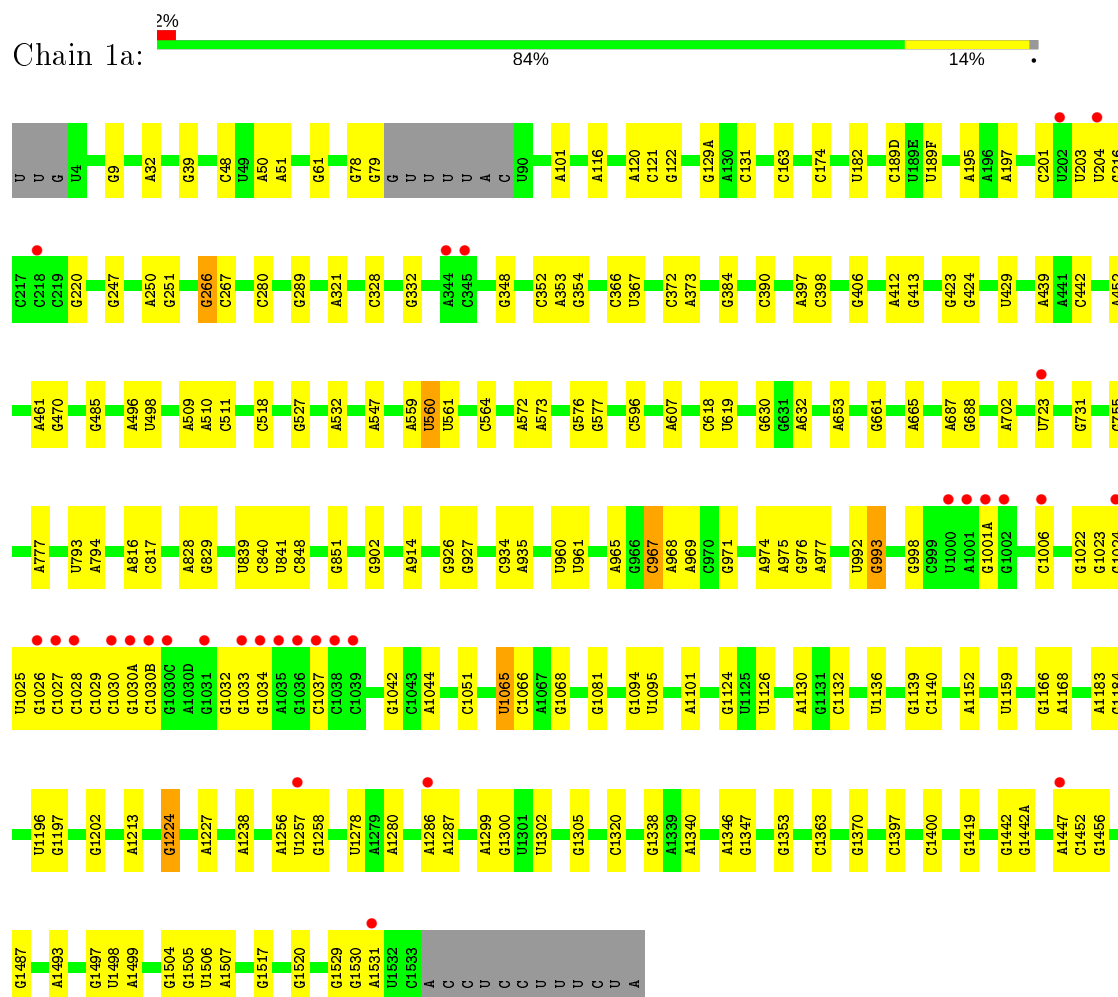
- Molecule 31: 50S ribosomal protein L36



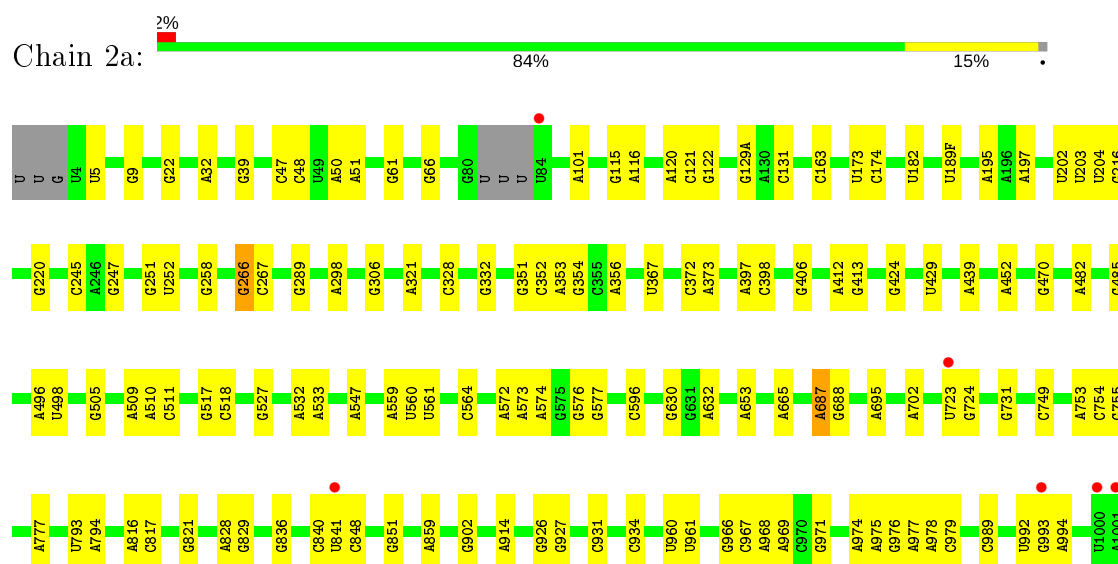
- Molecule 31: 50S ribosomal protein L36



- Molecule 32: 16S Ribosomal RNA



- Molecule 32: 16S Ribosomal RNA



ARG
PRO
ARG
ARG
ARG
ARG
PRO
ALA
VAL
ARG
VAL
LYS
GLU
GLU

- Molecule 35: 30S ribosomal protein S4

Chain 1d:  4% 97%

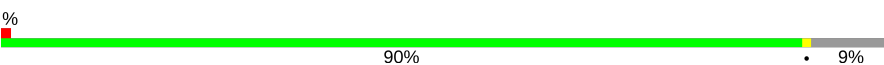
MET G2 R3 Y4 I5 C31 Y68 R86 R118 R122 R132 L135 P136 S137 Y138 L155 V178 L188 R209

- Molecule 35: 30S ribosomal protein S4

Chain 2d:  97%


MET G2 R3 Y4 V8 G12 C31 E34 L135 L155 R209

- Molecule 36: 30S ribosomal protein S5

Chain 1e:  % 90% 9%

MET PRO GLU THR D5 L12 V41 I118 L119 T120 R152 LYS GLY ALA HIS ALA GLN GLN GLY

- Molecule 36: 30S ribosomal protein S5

Chain 2e:  % 90% 9%

MET PRO GLU THR D5 L12 L31 V34 V41 F45 R152 LYS GLY ALA HIS ALA GLN GLN GLY

- Molecule 37: 30S ribosomal protein S6

Chain 1f:  % 99%

H1 E95 H100 ALA

- Molecule 37: 30S ribosomal protein S6

Chain 2f:  % 97%

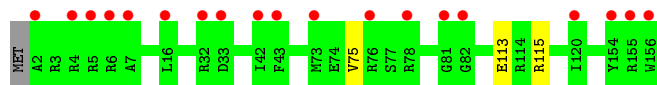
H1 E22 V72 V89 H100 ALA

- Molecule 38: 30S ribosomal protein S7

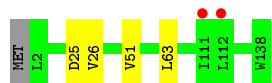
Chain 1g:  3% 99%



- Molecule 38: 30S ribosomal protein S7



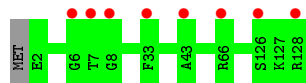
- Molecule 39: 30S ribosomal protein S8



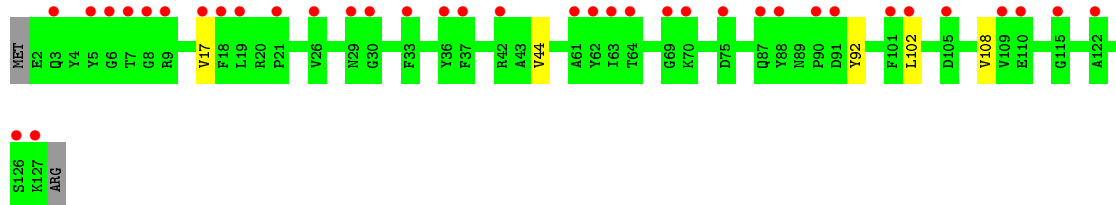
- Molecule 39: 30S ribosomal protein S8



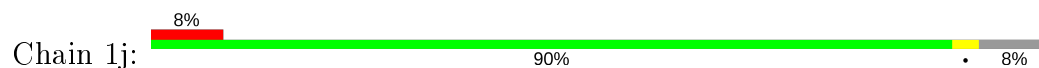
- Molecule 40: 30S ribosomal protein S9



- Molecule 40: 30S ribosomal protein S9

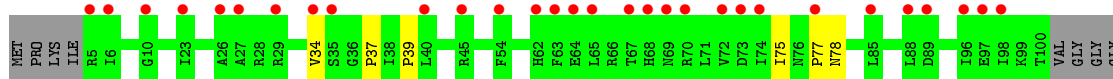
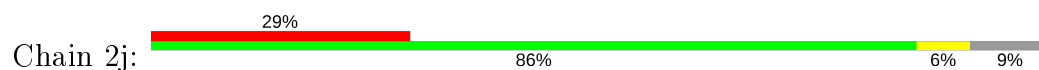


- Molecule 41: 30S ribosomal protein S10

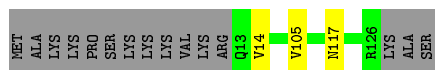
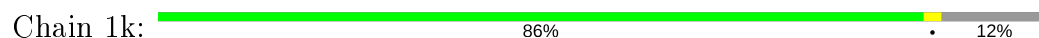




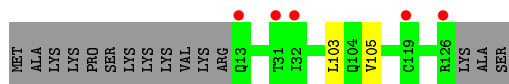
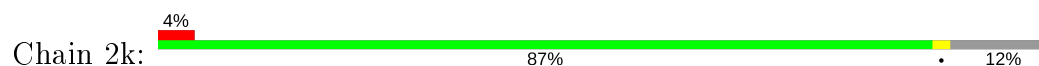
- Molecule 41: 30S ribosomal protein S10



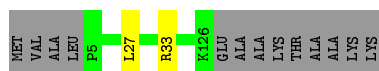
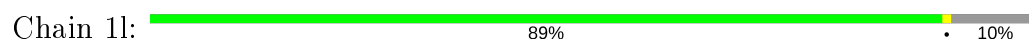
- Molecule 42: 30S ribosomal protein S11



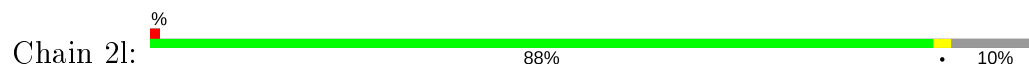
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12



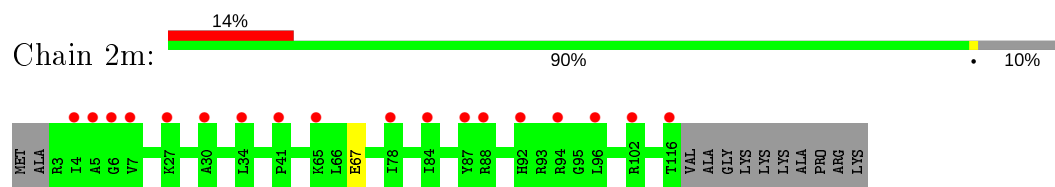
- Molecule 43: 30S ribosomal protein S12



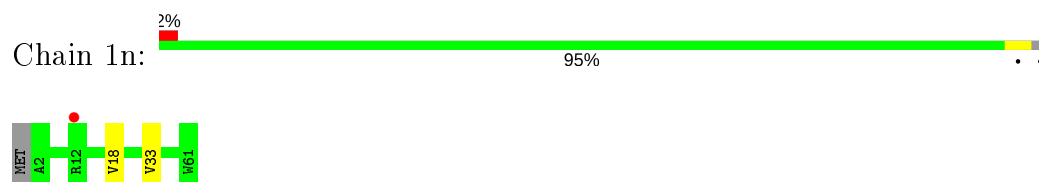
- Molecule 44: 30S ribosomal protein S13



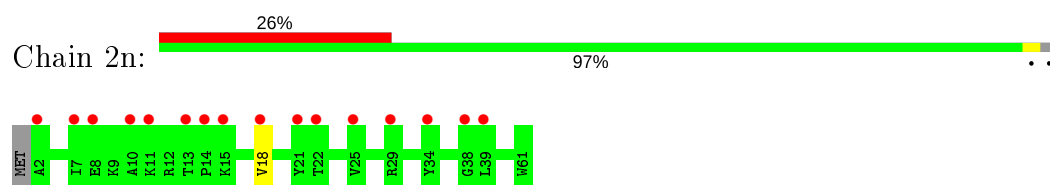
- Molecule 44: 30S ribosomal protein S13



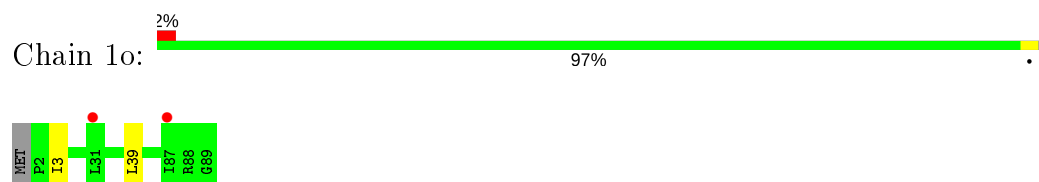
- Molecule 45: 30S ribosomal protein S14 type Z



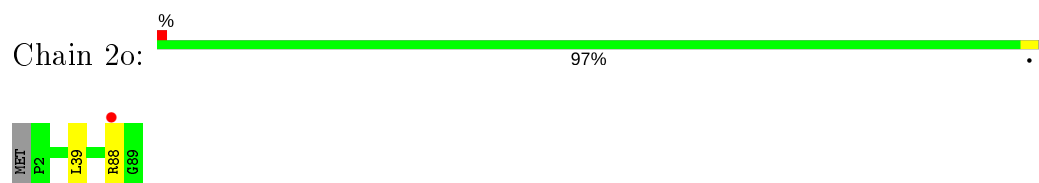
- Molecule 45: 30S ribosomal protein S14 type Z



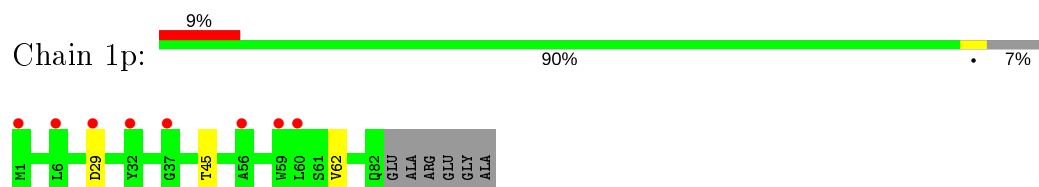
- Molecule 46: 30S ribosomal protein S15



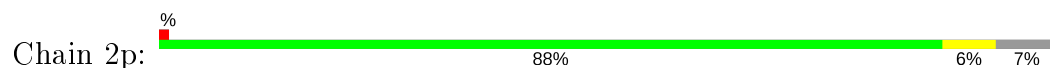
- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16

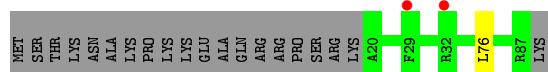
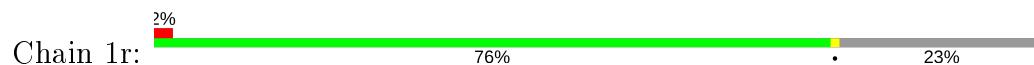


- Molecule 47: 30S ribosomal protein S16

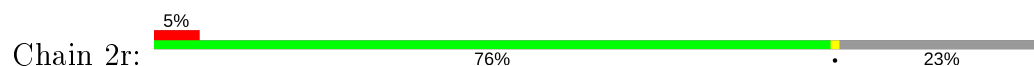




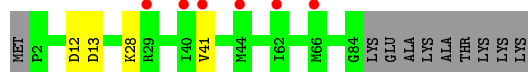
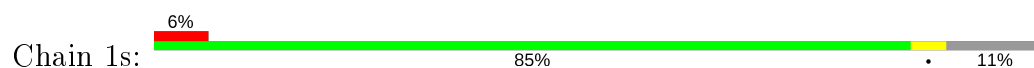
- Molecule 48: 30S ribosomal protein S18



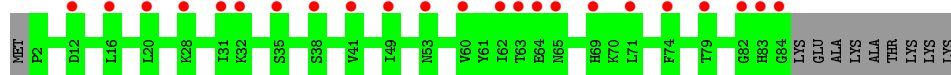
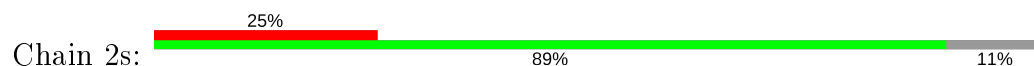
- Molecule 48: 30S ribosomal protein S18



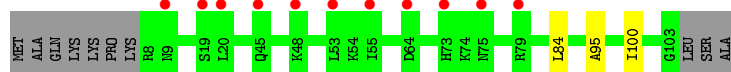
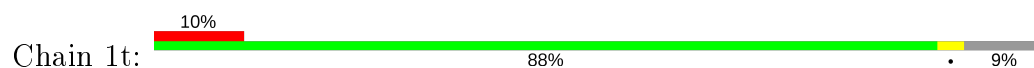
- Molecule 49: 30S ribosomal protein S19



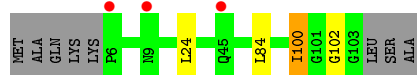
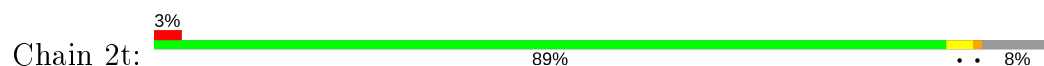
- Molecule 49: 30S ribosomal protein S19



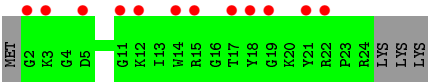
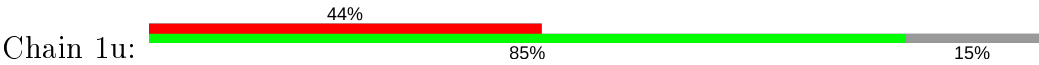
- Molecule 50: 30S ribosomal protein S20



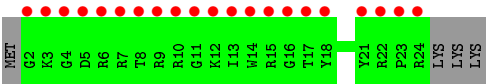
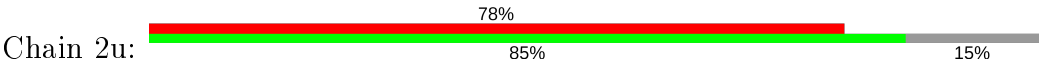
- Molecule 50: 30S ribosomal protein S20



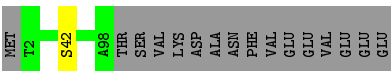
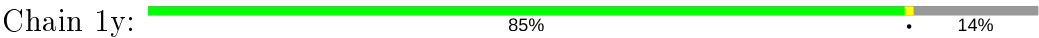
- Molecule 51: 30S ribosomal protein Thx



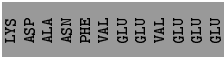
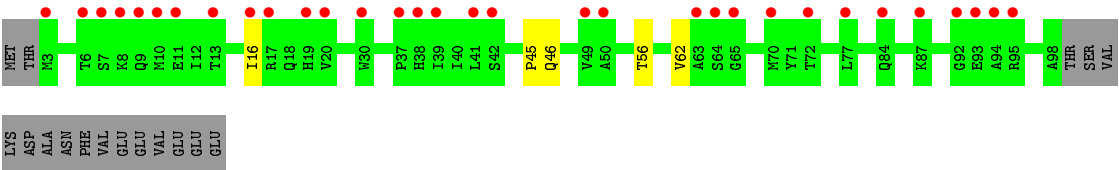
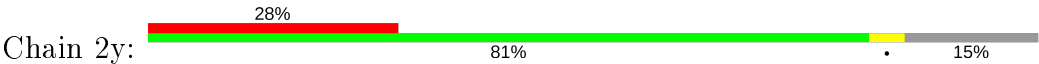
• Molecule 51: 30S ribosomal protein Thx



• Molecule 52: Ribosome-associated inhibitor A



• Molecule 52: Ribosome-associated inhibitor A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.81Å 450.83Å 621.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.93 – 3.25 49.93 – 3.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.93-3.25) 100.0 (49.93-3.25)	Depositor EDS
R_{merge}	0.47	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.25Å)	Xtriage
Refinement program	PHENIX dev_2747	Depositor
R, R_{free}	0.226 , 0.270 0.226 , 0.270	Depositor DCC
R_{free} test set	46129 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	290709	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, ZN, OMG, OMU, MA6, G7M, SF4, 0TD, MG, PSU, 2MA, 2MG, 5MC, UR3, 4OC, M2G, MPD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1A	0.30	0/68792	0.79	7/107386 (0.0%)
1	2A	0.25	0/68686	0.75	9/107216 (0.0%)
2	1B	0.29	0/2837	0.82	0/4426
2	2B	0.25	0/2837	0.81	1/4426 (0.0%)
3	1D	0.29	0/2181	0.49	0/2940
3	2D	0.27	0/2186	0.46	0/2944
4	1E	0.29	0/1592	0.46	0/2149
4	2E	0.26	0/1592	0.46	0/2149
5	1F	0.27	0/1621	0.45	0/2196
5	2F	0.25	0/1617	0.43	0/2191
6	1G	0.26	0/1452	0.45	0/1962
6	2G	0.25	0/1450	0.42	0/1958
7	1H	0.28	0/1356	0.44	0/1834
7	2H	0.25	0/1350	0.42	0/1826
8	1I	0.25	0/1110	0.44	0/1513
8	2I	0.24	0/1092	0.43	0/1491
9	1N	0.27	0/1148	0.45	0/1547
9	2N	0.25	0/1144	0.42	0/1543
10	1O	0.30	0/942	0.48	0/1268
10	2O	0.27	0/942	0.47	0/1268
11	1P	0.29	0/1152	0.47	0/1533
11	2P	0.27	0/1152	0.48	0/1533
12	1Q	0.28	0/1142	0.46	0/1525
12	2Q	0.27	0/1142	0.43	0/1525
13	1R	0.27	0/982	0.46	0/1312
13	2R	0.25	0/982	0.42	0/1312
14	1S	0.27	0/887	0.44	0/1180
14	2S	0.25	0/880	0.44	0/1172
15	1T	0.27	0/1105	0.44	0/1476
15	2T	0.25	0/1097	0.42	0/1467
16	1U	0.29	0/977	0.43	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.25	0/977	0.38	0/1301
17	1V	0.29	0/786	0.49	0/1053
17	2V	0.25	0/782	0.46	0/1049
18	1W	0.29	0/897	0.48	0/1205
18	2W	0.26	0/897	0.42	0/1205
19	1X	0.29	0/764	0.48	0/1025
19	2X	0.26	0/764	0.47	1/1025 (0.1%)
20	1Y	0.28	0/823	0.45	0/1099
20	2Y	0.26	0/823	0.45	0/1100
21	1Z	0.26	0/1620	0.44	0/2200
21	2Z	0.25	0/1590	0.42	0/2162
22	10	0.27	0/614	0.49	0/818
22	20	0.26	0/614	0.43	0/818
23	11	0.27	0/763	0.45	0/1016
23	21	0.26	0/768	0.44	0/1021
24	12	0.27	0/590	0.41	0/781
24	22	0.24	0/594	0.35	0/785
25	13	0.26	0/474	0.44	0/635
25	23	0.23	0/469	0.41	0/630
26	14	0.25	0/559	0.48	0/754
26	24	0.25	0/549	0.46	0/741
27	15	0.27	0/474	0.49	0/640
27	25	0.25	0/470	0.42	0/636
28	16	0.27	0/460	0.46	0/613
28	26	0.26	0/456	0.42	0/608
29	17	0.27	0/426	0.42	0/561
29	27	0.25	0/426	0.41	0/561
30	18	0.29	0/525	0.46	0/691
30	28	0.26	0/525	0.45	0/691
31	19	0.28	0/310	0.46	0/407
31	29	0.25	0/310	0.43	0/407
32	1a	0.25	0/35799	0.80	12/55871 (0.0%)
32	2a	0.25	0/35894	0.83	20/56019 (0.0%)
33	1b	0.24	0/1876	0.39	0/2533
33	2b	0.24	0/1860	0.41	0/2518
34	1c	0.24	0/1582	0.42	0/2137
34	2c	0.24	0/1566	0.42	0/2119
35	1d	0.24	0/1695	0.40	0/2274
35	2d	0.25	0/1698	0.40	0/2277
36	1e	0.26	0/1149	0.45	0/1548
36	2e	0.25	0/1149	0.44	0/1548
37	1f	0.25	0/827	0.41	0/1120
37	2f	0.24	0/829	0.41	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.24	0/1254	0.37	0/1683
38	2g	0.24	0/1248	0.38	0/1676
39	1h	0.25	0/1118	0.44	0/1506
39	2h	0.25	0/1108	0.43	0/1494
40	1i	0.25	0/1005	0.42	0/1350
40	2i	0.25	0/985	0.40	0/1328
41	1j	0.24	0/732	0.43	0/993
41	2j	0.24	0/723	0.45	0/984
42	1k	0.25	0/849	0.45	0/1150
42	2k	0.25	0/848	0.44	0/1149
43	1l	0.26	0/937	0.46	0/1260
43	2l	0.25	0/937	0.49	0/1260
44	1m	0.23	0/924	0.44	0/1242
44	2m	0.23	0/905	0.41	0/1217
45	1n	0.25	0/501	0.41	0/664
45	2n	0.25	0/501	0.41	0/664
46	1o	0.24	0/739	0.38	0/985
46	2o	0.24	0/739	0.38	0/985
47	1p	0.24	0/697	0.42	0/939
47	2p	0.24	0/693	0.42	0/935
48	1r	0.25	0/560	0.44	0/746
48	2r	0.24	0/560	0.40	0/746
49	1s	0.23	0/663	0.43	0/895
49	2s	0.24	0/660	0.44	0/893
50	1t	0.24	0/733	0.37	0/968
50	2t	0.24	0/735	0.36	0/975
51	1u	0.23	0/203	0.41	0/266
51	2u	0.22	0/203	0.41	0/266
52	1y	0.25	0/776	0.41	0/1048
52	2y	0.23	0/761	0.40	0/1030
All	All	0.27	0/307745	0.71	50/460191 (0.0%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2552	OMU	O3'-P-O5'	9.99	122.97	104.00
32	2a	754	C	C2-N1-C1'	7.50	127.05	118.80
32	2a	754	C	N1-C2-O2	7.10	123.16	118.90
1	1A	1313	U	C2-N1-C1'	6.41	125.40	117.70
32	1a	1224	G	N3-C4-N9	-6.24	122.26	126.00
32	2a	1003	G	C8-N9-C4	-6.24	103.91	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	754	C	N3-C2-O2	-6.21	117.55	121.90
32	1a	993	G	N3-C4-N9	6.16	129.70	126.00
32	2a	1003	G	N3-C4-C5	-6.15	125.53	128.60
1	1A	847	U	C2-N1-C1'	6.06	124.98	117.70
32	1a	993	G	C4-N9-C1'	6.02	134.32	126.50
1	2A	1313	U	C2-N1-C1'	5.94	124.83	117.70
32	2a	266	G	P-O3'-C3'	5.92	126.80	119.70
32	2a	1158	C	C2-N1-C1'	5.75	125.13	118.80
1	2A	1992	G	P-O3'-C3'	5.71	126.56	119.70
1	1A	1918	A	N1-C2-N3	5.68	132.14	129.30
1	1A	1300	U	P-O3'-C3'	5.68	126.51	119.70
1	2A	1082	U	C2-N1-C1'	5.67	124.50	117.70
32	1a	993	G	C8-N9-C1'	-5.66	119.64	127.00
32	2a	1003	G	C4-N9-C1'	5.66	133.86	126.50
19	2X	57	LEU	CA-CB-CG	5.65	128.29	115.30
32	1a	1224	G	C4-N9-C1'	-5.63	119.18	126.50
32	1a	1051	C	C5-C4-N4	5.62	124.14	120.20
32	2a	1224	G	N3-C4-N9	-5.45	122.73	126.00
32	2a	979	C	C6-N1-C2	-5.44	118.13	120.30
1	2A	1091	G	N3-C4-C5	-5.42	125.89	128.60
1	2A	1779	U	C2-N1-C1'	5.41	124.20	117.70
1	2A	1779	U	N1-C2-O2	5.40	126.58	122.80
32	2a	1003	G	N7-C8-N9	5.38	115.79	113.10
32	1a	1224	G	C8-N9-C1'	5.35	133.95	127.00
32	2a	252	U	C2-N1-C1'	5.31	124.08	117.70
32	2a	1054	C	N1-C2-O2	5.31	122.09	118.90
32	2a	754	C	C6-N1-C1'	-5.29	114.45	120.80
1	2A	1313	U	N1-C2-O2	5.25	126.48	122.80
1	1A	2552	OMU	P-O3'-C3'	-5.25	113.41	119.70
32	1a	1065	U	P-O3'-C3'	5.22	125.96	119.70
1	1A	1653	G	P-O3'-C3'	5.12	125.85	119.70
32	1a	560	U	C3'-C2'-C1'	5.12	105.59	101.50
2	2B	30	C	C2-N1-C1'	5.11	124.42	118.80
32	1a	967	5MC	P-O3'-C3'	5.08	125.80	119.70
1	2A	2321	G	C4-N9-C1'	5.08	133.10	126.50
32	2a	1158	C	N1-C2-O2	5.08	121.94	118.90
32	1a	266	G	P-O3'-C3'	5.07	125.79	119.70
32	2a	1067	A	P-O3'-C3'	5.06	125.77	119.70
32	2a	1224	G	C4-N9-C1'	-5.06	119.92	126.50
1	2A	1065	U	P-O3'-C3'	5.05	125.76	119.70
32	2a	687	A	P-O3'-C3'	5.05	125.75	119.70
32	2a	1030	C	C2-N1-C1'	5.03	124.33	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1224	G	N3-C4-C5	5.02	131.11	128.60
32	2a	115	G	P-O3'-C3'	5.01	125.71	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61654	0	31088	569	0
1	2A	61564	0	31051	664	0
2	1B	2536	0	1284	14	0
2	2B	2536	0	1284	32	0
3	1D	2131	0	2207	52	0
3	2D	2136	0	2218	41	0
4	1E	1559	0	1618	29	0
4	2E	1559	0	1618	27	0
5	1F	1586	0	1631	29	0
5	2F	1582	0	1626	34	0
6	1G	1427	0	1447	27	0
6	2G	1425	0	1443	24	0
7	1H	1330	0	1407	25	0
7	2H	1324	0	1402	18	0
8	1I	1095	0	1129	14	0
8	2I	1077	0	1096	12	0
9	1N	1121	0	1195	17	0
9	2N	1117	0	1184	17	0
10	1O	932	0	994	17	0
10	2O	932	0	994	20	0
11	1P	1135	0	1212	13	0
11	2P	1135	0	1212	20	0
12	1Q	1121	0	1179	24	0
12	2Q	1121	0	1179	31	0
13	1R	968	0	1033	15	0
13	2R	968	0	1033	16	0
14	1S	877	0	938	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	2S	870	0	923	17	0
15	1T	1091	0	1156	20	0
15	2T	1083	0	1141	12	0
16	1U	959	0	1019	15	0
16	2U	959	0	1019	20	0
17	1V	775	0	840	8	0
17	2V	771	0	830	11	0
18	1W	886	0	940	20	0
18	2W	886	0	939	16	0
19	1X	750	0	814	15	0
19	2X	750	0	814	11	0
20	1Y	810	0	893	14	0
20	2Y	810	0	888	18	0
21	1Z	1587	0	1598	26	0
21	2Z	1557	0	1564	24	0
22	10	606	0	622	10	0
22	20	606	0	622	11	0
23	11	756	0	823	9	0
23	21	761	0	837	23	0
24	12	588	0	643	8	0
24	22	592	0	654	12	0
25	13	469	0	518	12	0
25	23	464	0	514	8	0
26	14	546	0	523	13	0
26	24	536	0	518	16	0
27	15	460	0	480	10	0
27	25	456	0	469	7	0
28	16	453	0	473	10	0
28	26	449	0	469	6	0
29	17	418	0	467	6	0
29	27	418	0	467	10	0
30	18	517	0	582	8	0
30	28	517	0	582	16	0
31	19	307	0	335	7	0
31	29	307	0	336	8	0
32	1a	32249	0	16293	0	0
32	2a	32334	0	16338	0	0
33	1b	1842	0	1862	0	0
33	2b	1825	0	1828	0	0
34	1c	1558	0	1557	0	0
34	2c	1542	0	1517	0	0
35	1d	1665	0	1691	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	2d	1668	0	1707	0	0
36	1e	1133	0	1191	0	0
36	2e	1133	0	1191	0	0
37	1f	814	0	808	0	0
37	2f	816	0	808	0	0
38	1g	1235	0	1249	0	0
38	2g	1229	0	1238	0	0
39	1h	1098	0	1143	0	0
39	2h	1088	0	1126	0	0
40	1i	987	0	996	0	0
40	2i	967	0	959	0	0
41	1j	719	0	672	0	0
41	2j	710	0	661	0	0
42	1k	834	0	838	0	0
42	2k	833	0	836	0	0
43	1l	932	0	981	0	0
43	2l	932	0	981	0	0
44	1m	914	0	954	0	0
44	2m	895	0	920	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0
46	1o	728	0	760	0	0
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	677	0	686	0	0
48	1r	555	0	618	0	0
48	2r	555	0	618	0	0
49	1s	648	0	658	0	0
49	2s	645	0	635	0	0
50	1t	731	0	807	0	0
50	2t	732	0	793	0	0
51	1u	199	0	208	0	0
51	2u	199	0	208	0	0
52	1y	764	0	785	0	0
52	2y	749	0	757	0	0
53	18	8	0	14	1	0
53	1A	8	0	14	0	0
53	1T	8	0	14	0	0
53	1a	8	0	14	0	0
53	2A	16	0	28	1	0
53	2B	8	0	14	2	0
54	10	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	11	4	0	0	0	0
54	13	2	0	0	0	0
54	15	3	0	0	0	0
54	16	1	0	0	0	0
54	17	3	0	0	0	0
54	19	2	0	0	0	0
54	1A	900	0	0	0	0
54	1B	29	0	0	0	0
54	1D	12	0	0	0	0
54	1E	5	0	0	0	0
54	1F	12	0	0	0	0
54	1G	4	0	0	0	0
54	1H	2	0	0	0	0
54	1N	3	0	0	0	0
54	1O	1	0	0	0	0
54	1P	5	0	0	0	0
54	1Q	3	0	0	0	0
54	1R	7	0	0	0	0
54	1T	5	0	0	0	0
54	1U	3	0	0	0	0
54	1V	3	0	0	0	0
54	1W	4	0	0	0	0
54	1X	2	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	257	0	0	0	0
54	1b	1	0	0	0	0
54	1d	6	0	0	0	0
54	1e	3	0	0	0	0
54	1f	2	0	0	0	0
54	1g	3	0	0	0	0
54	1h	1	0	0	0	0
54	1l	2	0	0	0	0
54	1n	2	0	0	0	0
54	1o	1	0	0	0	0
54	1t	2	0	0	0	0
54	1y	4	0	0	0	0
54	20	1	0	0	0	0
54	21	4	0	0	0	0
54	23	1	0	0	0	0
54	28	1	0	0	0	0
54	2A	641	0	0	0	0
54	2B	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	2D	6	0	0	0	0
54	2E	2	0	0	0	0
54	2F	2	0	0	0	0
54	2G	3	0	0	0	0
54	2I	1	0	0	0	0
54	2O	2	0	0	0	0
54	2P	2	0	0	0	0
54	2Q	2	0	0	0	0
54	2R	3	0	0	0	0
54	2T	5	0	0	0	0
54	2V	1	0	0	0	0
54	2W	2	0	0	0	0
54	2X	1	0	0	0	0
54	2Y	1	0	0	0	0
54	2a	164	0	0	0	0
54	2e	1	0	0	0	0
54	2f	1	0	0	0	0
54	2i	1	0	0	0	0
54	2j	1	0	0	0	0
54	2k	1	0	0	0	0
54	2l	2	0	0	0	0
54	2p	1	0	0	0	0
54	2t	1	0	0	0	0
55	1B	12	0	12	0	0
55	1F	12	0	12	1	0
56	14	1	0	0	0	0
56	15	1	0	0	0	0
56	16	1	0	0	0	0
56	19	1	0	0	0	0
56	1Y	1	0	0	0	0
56	1n	1	0	0	0	0
56	24	1	0	0	0	0
56	25	1	0	0	0	0
56	26	1	0	0	0	0
56	29	1	0	0	0	0
56	2Y	1	0	0	0	0
56	2n	1	0	0	0	0
57	1d	8	0	0	0	0
57	2d	8	0	0	0	0
58	10	5	0	0	0	0
58	11	3	0	0	0	0
58	13	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	15	3	0	0	0	0
58	16	2	0	0	0	0
58	17	1	0	0	0	0
58	18	7	0	0	0	0
58	19	3	0	0	0	0
58	1A	1801	0	0	105	0
58	1B	56	0	0	3	0
58	1D	14	0	0	0	0
58	1E	17	0	0	0	0
58	1F	16	0	0	0	0
58	1G	5	0	0	0	0
58	1H	5	0	0	0	0
58	1N	7	0	0	0	0
58	1O	2	0	0	0	0
58	1P	17	0	0	0	0
58	1Q	5	0	0	0	0
58	1R	5	0	0	0	0
58	1T	8	0	0	0	0
58	1U	6	0	0	0	0
58	1V	5	0	0	0	0
58	1W	2	0	0	0	0
58	1X	6	0	0	0	0
58	1Y	1	0	0	0	0
58	1Z	1	0	0	0	0
58	1a	424	0	0	0	0
58	1c	1	0	0	0	0
58	1d	8	0	0	0	0
58	1e	4	0	0	0	0
58	1f	1	0	0	0	0
58	1h	1	0	0	0	0
58	1j	1	0	0	0	0
58	1l	3	0	0	0	0
58	1m	1	0	0	0	0
58	1o	3	0	0	0	0
58	1p	1	0	0	0	0
58	1t	2	0	0	0	0
58	1y	3	0	0	0	0
58	20	2	0	0	0	0
58	21	1	0	0	0	0
58	23	2	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	27	2	0	0	0	0
58	28	5	0	0	0	0
58	2A	1310	0	0	106	0
58	2B	32	0	0	3	0
58	2D	16	0	0	1	0
58	2E	10	0	0	0	0
58	2F	6	0	0	1	0
58	2G	1	0	0	0	0
58	2N	1	0	0	0	0
58	2O	3	0	0	0	0
58	2P	14	0	0	1	0
58	2Q	5	0	0	0	0
58	2R	1	0	0	0	0
58	2T	4	0	0	0	0
58	2V	2	0	0	0	0
58	2W	3	0	0	0	0
58	2X	4	0	0	1	0
58	2Y	1	0	0	0	0
58	2a	282	0	0	0	0
58	2e	1	0	0	0	0
58	2j	2	0	0	0	0
58	2l	1	0	0	0	0
58	2t	2	0	0	0	0
58	2y	3	0	0	0	0
All	All	290709	0	192529	1967	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1967) 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:2552:OMU:C4'	1:1A:2552:OMU:O4'	1.67	1.18
1:2A:2552:OMU:O4'	1:2A:2552:OMU:C4'	1.67	1.18
1:2A:2131:G:H5''	1:2A:2132:U:H5'	1.53	0.91
1:2A:1047:G:H21	1:2A:1111:A:H62	1.23	0.86
2:2B:8:U:H3	2:2B:113:G:H1	1.22	0.85
1:2A:1422:G:H5''	10:2O:48:PRO:HB3	100.05	0.83
1:1A:1422:G:H5''	10:1O:48:PRO:HB3	100.66	0.82
1:1A:198:C:OP2	58:1A:4001:HOH:O	1.98	0.81
1:1A:1085:A:HO2'	1:1A:1104:C:HO2'	1.20	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:55:ASN:H	15:1T:59:THR:HG22	1.46	0.80
1:1A:1441:G:H5''	1:1A:1442:G:H5'	5.57	0.80
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.63	0.80
20:1Y:92:ASN:HB2	20:1Y:94:LYS:H	1.47	0.80
1:1A:195:A:N7	58:1A:4001:HOH:O	2.14	0.80
1:1A:2116:G:OP2	1:1A:2166:G:N2	2.15	0.80
1:1A:2427:C:OP1	58:1A:4002:HOH:O	1.99	0.80
1:1A:1332:G:OP1	58:1A:4003:HOH:O	2.00	0.79
1:1A:1315:C:OP2	58:1A:4003:HOH:O	2.02	0.78
1:2A:195:A:N7	58:2A:3705:HOH:O	2.16	0.78
1:1A:1060:U:H4'	1:1A:1061:U:H5'	1.66	0.78
1:1A:2759:G:N7	58:1A:4040:HOH:O	2.16	0.78
1:1A:2137:C:O2	1:1A:2154:G:N2	2.18	0.77
1:1A:2430:A:OP1	58:1A:4004:HOH:O	2.03	0.76
1:1A:517:C:OP1	27:15:16:ARG:NH2	2.17	0.76
1:2A:1315:C:OP2	58:2A:3701:HOH:O	2.04	0.76
1:1A:2690:C:OP1	13:1R:17:ARG:NH2	2.20	0.75
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.18	0.75
1:1A:1057:A:N6	1:1A:1087:G:OP2	2.20	0.74
1:1A:2622:C:O2'	1:1A:2825:G:N2	2.20	0.74
1:2A:2602:A:N7	58:2A:3763:HOH:O	2.20	0.74
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.68	0.74
1:2A:2343:C:HO2'	1:2A:2373:G:HO2'	1.34	0.74
1:1A:11:G:H2'	1:1A:12:U:H5''	1.69	0.74
1:2A:2483:C:N3	12:2Q:124:LYS:NZ	2.34	0.74
12:1Q:30:GLY:HA2	12:1Q:107:ALA:HB2	1.70	0.74
1:1A:1267:U:OP1	58:1A:4005:HOH:O	2.05	0.74
1:1A:2499:C:OP1	58:1A:4006:HOH:O	2.06	0.73
1:2A:570:G:O6	58:2A:3702:HOH:O	2.07	0.73
1:1A:330:A:H2	1:1A:1210:A:HO2'	1.35	0.73
1:1A:1670:C:OP2	58:1A:4008:HOH:O	2.07	0.72
1:2A:198:C:OP2	58:2A:3705:HOH:O	2.07	0.72
1:1A:1010:A:OP2	58:1A:4007:HOH:O	2.07	0.72
1:2A:2602:A:H1'	1:2A:2603:G:H5''	1.70	0.72
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.70	0.72
2:2B:58:A:OP2	58:2B:301:HOH:O	2.08	0.72
1:1A:973:A:OP2	58:1A:4009:HOH:O	2.07	0.72
1:1A:2886:G:N7	58:1A:4081:HOH:O	2.21	0.72
1:1A:2583:G:OP2	58:1A:4010:HOH:O	2.08	0.71
1:1A:927:G:N7	58:1A:4095:HOH:O	2.23	0.71
2:1B:60:C:N4	58:1B:1103:HOH:O	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2058:A:N7	58:2A:3799:HOH:O	2.24	0.71
1:1A:981:A:OP1	58:1A:4011:HOH:O	2.09	0.71
1:1A:265:A:N1	1:1A:427:U:O2'	2.24	0.71
1:2A:1658:C:OP1	58:2A:3706:HOH:O	2.08	0.71
1:2A:1971:A:OP1	58:2A:3704:HOH:O	2.07	0.71
1:2A:2615:U:OP1	58:2A:3707:HOH:O	2.09	0.71
1:2A:422:A:OP2	58:2A:3703:HOH:O	2.07	0.71
6:1G:135:LEU:O	6:1G:154:GLY:HA3	1.91	0.70
1:2A:2753:A:N3	31:29:15:LYS:NZ	2.39	0.70
1:2A:740:U:OP2	58:2A:3709:HOH:O	2.09	0.70
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.08	0.70
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.23	0.70
3:1D:85:ASP:OD2	3:1D:88:ARG:NH1	2.22	0.70
3:2D:38:LYS:NZ	3:2D:39:LYS:O	2.25	0.70
18:2W:35:ILE:HG23	27:25:28:PRO:HD2	1.74	0.70
25:13:15:TYR:O	25:13:20:LYS:NZ	2.25	0.70
1:1A:400:G:N7	58:1A:4108:HOH:O	2.24	0.70
1:2A:1332:G:OP1	58:2A:3701:HOH:O	2.10	0.70
7:1H:86:GLU:OE2	7:1H:132:ARG:NH2	2.24	0.70
1:2A:1265:A:OP2	58:2A:3707:HOH:O	2.10	0.69
1:2A:2427:C:OP1	58:2A:3710:HOH:O	2.10	0.69
1:2A:2622:C:O2'	1:2A:2825:G:N2	2.25	0.69
1:2A:2430:A:OP2	58:2A:3708:HOH:O	2.09	0.69
1:1A:520:G:N7	58:1A:4115:HOH:O	2.25	0.69
4:2E:11:MET:HG2	4:2E:24:THR:HG22	1.73	0.69
1:2A:1063:G:H1	1:2A:1075:C:H42	1.39	0.69
1:2A:794:G:OP2	58:2A:3711:HOH:O	2.11	0.69
1:1A:1779:U:OP2	58:1A:4015:HOH:O	2.11	0.69
2:2B:115:G:O2'	14:2S:50:SER:OG	2.09	0.69
1:1A:526:A:O2'	1:1A:2043:C:O2	2.10	0.69
2:1B:106:G:H5'	21:1Z:31:ARG:HB3	1.74	0.69
1:2A:2439:A:N1	58:2A:3814:HOH:O	2.26	0.69
5:2F:135:LYS:HG2	5:2F:137:LYS:HG2	1.75	0.69
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.75	0.69
1:1A:945:A:N7	58:1A:4117:HOH:O	2.26	0.69
14:1S:15:ARG:O	14:1S:19:LYS:HG2	1.93	0.68
1:2A:2448:A:OP1	58:2A:3702:HOH:O	2.11	0.68
1:1A:2432:A:OP2	58:1A:4016:HOH:O	2.11	0.68
1:2A:1772:G:OP1	58:2A:3712:HOH:O	2.11	0.68
1:2A:2680:C:H5'	4:2E:189:PRO:HA	1.74	0.68
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:68:ILE:HG22	12:2Q:101:ARG:HE	1.59	0.68
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.75	0.68
1:1A:811:U:OP1	58:1A:4013:HOH:O	2.10	0.68
1:2A:827:U:OP1	58:2A:3708:HOH:O	2.11	0.68
31:19:25:VAL:HB	31:19:34:GLN:HB2	1.75	0.68
1:2A:963:U:OP2	58:2A:3716:HOH:O	2.12	0.68
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.27	0.68
22:20:10:THR:HG22	22:20:12:ASN:H	1.58	0.68
1:2A:2575:C:OP2	58:2A:3714:HOH:O	2.12	0.68
6:2G:142:PRO:HB2	26:24:31:ILE:HG21	1.76	0.68
1:2A:120:U:OP2	58:2A:3717:HOH:O	2.12	0.68
1:2A:34:C:H2'	1:2A:35:G:H8	5.30	0.68
1:2A:731:C:OP2	58:2A:3715:HOH:O	2.12	0.68
1:1A:759:G:N7	58:1A:4125:HOH:O	2.27	0.68
1:1A:271(M):G:H21	8:1I:50:ARG:HD3	1.57	0.67
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.27	0.67
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.27	0.67
1:2A:195:A:OP1	11:2P:46:LYS:NZ	2.26	0.67
7:1H:3:ARG:HA	7:1H:3:ARG:HH11	1.58	0.67
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.27	0.67
1:1A:2821:A:OP2	58:1A:4019:HOH:O	2.13	0.67
1:2A:785:G:OP2	58:2A:3713:HOH:O	2.11	0.67
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.27	0.67
12:1Q:34:LEU:HB2	12:1Q:118:LEU:HD22	1.77	0.67
1:1A:2292:C:OP1	14:1S:17:ARG:NH2	2.27	0.67
1:2A:2712(A):A:OP2	58:2A:3719:HOH:O	2.12	0.67
1:1A:1990:C:OP2	58:1A:4017:HOH:O	2.12	0.67
23:21:50:ARG:HG2	23:21:59:THR:HG22	1.76	0.67
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.76	0.67
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.77	0.67
21:1Z:77:ASP:OD2	21:1Z:80:ARG:NH1	2.25	0.67
28:26:14:THR:OG1	28:26:48:VAL:O	2.13	0.67
12:2Q:55:VAL:HG23	21:2Z:178:GLU:HB3	1.77	0.67
1:2A:2584:U:H2'	1:2A:2585:U:H2'	1.77	0.66
1:2A:1360:A:OP2	9:2N:35:ARG:NH2	118.35	0.66
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.78	0.66
25:23:5:LYS:HG3	25:23:36:VAL:HG22	1.77	0.66
1:2A:1286:A:H2'	1:2A:1287:A:H4'	6.45	0.66
1:2A:1334:G:N7	58:2A:3842:HOH:O	2.28	0.66
1:2A:495:G:N3	18:2W:61:ASN:ND2	2.44	0.66
1:1A:1023:U:OP2	58:1A:4014:HOH:O	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:144:LEU:HD21	21:1Z:150:LEU:HD13	1.77	0.66
1:2A:194:G:OP2	58:2A:3722:HOH:O	2.13	0.66
1:2A:2111:C:H42	1:2A:2147:G:H22	1.42	0.66
22:10:27:GLU:HG3	22:10:68:GLU:HA	1.77	0.66
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.75	0.66
1:2A:2432:A:OP2	58:2A:3721:HOH:O	2.13	0.66
1:2A:749:C:OP2	58:2A:3720:HOH:O	2.13	0.66
2:1B:87:G:N2	2:1B:90:A:OP2	2.23	0.66
1:1A:1007:C:OP2	58:1A:4022:HOH:O	2.13	0.66
1:1A:818:G:OP2	58:1A:4025:HOH:O	2.14	0.66
1:2A:1094:U:OP1	1:2A:1096:A:N6	2.29	0.66
3:2D:106:ILE:HD11	3:2D:144:ALA:HB2	1.78	0.66
1:2A:2375:G:N2	1:2A:2378:A:OP2	2.28	0.66
1:2A:331:A:N1	58:2A:3835:HOH:O	2.28	0.66
1:1A:2033:A:OP1	58:1A:4023:HOH:O	2.14	0.65
1:1A:380:U:OP1	58:1A:4028:HOH:O	2.15	0.65
1:1A:2062:A:OP1	58:1A:4024:HOH:O	2.14	0.65
1:1A:962:G:OP1	58:1A:4018:HOH:O	2.13	0.65
31:29:27:CYS:SG	31:29:28:GLU:N	2.69	0.65
1:2A:249:C:O2	30:28:12:LYS:NZ	2.27	0.65
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.76	0.65
1:1A:1911:PSU:C2	1:1A:1918:A:C5	2.80	0.65
1:2A:2823:A:O2'	58:2A:3718:HOH:O	2.12	0.65
1:2A:309:G:N3	1:2A:329:G:O2'	2.29	0.65
1:2A:2711:A:H5''	1:2A:2712:U:H5''	1.78	0.65
1:2A:818:G:OP2	58:2A:3726:HOH:O	2.15	0.65
12:2Q:39:PRO:HB3	12:2Q:99:PRO:HD3	1.77	0.65
25:13:6:VAL:HG13	25:13:56:VAL:HG22	1.78	0.65
1:1A:975:C:OP1	58:1A:4030:HOH:O	2.15	0.65
2:1B:56:G:O2'	58:1B:1101:HOH:O	2.15	0.65
20:1Y:92:ASN:N	20:1Y:93:GLY:HA2	2.10	0.65
1:2A:1314:C:OP1	58:2A:3701:HOH:O	2.14	0.65
1:2A:300:A:OP1	20:2Y:86:ARG:NH2	2.30	0.65
1:1A:2625:G:O6	58:1A:4021:HOH:O	2.13	0.65
1:2A:511:U:OP2	58:2A:3723:HOH:O	2.14	0.65
1:1A:668:G:H5'	1:1A:669:G:OP2	1.97	0.65
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	1.79	0.65
1:2A:1669:A:OP2	58:2A:3727:HOH:O	2.15	0.64
1:1A:1972:A:H2'	1:1A:1973:G:H8	1.62	0.64
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.79	0.64
1:2A:2499:C:OP1	58:2A:3702:HOH:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1828:G:OP1	58:1A:4026:HOH:O	2.14	0.64
1:2A:102:G:OP1	24:22:7:ARG:NH2	2.30	0.64
1:2A:2527:C:N4	58:2A:3746:HOH:O	2.26	0.64
1:2A:2292:C:OP1	14:2S:17:ARG:NH2	2.30	0.64
1:2A:1666:G:N7	58:2A:3848:HOH:O	2.30	0.64
1:2A:1038:C:H42	1:2A:1117:G:H1	1.44	0.64
1:2A:192:C:O2'	1:2A:802:A:N3	2.28	0.64
1:1A:1300:U:H4'	1:1A:1301:A:H5'	1.78	0.64
1:1A:1352:U:OP1	58:1A:4033:HOH:O	2.15	0.64
1:1A:2337:G:OP2	58:1A:4031:HOH:O	2.15	0.64
5:2F:164:ARG:HD2	5:2F:175:THR:HG23	1.78	0.64
1:1A:1056:G:N1	1:1A:1102:C:OP2	2.25	0.64
3:1D:136:ILE:O	3:1D:168:ARG:NH2	2.30	0.64
1:2A:1046:A:N6	1:2A:1211:U:O2	148.65	0.64
1:2A:1352:U:OP2	58:2A:3728:HOH:O	2.15	0.64
1:2A:910:A:OP1	58:2A:3724:HOH:O	2.14	0.64
1:1A:526:A:OP1	58:1A:4032:HOH:O	2.15	0.64
5:1F:143:ALA:HB1	5:1F:148:LEU:HB2	1.79	0.64
1:1A:2305:A:H5''	6:1G:134:GLY:HA3	1.79	0.64
1:2A:468:G:N7	29:27:39:ARG:NH2	2.46	0.64
26:14:40:HIS:HB3	26:14:43:TYR:HD1	1.62	0.64
1:1A:1094:U:H1'	1:1A:1097:U:H5	1.62	0.64
6:1G:161:THR:HG22	6:1G:163:ALA:H	1.62	0.64
1:1A:2441:C:OP2	1:1A:2586:C:O2'	2.17	0.63
1:1A:918:A:N3	2:1B:80:U:O2'	2.30	0.63
1:1A:1997:G:OP2	58:1A:4027:HOH:O	2.14	0.63
6:2G:112:PRO:HG3	26:24:43:TYR:HE2	1.63	0.63
1:2A:526:A:OP1	58:2A:3725:HOH:O	2.15	0.63
1:1A:2445:G:OP1	5:1F:74:ARG:NH2	2.31	0.63
1:1A:1064:C:H3'	1:1A:1065:U:H5''	1.80	0.63
1:1A:1865:G:OP1	58:1A:4029:HOH:O	2.15	0.63
6:1G:41:GLN:HB3	6:1G:43:LEU:HD13	1.80	0.63
7:1H:101:ARG:NH2	7:1H:121:ILE:O	2.31	0.63
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.19	0.63
23:21:51:VAL:HG11	23:21:74:VAL:HG21	1.80	0.63
1:2A:2424:C:O2	1:2A:2429:G:O2'	2.14	0.63
21:2Z:144:LEU:HD21	21:2Z:150:LEU:HD13	1.79	0.63
1:1A:1994:C:OP1	58:1A:4035:HOH:O	2.16	0.63
26:24:48:ARG:HG3	26:24:52:THR:HG23	1.80	0.63
21:1Z:19:ARG:NH1	21:1Z:84:GLU:O	2.31	0.63
7:2H:8:PRO:HB3	7:2H:51:ARG:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2Y:9:LYS:NZ	20:2Y:28:LYS:O	2.31	0.63
1:1A:34:C:H2'	1:1A:35:G:H8	3.45	0.63
1:2A:242:G:N2	1:2A:255:A:OP2	2.26	0.63
1:2A:2820:A:OP2	1:2A:2821:A:N6	2.24	0.63
1:1A:1068:G:HO2'	1:1A:1096:A:HO2'	1.42	0.62
8:1I:9:LEU:HD23	8:1I:12:LEU:HD13	1.80	0.62
1:1A:2503:2MA:O2'	58:1A:4034:HOH:O	2.15	0.62
1:1A:588:U:OP2	58:1A:4038:HOH:O	2.16	0.62
3:1D:75:ILE:HG21	3:1D:99:ASP:HB2	1.81	0.62
1:1A:2641:G:OP2	9:1N:83:LYS:NZ	2.32	0.62
15:1T:49:VAL:HG12	15:1T:63:VAL:HG22	1.82	0.62
1:2A:2126:A:H4'	1:2A:2127:G:O5'	1.98	0.62
10:2O:13:ASN:HD21	10:2O:96:THR:HG1	1.44	0.62
22:20:11:LYS:O	22:20:14:ARG:NH2	2.30	0.62
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.15	0.62
3:1D:180:GLY:HA3	3:1D:275:LYS:HG2	1.81	0.62
14:1S:28:VAL:HG11	14:1S:98:VAL:HG13	1.79	0.62
19:2X:60:ARG:HH22	29:27:47:ARG:HH12	1.48	0.62
1:2A:2353:G:N7	58:2A:3855:HOH:O	2.31	0.62
1:2A:1718:G:H1	1:2A:1744:U:H3	1.48	0.62
1:2A:1918:A:O2'	1:2A:1920:OMC:N4	2.33	0.62
11:1P:100:LEU:HD12	11:1P:112:LEU:HD11	1.82	0.62
1:1A:1286:A:H2'	1:1A:1287:A:H4'	6.64	0.62
4:1E:143:ASN:HD22	4:1E:147:PRO:HD3	1.64	0.62
1:2A:1779:U:OP2	1:2A:1784:A:N6	2.26	0.62
6:2G:131:TYR:HE2	6:2G:133:LEU:HD23	1.65	0.62
1:2A:1607:C:N4	1:2A:1622:G:OP2	2.30	0.61
1:1A:113:G:H2'	1:1A:114:U:H6	5.11	0.61
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.32	0.61
20:2Y:14:LEU:HB2	20:2Y:75:ILE:HD11	1.82	0.61
1:1A:2343:C:HO2'	1:1A:2373:G:HO2'	1.48	0.61
31:29:12:ASP:N	31:29:12:ASP:OD1	2.33	0.61
1:2A:1127:A:N7	1:2A:2488:A:O2'	2.34	0.61
1:2A:674:G:H2'	1:2A:675:A:H8	4.68	0.61
1:1A:270:A:OP2	1:1A:271(X):G:N2	2.33	0.61
26:24:59:PHE:HA	26:24:60:GLN:C	2.21	0.61
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.34	0.61
12:1Q:43:THR:HG22	12:1Q:94:VAL:HG12	1.82	0.61
23:21:76:ARG:HH22	23:21:97:LEU:HB3	1.66	0.61
1:2A:1891:G:N7	58:2A:3851:HOH:O	2.31	0.61
1:1A:687:C:H5''	29:17:2:LYS:HE2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:41:GLU:HG2	8:1I:45:LYS:HE3	1.82	0.61
1:2A:1006:C:OP2	58:2A:3733:HOH:O	2.16	0.61
1:2A:1062:G:N7	1:2A:1070:A:H1'	2.15	0.61
1:2A:2012:G:OP1	18:2W:11:ARG:NH2	2.22	0.61
1:1A:2126:A:H4'	1:1A:2127:G:O5'	2.00	0.61
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.34	0.61
1:2A:1119:C:H2'	1:2A:1120:G:H8	2.52	0.61
18:1W:73:ALA:HB3	18:1W:106:ILE:HB	1.82	0.60
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.36	0.60
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.36	0.60
18:1W:11:ARG:NH1	18:1W:99:ARG:O	2.32	0.60
1:2A:1530:C:O2'	1:2A:1531:C:O5'	2.17	0.60
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.66	0.60
1:1A:2012:G:P	18:1W:11:ARG:HH22	2.23	0.60
5:1F:185:ASP:OD1	5:1F:188:ARG:NH1	2.34	0.60
9:2N:25:ARG:O	9:2N:29:LYS:NZ	2.31	0.60
10:2O:1:MET:HG3	10:2O:67:LYS:HG2	1.81	0.60
26:14:24:THR:OG1	26:14:25:TYR:N	2.34	0.60
1:2A:1903:G:O2'	58:2A:3729:HOH:O	2.15	0.60
1:2A:2547:U:O2	10:2O:23:ARG:NH2	2.34	0.60
1:2A:826:U:OP1	58:2A:3710:HOH:O	2.17	0.60
1:1A:1265:A:OP1	58:1A:4039:HOH:O	2.16	0.60
7:1H:124:GLU:HG3	7:1H:132:ARG:HB3	1.83	0.60
5:2F:117:ARG:NH2	5:2F:189:THR:O	2.33	0.60
1:1A:1173:G:O2'	1:1A:1174:A:O5'	2.19	0.60
1:2A:1422:G:O3'	10:2O:49:ARG:NH1	99.84	0.60
1:2A:1665:A:OP2	58:2A:3736:HOH:O	2.16	0.60
1:2A:1994:C:OP1	58:2A:3739:HOH:O	2.17	0.60
25:13:4:LEU:O	25:13:36:VAL:HA	2.01	0.60
1:1A:2316:C:O2'	6:1G:128:ARG:NH2	2.35	0.60
4:1E:47:VAL:HG21	4:1E:86:PRO:HD2	1.83	0.60
12:1Q:21:THR:HG21	12:1Q:101:ARG:HB2	1.84	0.60
28:26:5:VAL:HA	28:26:27:LYS:HE2	1.84	0.60
1:2A:1271:G:OP2	58:2A:3731:HOH:O	2.16	0.60
1:2A:1853:A:N3	1:2A:2233:U:O2'	2.33	0.60
1:2A:979:G:N7	58:2A:3854:HOH:O	2.31	0.60
1:2A:631:A:OP2	30:28:47:LYS:NZ	2.29	0.60
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.37	0.60
1:2A:1073:A:H2'	1:2A:1074:G:C8	2.37	0.60
1:1A:120:U:OP2	58:1A:4036:HOH:O	2.16	0.59
1:1A:2584:U:H2'	1:1A:2585:U:H2'	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1816:G:O6	3:1D:35:LYS:NZ	2.32	0.59
1:2A:1418:G:OP2	58:2A:3738:HOH:O	2.17	0.59
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.35	0.59
1:2A:521:G:O6	58:2A:3732:HOH:O	2.16	0.59
30:18:15:LYS:HB2	53:18:101:MPD:H31	1.83	0.59
1:1A:1607:C:N4	1:1A:1622:G:OP2	2.29	0.59
1:2A:2189:U:H2'	1:2A:2190:G:C8	2.36	0.59
7:2H:85:LYS:HD3	7:2H:141:VAL:HG12	1.84	0.59
1:2A:2448:A:OP1	58:2A:3735:HOH:O	2.16	0.59
1:1A:958:U:H5''	12:1Q:14:ARG:HD3	1.84	0.59
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.83	0.59
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.30	0.59
1:2A:2538:C:N4	58:2A:3867:HOH:O	2.33	0.59
1:2A:2640:G:O3'	9:2N:74:ARG:NH2	2.27	0.59
1:2A:785:G:OP2	58:2A:3730:HOH:O	2.16	0.59
1:2A:822:U:H2'	1:2A:823:G:H8	1.67	0.59
1:1A:338:G:OP2	58:1A:4041:HOH:O	2.17	0.59
6:1G:114:ILE:HG12	6:1G:140:ILE:HD13	1.85	0.59
10:1O:115:VAL:HG13	10:1O:121:VAL:HG21	1.83	0.59
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.85	0.59
7:1H:40:GLU:OE2	7:1H:60:ARG:NH1	2.35	0.59
1:1A:2022:U:OP1	58:1A:4045:HOH:O	2.17	0.59
1:2A:1495:A:OP2	58:2A:3740:HOH:O	2.17	0.59
3:1D:17:THR:O	3:1D:211:ARG:NH2	2.35	0.59
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.38	0.59
1:2A:326:G:N7	58:2A:3865:HOH:O	2.32	0.59
1:2A:637:A:H8	11:2P:117:GLU:HG3	1.67	0.59
1:1A:637:A:OP1	11:1P:133:SER:OG	2.20	0.59
1:2A:958:U:OP2	12:2Q:14:ARG:NH1	2.36	0.59
1:1A:2239:G:OP2	58:1A:4043:HOH:O	2.17	0.59
1:1A:971:C:OP2	58:1A:4042:HOH:O	2.17	0.58
1:2A:1349:A:OP1	58:2A:3742:HOH:O	2.17	0.58
5:2F:178:PRO:HB2	5:2F:201:VAL:HG21	1.84	0.58
1:1A:1024:G:OP2	58:1A:4014:HOH:O	2.17	0.58
1:1A:942:G:O2'	1:1A:1189:A:N3	2.36	0.58
1:1A:2893:G:H4'	1:1A:2894:G:O5'	2.02	0.58
1:2A:1356:G:OP2	58:2A:3734:HOH:O	2.16	0.58
1:2A:2255:G:OP2	58:2A:3737:HOH:O	2.17	0.58
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.35	0.58
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.85	0.58
1:2A:637:A:OP1	11:2P:133:SER:OG	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:889:C:O2'	1:2A:890:A:O5'	2.21	0.58
1:2A:861:A:N3	2:2B:79:C:O2'	2.36	0.58
1:1A:2319:G:H22	14:1S:3:ARG:HD3	1.67	0.58
1:2A:2360:A:OP2	58:2A:3744:HOH:O	2.17	0.58
4:2E:181:LEU:HD11	15:2T:6:LEU:HD23	1.85	0.58
6:1G:179:PRO:HB2	26:14:42:PHE:HE2	1.67	0.58
1:1A:2010:G:H5''	18:1W:42:ARG:HB2	1.86	0.58
1:1A:2130:U:O2'	1:1A:2133:G:O2'	2.22	0.58
1:2A:514:A:N3	1:2A:581:C:O2'	2.36	0.58
19:2X:65:ARG:HB3	19:2X:70:LEU:HD23	1.86	0.58
1:1A:1345:C:OP2	58:1A:4048:HOH:O	2.17	0.58
1:1A:1856:G:OP2	58:1A:4046:HOH:O	2.17	0.58
1:2A:1385:G:O2'	1:2A:1396:U:O2	2.19	0.58
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.36	0.58
1:1A:307:G:H21	1:1A:330:A:H62	1.49	0.58
1:1A:764:A:H5'	3:1D:210:GLY:HA2	1.85	0.58
22:20:36:ILE:HD13	22:20:60:PHE:HB3	1.86	0.58
2:2B:22:U:H2'	2:2B:23:G:C8	2.39	0.58
11:2P:2:LYS:NZ	11:2P:4:SER:OG	2.31	0.58
1:1A:102:G:OP1	24:12:7:ARG:NH2	2.37	0.58
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.37	0.58
6:2G:7:LEU:HD23	6:2G:100:TRP:HE3	1.68	0.58
1:1A:2548:G:O6	58:1A:4037:HOH:O	2.16	0.58
26:24:16:CYS:SG	26:24:17:GLY:N	2.77	0.58
1:2A:886:C:O2'	1:2A:889:C:N4	2.36	0.57
28:16:9:LEU:HD13	28:16:51:GLU:HG3	1.87	0.57
1:1A:1173:G:O2'	1:1A:1174:A:O4'	2.19	0.57
1:1A:2810:A:N6	1:1A:2891:G:O2'	2.36	0.57
9:1N:89:LYS:O	9:1N:93:THR:OG1	2.18	0.57
12:1Q:39:PRO:HB3	12:1Q:99:PRO:HD3	1.84	0.57
13:1R:38:VAL:HG22	13:1R:112:ALA:HB2	1.86	0.57
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.39	0.57
1:2A:864:G:H21	1:2A:866:A:H61	1.49	0.57
31:19:27:CYS:SG	31:19:28:GLU:N	2.77	0.57
1:2A:1470:G:N2	1:2A:1520:G:OP2	2.36	0.57
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.38	0.57
1:2A:452:G:OP2	58:2A:3743:HOH:O	2.17	0.57
1:1A:807:U:OP2	11:1P:41:ARG:NH2	2.37	0.57
1:2A:1002:G:N3	1:2A:1003:G:H8	4.16	0.57
1:2A:1267:U:O2'	58:2A:3747:HOH:O	2.18	0.57
1:2A:1426:G:O2'	1:2A:1572:A:N6	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2119:A:H61	1:2A:2168:G:H21	1.51	0.57
1:2A:2572:A:OP1	1:2A:2574:G:O2'	2.18	0.57
1:2A:601:C:O2'	1:2A:605:C:OP1	2.17	0.57
5:2F:85:GLY:O	58:2F:5901:HOH:O	2.18	0.57
6:1G:122:PRO:HD3	6:1G:181:ARG:HG2	1.86	0.57
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.85	0.57
1:1A:64:A:C5	19:1X:66:LEU:HD12	2.40	0.57
29:27:13:ALA:HB2	29:27:46:VAL:HG21	1.86	0.57
1:2A:2823:A:OP1	4:2E:159:HIS:NE2	2.35	0.57
1:1A:1701:A:OP2	58:1A:4050:HOH:O	2.18	0.57
1:1A:2308:G:O2'	1:1A:2310:A:N7	2.38	0.57
1:1A:113:G:H2'	1:1A:114:U:C6	5.51	0.56
1:1A:568:U:O2'	58:1A:4012:HOH:O	2.09	0.56
2:1B:77:U:OP1	21:1Z:19:ARG:NH2	2.38	0.56
1:2A:1590:U:H2'	1:2A:1591:G:H8	1.68	0.56
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.87	0.56
2:2B:98:G:N7	58:2B:303:HOH:O	2.32	0.56
1:1A:2285:C:OP2	28:16:6:ARG:NH1	2.37	0.56
1:1A:1410:G:H2'	1:1A:1411:C:H6	2.02	0.56
8:1I:77:LEU:HD22	8:1I:101:LEU:HG	1.86	0.56
1:2A:2536:G:O6	58:2A:3746:HOH:O	2.17	0.56
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.40	0.56
1:1A:657:U:H2'	1:1A:658:C:C6	2.40	0.56
13:1R:96:ARG:NH2	13:1R:118:GLU:OE2	2.39	0.56
1:2A:1084:A:N6	1:2A:1086:A:N7	2.53	0.56
1:2A:848:G:OP1	58:2A:3749:HOH:O	2.18	0.56
15:1T:91:ARG:HB2	15:1T:121:ILE:HG13	1.86	0.56
1:2A:2347:C:O2'	28:26:21:TYR:OH	2.23	0.56
1:2A:2499:C:OP2	58:2A:3750:HOH:O	2.18	0.56
6:2G:113:ARG:HD2	6:2G:140:ILE:HA	1.87	0.56
1:1A:1410:G:H2'	1:1A:1411:C:C6	2.71	0.56
1:1A:751:A:OP1	58:1A:4051:HOH:O	2.18	0.56
5:2F:155:LEU:HD11	5:2F:176:LEU:HD12	1.88	0.56
1:2A:2206:G:H8	1:2A:2207:G:N7	2.03	0.56
1:2A:751:A:OP1	58:2A:3741:HOH:O	2.17	0.56
1:1A:1968:G:OP1	58:1A:4049:HOH:O	2.17	0.56
1:1A:963:U:H2'	1:1A:964:C:C6	2.40	0.56
6:2G:15:VAL:HG21	6:2G:176:LEU:HD23	1.86	0.56
1:1A:746:A:N7	58:1A:4176:HOH:O	2.33	0.56
8:1I:38:LEU:HB3	8:1I:40:THR:HG23	1.87	0.56
1:2A:2347:C:HO2'	28:26:21:TYR:HH	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1041:C:H42	1:2A:1114:G:H1	1.52	0.56
6:2G:41:GLN:HB3	6:2G:43:LEU:HD13	1.86	0.56
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.86	0.56
15:1T:28:VAL:O	15:1T:46:GLU:HA	2.05	0.56
1:2A:1300:U:H4'	1:2A:1301:A:H5'	1.87	0.56
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.41	0.56
3:2D:69:ARG:NH2	3:2D:128:GLY:O	2.28	0.56
6:2G:19:LEU:HD13	6:2G:32:PRO:HD2	1.88	0.56
18:2W:11:ARG:NH1	18:2W:99:ARG:O	2.38	0.56
1:1A:986:C:HO2'	1:1A:1001:A:HO2'	1.52	0.56
1:2A:2156:G:N7	1:2A:2157:G:N2	2.54	0.56
2:2B:49:C:OP2	14:2S:30:ARG:NH1	2.39	0.56
3:2D:17:THR:O	3:2D:211:ARG:NH2	2.37	0.56
1:1A:1075:C:N4	1:1A:1077:A:N1	2.54	0.56
1:1A:1347:G:H1	1:1A:1599:C:H42	1.54	0.56
1:1A:2031:A:N3	1:1A:2455:G:O2'	2.35	0.56
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.06	0.56
1:1A:848:G:H2'	1:1A:849:A:C8	2.41	0.56
1:2A:811:U:OP1	58:2A:3751:HOH:O	2.18	0.56
17:2V:59:ALA:HB2	17:2V:96:ILE:HD13	1.88	0.56
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.21	0.55
1:1A:582:G:H2'	1:1A:583:G:C8	2.41	0.55
6:1G:66:GLN:OE1	6:1G:98:ARG:NE	2.36	0.55
11:1P:141:ALA:HA	25:23:38:GLU:HG2	1.88	0.55
5:2F:95:ARG:HD3	5:2F:97:TYR:CZ	2.41	0.55
12:1Q:55:VAL:HG12	12:1Q:64:ILE:HD12	1.88	0.55
21:1Z:69:THR:HG22	21:1Z:90:VAL:HA	1.89	0.55
1:2A:1525:G:H2'	1:2A:1526:G:H8	1.72	0.55
3:2D:142:VAL:HG23	3:2D:193:VAL:HA	1.88	0.55
1:1A:1683:C:H2'	1:1A:1684:C:C6	2.41	0.55
1:1A:185:U:H4'	1:1A:218:A:H4'	1.88	0.55
10:1O:66:LYS:N	10:1O:82:ASN:OD1	2.31	0.55
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.88	0.55
1:2A:630:G:OP2	30:28:15:LYS:NZ	2.31	0.55
7:2H:164:TYR:HB2	7:2H:167:GLU:HB2	1.87	0.55
15:1T:16:ARG:NH1	15:1T:83:ILE:O	2.39	0.55
24:22:66:GLU:HG2	24:22:69:ARG:HH22	1.70	0.55
3:2D:41:GLY:O	3:2D:43:ARG:NH1	2.40	0.55
22:10:27:GLU:HB2	22:10:69:PHE:HD1	1.72	0.55
1:1A:674:G:H2'	1:1A:675:A:C8	5.29	0.55
9:1N:9:VAL:HG21	9:1N:39:ARG:NH2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:24:PRO:HA	15:1T:49:VAL:HG23	1.87	0.55
20:1Y:15:VAL:HG21	20:1Y:42:VAL:HG11	1.88	0.55
1:2A:1799:G:O2'	3:2D:183:ARG:NH1	2.40	0.55
1:1A:1141:U:OP2	9:1N:63:THR:OG1	2.21	0.55
1:1A:1912:A:C5	1:1A:1918:A:H2	2.25	0.55
1:1A:458:G:O2'	1:1A:469:G:O6	2.21	0.55
7:1H:11:VAL:HG21	7:1H:50:VAL:HG23	1.88	0.55
24:22:19:VAL:HG12	24:22:23:LYS:HE3	1.87	0.55
1:2A:1003:G:N3	1:2A:1003:G:H3'	4.49	0.55
28:16:36:LEU:O	28:16:48:VAL:HA	2.06	0.55
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.41	0.55
1:2A:399:G:OP2	58:2A:3752:HOH:O	2.18	0.55
1:2A:635:C:O2'	1:2A:639:U:OP1	2.23	0.55
1:2A:820:A:N3	1:2A:943:U:O2'	2.36	0.55
1:1A:2825:G:O5'	1:1A:2825:G:H8	1.89	0.55
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.42	0.55
9:1N:110:GLY:O	9:1N:114:ARG:HG3	2.06	0.55
1:2A:84:A:N1	1:2A:98:G:O2'	2.37	0.55
3:2D:67:PHE:HD1	3:2D:153:ALA:HB3	1.72	0.55
1:1A:674:G:H2'	1:1A:675:A:H8	5.01	0.55
1:1A:1279:G:H4'	13:1R:31:HIS:CD2	2.42	0.55
3:2D:143:HIS:ND1	3:2D:194:GLY:O	2.32	0.55
1:1A:1508:A:H4'	1:1A:1509:A:C4	2.42	0.55
1:1A:1651:G:OP1	13:1R:40:LYS:NZ	2.39	0.55
1:1A:1911:PSU:N3	1:1A:1918:A:C4	2.75	0.55
1:1A:299:A:N1	1:1A:322:A:O2'	2.33	0.55
7:1H:159:GLU:HG2	7:1H:169:VAL:HG11	1.88	0.55
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.42	0.55
1:2A:2561:A:H2	10:2O:23:ARG:HH21	1.54	0.55
3:2D:85:ASP:OD2	3:2D:88:ARG:NH1	2.38	0.54
31:29:2:LYS:HB2	31:29:34:GLN:HG2	1.88	0.54
6:2G:170:ARG:NH2	6:2G:182:LYS:O	2.40	0.54
2:2B:42:C:O2	6:2G:93:THR:N	2.30	0.54
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.87	0.54
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.39	0.54
1:1A:521:G:O6	58:1A:4047:HOH:O	2.17	0.54
1:1A:577:G:O2'	1:1A:1254:A:OP1	2.26	0.54
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.89	0.54
1:2A:1063:G:H1	1:2A:1075:C:N4	2.04	0.54
1:2A:2444:G:OP2	58:2A:3745:HOH:O	2.17	0.54
1:2A:307:G:N1	1:2A:310:A:OP2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1637:A:OP2	58:2A:3753:HOH:O	2.19	0.54
1:2A:2140:C:H2'	1:2A:2141:G:H8	1.72	0.54
23:11:52:ARG:NH2	23:11:55:GLY:O	2.40	0.54
1:1A:1175:U:H5''	1:1A:1177:A:H2	1.72	0.54
12:1Q:39:PRO:HD3	12:1Q:99:PRO:HG3	1.90	0.54
26:24:36:CYS:SG	26:24:37:SER:N	2.80	0.54
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.89	0.54
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.21	0.54
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.73	0.54
1:1A:885:C:H1'	1:1A:892:G:H22	1.73	0.54
20:1Y:13:VAL:HG12	20:1Y:74:PRO:HA	1.90	0.54
1:2A:1066:U:O2'	1:2A:1068:G:OP2	2.23	0.54
1:2A:2503:2MA:O2'	1:2A:2505:G:OP2	2.20	0.54
1:2A:1983:C:H4'	1:2A:2606:C:H4'	1.89	0.54
2:1B:12:C:H2'	22:10:73:GLY:HA3	1.90	0.54
1:1A:2058:A:N7	58:1A:4183:HOH:O	2.34	0.54
1:1A:2467:C:O2	12:1Q:124:LYS:NZ	2.41	0.54
1:2A:1991:U:H2'	1:2A:1992:G:H5''	1.90	0.54
1:2A:212:G:H2'	1:2A:213:A:O4'	2.08	0.54
1:2A:2206:G:H5''	1:2A:2207:G:C8	2.43	0.54
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.42	0.54
1:2A:1446:C:H42	1:2A:1465:G:H1	1.55	0.54
1:1A:1048:A:OP2	1:1A:1109:C:N4	2.41	0.54
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.23	0.54
1:1A:2197:U:H1'	1:1A:2198:A:C8	2.43	0.54
1:1A:2612:C:OP1	58:1A:4055:HOH:O	2.19	0.54
3:1D:69:ARG:HH11	3:1D:105:ILE:HG21	1.73	0.54
1:2A:2321:G:O2'	1:2A:2322:A:OP1	2.25	0.54
11:2P:95:VAL:HG22	11:2P:125:VAL:HA	1.88	0.54
26:14:16:CYS:SG	26:14:17:GLY:N	2.81	0.53
1:1A:579:G:O2'	1:1A:2019:A:OP1	2.25	0.53
1:2A:1147:C:H2'	1:2A:1148:A:H8	1.72	0.53
2:2B:112:U:H2'	2:2B:113:G:H8	1.72	0.53
18:1W:67:ASP:N	18:1W:67:ASP:OD1	2.40	0.53
2:2B:40:U:H2'	26:24:2:LYS:HE3	1.90	0.53
1:2A:2551:C:OP2	58:2A:3748:HOH:O	2.18	0.53
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.19	0.53
9:1N:35:ARG:HH21	9:1N:42:TRP:HZ2	1.57	0.53
1:2A:1045:A:H8	1:2A:1047:G:N3	2.06	0.53
1:2A:300:A:H2'	1:2A:334:C:H1'	1.89	0.53
1:2A:34:C:H2'	1:2A:35:G:C8	6.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:4:ILE:HD11	8:2I:44:LEU:HD12	1.90	0.53
28:16:23:THR:OG1	28:16:24:GLU:N	2.41	0.53
1:1A:2059:A:C8	1:1A:2503:2MA:HM23	2.43	0.53
1:1A:370:G:OP2	58:1A:4054:HOH:O	2.18	0.53
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.09	0.53
1:2A:1508:A:H4'	1:2A:1509:A:C4	2.43	0.53
1:2A:55:G:H2'	1:2A:56:A:H8	1.72	0.53
1:2A:571:A:N6	1:2A:2499:C:O3'	2.40	0.53
1:2A:615:G:OP2	5:2F:43:LYS:NZ	2.33	0.53
1:2A:953:A:OP2	12:2Q:16:ARG:NH2	2.42	0.53
1:1A:982:C:OP2	58:1A:4053:HOH:O	2.18	0.53
3:1D:173:VAL:O	3:1D:184:LYS:HA	2.09	0.53
27:25:41:PRO:O	27:25:44:THR:OG1	2.24	0.53
1:2A:2128:C:H42	1:2A:2160:G:H1	1.54	0.53
1:2A:2882:A:OP1	13:2R:96:ARG:NH1	2.42	0.53
1:1A:220:G:O2'	1:1A:233:A:N3	2.36	0.53
6:1G:18:GLU:OE2	6:1G:22:ARG:NH2	2.40	0.53
30:28:6:THR:HG22	30:28:63:PRO:HD2	1.89	0.53
1:2A:1064:C:H3'	1:2A:1065:U:C5'	2.39	0.53
1:2A:1355:G:H2'	1:2A:1356:G:C8	2.97	0.53
10:1O:64:ARG:HB2	10:1O:79:PHE:CD1	2.43	0.53
18:1W:25:ARG:NH2	18:1W:74:ALA:O	2.41	0.53
1:2A:1073:A:H2'	1:2A:1074:G:H8	1.72	0.53
1:2A:764:A:H5''	3:2D:210:GLY:HA2	1.91	0.53
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.44	0.53
19:2X:44:GLU:OE1	58:2X:201:HOH:O	2.18	0.53
1:1A:573:G:O2'	1:1A:574:C:H3'	2.09	0.53
10:1O:13:ASN:ND2	10:1O:96:THR:OG1	2.39	0.53
1:2A:1278:A:H2'	1:2A:1279:G:C8	2.43	0.53
6:2G:108:ASN:HA	26:24:37:SER:HB3	1.90	0.53
12:2Q:75:THR:HG21	12:2Q:87:LYS:HG2	1.91	0.53
13:2R:36:THR:HG22	13:2R:37:THR:H	1.74	0.53
1:1A:2668:G:N7	58:1A:4185:HOH:O	2.34	0.53
1:1A:1791:A:H5'	3:1D:206:LEU:HD12	1.90	0.53
1:2A:2398:U:H2'	1:2A:2399:G:C8	2.44	0.53
8:1I:72:LEU:HD23	8:1I:75:LEU:HD21	1.90	0.53
15:1T:54:ARG:HA	15:1T:59:THR:HG22	1.90	0.53
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.74	0.53
1:2A:247:G:H4'	1:2A:386:G:C5	2.44	0.53
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.42	0.53
1:1A:1045:A:H5'	1:1A:1046:A:H5'	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2314:C:H2'	1:1A:2315:G:H8	1.74	0.52
1:2A:1086:A:OP1	1:2A:1104:C:O2'	2.27	0.52
1:2A:144:C:H2'	1:2A:145:G:H8	1.74	0.52
13:2R:98:LEU:HD12	27:25:57:VAL:HG11	1.92	0.52
1:1A:1142(A):A:O2'	1:1A:1143:A:H3'	2.10	0.52
1:2A:383:U:H2'	1:2A:385:C:H5	1.75	0.52
1:2A:2574:G:N3	4:2E:143:ASN:ND2	2.57	0.52
24:12:32:LEU:HD22	24:12:36:ARG:HH11	1.75	0.52
31:19:2:LYS:NZ	31:19:31:LYS:O	2.41	0.52
1:1A:2061:G:H5''	1:1A:2503:2MA:C2	2.39	0.52
1:1A:330:A:H2	1:1A:1210:A:O2'	1.92	0.52
1:2A:84:A:H5'	20:2Y:8:LYS:HB3	1.91	0.52
12:2Q:63:LYS:HD2	21:2Z:175:VAL:HG21	1.92	0.52
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.43	0.52
15:1T:76:PHE:HB3	15:1T:83:ILE:HD11	1.90	0.52
8:2I:26:ALA:HA	8:2I:30:LEU:HB2	1.90	0.52
17:2V:57:VAL:HG12	17:2V:99:ILE:HG23	1.91	0.52
17:2V:30:GLY:H	17:2V:61:VAL:HG23	1.74	0.52
1:1A:574:C:OP2	58:1A:4057:HOH:O	2.19	0.52
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.45	0.52
6:2G:80:PHE:O	6:2G:82:LEU:N	2.43	0.52
1:1A:1074:G:H2'	1:1A:1075:C:H6	3.87	0.52
1:1A:2448:A:OP1	58:1A:4006:HOH:O	2.19	0.52
1:1A:581:C:H2'	1:1A:582:G:C8	2.45	0.52
1:1A:826:U:OP1	58:1A:4002:HOH:O	2.18	0.52
1:2A:1081:U:H2'	1:2A:1082:U:H5''	1.91	0.52
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.44	0.52
1:2A:559:G:H22	16:2U:49:HIS:CE1	2.28	0.52
1:1A:2349:G:OP2	30:18:42:ARG:NE	2.35	0.52
1:2A:2312:U:H5'	6:2G:88:ILE:HD11	1.92	0.52
1:2A:2749:A:OP1	7:2H:3:ARG:NH1	2.43	0.52
10:2O:73:ASP:OD2	15:2T:32:TYR:OH	2.24	0.52
14:2S:41:ASP:OD2	14:2S:44:LYS:NZ	2.37	0.52
24:12:39:ALA:HB2	24:12:44:LEU:HD23	1.90	0.52
1:1A:1530:C:HO2'	1:1A:1531:C:H6	1.56	0.52
1:1A:1826:G:H4'	3:1D:242:ARG:NH1	2.24	0.52
1:1A:2064:C:H2'	1:1A:2065:C:C6	2.44	0.52
1:1A:2637:U:H5''	4:1E:82:ARG:NH1	2.25	0.52
3:2D:108:PRO:HD2	3:2D:111:LEU:HD12	1.92	0.52
1:1A:37:C:H2'	1:1A:38:A:C8	2.45	0.52
1:1A:651:G:OP1	30:18:19:SER:OG	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.45	0.52
1:2A:2369:A:H2'	1:2A:2370:G:H8	1.75	0.52
3:2D:244:ARG:NH2	58:2D:404:HOH:O	2.41	0.52
25:13:35:ARG:HE	25:13:37:LEU:HD21	1.74	0.51
1:1A:190:A:N3	1:1A:679:C:O2'	2.41	0.51
1:1A:2615:U:OP2	58:1A:4060:HOH:O	2.19	0.51
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.92	0.51
21:1Z:144:LEU:HD11	21:1Z:150:LEU:HD22	1.92	0.51
1:2A:149:A:H2'	1:2A:150:C:C6	2.88	0.51
12:1Q:51:ARG:O	12:1Q:55:VAL:HG13	2.10	0.51
1:1A:436:C:H2'	1:1A:437:G:H8	1.73	0.51
19:1X:26:TYR:OH	19:1X:93:GLU:OE2	2.24	0.51
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.25	0.51
1:2A:2817:G:O2'	1:2A:2836:U:O2	2.25	0.51
1:2A:333:G:H2'	1:2A:334:C:H6	3.23	0.51
17:2V:72:VAL:HG13	17:2V:85:LYS:HB3	1.92	0.51
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.10	0.51
1:2A:2299:G:H2'	1:2A:2300:G:H8	1.74	0.51
1:2A:252:G:OP1	11:2P:50:ARG:NH1	2.35	0.51
1:2A:2590:A:H5''	3:2D:239:ARG:HG3	1.92	0.51
1:2A:2584:U:H5''	1:2A:2602:A:C2	2.45	0.51
1:1A:1336:A:H2'	1:1A:1337:G:C8	2.46	0.51
1:1A:876:C:H2'	1:1A:877:U:O4'	2.11	0.51
28:26:10:LEU:HD23	28:26:22:ALA:HB2	1.93	0.51
3:2D:182:LEU:HB2	3:2D:272:ALA:H	1.76	0.51
6:2G:94:LEU:HD22	6:2G:98:ARG:HB3	1.93	0.51
1:1A:2046:G:H5'	27:15:19:ARG:HG3	1.93	0.51
1:1A:1952:A:OP1	10:1O:44:LYS:NZ	2.28	0.51
1:1A:1490:A:O2'	3:1D:99:ASP:OD1	2.29	0.51
9:2N:62:VAL:HG11	9:2N:66:LYS:HB2	1.93	0.51
14:2S:50:SER:O	14:2S:76:LYS:NZ	2.34	0.51
1:2A:904:C:O2'	21:2Z:169:GLU:OE2	2.25	0.51
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.46	0.51
1:1A:2595:G:N2	1:1A:2598:A:OP2	2.37	0.51
1:2A:1096:A:C8	1:2A:1097:U:H5	2.28	0.51
1:2A:1590:U:H2'	1:2A:1591:G:C8	2.46	0.51
21:2Z:45:ASP:OD1	21:2Z:49:ARG:NE	2.44	0.51
1:2A:2299:G:H2'	1:2A:2300:G:C8	2.46	0.51
20:2Y:68:HIS:HB3	20:2Y:71:LYS:HG3	1.92	0.51
29:17:12:ARG:NH2	29:17:44:PRO:HB3	2.25	0.51
1:1A:436:C:H2'	1:1A:437:G:C8	2.47	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1842:G:O2'	3:2D:253:GLN:OE1	2.26	0.51
1:1A:1707:G:O6	58:1A:4044:HOH:O	2.17	0.50
1:2A:2527:C:H5''	31:29:30:PRO:HB3	1.93	0.50
7:2H:87:LEU:HD23	7:2H:164:TYR:HA	1.93	0.50
18:2W:29:LEU:HD22	18:2W:69:LEU:HD12	1.92	0.50
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	1.92	0.50
1:1A:1300:U:H4'	1:1A:1301:A:C5'	2.40	0.50
1:1A:1911:PSU:C2	1:1A:1918:A:C4	2.96	0.50
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.44	0.50
1:2A:1027:A:C2	1:2A:2488:A:H5'	2.46	0.50
1:2A:1067:A:O2'	1:2A:1068:G:OP2	5.17	0.50
1:2A:817:C:O2'	1:2A:839:U:H5''	2.11	0.50
10:2O:36:GLY:HA3	10:2O:109:LYS:HD2	1.92	0.50
12:2Q:54:MET:HG2	12:2Q:117:ALA:HB1	1.93	0.50
24:12:35:LEU:HD12	24:12:53:LEU:HD12	1.93	0.50
1:1A:1794:U:H2'	1:1A:1795:C:H6	1.75	0.50
1:1A:271(Z):C:H1'	1:1A:272(C):G:H1'	1.92	0.50
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.11	0.50
19:1X:29:TRP:CE3	19:1X:78:LYS:HB3	2.46	0.50
1:2A:530:G:N1	1:2A:2023:G:OP1	2.43	0.50
1:2A:2375:G:O2'	1:2A:2377:A:N7	2.34	0.50
2:2B:37:C:O2	14:2S:95:HIS:NE2	2.44	0.50
9:2N:58:ASP:N	9:2N:58:ASP:OD1	2.44	0.50
13:2R:79:LEU:HA	13:2R:83:ILE:HD12	1.93	0.50
1:1A:1266:G:O2'	1:1A:2012:G:O6	2.21	0.50
1:2A:335:C:H2'	1:2A:336:C:H6	2.03	0.50
1:1A:1114:G:H2'	1:1A:1115:G:H8	1.75	0.50
10:1O:105:GLU:OE1	10:1O:105:GLU:N	2.42	0.50
10:1O:22:ILE:HD11	10:1O:40:VAL:HG12	1.93	0.50
20:1Y:99:CYS:SG	20:1Y:100:ALA:N	2.85	0.50
1:2A:1365:A:O5'	23:21:41:ARG:NH2	2.44	0.50
1:2A:1847:A:H3'	1:2A:1848:A:H5'	1.94	0.50
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.47	0.50
1:2A:566:U:H5''	11:2P:29:LYS:HE3	1.94	0.50
23:11:3:LYS:HG3	23:11:4:VAL:H	1.76	0.50
1:1A:1009:A:OP2	9:1N:37:LYS:NZ	2.36	0.50
1:2A:210:C:H4'	1:2A:1367:A:H1'	1.93	0.50
1:2A:586:A:N1	1:2A:809:G:O2'	2.39	0.50
1:2A:876:C:H2'	1:2A:877:U:O4'	2.12	0.50
13:2R:95:THR:HG22	13:2R:116:LEU:HD23	1.94	0.50
1:1A:1022:G:N7	9:1N:66:LYS:HE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:189:G:O6	1:1A:205:G:O2'	2.24	0.50
1:1A:2836:U:H2'	1:1A:2837:G:C8	2.47	0.50
6:1G:16:ARG:HB2	6:1G:17:PRO:HD3	1.93	0.50
15:1T:55:ASN:N	15:1T:59:THR:HG22	2.22	0.50
5:2F:46:ARG:HB3	5:2F:48:THR:HG23	1.93	0.50
7:2H:144:VAL:O	7:2H:148:ILE:HG12	2.12	0.50
13:2R:103:ARG:NH1	13:2R:108:GLY:O	2.42	0.50
19:2X:26:TYR:HB3	19:2X:92:LEU:HD22	1.94	0.50
3:1D:108:PRO:HD2	3:1D:111:LEU:HD12	1.94	0.50
1:2A:1899:G:N3	1:2A:1899:G:H2'	2.27	0.50
1:2A:790:C:OP2	58:2A:3761:HOH:O	2.20	0.50
15:2T:53:ARG:O	15:2T:59:THR:HG23	2.11	0.50
1:1A:1889:A:H2'	1:1A:1890:A:C8	2.47	0.50
19:1X:44:GLU:HG2	19:1X:51:VAL:HG23	1.93	0.50
30:28:62:LEU:HB3	30:28:65:GLU:HG3	1.94	0.50
1:2A:1025:G:O2'	58:2A:3756:HOH:O	2.20	0.50
1:2A:2502:G:OP2	58:2A:3754:HOH:O	2.19	0.50
5:2F:158:THR:O	5:2F:164:ARG:NH1	2.39	0.50
1:1A:1482:G:H1	1:1A:1506:C:H42	1.60	0.49
2:1B:22:U:H2'	2:1B:23:G:C8	2.46	0.49
4:1E:34:VAL:HG23	4:1E:48:GLN:HE21	1.77	0.49
1:2A:1525:G:H2'	1:2A:1526:G:C8	2.46	0.49
1:2A:270:A:OP2	1:2A:271(X):G:N1	2.36	0.49
1:2A:668:G:H5'	1:2A:669:G:OP2	2.12	0.49
10:2O:34:THR:OG1	10:2O:35:VAL:N	2.45	0.49
1:1A:2227:A:OP2	58:1A:4067:HOH:O	2.20	0.49
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.95	0.49
1:1A:2784:C:H1'	4:1E:37:ARG:HH12	1.77	0.49
1:2A:942:G:O2'	1:2A:1189:A:N3	2.38	0.49
1:2A:1248:G:C5	16:2U:3:ARG:HB2	2.48	0.49
1:2A:1856:G:O6	58:2A:3762:HOH:O	2.20	0.49
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.12	0.49
9:1N:62:VAL:HG22	9:1N:66:LYS:HD2	1.93	0.49
1:2A:1442:G:N3	1:2A:1442:G:H2'	3.00	0.49
1:2A:1779:U:OP2	58:2A:3760:HOH:O	2.20	0.49
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.12	0.49
12:2Q:39:PRO:HD3	12:2Q:99:PRO:HG3	1.94	0.49
13:2R:70:LEU:O	13:2R:72:ASP:N	2.44	0.49
22:10:53:MET:HG3	22:10:59:LEU:HD12	1.95	0.49
29:17:24:THR:HG23	29:17:27:GLY:H	1.77	0.49
1:1A:2038:G:O6	58:1A:4056:HOH:O	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:164:ARG:HE	55:1F:303:ARG:HH12	1.59	0.49
18:1W:9:TYR:H	18:1W:102:HIS:CE1	2.31	0.49
20:1Y:9:LYS:HA	20:1Y:27:VAL:HB	1.94	0.49
1:2A:441:U:H2'	1:2A:442:G:C8	2.46	0.49
8:2I:77:LEU:HD13	8:2I:101:LEU:HD23	1.94	0.49
11:2P:126:VAL:HG12	11:2P:148:LEU:HD23	1.94	0.49
12:2Q:41:TRP:HB3	12:2Q:94:VAL:HB	1.93	0.49
1:1A:1912:A:C5	1:1A:1918:A:C2	3.01	0.49
1:1A:2464:C:O2'	58:1A:4062:HOH:O	2.19	0.49
3:1D:130:ALA:HA	3:1D:191:ALA:O	2.12	0.49
6:1G:98:ARG:NH1	26:14:1:MET:SD	2.86	0.49
7:1H:101:ARG:HG2	7:1H:117:PRO:HG2	1.94	0.49
20:1Y:10:GLY:HA2	20:1Y:27:VAL:HB	1.94	0.49
29:27:30:VAL:HG22	29:27:33:ARG:HH22	1.76	0.49
1:2A:1911:PSU:N3	1:2A:1918:A:C4	2.81	0.49
1:2A:1916:A:H2'	1:2A:1917:PSU:O4'	2.13	0.49
5:2F:101:LEU:HD12	5:2F:102:PRO:HD2	1.95	0.49
18:2W:18:ARG:NH1	18:2W:76:VAL:O	2.45	0.49
2:2B:75:G:O3'	21:2Z:10:ARG:NH2	2.45	0.49
1:1A:535:C:O3'	16:1U:53:ARG:NH1	2.45	0.49
5:1F:117:ARG:NH2	5:1F:189:THR:O	2.43	0.49
16:1U:97:ASP:O	16:1U:101:ARG:HB2	2.12	0.49
1:2A:397:G:N7	58:2A:3888:HOH:O	2.35	0.49
3:2D:260:ARG:NH1	3:2D:267:SER:OG	2.40	0.49
5:2F:24:LEU:HD23	5:2F:115:ALA:HA	1.94	0.49
12:2Q:55:VAL:HG11	21:2Z:183:LEU:HD21	1.95	0.49
18:2W:6:ILE:HG22	18:2W:8:ARG:HG3	1.94	0.49
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.47	0.49
1:1A:1407:C:H2'	1:1A:1408:C:H6	1.76	0.49
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.48	0.49
2:1B:48:A:H4'	14:1S:95:HIS:HD2	1.77	0.49
3:1D:71:ASP:HB3	3:1D:103:ARG:HH22	1.78	0.49
1:1A:483:A:O2'	20:1Y:49:VAL:O	2.22	0.49
4:2E:4:ILE:HD13	4:2E:28:ALA:HB1	1.94	0.49
5:2F:33:LEU:HD13	5:2F:112:MET:HE1	1.95	0.49
1:2A:2313:C:H5''	6:2G:91:ARG:HD3	1.94	0.49
12:2Q:30:GLY:HA2	12:2Q:107:ALA:HB2	1.95	0.49
1:1A:615:G:OP1	5:1F:40:GLN:NE2	2.43	0.49
6:1G:139:LEU:HD21	6:1G:149:VAL:HG11	1.93	0.49
15:1T:24:PRO:HD3	15:1T:52:ILE:HD12	1.94	0.49
18:1W:46:PHE:O	18:1W:50:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2659:G:N2	1:2A:2662:A:OP2	2.43	0.49
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.48	0.49
1:2A:1155:A:H5''	16:2U:55:ARG:HD3	1.94	0.49
18:2W:6:ILE:HG12	18:2W:104:THR:HG23	1.95	0.49
1:1A:1334:G:OP2	58:1A:4068:HOH:O	2.20	0.49
1:1A:1608:A:H1'	1:1A:1610:A:OP2	2.12	0.49
1:1A:2096:U:H2'	1:1A:2097:C:C6	2.48	0.49
1:1A:271(E):U:H2'	1:1A:271(F):C:C6	2.48	0.49
1:1A:776:G:N7	1:1A:793:A:O2'	2.39	0.49
18:1W:57:ASN:O	18:1W:61:ASN:HB2	2.11	0.49
1:2A:1200:C:O2	1:2A:1205:U:N3	23.48	0.49
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.30	0.49
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	1.95	0.49
1:2A:95:G:H4'	24:22:46:GLN:HA	1.93	0.49
5:2F:101:LEU:HD23	5:2F:106:ARG:HG2	1.95	0.49
20:2Y:6:HIS:CD2	20:2Y:7:VAL:HG23	2.48	0.49
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.48	0.49
1:1A:1452:A:OP2	58:1A:4063:HOH:O	2.19	0.49
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	1.95	0.49
4:1E:109:LYS:O	4:1E:111:ARG:NH1	2.45	0.49
1:1A:2313:C:H5''	6:1G:91:ARG:HD3	1.94	0.49
8:1I:68:LEU:HD21	8:1I:109:ILE:HD11	1.94	0.49
1:2A:189:G:H1	1:2A:205:G:HO2'	1.61	0.49
1:2A:2171:A:H4'	1:2A:2172:U:OP1	2.10	0.49
6:2G:72:ARG:HG2	6:2G:87:PRO:HA	1.94	0.49
31:19:15:LYS:HG2	31:19:17:ILE:HD11	1.95	0.48
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.48	0.48
1:1A:1406:U:O2	1:1A:1517:G:N2	33.15	0.48
1:1A:2312:U:H5'	6:1G:88:ILE:HD11	1.95	0.48
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.47	0.48
1:1A:34:C:H2'	1:1A:35:G:C8	3.89	0.48
1:1A:571:A:O2'	17:1V:78:LYS:HE2	2.13	0.48
1:1A:897:C:H2'	1:1A:898:C:C6	2.48	0.48
3:1D:10:THR:OG1	3:1D:13:ARG:HG2	2.13	0.48
4:1E:101:ARG:HB3	4:1E:201:THR:HG21	1.95	0.48
7:1H:84:SER:HA	7:1H:133:VAL:O	2.13	0.48
1:2A:1827:C:O2'	1:2A:1970:A:N3	2.34	0.48
1:2A:77:C:H42	1:2A:109:G:H1	1.61	0.48
1:2A:806:C:O2	1:2A:2444:G:O2'	2.29	0.48
53:2B:201:MPD:O4	53:2B:201:MPD:O2	2.27	0.48
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1203:G:O2'	1:1A:1242:A:N6	2.45	0.48
1:1A:686:G:N2	1:1A:788:A:H61	2.10	0.48
1:2A:1670:C:OP1	58:2A:3765:HOH:O	2.20	0.48
1:2A:2705:A:N7	58:2A:3877:HOH:O	2.34	0.48
1:2A:822:U:H2'	1:2A:823:G:C8	2.46	0.48
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.95	0.48
1:1A:833:U:O2	11:1P:55:ARG:NH1	2.46	0.48
1:1A:889:C:O2'	1:1A:890:A:O4'	2.31	0.48
7:1H:27:LYS:HG2	7:1H:32:GLU:HG2	1.95	0.48
7:1H:3:ARG:HB3	7:1H:6:ARG:HG2	1.95	0.48
21:1Z:95:PRO:HA	21:1Z:129:SER:HA	1.95	0.48
1:2A:630:G:N2	1:2A:633:A:OP2	2.33	0.48
8:2I:101:LEU:O	8:2I:106:GLY:N	2.45	0.48
1:1A:1981:A:OP1	58:1A:4058:HOH:O	2.19	0.48
1:1A:2445:G:OP2	58:1A:4066:HOH:O	2.20	0.48
5:1F:178:PRO:HB2	5:1F:201:VAL:HG21	1.96	0.48
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.13	0.48
17:1V:72:VAL:HG13	17:1V:85:LYS:HB3	1.95	0.48
26:24:46:GLN:O	26:24:48:ARG:N	2.40	0.48
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.44	0.48
1:2A:2243:U:OP1	58:2A:3759:HOH:O	2.20	0.48
1:2A:2576:G:O2'	58:2A:3755:HOH:O	2.20	0.48
1:2A:78:A:H2'	1:2A:79:G:H8	1.79	0.48
10:2O:68:GLU:HB3	10:2O:78:ARG:HB2	1.96	0.48
1:1A:1022:G:N2	1:1A:1023:U:O4	2.33	0.48
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.94	0.48
7:1H:117:PRO:HG3	7:1H:123:PHE:CD2	2.48	0.48
12:1Q:125:LEU:HD12	12:1Q:129:THR:HG21	1.96	0.48
14:1S:65:VAL:O	14:1S:69:VAL:HG13	2.12	0.48
1:2A:1359:A:N3	1:2A:1359:A:H5'	2.28	0.48
1:2A:1818:U:O2'	3:2D:154:LYS:O	2.17	0.48
2:2B:105:A:O2'	21:2Z:30:ASN:O	2.29	0.48
1:2A:579:G:O2'	1:2A:2019:A:OP1	2.24	0.48
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.29	0.48
1:2A:964:C:O2'	1:2A:2273:A:N3	2.37	0.48
1:2A:2552:OMU:H6	1:2A:2552:OMU:O5'	2.13	0.48
1:2A:563:G:H22	1:2A:578:A:H2	1.62	0.48
1:2A:729:G:C5	3:2D:208:LYS:HB2	2.49	0.48
4:2E:26:ILE:HD11	4:2E:188:VAL:HG21	1.96	0.48
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.14	0.48
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.95	0.48
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.96	0.48
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.94	0.48
1:2A:903:C:H2'	1:2A:904:C:C6	2.49	0.48
4:2E:34:VAL:HG12	4:2E:72:VAL:HG11	1.95	0.48
5:2F:29:ASN:HB3	5:2F:112:MET:HE3	1.96	0.48
6:2G:145:THR:OG1	6:2G:146:TYR:N	2.45	0.48
1:1A:1114:G:H2'	1:1A:1115:G:C8	2.49	0.48
1:1A:2031:A:C6	1:1A:2498:C:H1'	2.49	0.48
1:1A:2712:U:OP1	1:1A:2714:G:H4'	2.13	0.48
1:1A:483:A:H5''	20:1Y:50:ARG:HD3	1.95	0.48
3:1D:146:GLU:HB2	3:1D:189:CYS:HB3	1.95	0.48
7:1H:88:LEU:HD23	7:1H:130:ARG:HG3	1.96	0.48
19:1X:57:LEU:HD11	19:1X:78:LYS:HE2	1.96	0.48
1:2A:2128:C:H1'	1:2A:2173:A:H2	1.78	0.48
1:2A:919:G:N2	1:2A:2269:A:OP2	2.46	0.48
1:2A:2602:A:C1'	1:2A:2603:G:H5''	2.41	0.48
1:2A:2857:G:N2	1:2A:2860:A:OP2	2.39	0.48
1:2A:869:G:O2'	1:2A:872:A:N7	14.33	0.48
1:2A:70:G:H1	1:2A:99:U:H3	37.54	0.48
7:2H:55:PRO:HG2	7:2H:61:HIS:ND1	2.28	0.48
22:10:33:ALA:N	22:10:64:ASP:OD1	2.46	0.48
1:1A:709:U:H2'	1:1A:710:G:C8	2.49	0.48
4:1E:34:VAL:HG21	4:1E:78:LEU:HD11	1.96	0.48
4:1E:82:ARG:HG3	4:1E:83:ASP:N	2.27	0.48
5:1F:18:ARG:NH1	5:1F:127:GLU:OE2	2.46	0.48
1:1A:747:U:H1'	18:1W:92:ARG:HH22	1.79	0.48
1:2A:1821:A:H2'	1:2A:1822:G:C8	2.49	0.48
1:2A:1649:G:O2'	13:2R:107:ASP:OD2	2.30	0.48
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.78	0.48
1:1A:1972:A:H2'	1:1A:1973:G:C8	2.45	0.48
1:1A:242:G:C8	30:18:5:LYS:HG2	2.49	0.48
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.95	0.48
1:2A:1355:G:H2'	1:2A:1356:G:H8	2.27	0.48
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.49	0.48
1:2A:539:G:H2'	1:2A:540:C:C6	2.49	0.48
25:13:13:ILE:O	58:13:201:HOH:O	2.20	0.47
1:1A:1552:G:N7	58:1A:4193:HOH:O	2.35	0.47
1:1A:1773:A:OP2	58:1A:4061:HOH:O	2.19	0.47
1:1A:2119:A:H61	1:1A:2168:G:H21	1.61	0.47
1:1A:2575:C:OP2	58:1A:4072:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:69:ARG:HE	3:1D:130:ALA:HB2	1.78	0.47
1:1A:2495:G:H5''	12:1Q:82:ARG:HG2	1.96	0.47
1:2A:1936:A:OP2	1:2A:1962:5MC:N4	2.40	0.47
1:2A:538:G:H2'	1:2A:539:G:H8	1.79	0.47
1:2A:731:C:OP1	58:2A:3766:HOH:O	2.20	0.47
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.47	0.47
1:1A:2086:U:H2'	1:1A:2087:G:H8	1.78	0.47
1:1A:858:U:O2	1:1A:2268:A:H2'	2.13	0.47
1:1A:247:G:H4'	1:1A:386:G:C5	2.49	0.47
1:2A:1509(A):A:H2'	1:2A:1510:G:O4'	2.14	0.47
1:2A:184:C:H2'	1:2A:185:U:C6	2.48	0.47
1:2A:2529:G:H5''	1:2A:2530:A:H5''	1.96	0.47
1:2A:578:A:OP2	58:2A:3767:HOH:O	2.20	0.47
16:2U:108:GLU:O	16:2U:112:ARG:HG2	2.14	0.47
1:1A:151:C:H2'	1:1A:152:G:H8	1.79	0.47
1:1A:1790:C:H5''	1:1A:1791:A:OP1	2.15	0.47
1:1A:2286:A:N6	28:16:23:THR:OG1	2.47	0.47
1:1A:800:A:OP1	1:1A:800:A:H8	1.97	0.47
1:2A:840:C:H2'	1:2A:841:A:C8	2.48	0.47
1:2A:942:G:OP2	11:2P:39:LYS:NZ	2.29	0.47
1:1A:2140:C:H2'	1:1A:2141:G:H8	1.78	0.47
1:1A:679:C:OP1	58:1A:4059:HOH:O	2.19	0.47
19:1X:43:VAL:HG21	19:1X:81:VAL:HG11	1.96	0.47
1:2A:1541:G:O6	58:2A:3764:HOH:O	2.20	0.47
1:2A:304:G:O6	58:2A:3758:HOH:O	2.20	0.47
9:2N:53:VAL:HG22	9:2N:121:LYS:HB2	1.95	0.47
1:1A:690:G:O2'	3:1D:43:ARG:NH2	2.47	0.47
1:2A:1365:A:O2'	23:21:11:ARG:NH2	2.47	0.47
1:2A:1568:G:P	3:2D:63:ARG:HH12	2.38	0.47
1:2A:385:C:O2'	1:2A:388:G:N2	2.47	0.47
1:2A:599:G:H4'	5:2F:31:HIS:HD2	1.79	0.47
7:2H:137:ASP:HB3	7:2H:140:LYS:HB3	1.97	0.47
1:1A:1171:G:H3'	1:1A:1173:G:H5'	1.96	0.47
1:1A:2008:C:OP2	58:1A:4073:HOH:O	2.21	0.47
1:1A:530:G:H4'	1:1A:531:C:OP1	2.14	0.47
16:1U:21:ALA:HA	16:1U:24:TYR:CE2	2.50	0.47
1:2A:1154:G:P	16:2U:58:ARG:HE	2.37	0.47
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.49	0.47
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.49	0.47
1:2A:320:A:H4'	1:2A:322:A:N7	2.30	0.47
4:2E:52:LEU:HB3	4:2E:53:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1512:U:H2'	1:1A:1513:C:C6	2.50	0.47
1:1A:1779:U:OP2	1:1A:1784:A:N6	2.28	0.47
1:1A:2142:C:H2'	1:1A:2143:C:C6	2.50	0.47
1:1A:527:C:OP1	58:1A:4032:HOH:O	2.20	0.47
1:2A:1266:G:N2	1:2A:1269:A:OP2	13.97	0.47
12:2Q:23:GLY:O	12:2Q:101:ARG:NH1	2.48	0.47
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.14	0.47
21:2Z:179:ASP:OD1	21:2Z:180:VAL:N	2.48	0.47
22:10:11:LYS:O	22:10:14:ARG:NH2	2.41	0.47
1:1A:1074:G:H2'	1:1A:1075:C:C6	4.60	0.47
10:1O:64:ARG:HB2	10:1O:79:PHE:CG	2.50	0.47
1:1A:907:U:O2'	12:1Q:101:ARG:NH2	2.47	0.47
1:1A:2319:G:H22	14:1S:3:ARG:CD	2.27	0.47
22:20:23:VAL:HG22	22:20:38:VAL:HG22	1.97	0.47
1:2A:177:G:H3'	1:2A:178:G:C8	2.49	0.47
1:2A:2110:G:OP1	1:2A:2118:U:N3	2.42	0.47
1:2A:2758:A:C4	7:2H:67:LEU:HD21	2.49	0.47
1:2A:434:U:H2'	1:2A:435:C:C6	6.37	0.47
8:2I:50:ARG:O	8:2I:54:GLN:HG2	2.15	0.47
14:2S:15:ARG:O	14:2S:19:LYS:HG2	2.15	0.47
1:2A:2849:U:OP2	15:2T:95:ARG:NH1	2.48	0.47
23:11:18:ILE:HG12	23:11:37:ILE:HG12	1.97	0.47
27:15:49:CYS:SG	27:15:51:TYR:HB2	2.54	0.47
1:1A:1468:C:H2'	1:1A:1469:A:C8	2.50	0.47
1:1A:2345:G:N3	1:1A:2381:C:H2'	2.30	0.47
1:1A:2759:G:OP2	58:1A:4065:HOH:O	2.20	0.47
2:1B:22:U:H2'	2:1B:23:G:H8	1.80	0.47
4:1E:110:GLY:HA2	4:1E:161:GLY:HA3	1.97	0.47
4:1E:120:TRP:CD1	4:1E:155:LYS:HB3	2.50	0.47
18:1W:12:ILE:HD13	18:1W:17:VAL:HG13	1.97	0.47
1:1A:24:G:O2'	18:1W:78:GLU:O	2.28	0.47
23:21:64:ALA:HA	23:21:67:ILE:HG13	1.97	0.47
1:2A:1076:C:H4'	1:2A:1077:A:OP1	2.15	0.47
1:2A:2251:OMG:HM23	1:2A:2251:OMG:H1'	1.62	0.47
1:2A:1022:G:N7	9:2N:66:LYS:HE2	2.29	0.47
1:1A:1040:C:H2'	1:1A:1041:C:O4'	2.15	0.47
1:1A:1336:A:H2'	1:1A:1337:G:H8	1.80	0.47
1:1A:2119:A:O2'	1:1A:2120:G:H5'	2.15	0.47
1:1A:329:G:O4'	1:1A:477:A:H1'	2.15	0.47
22:20:9:SER:OG	22:20:10:THR:N	2.48	0.47
1:2A:2115:G:N1	1:2A:2119:A:OP2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2193:G:H2'	1:2A:2194:G:C8	2.50	0.47
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.50	0.47
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.97	0.47
5:2F:148:LEU:HD13	5:2F:154:VAL:HG21	1.96	0.47
23:11:69:LYS:O	23:11:72:GLU:HB3	2.15	0.47
2:1B:25:A:OP2	58:1B:1102:HOH:O	2.21	0.47
3:1D:154:LYS:HB2	3:1D:155:LEU:HD12	1.97	0.47
7:1H:26:VAL:HG12	7:1H:79:VAL:HG21	1.96	0.47
22:20:27:GLU:HB2	22:20:69:PHE:HD1	1.79	0.47
1:2A:2458:G:H21	1:2A:2459:A:N6	2.13	0.47
1:2A:1953:A:HO2'	1:2A:2559:C:HO2'	1.61	0.47
1:2A:320:A:H4'	1:2A:322:A:C8	2.50	0.47
1:2A:342:G:O6	58:2A:3757:HOH:O	2.20	0.47
1:2A:779:U:OP1	3:2D:49:ILE:HG13	2.15	0.47
1:1A:1056:G:H5''	1:1A:1057:A:O4'	2.14	0.46
1:1A:1199:U:H2'	1:1A:1200:C:C6	2.51	0.46
1:1A:1509:A:H2'	1:1A:1509(A):A:C8	2.50	0.46
1:1A:731:C:OP1	58:1A:4071:HOH:O	2.20	0.46
5:1F:161:GLU:HG2	5:1F:164:ARG:NH2	2.29	0.46
8:1I:38:LEU:HD12	8:1I:38:LEU:HA	1.81	0.46
21:1Z:198:LYS:HD3	21:1Z:202:GLU:HB3	1.97	0.46
1:2A:851:U:OP1	25:23:49:LYS:NZ	2.38	0.46
1:2A:990:A:N6	1:2A:1186:G:H1'	2.30	0.46
24:12:1:MET:HE1	24:12:56:GLN:HG2	1.96	0.46
1:1A:190:A:P	1:1A:205:G:H22	2.37	0.46
1:1A:1971:A:C4	3:1D:241:PRO:HD3	2.50	0.46
1:1A:27:G:O2'	1:1A:28:A:OP2	2.32	0.46
10:1O:36:GLY:HA3	10:1O:109:LYS:HD2	1.97	0.46
19:1X:66:LEU:HA	19:1X:66:LEU:HD23	1.69	0.46
1:2A:2189:U:H2'	1:2A:2190:G:H8	1.80	0.46
1:2A:2469:A:H4'	12:2Q:56:ARG:HG2	1.97	0.46
9:2N:42:TRP:HA	9:2N:48:MET:SD	2.56	0.46
10:2O:120:GLU:OE1	15:2T:67:SER:OG	2.31	0.46
2:1B:91:C:OP2	12:1Q:16:ARG:NH1	2.49	0.46
12:1Q:116:GLU:OE2	12:1Q:119:ARG:NH2	2.43	0.46
19:1X:34:ALA:O	19:1X:77:LYS:NZ	2.48	0.46
21:1Z:91:LEU:HD23	21:1Z:130:PRO:HB3	1.96	0.46
1:2A:397:G:H5''	23:21:45:ASN:HB2	1.97	0.46
26:24:41:PRO:HG3	26:24:49:PHE:CE2	2.50	0.46
26:24:40:HIS:O	26:24:44:THR:HG22	2.14	0.46
1:2A:1441:G:H4'	1:2A:1442:G:C2	10.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:39:TRP:NE1	5:2F:99:TYR:O	2.47	0.46
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.96	0.46
1:1A:1023:U:O2'	1:1A:1122:G:H5'	2.16	0.46
1:1A:1442:G:H2'	1:1A:1442:G:N3	3.05	0.46
1:1A:1927:A:H2'	1:1A:1928:A:C8	2.51	0.46
1:1A:251:A:C5	1:1A:252:G:H1'	2.50	0.46
1:1A:2814:C:O2'	27:15:29:ILE:HG12	2.15	0.46
1:1A:27:G:N2	1:1A:512:G:H1'	2.30	0.46
1:1A:793:A:OP2	1:1A:2071:A:O2'	2.32	0.46
16:1U:92:ARG:HA	16:1U:95:LEU:HB2	1.96	0.46
2:2B:83:G:H4'	25:23:52:HIS:CG	2.51	0.46
1:2A:1509:A:H2'	1:2A:1509(A):A:O4'	2.15	0.46
1:2A:177:G:H3'	1:2A:178:G:H8	1.80	0.46
1:2A:2062:A:OP1	58:2A:3768:HOH:O	2.20	0.46
1:2A:2240:C:H2'	1:2A:2241:A:H8	1.80	0.46
1:2A:956:G:H2'	1:2A:957:A:H2'	1.97	0.46
2:2B:60:C:H2'	2:2B:61:G:H8	1.80	0.46
22:10:15:ASP:OD1	22:10:16:SER:N	2.40	0.46
28:16:25:LYS:HE3	28:16:27:LYS:HA	1.96	0.46
1:1A:1185:C:OP2	58:1A:4074:HOH:O	2.21	0.46
4:1E:9:VAL:HG22	4:1E:25:VAL:HB	1.97	0.46
1:1A:1257:C:H4'	5:1F:83:PHE:CD1	2.51	0.46
15:1T:112:ARG:HG2	15:1T:115:ARG:HH21	1.80	0.46
15:1T:9:LEU:O	15:1T:12:SER:OG	2.25	0.46
19:1X:60:ARG:NH1	29:17:47:ARG:HH22	2.14	0.46
21:1Z:54:HIS:ND1	21:1Z:101:PRO:HG3	2.31	0.46
25:23:8:LEU:HG	25:23:31:LEU:HD23	1.98	0.46
1:2A:1580:A:H3'	1:2A:1581:G:H8	1.80	0.46
1:2A:595:C:H2'	1:2A:596:G:H8	1.81	0.46
1:2A:1224:C:O2'	17:2V:85:LYS:HA	2.15	0.46
1:1A:1338:G:N7	19:1X:62:LYS:NZ	2.62	0.46
1:1A:184:C:H2'	1:1A:185:U:C6	2.51	0.46
1:1A:2241:A:N7	58:1A:4202:HOH:O	2.36	0.46
1:1A:624:C:H2'	1:1A:625:G:C8	2.94	0.46
1:1A:889:C:O2'	1:1A:890:A:O5'	2.33	0.46
3:1D:16:MET:HG3	3:1D:206:LEU:O	2.16	0.46
21:1Z:99:TYR:HA	21:1Z:124:ILE:O	2.16	0.46
1:2A:2218:U:O2	23:21:52:ARG:NH1	2.49	0.46
1:2A:975(A):G:O2'	1:2A:1156:A:N1	2.39	0.46
1:2A:11:G:H2'	1:2A:12:U:H5'	1.98	0.46
1:2A:1686:C:H2'	1:2A:1687:G:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2752:C:OP2	7:2H:4:ILE:HD11	2.15	0.46
1:2A:335:C:H4'	20:2Y:73:ARG:HD2	1.97	0.46
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.89	0.46
1:1A:1230:C:H2'	1:1A:1231:G:C8	2.50	0.46
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.50	0.46
1:1A:1475:G:O6	58:1A:4069:HOH:O	2.20	0.46
1:1A:2512:C:H2'	1:1A:2513:G:O4'	2.16	0.46
18:1W:71:VAL:HA	18:1W:107:LEU:HD12	1.98	0.46
23:21:40:ARG:NH2	23:21:42:GLN:HG2	2.31	0.46
23:21:77:ALA:HA	23:21:80:LEU:HD13	1.98	0.46
1:2A:971:C:H2'	1:2A:972:G:O4'	2.16	0.46
2:2B:22:U:H2'	2:2B:23:G:H8	1.79	0.46
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.97	0.46
23:11:40:ARG:NH2	23:11:42:GLN:HG2	2.30	0.46
1:1A:1908:C:H2'	1:1A:1909:C:H6	1.81	0.46
21:1Z:33:LEU:HD11	21:1Z:90:VAL:HG21	1.97	0.46
1:2A:839:U:O2'	1:2A:1191:G:N3	2.48	0.46
1:2A:266:G:O2'	1:2A:267:C:OP2	4.83	0.46
1:2A:29:U:H2'	1:2A:30:G:C8	2.51	0.46
1:1A:1357:U:H2'	1:1A:1358:G:O4'	2.16	0.46
1:1A:307:G:H21	1:1A:330:A:N6	2.13	0.46
3:1D:106:ILE:O	3:1D:108:PRO:HD3	2.16	0.46
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.97	0.46
4:1E:5:LEU:HD12	4:1E:51:PHE:HB2	1.98	0.46
4:1E:7:VAL:HG13	4:1E:27:LEU:HB3	1.97	0.46
8:1I:72:LEU:HD12	8:1I:138:ILE:HG21	1.97	0.46
1:2A:2224:G:H4'	1:2A:2226:C:C2	2.51	0.46
5:2F:132:VAL:HG21	5:2F:163:VAL:HG22	1.98	0.46
8:2I:14:ASP:OD1	8:2I:15:VAL:N	2.45	0.46
9:2N:15:LEU:HB2	9:2N:135:PRO:HB2	1.96	0.46
10:2O:9:GLU:O	10:2O:83:ALA:HA	2.15	0.46
18:2W:76:VAL:HG22	18:2W:103:ILE:HG12	1.98	0.46
28:16:12:GLU:O	28:16:49:HIS:HA	2.16	0.46
1:1A:534:U:H5'	16:1U:42:ALA:HB1	1.98	0.46
1:1A:859:G:O2'	1:1A:916:G:O6	2.23	0.46
24:22:13:ALA:HA	24:22:16:LEU:HD12	1.98	0.46
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.50	0.46
1:2A:729:G:H2'	1:2A:1775:U:H1'	1.98	0.46
1:2A:856:C:H2'	1:2A:857:C:C6	2.51	0.46
8:2I:130:TYR:CE2	8:2I:132:PRO:HB3	2.51	0.46
16:2U:46:ALA:O	16:2U:50:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:15:18:ALA:O	27:15:21:SER:HB3	2.16	0.45
1:1A:1278:A:H2'	1:1A:1279:G:H8	1.81	0.45
4:1E:11:MET:HB3	4:1E:11:MET:HE2	1.94	0.45
1:2A:2438:U:O2'	1:2A:2440:C:OP1	2.27	0.45
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.16	0.45
1:2A:323:G:C8	5:2F:171:PRO:HG3	2.51	0.45
1:1A:973:A:OP1	1:1A:973:A:H8	1.99	0.45
3:1D:121:PRO:HB3	3:1D:135:PHE:CE2	2.50	0.45
9:1N:24:GLY:O	9:1N:28:THR:HG23	2.17	0.45
15:1T:13:ARG:NH2	15:1T:14:TYR:OH	2.49	0.45
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.97	0.45
1:2A:1265:A:H61	1:2A:2013:A:H5''	1.81	0.45
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.34	0.45
1:2A:744:G:H2'	1:2A:745:G:O4'	2.16	0.45
1:2A:774:A:N3	1:2A:774:A:H2'	2.30	0.45
2:2B:59:A:N6	58:2B:302:HOH:O	2.42	0.45
1:2A:566:U:P	17:2V:80:GLN:HE21	2.39	0.45
1:1A:1278:A:H2'	1:1A:1279:G:C8	2.51	0.45
1:1A:2233:U:H2'	1:1A:2234:G:C8	2.51	0.45
1:1A:2262:U:OP1	1:1A:2387:U:O2'	2.33	0.45
1:1A:2273:A:H2'	1:1A:2274:A:C8	2.52	0.45
1:1A:2314:C:H2'	1:1A:2315:G:C8	2.50	0.45
1:1A:2784:C:H1'	4:1E:37:ARG:NH1	2.32	0.45
1:2A:667:U:O2	30:28:2:PRO:HD2	2.15	0.45
1:2A:1486:A:H2'	1:2A:1487:G:C8	2.51	0.45
1:2A:184:C:H2'	1:2A:185:U:H6	1.82	0.45
1:2A:2448:A:HO2'	1:2A:2449:U:H5	1.61	0.45
1:2A:671:C:H2'	1:2A:672:C:C6	2.51	0.45
1:1A:2420:C:H5'	28:16:54:ILE:HD11	1.97	0.45
1:1A:588:U:H2'	1:1A:589:C:C6	2.51	0.45
5:1F:197:ASP:O	5:1F:201:VAL:HG13	2.17	0.45
11:1P:126:VAL:HG22	11:1P:146:VAL:HB	1.99	0.45
1:1A:560:C:H4'	16:1U:52:ARG:CZ	2.47	0.45
1:2A:1047:G:H21	1:2A:1111:A:N6	2.03	0.45
1:2A:1321:A:H2'	1:2A:1322:A:O4'	2.17	0.45
1:2A:2150:U:H2'	1:2A:2151:G:C8	2.51	0.45
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.17	0.45
12:2Q:38:GLU:HG3	12:2Q:127:ILE:HB	1.99	0.45
12:2Q:93:TYR:OH	21:2Z:194:PRO:HG2	2.16	0.45
1:1A:1045:A:H1'	1:1A:1047:G:C2	2.52	0.45
1:1A:1270:C:H2'	1:1A:1271:G:H8	5.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:29:U:H2'	1:1A:30:G:C8	2.51	0.45
1:1A:359:A:H2'	1:1A:360:G:O4'	2.17	0.45
1:1A:840:C:H2'	1:1A:841:A:C8	2.51	0.45
8:1I:72:LEU:C	8:1I:74:ASN:H	2.20	0.45
23:21:73:LEU:HD21	23:21:98:LEU:HD23	1.99	0.45
1:2A:2385:C:OP1	58:2A:3774:HOH:O	2.21	0.45
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.82	0.45
3:2D:70:TRP:HB3	3:2D:190:TYR:CE1	2.52	0.45
9:2N:21:LYS:HE3	9:2N:140:VAL:HG23	1.99	0.45
1:2A:952:G:P	12:2Q:16:ARG:HH22	2.39	0.45
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.16	0.45
1:1A:1762:A:H2'	58:1A:5335:HOH:O	2.15	0.45
3:1D:232:PRO:HB3	3:1D:244:ARG:NH2	2.32	0.45
1:2A:1002:G:H2'	1:2A:1003:G:C8	3.73	0.45
1:2A:79:G:H1	1:2A:90:U:H3	29.36	0.45
3:2D:12:SER:HB3	3:2D:208:LYS:HB3	1.99	0.45
6:2G:16:ARG:CZ	6:2G:31:VAL:HG21	2.47	0.45
16:2U:11:ARG:O	16:2U:15:LYS:HG3	2.17	0.45
1:1A:1434:A:H2'	1:1A:1435:G:O4'	2.40	0.45
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.16	0.45
1:1A:957:A:N1	1:1A:2458:G:H4'	2.32	0.45
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.49	0.45
20:1Y:56:PRO:C	20:1Y:58:GLY:H	2.19	0.45
1:2A:1333:C:H2'	1:2A:1334:G:H8	1.80	0.45
1:2A:1386:C:H2'	1:2A:1387:C:C6	2.52	0.45
1:2A:1598:C:H2'	1:2A:1599:C:C6	2.52	0.45
1:2A:1647:G:H3'	1:2A:1647:G:OP2	2.15	0.45
1:2A:1911:PSU:H2'	1:2A:1918:A:N1	2.32	0.45
6:2G:97:ASP:HA	6:2G:100:TRP:HD1	1.81	0.45
11:2P:100:LEU:HD12	11:2P:112:LEU:HD11	1.98	0.45
16:2U:27:LEU:HA	16:2U:30:LYS:HB2	1.98	0.45
1:1A:186:G:H2'	1:1A:187:G:H8	1.82	0.45
1:1A:530:G:O6	58:1A:4045:HOH:O	2.19	0.45
4:1E:101:ARG:HG3	4:1E:169:ASN:HA	1.97	0.45
13:1R:86:ARG:HH12	13:1R:118:GLU:HA	1.81	0.45
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.99	0.45
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.26	0.45
1:2A:571:A:O2'	1:2A:575:A:N6	2.50	0.45
7:2H:3:ARG:HE	7:2H:54:ARG:HH12	1.65	0.45
11:2P:54:GLY:O	58:2P:301:HOH:O	2.20	0.45
1:1A:1464:C:H2'	1:1A:1465:G:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1073:A:O2'	1:2A:1074:G:O5'	2.35	0.45
1:2A:1117:G:H2'	1:2A:1118:C:C6	2.51	0.45
1:2A:1186:G:OP1	58:2A:3773:HOH:O	2.21	0.45
1:2A:370:G:OP2	1:2A:370:G:H8	2.00	0.45
1:2A:698:C:O2'	1:2A:734:A:N6	2.50	0.45
1:2A:898:C:H2'	1:2A:899:A:O4'	2.16	0.45
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	1.98	0.45
16:2U:49:HIS:O	16:2U:53:ARG:N	2.43	0.45
1:1A:1441:G:H2'	1:1A:1442:G:H8	1.82	0.45
1:1A:199:A:OP1	58:1A:4075:HOH:O	2.21	0.45
1:1A:2696:U:H2'	1:1A:2697:G:C8	2.52	0.45
1:1A:2712:U:H1'	1:1A:2712(A):A:C8	2.52	0.45
1:1A:570:G:OP1	58:1A:4076:HOH:O	2.21	0.45
3:1D:134:ARG:HG3	3:1D:135:PHE:CD1	2.51	0.45
6:1G:27:ASN:OD1	6:1G:28:VAL:N	2.50	0.45
16:1U:105:VAL:HG11	17:1V:39:LEU:HD21	1.98	0.45
18:1W:19:LEU:HD23	27:15:25:LEU:HD21	1.98	0.45
23:21:2:SER:HB3	23:21:46:LEU:HD12	1.99	0.45
26:24:41:PRO:HG3	26:24:49:PHE:HE2	1.82	0.45
1:2A:1007:C:H5''	9:2N:35:ARG:NH1	2.32	0.45
1:2A:108:U:H2'	1:2A:109:G:H8	1.81	0.45
1:2A:2140:C:H2'	1:2A:2141:G:C8	2.50	0.45
1:2A:2336:A:H61	22:20:43:THR:CG2	2.29	0.45
1:2A:250:G:C6	1:2A:251:A:C6	3.04	0.45
1:2A:473:G:H2'	1:2A:474:G:H8	2.90	0.45
1:2A:671:C:H2'	1:2A:672:C:H6	1.82	0.45
17:2V:29:PRO:HG3	17:2V:64:HIS:HD2	1.82	0.45
1:1A:738:G:C6	1:1A:739:G:C2	3.06	0.44
24:22:35:LEU:HB3	24:22:50:ILE:HG12	1.98	0.44
1:2A:243:U:OP1	30:28:6:THR:OG1	2.27	0.44
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.17	0.44
7:2H:115:VAL:HG11	7:2H:148:ILE:HD11	1.99	0.44
16:2U:65:ILE:HD11	16:2U:95:LEU:HB3	1.99	0.44
21:2Z:54:HIS:HB3	21:2Z:101:PRO:HD3	1.99	0.44
1:1A:2150:U:H2'	1:1A:2151:G:H8	1.82	0.44
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.17	0.44
4:1E:144:ARG:HB3	4:1E:145:LYS:H	1.56	0.44
6:1G:106:LEU:HD12	6:1G:110:ALA:HB3	1.99	0.44
6:1G:25:TYR:CZ	6:1G:32:PRO:HD3	2.52	0.44
18:1W:13:SER:HB3	18:1W:16:LYS:HD2	1.99	0.44
30:28:43:GLN:O	30:28:46:ARG:NE	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1656:C:H2'	1:2A:1657:C:C6	2.52	0.44
1:2A:1827:C:OP2	3:2D:222:ARG:NH1	2.51	0.44
1:2A:2716:U:H2'	1:2A:2717:G:C8	2.51	0.44
2:2B:8:U:O4	2:2B:113:G:O6	2.34	0.44
1:1A:1664:A:O2'	10:1O:67:LYS:NZ	2.42	0.44
1:1A:2732:G:H3'	1:1A:2733:A:O4'	2.18	0.44
7:1H:121:ILE:HD11	7:1H:140:LYS:HG2	2.00	0.44
14:1S:84:GLN:HA	14:1S:111:GLU:HB2	1.98	0.44
1:2A:245:G:N7	30:28:8:LYS:NZ	2.65	0.44
1:2A:1404:C:H2'	1:2A:1405:U:H6	1.82	0.44
1:2A:2261:C:C6	22:20:16:SER:HB3	2.53	0.44
1:2A:492:A:H2'	1:2A:493:G:O4'	2.17	0.44
1:2A:506:G:O3'	1:2A:507:A:H8	2.00	0.44
9:2N:108:PRO:O	9:2N:113:GLY:HA3	2.17	0.44
1:1A:131:G:OP1	58:1A:4080:HOH:O	2.21	0.44
1:1A:1355:G:H2'	1:1A:1356:G:H8	2.05	0.44
1:1A:278:A:H4'	1:1A:279:C:OP1	2.18	0.44
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.54	0.44
7:1H:7:LEU:HG	7:1H:69:ARG:HH21	1.82	0.44
21:1Z:77:ASP:O	21:1Z:81:ARG:N	2.46	0.44
21:1Z:54:HIS:O	21:1Z:98:MET:HE1	2.18	0.44
1:2A:1199:U:O2'	58:2A:3771:HOH:O	2.20	0.44
1:2A:2541:A:N7	58:2A:3895:HOH:O	2.36	0.44
1:2A:565:C:H2'	1:2A:566:U:O4'	2.16	0.44
1:2A:922:U:H2'	1:2A:923:C:C6	2.53	0.44
8:2I:57:ARG:O	8:2I:61:ARG:HG2	2.17	0.44
12:2Q:52:VAL:HA	12:2Q:55:VAL:HG12	1.99	0.44
12:2Q:58:PHE:O	12:2Q:60:ARG:N	2.51	0.44
15:2T:114:LEU:HA	15:2T:114:LEU:HD23	1.82	0.44
31:19:2:LYS:HD3	31:19:4:ARG:NH2	2.32	0.44
1:1A:1068:G:O2'	1:1A:1096:A:O2'	2.18	0.44
1:1A:2398:U:H2'	1:1A:2399:G:C8	2.52	0.44
1:1A:314:A:H2'	1:1A:315:G:C8	2.52	0.44
1:1A:428:A:H3'	1:1A:429:A:C8	2.53	0.44
1:1A:774:A:N3	1:1A:774:A:H2'	2.32	0.44
7:1H:15:VAL:HG12	7:1H:29:PRO:HD3	2.00	0.44
10:1O:64:ARG:HG2	10:1O:83:ALA:HB3	1.99	0.44
13:1R:79:LEU:HD12	13:1R:83:ILE:HB	2.00	0.44
1:2A:1069:A:H5'	1:2A:1096:A:H5'	2.00	0.44
1:2A:1759:A:H1'	1:2A:2711:A:C2	2.52	0.44
1:2A:2074:U:OP1	58:2A:3776:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:55:G:H2'	1:2A:56:A:C8	2.52	0.44
2:2B:87:G:N2	2:2B:90:A:OP2	2.37	0.44
1:2A:2579:C:H4'	4:2E:134:ILE:HG12	1.99	0.44
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.99	0.44
7:2H:117:PRO:HA	7:2H:118:PRO:HD3	1.91	0.44
13:2R:96:ARG:HG2	13:2R:115:GLU:HG2	1.98	0.44
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.18	0.44
26:14:40:HIS:HB3	26:14:43:TYR:CD1	2.49	0.44
1:1A:2065:C:H2'	1:1A:2066:C:C6	2.53	0.44
1:1A:2134:A:O2'	1:1A:2159:G:N3	2.49	0.44
1:1A:2183:C:H2'	1:1A:2184:G:C8	2.53	0.44
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.51	0.44
7:1H:46:GLU:HB2	7:1H:49:VAL:O	2.18	0.44
21:1Z:54:HIS:HB3	21:1Z:101:PRO:HD3	2.00	0.44
1:2A:1153:C:H2'	1:2A:1154:G:O4'	2.18	0.44
1:2A:1756:G:H4'	1:2A:1758:G:O4'	2.17	0.44
1:2A:2585:U:OP2	1:2A:2602:A:N6	2.50	0.44
1:2A:827:U:O2'	1:2A:2068:U:C2	2.71	0.44
16:2U:34:LYS:HA	16:2U:34:LYS:HD3	1.67	0.44
21:2Z:28:MET:HE1	21:2Z:61:LEU:HD11	1.99	0.44
1:1A:1939:5MU:H3'	1:1A:1940:U:H5'	1.98	0.44
1:1A:2667:C:H2'	1:1A:2668:G:O4'	2.18	0.44
1:1A:38:A:H2'	1:1A:39:C:C6	2.53	0.44
1:1A:483:A:O4'	20:1Y:48:ALA:HB1	2.18	0.44
1:1A:730:C:H5'	58:1A:4492:HOH:O	2.17	0.44
1:1A:740:U:H2'	1:1A:741:G:C8	2.52	0.44
1:1A:1824:G:N3	3:1D:254:THR:OG1	2.50	0.44
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.82	0.44
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.53	0.44
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.18	0.44
1:2A:2467:C:OP1	31:29:6:SER:OG	2.34	0.44
7:2H:117:PRO:HG3	7:2H:123:PHE:CD2	2.53	0.44
25:13:28:LEU:HD23	25:13:35:ARG:HD3	1.99	0.44
1:1A:1508:A:H4'	1:1A:1509:A:N9	2.33	0.44
1:1A:1853:A:H2'	1:1A:1854:A:C8	2.52	0.44
1:1A:1662:C:O2'	1:1A:2687:U:OP1	2.35	0.44
1:1A:2805:G:H2'	1:1A:2807:G:H8	1.82	0.44
1:1A:675:A:H2'	1:1A:676:A:C8	3.32	0.44
3:1D:83:GLU:OE1	3:1D:104:TYR:OH	2.22	0.44
14:1S:27:SER:O	14:1S:37:ALA:HA	2.18	0.44
1:2A:121:G:H4'	1:2A:149:A:H5'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.17	0.44
1:2A:422:A:H2'	1:2A:423:A:C8	2.53	0.44
1:2A:595:C:H2'	1:2A:596:G:C8	2.52	0.44
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.18	0.44
5:2F:74:ARG:O	5:2F:75:HIS:ND1	2.50	0.44
12:2Q:57:HIS:CE1	12:2Q:116:GLU:HB3	2.53	0.44
1:2A:955:C:OP2	12:2Q:14:ARG:HG3	2.18	0.44
13:2R:56:LYS:NZ	13:2R:90:ARG:O	2.51	0.44
21:2Z:53:ILE:H	21:2Z:53:ILE:HG13	1.67	0.44
30:18:62:LEU:HB3	30:18:65:GLU:CG	2.48	0.44
30:18:6:THR:HB	30:18:8:LYS:HE2	2.00	0.44
1:1A:1045:A:H1'	1:1A:1047:G:N3	2.33	0.44
1:1A:1056:G:H4'	1:1A:1086:A:H8	1.82	0.44
1:1A:1299:G:H5'	1:1A:1301:A:O4'	2.18	0.44
1:1A:2272:U:H5''	1:1A:2273:A:OP1	2.17	0.44
1:1A:2721:A:H1'	1:1A:2873:A:O2'	2.18	0.44
3:1D:146:GLU:HG2	3:1D:152:GLY:C	2.38	0.44
21:1Z:182:LYS:HB3	21:1Z:182:LYS:HE2	1.79	0.44
25:23:46:ASN:O	25:23:50:VAL:HG22	2.18	0.44
1:2A:2419:U:H2'	1:2A:2420:C:C6	2.53	0.44
1:2A:300:A:H8	20:2Y:84:ARG:HH12	1.65	0.44
1:2A:568:U:H5'	1:2A:945:A:N6	2.33	0.44
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	2.00	0.44
25:13:31:LEU:HD23	25:13:31:LEU:HA	1.74	0.43
1:1A:1636:C:H2'	1:1A:1637:A:C8	2.53	0.43
1:2A:1365:A:P	23:21:41:ARG:HH22	2.41	0.43
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.53	0.43
1:2A:1032:A:H2	1:2A:1122:G:H22	1.66	0.43
1:2A:30:G:O2'	1:2A:1214:A:N3	2.41	0.43
1:2A:1278:A:H2'	1:2A:1279:G:H8	1.81	0.43
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.82	0.43
3:2D:53:PHE:HA	3:2D:218:ARG:HB2	1.99	0.43
1:1A:1499:C:H2'	1:1A:1500:G:H8	1.83	0.43
1:1A:586:A:N1	1:1A:809:G:O2'	2.50	0.43
1:1A:796:C:H2'	1:1A:797:C:C6	2.54	0.43
20:1Y:43:ASN:HB3	20:1Y:65:ALA:HB3	1.98	0.43
1:2A:1057:A:O2'	1:2A:1058:G:OP1	2.31	0.43
1:2A:210:C:OP2	29:27:29:LYS:NZ	2.44	0.43
1:2A:2556:C:H2'	1:2A:2557:G:O4'	2.18	0.43
1:2A:2578:G:OP1	58:2A:3778:HOH:O	2.21	0.43
1:2A:57:C:H2'	1:2A:58:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:76:G:H2'	2:2B:77:U:H6	1.83	0.43
5:2F:110:LEU:HD11	5:2F:181:LEU:HG	2.00	0.43
9:2N:34:LEU:O	9:2N:49:GLY:HA3	2.18	0.43
25:13:26:LEU:HD21	25:13:46:ASN:HB3	2.00	0.43
1:1A:1423:G:H2'	1:1A:1424:G:C8	2.53	0.43
1:1A:2737:G:H2'	1:1A:2738:A:C8	2.53	0.43
1:1A:484:C:H2'	1:1A:485:C:C6	2.54	0.43
4:1E:176:ILE:HB	4:1E:181:LEU:HB2	2.00	0.43
12:1Q:21:THR:HG21	12:1Q:101:ARG:N	2.33	0.43
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.66	0.43
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.53	0.43
1:2A:570:G:H2'	1:2A:2030:A:C5	2.52	0.43
1:2A:2270:G:H2'	1:2A:2271:G:O4'	2.19	0.43
1:2A:793:A:OP2	1:2A:2071:A:O2'	2.36	0.43
5:2F:102:PRO:HB2	5:2F:105:VAL:HG23	1.99	0.43
1:2A:1653:G:H3'	13:2R:2:ARG:HB2	1.99	0.43
16:2U:83:LEU:HD12	16:2U:113:ALA:HB2	2.00	0.43
17:2V:35:LEU:HB2	17:2V:57:VAL:HG22	2.01	0.43
1:1A:1124:C:OP1	58:1A:4070:HOH:O	2.20	0.43
1:1A:1449:A:H2'	1:1A:1450:G:O4'	2.18	0.43
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.18	0.43
1:1A:2689:U:H4'	1:1A:2690:C:H5'	1.99	0.43
3:1D:166:GLN:HB2	3:1D:174:ILE:HG22	2.01	0.43
11:1P:121:LYS:O	11:1P:123:LEU:N	2.52	0.43
13:1R:53:HIS:HB2	13:1R:94:TYR:HE2	1.82	0.43
19:1X:11:PRO:HB3	19:1X:92:LEU:HD11	1.99	0.43
1:2A:521:G:N7	58:2A:3905:HOH:O	2.37	0.43
1:2A:571:A:O5'	1:2A:2030:A:N6	2.48	0.43
3:2D:79:VAL:HB	3:2D:114:GLY:H	1.83	0.43
14:2S:64:GLU:HB2	26:24:59:PHE:CE1	85.43	0.43
15:2T:92:GLY:O	15:2T:120:ARG:NH2	2.51	0.43
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.51	0.43
21:2Z:93:ASP:OD1	21:2Z:93:ASP:N	2.52	0.43
27:15:16:ARG:HG3	27:15:17:ASP:N	2.34	0.43
1:1A:2157:G:H5''	1:1A:2158:A:OP1	2.19	0.43
3:1D:155:LEU:HD23	3:1D:177:LEU:HD22	1.99	0.43
10:1O:70:LYS:HE2	10:1O:70:LYS:HB3	1.74	0.43
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.48	0.43
26:24:53:GLU:H	26:24:53:GLU:CD	2.21	0.43
1:2A:827:U:O2'	1:2A:2068:U:N3	2.50	0.43
1:2A:2391:G:O6	1:2A:2425:A:H8	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2552:OMU:H2'	1:2A:2554:U:OP2	2.19	0.43
12:2Q:8:LYS:HG2	21:2Z:197:ILE:HD12	1.99	0.43
1:1A:217:G:OP2	58:1A:4077:HOH:O	2.21	0.43
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.34	0.43
1:1A:2679:A:H4'	4:1E:165:VAL:HG11	2.01	0.43
2:1B:48:A:H2'	2:1B:49:C:C6	2.53	0.43
6:1G:114:ILE:HB	6:1G:117:PHE:HB2	2.01	0.43
1:1A:2748:A:N3	7:1H:63:SER:HB3	2.34	0.43
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.54	0.43
1:2A:1889:A:C6	1:2A:1890:A:C6	3.06	0.43
1:2A:2614:A:OP1	58:2A:3779:HOH:O	2.22	0.43
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.53	0.43
1:2A:2773:C:OP1	4:2E:164:ARG:NE	2.49	0.43
2:2B:19:G:H2'	2:2B:20:C:H6	1.83	0.43
3:2D:205:VAL:O	3:2D:211:ARG:NH2	2.49	0.43
11:2P:48:PRO:O	30:28:57:ARG:NH2	2.52	0.43
21:2Z:180:VAL:HG13	21:2Z:183:LEU:HD12	2.00	0.43
28:16:33:LYS:HA	28:16:33:LYS:HD3	1.80	0.43
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.53	0.43
1:1A:910:A:N1	1:1A:2277:G:H1'	2.34	0.43
13:1R:29:LEU:HG	13:1R:79:LEU:HD13	1.99	0.43
1:2A:1033:U:O2'	1:2A:2750:A:N6	2.52	0.43
1:2A:1669:A:H5''	1:2A:2550:G:OP1	2.18	0.43
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.53	0.43
1:2A:2807:G:N2	1:2A:2893:G:O6	2.52	0.43
1:2A:361:G:O2'	1:2A:362:U:H5'	2.19	0.43
1:2A:27:G:N2	1:2A:512:G:H1'	2.33	0.43
1:2A:576:U:OP1	58:2A:3777:HOH:O	2.21	0.43
25:13:39:ASP:OD2	25:13:44:ARG:NH2	2.52	0.43
1:1A:1371:G:H2'	1:1A:1372:U:C5	2.54	0.43
1:1A:2096:U:H2'	1:1A:2097:C:H6	1.84	0.43
1:1A:753:C:H2'	1:1A:754:C:H6	1.84	0.43
5:1F:74:ARG:H	5:1F:74:ARG:HG3	1.48	0.43
23:21:8:SER:HB3	23:21:66:HIS:CE1	2.53	0.43
30:28:14:VAL:HG22	30:28:24:ALA:HB2	2.00	0.43
1:2A:674:G:H2'	1:2A:675:A:C8	5.00	0.43
2:2B:84:C:OP1	25:23:15:TYR:OH	2.32	0.43
1:2A:468:G:O2'	5:2F:62:ARG:NH2	2.52	0.43
14:2S:66:ALA:HB1	14:2S:101:LEU:HB2	2.00	0.43
1:1A:36:G:H4'	1:1A:451:C:C2	2.54	0.43
1:1A:492:A:H2'	1:1A:493:G:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:668:G:H2'	1:1A:670:A:H62	1.84	0.43
1:1A:675:A:H2'	1:1A:676:A:H8	3.30	0.43
58:1A:4035:HOH:O	4:1E:127:ASP:OD2	2.22	0.43
12:1Q:14:ARG:HG2	12:1Q:41:TRP:HH2	1.84	0.43
21:1Z:104:PHE:HD1	21:1Z:141:VAL:HG11	1.84	0.43
23:21:8:SER:HB3	23:21:66:HIS:ND1	2.34	0.43
1:2A:1102:C:H2'	1:2A:1103:A:C8	2.54	0.43
1:2A:2000:G:OP1	13:2R:5:LYS:NZ	2.52	0.43
1:2A:594:U:H2'	1:2A:595:C:C6	2.54	0.43
5:2F:176:LEU:HD23	5:2F:176:LEU:HA	1.81	0.43
1:2A:956:G:H5''	12:2Q:77:LYS:HD2	2.00	0.43
26:14:43:TYR:O	26:14:45:GLY:N	2.51	0.43
1:1A:1578:U:C2'	1:1A:1579:A:H5'	2.49	0.43
1:1A:1999:C:H4'	1:1A:2723:C:O2	2.19	0.43
1:1A:222:A:H3'	1:1A:421:U:H5''	2.00	0.43
1:1A:2654:A:N1	1:1A:2665:A:H5''	2.34	0.43
1:1A:2680:C:H5'	4:1E:189:PRO:HA	2.01	0.43
1:1A:286:C:H2'	1:1A:287:C:C6	2.54	0.43
3:1D:147:LEU:HD13	3:1D:155:LEU:HD11	2.01	0.43
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.18	0.43
1:2A:1574:C:H2'	1:2A:1575:C:C6	2.54	0.43
1:2A:218:A:C2	1:2A:235:U:H4'	2.52	0.43
2:2B:72:G:OP2	53:2B:201:MPD:O2	2.29	0.43
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	2.00	0.43
7:2H:105:LEU:HD21	7:2H:162:ILE:HD11	2.01	0.43
8:2I:114:LEU:HD11	8:2I:128:LEU:HB3	2.01	0.43
1:2A:1007:C:H5''	9:2N:35:ARG:HH11	1.84	0.43
1:1A:1616:A:H2'	58:1A:4538:HOH:O	2.17	0.42
1:1A:239:U:H2'	1:1A:240:G:O4'	2.18	0.42
1:1A:2529:G:H5''	1:1A:2530:A:H5''	2.00	0.42
1:1A:2711:A:OP1	1:1A:2712:U:H3'	2.18	0.42
1:1A:464:U:H2'	1:1A:465:G:O4'	2.19	0.42
1:2A:2695:C:H2'	1:2A:2696:U:H6	1.84	0.42
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.18	0.42
19:2X:35:THR:O	19:2X:39:ILE:N	2.48	0.42
1:1A:1006:C:H2'	1:1A:1007:C:C6	3.12	0.42
1:1A:1703:G:H2'	1:1A:1704:G:C8	2.54	0.42
1:1A:2012:G:OP1	18:1W:11:ARG:NH2	2.39	0.42
1:1A:2718:G:O3'	15:1T:98:LYS:HG3	2.19	0.42
1:1A:588:U:H1'	5:1F:90:PHE:CG	2.54	0.42
9:1N:34:LEU:HD21	9:1N:120:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1S:66:ALA:HA	14:1S:69:VAL:HG22	2.01	0.42
21:1Z:123:ASP:N	21:1Z:123:ASP:OD1	2.52	0.42
26:24:45:GLY:O	26:24:47:GLN:N	2.46	0.42
30:28:4:MET:HB3	30:28:4:MET:HE2	1.93	0.42
1:2A:1233:C:H2'	1:2A:1234:U:C6	2.54	0.42
1:2A:858:U:O2	1:2A:2268:A:H2'	2.19	0.42
1:2A:2853:C:H2'	1:2A:2854:G:H8	1.83	0.42
1:2A:77:C:O3'	24:22:14:ARG:NH2	2.52	0.42
1:2A:2679:A:H4'	4:2E:165:VAL:HG11	2.02	0.42
1:2A:2846:G:P	15:2T:54:ARG:HB2	2.58	0.42
1:2A:996:A:H4'	16:2U:91:ASP:OD2	2.19	0.42
18:2W:39:THR:HG22	18:2W:41:LYS:HB2	2.01	0.42
19:2X:44:GLU:HG3	19:2X:51:VAL:HG23	2.01	0.42
12:2Q:52:VAL:HG13	21:2Z:183:LEU:HD13	2.01	0.42
24:12:32:LEU:HD22	24:12:36:ARG:NH1	2.33	0.42
1:1A:1003:G:N2	1:1A:1038:C:N3	40.94	0.42
1:1A:1186:G:H2'	1:1A:1187:G:O4'	2.18	0.42
1:1A:1226:A:OP1	17:1V:84:LYS:NZ	2.33	0.42
1:1A:1430:C:H2'	1:1A:1431:U:C6	2.54	0.42
1:1A:1923:U:H2'	1:1A:1924:C:C6	2.53	0.42
1:1A:2270:G:H2'	1:1A:2271:G:O4'	2.19	0.42
1:1A:993:G:N7	1:1A:1213:A:N6	48.96	0.42
1:1A:1790:C:H4'	3:1D:209:ALA:HB2	2.02	0.42
21:1Z:98:MET:O	21:1Z:125:LEU:HD12	2.19	0.42
1:2A:1147:C:H2'	1:2A:1148:A:C8	2.52	0.42
1:2A:1436:G:H2'	1:2A:1437:C:O4'	2.19	0.42
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.20	0.42
1:2A:700:G:O2'	1:2A:1632:A:N3	2.45	0.42
1:2A:2638:G:P	4:2E:82:ARG:HH12	2.40	0.42
10:2O:12:ASP:OD1	10:2O:14:THR:OG1	2.26	0.42
14:2S:26:LEU:N	14:2S:86:ALA:O	2.51	0.42
18:2W:9:TYR:H	18:2W:102:HIS:CE1	2.37	0.42
26:14:41:PRO:HB3	26:14:47:GLN:O	2.20	0.42
1:1A:1239:G:H2'	1:1A:1240:U:O4'	2.19	0.42
1:1A:1270:C:H2'	1:1A:1271:G:C8	6.58	0.42
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.54	0.42
1:1A:2001:A:H2'	1:1A:2002:G:C8	2.54	0.42
1:1A:2715:C:H2'	1:1A:2716:U:H6	1.84	0.42
1:1A:459:U:H2'	1:1A:460:A:C8	2.55	0.42
1:1A:56:A:H2'	1:1A:57:C:O4'	2.19	0.42
1:1A:724:U:H2'	1:1A:725:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:811:U:H2'	11:1P:21:ARG:HA	2.01	0.42
1:1A:824:A:H1'	1:1A:2358:G:N7	2.33	0.42
5:1F:150:GLY:HA2	5:1F:172:TRP:CE3	2.54	0.42
15:1T:91:ARG:HD2	15:1T:120:ARG:NH1	2.35	0.42
18:1W:45:TYR:CE2	18:1W:49:LYS:HD2	2.55	0.42
1:2A:1057:A:HO2'	1:2A:1058:G:P	2.42	0.42
1:2A:1067:A:O5'	1:2A:1067:A:H8	4.10	0.42
1:2A:1312:U:H4'	1:2A:1313:U:O5'	2.19	0.42
1:2A:1920:OMC:H1'	1:2A:1920:OMC:HM22	1.74	0.42
1:2A:2591:C:OP1	3:2D:239:ARG:HD2	2.19	0.42
1:2A:2601:C:C3'	1:2A:2602:A:H5''	2.49	0.42
1:2A:2690:C:N4	1:2A:2713:A:H1'	2.34	0.42
4:2E:59:VAL:HG21	4:2E:74:PRO:HB3	2.00	0.42
18:2W:78:GLU:OE2	18:2W:99:ARG:NH1	2.44	0.42
1:1A:111:A:H4'	24:12:69:ARG:NH1	2.35	0.42
1:1A:1721:G:H8	1:1A:1741:A:H62	1.67	0.42
1:1A:2550:G:OP1	58:1A:4008:HOH:O	2.22	0.42
1:1A:2704:C:H2'	1:1A:2705:A:O4'	2.19	0.42
1:1A:270:A:H1'	1:1A:370:G:C2	2.54	0.42
1:1A:272:G:O2'	1:1A:421:U:OP2	2.27	0.42
1:1A:948:G:OP2	58:1A:4079:HOH:O	2.21	0.42
4:1E:32:PRO:HA	4:1E:90:THR:HA	2.02	0.42
7:1H:40:GLU:OE1	7:1H:61:HIS:NE2	2.51	0.42
10:1O:120:GLU:OE1	15:1T:67:SER:OG	2.33	0.42
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.52	0.42
1:2A:1102:C:H2'	1:2A:1103:A:H8	1.85	0.42
1:2A:1225:G:H4'	17:2V:84:LYS:HG2	2.02	0.42
1:2A:2712:U:H1'	1:2A:2712(A):A:C8	2.55	0.42
1:2A:795:C:H2'	1:2A:796:C:C6	2.55	0.42
1:2A:800:A:OP1	1:2A:800:A:H8	2.03	0.42
3:2D:206:LEU:HD22	3:2D:211:ARG:HG2	2.00	0.42
5:2F:107:LYS:HG3	5:2F:206:ILE:HA	2.02	0.42
5:2F:164:ARG:O	5:2F:168:ARG:HG3	2.20	0.42
1:1A:1309:G:H4'	29:17:7:PRO:HG2	2.00	0.42
1:1A:1557:C:H5''	1:1A:1558:A:OP2	2.20	0.42
1:1A:2064:C:H2'	1:1A:2065:C:H6	1.85	0.42
1:1A:207:A:H2'	1:1A:208:C:O4'	2.20	0.42
3:1D:13:ARG:NH1	3:1D:16:MET:SD	2.92	0.42
3:1D:67:PHE:HD1	3:1D:153:ALA:HB3	1.84	0.42
17:1V:52:VAL:HG23	17:1V:55:ALA:HB3	2.01	0.42
21:1Z:30:ASN:O	21:1Z:32:HIS:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:27:30:VAL:HG22	29:27:33:ARG:NH2	2.35	0.42
1:2A:1068:G:H3'	1:2A:1096:A:OP2	2.19	0.42
1:2A:108:U:H2'	1:2A:109:G:C8	2.55	0.42
1:2A:1508:A:H4'	1:2A:1509:A:N9	2.35	0.42
1:2A:2321:G:HO2'	1:2A:2322:A:P	2.42	0.42
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.53	0.42
1:2A:333:G:H2'	1:2A:334:C:C6	3.72	0.42
1:2A:391:G:O2'	1:2A:410:G:OP1	2.28	0.42
1:2A:451:C:H5'	58:2A:3743:HOH:O	2.19	0.42
1:2A:78:A:H2'	1:2A:79:G:C8	2.54	0.42
4:2E:51:PHE:HA	4:2E:52:LEU:HA	1.88	0.42
1:2A:335:C:H4'	20:2Y:73:ARG:HH11	1.85	0.42
21:2Z:31:ARG:NH1	21:2Z:94:GLU:OE1	2.53	0.42
23:11:67:ILE:N	23:11:68:PRO:HD2	2.35	0.42
1:1A:987:G:O2'	1:1A:1000:A:N3	2.43	0.42
1:1A:2356:C:H2'	1:1A:2357:U:O4'	2.20	0.42
1:1A:36:G:N3	1:1A:450:G:O2'	2.52	0.42
1:1A:581:C:H2'	1:1A:582:G:H8	1.82	0.42
4:1E:178:GLU:CD	4:1E:178:GLU:H	2.22	0.42
1:2A:2080:G:H5'	23:21:35:THR:O	2.20	0.42
23:21:53:VAL:HG22	23:21:74:VAL:HG13	2.02	0.42
1:2A:1269:A:H2'	1:2A:1270:C:C6	2.55	0.42
1:2A:1486:A:H2'	1:2A:1487:G:H8	1.84	0.42
1:2A:1614:A:P	1:2A:1614:A:H8	2.42	0.42
1:2A:1645:G:H5''	1:2A:1646:C:H5'	2.00	0.42
1:2A:2643:G:H2'	1:2A:2644:G:O4'	2.20	0.42
1:2A:2823:A:OP1	4:2E:113:PHE:HB2	2.19	0.42
1:2A:2886:G:H2'	1:2A:2887:U:H6	1.84	0.42
1:2A:455:C:H2'	1:2A:456:C:H6	7.20	0.42
1:2A:473:G:H2'	1:2A:474:G:C8	3.42	0.42
1:2A:536:A:H2'	1:2A:537:C:C6	2.54	0.42
12:2Q:45:GLN:N	12:2Q:45:GLN:OE1	2.50	0.42
1:1A:1447:G:N7	58:1A:4216:HOH:O	2.37	0.42
1:1A:1481:U:H2'	1:1A:1482:G:C8	6.50	0.42
1:1A:1517:G:N3	1:1A:1919:A:O2'	106.77	0.42
1:1A:1590:U:H2'	1:1A:1591:G:C8	2.55	0.42
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.34	0.42
1:1A:1920:OMC:H1'	1:1A:1920:OMC:HM23	1.74	0.42
1:1A:614(C):A:C4	5:1F:180:GLY:HA3	2.54	0.42
1:2A:2741:A:H5''	31:29:22:ARG:HH12	1.84	0.42
1:2A:1153:C:H5'	16:2U:76:TYR:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1184:G:OP1	25:23:30:ARG:NH1	2.52	0.42
1:2A:199:A:OP1	58:2A:3775:HOH:O	2.21	0.42
1:2A:807:U:OP2	11:2P:41:ARG:NH2	2.50	0.42
10:2O:17:ARG:HA	10:2O:17:ARG:HD3	1.74	0.42
11:2P:39:LYS:HB2	11:2P:45:LEU:HD21	2.01	0.42
19:2X:11:PRO:HA	19:2X:28:PHE:HA	2.02	0.42
26:14:14:ILE:HB	26:14:22:ILE:HB	2.01	0.42
27:15:55:ARG:NH1	27:15:57:VAL:HG22	2.35	0.42
31:19:4:ARG:O	31:19:36:GLN:HA	2.20	0.42
1:1A:1509:A:H2'	1:1A:1509(A):A:O4'	2.20	0.42
1:1A:2320:A:H2'	1:1A:2320:A:N3	2.35	0.42
1:1A:531:C:H4'	1:1A:532:A:H5''	2.01	0.42
1:1A:924:C:H2'	1:1A:925:C:C6	2.54	0.42
5:1F:10:PRO:HB3	5:1F:17:ARG:NH2	2.35	0.42
1:2A:1050:A:H2'	1:2A:1051:G:C8	2.54	0.42
1:2A:2130:U:H2'	1:2A:2158:A:N1	2.35	0.42
1:2A:2629:A:H1'	1:2A:2630:G:H5''	2.01	0.42
1:2A:2747:G:H21	1:2A:2757:A:H62	1.68	0.42
1:2A:390:A:H4'	1:2A:391:G:H5'	2.02	0.42
1:2A:615:G:OP1	5:2F:40:GLN:NE2	2.53	0.42
2:2B:18:G:H2'	2:2B:19:G:H8	1.85	0.42
9:2N:103:VAL:HG11	9:2N:120:LEU:HD22	2.02	0.42
1:2A:534:U:O2'	16:2U:49:HIS:ND1	2.35	0.42
20:2Y:39:VAL:HB	20:2Y:42:VAL:HB	2.01	0.42
1:1A:1805:U:O2	3:1D:50:THR:HB	2.20	0.42
1:1A:2150:U:H2'	1:1A:2151:G:C8	2.55	0.42
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.84	0.42
1:1A:2398:U:H2'	1:1A:2399:G:H8	1.85	0.42
1:1A:438:G:H2'	1:1A:440:G:C8	2.55	0.42
1:1A:491:G:O6	18:1W:49:LYS:HE2	2.19	0.42
1:1A:821:A:H5'	1:1A:822:U:C6	2.55	0.42
1:1A:729:G:C5	3:1D:208:LYS:HB2	2.54	0.42
8:1I:101:LEU:HD11	8:1I:140:LEU:HD11	2.02	0.42
1:2A:459:U:H5''	29:27:40:TRP:CD2	2.55	0.42
1:2A:116:C:H2'	1:2A:117:G:O4'	2.20	0.42
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.55	0.42
1:2A:2358:G:H22	11:2P:55:ARG:NH2	2.17	0.42
1:2A:2023:G:H4'	1:2A:2617:C:O3'	2.20	0.42
1:2A:2716:U:H2'	1:2A:2717:G:H8	1.84	0.42
1:2A:2781:A:H5''	1:2A:2782:G:H5'	2.02	0.42
6:2G:54:GLU:O	6:2G:58:GLN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2O:15:GLY:O	10:2O:47:ILE:HG13	2.19	0.42
10:2O:71:ARG:HH22	10:2O:122:LEU:C	2.23	0.42
16:2U:83:LEU:HG	16:2U:88:ILE:HD12	2.02	0.42
20:2Y:56:PRO:C	20:2Y:58:GLY:H	2.23	0.42
31:19:12:ASP:OD1	31:19:13:LYS:N	2.53	0.41
1:1A:1056:G:H4'	1:1A:1086:A:C8	2.55	0.41
1:1A:1272:A:OP2	58:1A:4082:HOH:O	2.22	0.41
1:1A:1578:U:H2'	1:1A:1579:A:H5'	2.01	0.41
1:1A:2100:G:H1	1:1A:2189:U:H3	1.67	0.41
1:1A:2805:G:H2'	1:1A:2807:G:C8	2.55	0.41
1:1A:879:G:H22	1:1A:899:A:H1'	1.85	0.41
1:1A:1141:U:OP1	9:1N:25:ARG:NH1	2.53	0.41
12:1Q:54:MET:HG3	12:1Q:121:ALA:HB2	2.01	0.41
13:1R:86:ARG:NH1	13:1R:118:GLU:O	2.53	0.41
19:1X:26:TYR:HB3	19:1X:92:LEU:HD22	2.01	0.41
1:2A:196:A:N3	1:2A:196:A:H2'	2.35	0.41
1:2A:2287:A:H61	1:2A:2344:U:H3	1.68	0.41
2:2B:28:C:H2'	2:2B:29:A:C8	2.55	0.41
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	2.02	0.41
15:2T:51:ARG:HB3	15:2T:62:THR:HB	2.00	0.41
22:10:43:THR:OG1	22:10:46:LYS:HG2	2.19	0.41
25:13:26:LEU:O	25:13:35:ARG:NE	2.53	0.41
1:1A:1118:C:H2'	1:1A:1119:C:H6	2.58	0.41
1:1A:1703:G:H2'	1:1A:1704:G:H8	1.85	0.41
1:1A:840:C:H2'	1:1A:841:A:H8	1.85	0.41
1:1A:970:C:H2'	1:1A:971:C:H6	1.85	0.41
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.85	0.41
12:1Q:137:TYR:O	12:1Q:141:GLN:HG2	2.21	0.41
13:1R:38:VAL:HG23	13:1R:110:PRO:O	2.21	0.41
23:21:83:GLU:HA	23:21:84:GLY:HA2	1.57	0.41
1:2A:1468:C:H2'	1:2A:1469:A:C8	2.55	0.41
1:2A:421:U:O2'	58:2A:3784:HOH:O	2.22	0.41
1:2A:724:U:H2'	1:2A:725:G:O4'	2.20	0.41
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	2.02	0.41
27:15:40:LYS:HD3	27:15:46:CYS:HA	2.01	0.41
1:1A:1246:A:OP1	5:1F:38:ARG:NH1	2.51	0.41
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.20	0.41
1:1A:2369:A:H2'	1:1A:2370:G:H8	1.85	0.41
1:1A:465:G:C6	1:1A:466:A:N6	2.88	0.41
4:1E:170:LEU:HB3	4:1E:184:VAL:HG22	2.02	0.41
5:1F:40:GLN:NE2	5:1F:182:ASN:HB2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:21:THR:HG23	12:1Q:99:PRO:O	2.19	0.41
19:1X:36:LYS:HG2	19:1X:56:THR:HG23	2.02	0.41
1:2A:991:C:H42	1:2A:1163:G:H1	1.66	0.41
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.19	0.41
1:2A:1656:C:H2'	1:2A:1657:C:H6	1.85	0.41
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.55	0.41
1:2A:218:A:H2	1:2A:235:U:H4'	1.85	0.41
1:2A:27:G:O2'	1:2A:28:A:OP2	2.34	0.41
1:2A:335:C:C2	1:2A:336:C:C5	3.60	0.41
2:2B:19:G:H2'	2:2B:20:C:C6	2.55	0.41
3:2D:181:GLU:HG3	3:2D:272:ALA:O	2.21	0.41
4:2E:28:ALA:HB3	4:2E:93:VAL:HG13	2.02	0.41
11:2P:49:ARG:HH12	30:28:4:MET:HE1	1.86	0.41
1:1A:1153:C:H2'	1:1A:1154:G:O4'	2.21	0.41
1:1A:376:C:H2'	1:1A:377:C:C6	2.56	0.41
1:1A:960:A:C8	1:1A:962:G:C8	3.09	0.41
3:1D:111:LEU:HA	3:1D:111:LEU:HD23	1.80	0.41
3:1D:211:ARG:HG3	3:1D:214:TRP:CE3	2.55	0.41
3:1D:246:PRO:O	3:1D:254:THR:HG22	2.20	0.41
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.20	0.41
6:1G:16:ARG:NE	6:1G:31:VAL:HG21	2.35	0.41
9:1N:112:LEU:O	9:1N:116:LEU:HG	2.21	0.41
14:1S:18:ILE:HD13	14:1S:18:ILE:HA	1.90	0.41
21:1Z:30:ASN:C	21:1Z:32:HIS:H	2.23	0.41
23:21:23:LYS:HB3	23:21:29:GLY:HA3	2.02	0.41
1:2A:1638:C:OP1	1:2A:2710:C:O2'	2.35	0.41
1:2A:519:U:H2'	1:2A:520:G:H8	1.84	0.41
2:2B:24:G:N7	2:2B:56:G:H2'	2.36	0.41
7:2H:5:GLY:O	7:2H:65:HIS:NE2	2.54	0.41
1:2A:336:C:H4'	20:2Y:6:HIS:CE1	2.56	0.41
23:11:70:VAL:O	23:11:73:LEU:HB2	2.20	0.41
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.56	0.41
1:1A:1857:G:C6	1:1A:1858:G:C6	3.08	0.41
1:1A:26:G:H1'	1:1A:515:A:H61	1.85	0.41
3:1D:233:HIS:CE1	3:1D:242:ARG:HG2	2.56	0.41
4:1E:173:VAL:HG22	4:1E:185:LYS:HB2	2.02	0.41
1:1A:2019:A:O4'	16:1U:34:LYS:HE3	2.21	0.41
21:1Z:136:PHE:HE1	21:1Z:138:GLU:HG3	1.84	0.41
27:25:49:CYS:SG	27:25:51:TYR:HB2	2.60	0.41
1:2A:1301:A:N1	1:2A:1626:G:O2'	2.40	0.41
1:2A:1316:U:H2'	1:2A:1317:A:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1980:G:O2'	1:2A:1982:C:OP2	2.34	0.41
1:2A:2232:U:P	23:21:40:ARG:HH12	2.43	0.41
1:2A:2295:C:OP1	14:2S:10:ARG:NH1	2.53	0.41
1:2A:2320:A:H2'	1:2A:2320:A:N3	2.35	0.41
1:2A:2706:G:N7	58:2A:3906:HOH:O	2.37	0.41
1:2A:634:C:H2'	1:2A:635:C:C6	2.56	0.41
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.21	0.41
4:2E:104:VAL:HG13	4:2E:198:VAL:HG22	2.01	0.41
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.51	0.41
1:1A:2046:G:O5'	27:15:19:ARG:HA	2.21	0.41
1:1A:1101:U:H2'	1:1A:1102:C:C6	2.56	0.41
1:1A:1439:A:H2'	1:1A:1440:G:O4'	2.21	0.41
1:1A:1448:G:H5''	1:1A:1542:A:OP1	2.21	0.41
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.20	0.41
1:1A:2660:A:H2'	1:1A:2661:G:O4'	2.20	0.41
1:1A:30:G:H2'	1:1A:31:C:C6	2.56	0.41
1:1A:335:C:H2'	1:1A:336:C:C6	3.16	0.41
1:1A:987:G:H2'	1:1A:988:A:O4'	2.20	0.41
5:1F:155:LEU:HD11	5:1F:176:LEU:HD12	2.01	0.41
5:1F:196:LEU:HA	5:1F:196:LEU:HD23	1.89	0.41
5:1F:23:ASP:N	5:1F:23:ASP:OD1	2.50	0.41
5:1F:51:THR:HB	5:1F:88:VAL:HG11	2.02	0.41
12:1Q:79:LEU:HD23	12:1Q:79:LEU:HA	1.89	0.41
15:1T:30:VAL:HG22	15:1T:86:ILE:HG12	2.02	0.41
1:2A:113:G:H2'	1:2A:114:U:H6	4.61	0.41
1:2A:1277:G:O2'	13:2R:24:GLN:HG2	2.20	0.41
1:2A:768:G:O2'	1:2A:1379:A:N1	2.49	0.41
1:2A:1821:A:H2'	1:2A:1822:G:H8	1.84	0.41
1:2A:1866:C:H2'	1:2A:1876:A:O4'	2.20	0.41
1:2A:195:A:H2'	1:2A:198:C:N4	2.36	0.41
1:2A:2350:C:H2'	1:2A:2351:G:O4'	2.21	0.41
1:2A:2489:G:C6	1:2A:2490:G:C6	3.09	0.41
1:2A:328:U:H4'	20:2Y:68:HIS:CD2	2.56	0.41
1:2A:509:C:OP1	58:2A:3780:HOH:O	2.22	0.41
1:2A:582:G:H2'	1:2A:583:G:C8	2.56	0.41
1:2A:747:U:O2	1:2A:2014:A:H1'	2.20	0.41
2:2B:8:U:OP1	14:2S:15:ARG:NH2	2.49	0.41
3:2D:37:LEU:HD23	3:2D:60:ARG:HB2	2.01	0.41
1:2A:2302:G:N2	6:2G:126:ASP:OD2	2.41	0.41
14:2S:23:ARG:HD2	14:2S:86:ALA:HB2	2.02	0.41
17:2V:29:PRO:HG3	17:2V:64:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:5:LEU:O	21:2Z:59:LEU:HA	2.20	0.41
23:11:50:ARG:HG2	23:11:59:THR:HG22	2.03	0.41
29:17:24:THR:O	29:17:28:ARG:HG3	2.20	0.41
1:1A:1050:A:H2'	1:1A:1051:G:O4'	2.21	0.41
1:1A:1540:U:H2'	1:1A:1541:G:O4'	2.21	0.41
1:1A:2167:U:H2'	1:1A:2168:G:C8	2.55	0.41
1:1A:2552:OMU:H2'	1:1A:2554:U:OP2	2.20	0.41
1:1A:2846:G:P	15:1T:54:ARG:HB2	2.60	0.41
1:1A:41:C:H2'	1:1A:42:G:O4'	2.21	0.41
1:1A:438:G:H2'	1:1A:440:G:H8	1.86	0.41
1:1A:675:A:OP1	5:1F:63:LYS:NZ	2.45	0.41
3:1D:18:VAL:HG12	3:1D:211:ARG:HH12	1.86	0.41
13:1R:2:ARG:NH1	13:1R:5:LYS:O	2.53	0.41
21:1Z:132:ASN:ND2	21:1Z:160:GLY:HA3	2.36	0.41
1:2A:2056:G:N2	27:25:4:HIS:O	2.48	0.41
1:2A:1006:C:H2'	1:2A:1007:C:C6	3.27	0.41
1:2A:1186:G:H2'	1:2A:1187:G:O4'	2.20	0.41
1:2A:1374:G:H2'	1:2A:1375:C:C6	2.56	0.41
1:2A:271(Q):G:H2'	1:2A:271(R):G:H8	1.86	0.41
1:2A:286:C:H2'	1:2A:287:C:C6	2.55	0.41
1:2A:635:C:H2'	1:2A:636:G:O4'	2.21	0.41
3:2D:68:LYS:O	3:2D:70:TRP:N	2.49	0.41
10:2O:97:ARG:HA	10:2O:117:LEU:HD22	2.03	0.41
11:2P:99:LEU:HD23	11:2P:100:LEU:HD23	2.03	0.41
20:2Y:40:GLU:O	20:2Y:42:VAL:HG23	2.19	0.41
1:1A:1371:G:H2'	1:1A:1372:U:H5	1.86	0.41
1:1A:2023:G:H4'	1:1A:2617:C:O3'	2.21	0.41
1:1A:2492:U:H2'	1:1A:2493:U:C6	2.56	0.41
1:1A:266:G:H2'	1:1A:266:G:N3	3.24	0.41
1:1A:2698:U:H2'	1:1A:2699:C:C6	2.56	0.41
1:1A:644:A:N6	1:1A:2349:G:H1'	2.35	0.41
6:1G:77:ILE:HG22	6:1G:80:PHE:H	1.86	0.41
9:1N:15:LEU:HB2	9:1N:135:PRO:HB2	2.02	0.41
1:2A:2336:A:H61	22:20:43:THR:HG21	1.85	0.41
23:21:3:LYS:HB3	23:21:4:VAL:H	1.64	0.41
24:22:12:GLU:O	24:22:16:LEU:HG	2.20	0.41
29:27:12:ARG:NH2	29:27:44:PRO:HB3	2.35	0.41
1:2A:1358:G:N1	1:2A:1372:U:OP2	2.42	0.41
1:2A:2180:U:H2'	1:2A:2181:G:C8	2.56	0.41
1:2A:2472:G:H22	1:2A:2477:C:H5''	1.86	0.41
1:2A:271(A):A:N7	1:2A:271(W):G:N2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2820:A:HO2'	1:2A:2821:A:P	2.39	0.41
1:2A:355:G:H2'	1:2A:356:G:C8	2.55	0.41
1:2A:530:G:H4'	1:2A:531:C:OP1	2.21	0.41
11:2P:59:LEU:HD21	30:28:10:ALA:HA	2.03	0.41
13:2R:104:ARG:HD2	13:2R:107:ASP:OD1	2.21	0.41
2:2B:37:C:O2'	14:2S:95:HIS:HE1	2.03	0.41
16:2U:89:GLU:HG3	17:2V:50:PRO:HB3	2.03	0.41
22:10:12:ASN:O	22:10:14:ARG:N	2.54	0.41
1:1A:1423:G:H2'	1:1A:1424:G:H8	1.85	0.41
1:1A:2516:G:C5	1:1A:2517:C:C4	3.09	0.41
1:1A:266:G:H1'	1:1A:267:C:OP2	5.84	0.41
1:1A:459:U:H2'	1:1A:460:A:H8	1.86	0.41
1:1A:998:C:OP1	58:1A:4084:HOH:O	2.22	0.41
3:1D:133:LEU:HD13	3:1D:173:VAL:HG21	2.03	0.41
15:1T:51:ARG:HG3	15:1T:98:LYS:HE3	2.01	0.41
17:1V:97:LYS:HD3	17:1V:97:LYS:HA	1.91	0.41
21:1Z:136:PHE:CE1	21:1Z:138:GLU:HG3	2.56	0.41
24:22:1:MET:SD	24:22:56:GLN:NE2	2.94	0.41
1:2A:1050:A:H2'	1:2A:1051:G:H8	1.86	0.41
1:2A:1064:C:H3'	1:2A:1065:U:H5'	2.02	0.41
1:2A:17:G:H4'	16:2U:25:TRP:NE1	2.35	0.41
1:2A:25:U:H2'	1:2A:26:G:O4'	2.21	0.41
1:2A:732:C:H2'	1:2A:733:G:O4'	2.21	0.41
8:2I:104:GLN:HG2	8:2I:105:HIS:CD2	2.55	0.41
14:2S:93:LYS:NZ	14:2S:95:HIS:HB2	2.36	0.41
20:2Y:87:LYS:HB3	20:2Y:95:LYS:HD2	2.03	0.41
22:10:50:ASN:HB3	22:10:63:VAL:HG22	2.02	0.41
1:1A:1783:A:H5'	1:1A:2608:G:H4'	2.02	0.41
1:1A:530:G:N1	1:1A:2023:G:OP1	2.51	0.41
1:1A:2228:G:OP1	3:1D:261:LYS:NZ	2.41	0.41
1:1A:2359:C:H2'	1:1A:2360:A:O4'	2.21	0.41
1:1A:2821:A:H2'	1:1A:2822:G:C8	2.56	0.41
10:1O:23:ARG:HD3	10:1O:24:VAL:N	2.36	0.41
14:1S:43:GLU:OE1	14:1S:43:GLU:N	3.94	0.41
1:2A:1055:G:H2'	1:2A:1056:G:O4'	2.21	0.41
1:2A:113:G:H2'	1:2A:114:U:C6	5.18	0.41
1:2A:1187:G:N2	1:2A:1188:U:O4	2.54	0.41
1:2A:1266:G:O6	18:2W:13:SER:OG	2.28	0.41
1:2A:1587:A:H2'	1:2A:1588:C:C6	2.56	0.41
1:2A:1941:C:C5	1:2A:1942:5MC:HM52	2.56	0.41
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:910:A:N3	1:2A:2264:C:O2'	2.46	0.41
12:2Q:137:TYR:O	12:2Q:141:GLN:HG2	2.20	0.41
1:1A:1321:A:H2'	1:1A:1322:A:O4'	2.21	0.41
1:1A:1798:U:H5'	3:1D:259:THR:CG2	2.49	0.41
1:1A:305:U:H2'	1:1A:306:U:C6	2.56	0.41
1:1A:272(D):G:H1	1:1A:364:C:H42	1.69	0.41
1:1A:630:G:N2	1:1A:633:A:OP2	2.46	0.41
13:1R:26:LYS:HE2	13:1R:70:LEU:O	2.21	0.41
29:27:3:ARG:HA	29:27:3:ARG:HD3	1.79	0.41
1:2A:1431:U:H2'	1:2A:1432:C:C6	2.56	0.41
1:2A:2014:A:OP2	58:2A:3772:HOH:O	2.21	0.41
1:2A:2109:U:H1'	1:2A:2181:G:N2	2.36	0.41
1:2A:2298:A:H2'	1:2A:2299:G:O4'	2.20	0.41
1:2A:2584:U:H5''	1:2A:2602:A:N1	2.35	0.41
1:2A:2602:A:H4'	1:2A:2603:G:OP1	2.20	0.41
1:2A:628:G:O2'	1:2A:651:G:O2'	2.21	0.41
1:2A:655:A:H2'	1:2A:656:G:O4'	2.20	0.41
1:2A:725:G:O5'	1:2A:725:G:H8	2.04	0.41
1:2A:821:A:H2'	1:2A:946:G:H5''	2.03	0.41
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.56	0.41
24:12:32:LEU:HD12	24:12:57:ILE:HD12	2.03	0.40
25:13:3:ARG:NH1	25:13:60:GLU:OE2	2.54	0.40
1:1A:1486:A:H2'	1:1A:1487:G:C8	2.56	0.40
1:1A:1641:A:H2'	1:1A:1642:G:O4'	2.21	0.40
2:1B:115:G:O2'	14:1S:50:SER:OG	2.30	0.40
3:1D:79:VAL:HG12	3:1D:113:VAL:HA	2.04	0.40
16:1U:34:LYS:HD3	16:1U:34:LYS:HA	1.72	0.40
28:26:18:ARG:HD2	28:26:42:TRP:CD1	2.56	0.40
1:2A:1464:C:H2'	1:2A:1465:G:C8	2.56	0.40
1:2A:2017:U:O2	27:25:10:LYS:HB2	2.22	0.40
1:2A:2152:G:H2'	1:2A:2153:G:C8	2.56	0.40
1:2A:2134:A:N6	1:2A:2156:G:O2'	2.43	0.40
1:2A:2887:U:H2'	1:2A:2888:C:C6	2.57	0.40
1:2A:716:A:C2	1:2A:717:G:H1'	2.56	0.40
2:2B:29:A:H2'	2:2B:30:C:C6	2.56	0.40
25:13:5:LYS:HG3	25:13:36:VAL:HG22	2.02	0.40
1:1A:2371:G:H21	28:16:46:HIS:HE1	1.69	0.40
1:1A:1671:U:O4	58:1A:4008:HOH:O	2.22	0.40
1:1A:2189:U:H2'	1:1A:2190:G:H8	1.87	0.40
3:1D:134:ARG:HG3	3:1D:135:PHE:CE1	2.56	0.40
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:108:ASN:HB3	26:14:22:ILE:HD13	2.03	0.40
6:1G:43:LEU:HB3	6:1G:44:GLY:H	1.65	0.40
12:1Q:68:ILE:HD13	12:1Q:103:MET:HG2	2.03	0.40
13:1R:118:GLU:H	13:1R:118:GLU:CD	2.25	0.40
1:2A:1002:G:C4	1:2A:1003:G:H8	3.60	0.40
1:2A:1091:G:N3	1:2A:1091:G:H2'	2.37	0.40
1:2A:1296:G:OP1	1:2A:2709:G:O2'	2.28	0.40
1:2A:1453:U:O2'	1:2A:1455:G:N7	2.51	0.40
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.57	0.40
1:2A:2037:G:C6	1:2A:2038:G:C6	3.10	0.40
1:2A:2619:C:H4'	4:2E:151:TYR:O	2.21	0.40
1:2A:1772:G:O6	53:2A:3001:MPD:H32	2.20	0.40
1:2A:609:A:C5	1:2A:610:G:C8	3.90	0.40
4:2E:175:VAL:HB	4:2E:182:LEU:HD12	2.02	0.40
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	2.04	0.40
9:2N:67:LEU:O	9:2N:88:GLU:HG3	2.21	0.40
10:2O:70:LYS:HB3	10:2O:70:LYS:HE2	1.78	0.40
11:2P:63:PRO:HD3	30:28:27:THR:HG22	2.03	0.40
15:2T:24:PRO:HD3	15:2T:52:ILE:HD12	2.03	0.40
18:2W:86:LEU:HD22	18:2W:96:ILE:HD11	2.03	0.40
12:2Q:59:ARG:HA	21:2Z:180:VAL:HG23	2.03	0.40
1:1A:1210:A:H5''	1:1A:1212:G:O4'	2.22	0.40
1:1A:1272:A:H3'	1:1A:1273:U:H5''	2.02	0.40
1:1A:189:G:OP1	23:11:39:LYS:HD3	2.21	0.40
1:1A:2259:G:N7	58:1A:4220:HOH:O	2.37	0.40
1:1A:2432:A:H5''	58:1A:5422:HOH:O	2.20	0.40
1:1A:2809:A:H62	1:1A:2891:G:H2'	1.85	0.40
1:1A:583:G:OP2	16:1U:10:ARG:HD2	2.22	0.40
4:1E:101:ARG:HD3	4:1E:101:ARG:HA	1.58	0.40
9:1N:138:LEU:HA	9:1N:138:LEU:HD23	1.90	0.40
11:1P:71:VAL:HG23	11:1P:72:PRO:HA	2.04	0.40
1:2A:1410:G:H2'	1:2A:1411:C:H6	1.86	0.40
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.22	0.40
1:2A:2109:U:N3	1:2A:2110:G:O6	2.55	0.40
1:2A:2497:A:H5''	58:2A:4329:HOH:O	2.21	0.40
2:2B:7:G:H3'	2:2B:8:U:H5''	2.03	0.40
1:2A:729:G:C8	3:2D:208:LYS:HD2	2.56	0.40
1:2A:956:G:OP2	12:2Q:14:ARG:NH2	2.54	0.40
26:14:54:GLY:C	26:14:56:VAL:HA	2.42	0.40
1:1A:392:C:H5''	1:1A:409:C:H5''	2.02	0.40
1:1A:875:G:H2'	1:1A:876:C:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:885:C:H1'	1:1A:892:G:N2	2.36	0.40
1:1A:972:G:H3'	1:1A:973:A:H2'	2.03	0.40
9:1N:73:THR:HA	9:1N:83:LYS:O	2.22	0.40
1:1A:2405:G:H4'	11:1P:75:ILE:HD13	2.02	0.40
14:1S:87:PHE:HZ	14:1S:98:VAL:HG12	1.85	0.40
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.56	0.40
18:1W:24:ILE:HA	18:1W:27:LYS:HG3	2.03	0.40
26:24:57:GLU:HA	26:24:58:ARG:HA	1.68	0.40
1:2A:1047:G:H2'	1:2A:1110:G:H22	1.85	0.40
1:2A:411:G:H5''	58:2A:3833:HOH:O	2.21	0.40
2:2B:42:C:O2'	6:2G:66:GLN:HG2	2.22	0.40
8:2I:116:LEU:HD23	8:2I:116:LEU:HA	1.87	0.40
13:2R:26:LYS:HE2	13:2R:70:LEU:O	2.21	0.40
1:1A:1066:U:H3	1:1A:1073:A:N6	2.19	0.40
1:1A:1152:C:H4'	16:1U:77:SER:HA	2.04	0.40
1:1A:1935:G:H1'	1:1A:1964:G:N2	2.36	0.40
1:1A:557:U:H2'	1:1A:558:G:C8	2.56	0.40
19:1X:29:TRP:CZ3	19:1X:78:LYS:HB3	2.57	0.40
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.95	0.40
1:2A:466:A:P	29:27:34:ARG:HH21	2.43	0.40
11:2P:63:PRO:HG2	30:28:25:MET:HB2	2.03	0.40
1:2A:1006:C:H2'	1:2A:1007:C:H6	2.58	0.40
1:2A:1639:U:H2'	1:2A:1640:C:H5''	2.04	0.40
1:2A:299:A:N1	1:2A:322:A:O2'	2.43	0.40
1:2A:476:G:H2'	1:2A:477:A:H8	3.63	0.40
1:2A:593:G:H2'	1:2A:594:U:C6	2.56	0.40
1:2A:864:G:N2	1:2A:866:A:H61	2.18	0.40
6:2G:136:ARG:HG3	6:2G:137:GLU:HG3	2.03	0.40
7:2H:86:GLU:OE2	7:2H:132:ARG:NH2	2.55	0.40
12:2Q:64:ILE:N	21:2Z:178:GLU:OE2	2.48	0.40
21:2Z:4:ARG:HH21	21:2Z:60:GLU:HG2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	259 (95%)	14 (5%)	0	100	100
3	2D	273/276 (99%)	257 (94%)	16 (6%)	0	100	100
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	29	62
4	2E	202/206 (98%)	187 (93%)	13 (6%)	2 (1%)	15	47
5	1F	201/210 (96%)	193 (96%)	8 (4%)	0	100	100
5	2F	201/210 (96%)	189 (94%)	12 (6%)	0	100	100
6	1G	179/182 (98%)	164 (92%)	13 (7%)	2 (1%)	14	46
6	2G	179/182 (98%)	162 (90%)	15 (8%)	2 (1%)	14	46
7	1H	172/180 (96%)	161 (94%)	7 (4%)	4 (2%)	6	29
7	2H	171/180 (95%)	156 (91%)	13 (8%)	2 (1%)	13	43
8	1I	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
8	2I	144/148 (97%)	138 (96%)	5 (4%)	1 (1%)	22	56
9	1N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
9	2N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
10	1O	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
10	2O	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
11	1P	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
11	2P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	22	56
12	1Q	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
12	2Q	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	22	56
13	1R	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
13	2R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	7 (6%)	2 (2%)	8	34
14	2S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
15	1T	129/146 (88%)	115 (89%)	12 (9%)	2 (2%)	9	37
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	15	47
17	2V	99/101 (98%)	93 (94%)	4 (4%)	2 (2%)	7	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	1W	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
18	2W	110/113 (97%)	105 (96%)	5 (4%)	0	100	100
19	1X	93/96 (97%)	87 (94%)	4 (4%)	2 (2%)	6	31
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	14	46
20	1Y	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
21	1Z	201/206 (98%)	191 (95%)	9 (4%)	1 (0%)	29	62
21	2Z	199/206 (97%)	187 (94%)	11 (6%)	1 (0%)	29	62
22	10	75/85 (88%)	71 (95%)	3 (4%)	1 (1%)	12	41
22	20	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	46
24	12	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
26	14	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	10
26	24	67/71 (94%)	52 (78%)	13 (19%)	2 (3%)	4	24
27	15	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
27	25	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
30	28	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
31	19	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	199 (87%)	22 (10%)	8 (4%)	3	21
33	2b	229/256 (90%)	203 (89%)	22 (10%)	4 (2%)	9	36
34	1c	204/239 (85%)	190 (93%)	13 (6%)	1 (0%)	29	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	2c	204/239 (85%)	192 (94%)	11 (5%)	1 (0%)	29	62
35	1d	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	29	62
35	2d	206/209 (99%)	193 (94%)	13 (6%)	0	100	100
36	1e	146/162 (90%)	137 (94%)	9 (6%)	0	100	100
36	2e	146/162 (90%)	141 (97%)	5 (3%)	0	100	100
37	1f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
38	2g	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
40	1i	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
40	2i	124/128 (97%)	111 (90%)	12 (10%)	1 (1%)	19	52
41	1j	95/105 (90%)	83 (87%)	9 (10%)	3 (3%)	4	23
41	2j	94/105 (90%)	85 (90%)	4 (4%)	5 (5%)	2	12
42	1k	112/129 (87%)	104 (93%)	7 (6%)	1 (1%)	17	50
42	2k	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	17	50
43	1l	119/135 (88%)	111 (93%)	8 (7%)	0	100	100
43	2l	119/135 (88%)	109 (92%)	10 (8%)	0	100	100
44	1m	114/126 (90%)	106 (93%)	7 (6%)	1 (1%)	17	50
44	2m	112/126 (89%)	106 (95%)	5 (4%)	1 (1%)	17	50
45	1n	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
45	2n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
46	1o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
46	2o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	13	43
47	1p	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
47	2p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	12	41
48	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
48	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
49	1s	81/93 (87%)	74 (91%)	5 (6%)	2 (2%)	5	28
49	2s	81/93 (87%)	74 (91%)	7 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	1t	94/106 (89%)	91 (97%)	2 (2%)	1 (1%)	14	46
50	2t	96/106 (91%)	90 (94%)	4 (4%)	2 (2%)	7	32
51	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
51	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	1y	95/113 (84%)	92 (97%)	3 (3%)	0	100	100
52	2y	94/113 (83%)	91 (97%)	2 (2%)	1 (1%)	14	46
All	All	11435/12150 (94%)	10717 (94%)	646 (6%)	72 (1%)	25	59

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	10	13	GLY
26	14	55	ARG
33	1b	125	PRO
41	1j	77	PRO
33	2b	17	PHE
6	1G	52	ILE
7	1H	47	GLU
14	1S	59	LYS
14	1S	94	TYR
15	1T	127	ALA
19	1X	67	GLY
19	1X	94	GLY
26	14	61	ARG
33	1b	36	ARG
41	1j	55	LYS
4	2E	51	PHE
6	2G	81	LYS
12	2Q	59	ARG
17	2V	79	VAL
33	2b	95	GLN
41	2j	75	ILE
44	2m	67	GLU
50	2t	100	ILE
7	1H	92	ILE
26	14	44	THR
26	14	49	PHE
33	1b	17	PHE
33	1b	21	ARG
33	1b	95	GLN

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Mol	Chain	Res	Type
34	1c	3	ASN
41	1j	78	ASN
44	1m	23	TYR
8	2I	85	GLU
17	2V	53	GLU
19	2X	94	GLY
23	21	3	LYS
26	24	55	ARG
33	2b	123	ALA
41	2j	78	ASN
4	1E	52	LEU
6	1G	47	LYS
33	1b	20	GLU
35	1d	5	ILE
50	1t	95	ALA
21	2Z	30	ASN
26	24	44	THR
33	2b	125	PRO
40	2i	44	VAL
46	2o	88	ARG
7	1H	126	PRO
21	1Z	31	ARG
33	1b	127	ILE
33	1b	231	GLU
49	1s	13	ASP
4	2E	113	PHE
6	2G	43	LEU
49	1s	12	ASP
11	2P	29	LYS
34	2c	99	VAL
7	1H	21	PRO
17	1V	79	VAL
42	1k	105	VAL
41	2j	37	PRO
41	2j	39	PRO
41	2j	77	PRO
7	2H	21	PRO
42	2k	105	VAL
47	2p	63	GLY
7	2H	126	PRO
50	2t	102	GLY
52	2y	45	PRO

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Mol	Chain	Res	Type
15	1T	56	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	214/218 (98%)	200 (94%)	14 (6%)	17	46
3	2D	215/218 (99%)	204 (95%)	11 (5%)	24	54
4	1E	164/166 (99%)	152 (93%)	12 (7%)	14	40
4	2E	164/166 (99%)	152 (93%)	12 (7%)	14	40
5	1F	161/166 (97%)	154 (96%)	7 (4%)	29	59
5	2F	160/166 (96%)	154 (96%)	6 (4%)	33	62
6	1G	144/156 (92%)	140 (97%)	4 (3%)	43	69
6	2G	142/156 (91%)	137 (96%)	5 (4%)	36	64
7	1H	144/148 (97%)	142 (99%)	2 (1%)	67	81
7	2H	143/148 (97%)	140 (98%)	3 (2%)	53	75
8	1I	111/124 (90%)	105 (95%)	6 (5%)	22	53
8	2I	108/124 (87%)	105 (97%)	3 (3%)	43	69
9	1N	119/119 (100%)	111 (93%)	8 (7%)	16	45
9	2N	118/119 (99%)	109 (92%)	9 (8%)	13	39
10	1O	100/100 (100%)	100 (100%)	0	100	100
10	2O	100/100 (100%)	98 (98%)	2 (2%)	55	76
11	1P	115/116 (99%)	112 (97%)	3 (3%)	46	71
11	2P	115/116 (99%)	113 (98%)	2 (2%)	60	78
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	44	70
12	2Q	111/111 (100%)	109 (98%)	2 (2%)	59	77
13	1R	101/101 (100%)	93 (92%)	8 (8%)	12	37
13	2R	101/101 (100%)	95 (94%)	6 (6%)	19	50
14	1S	87/88 (99%)	85 (98%)	2 (2%)	50	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	2S	85/88 (97%)	84 (99%)	1 (1%)	71	83
15	1T	115/128 (90%)	114 (99%)	1 (1%)	78	87
15	2T	113/128 (88%)	109 (96%)	4 (4%)	36	64
16	1U	93/94 (99%)	87 (94%)	6 (6%)	17	46
16	2U	93/94 (99%)	89 (96%)	4 (4%)	29	59
17	1V	81/82 (99%)	78 (96%)	3 (4%)	34	62
17	2V	80/82 (98%)	77 (96%)	3 (4%)	33	62
18	1W	90/92 (98%)	85 (94%)	5 (6%)	21	52
18	2W	90/92 (98%)	89 (99%)	1 (1%)	73	84
19	1X	77/78 (99%)	76 (99%)	1 (1%)	69	82
19	2X	77/78 (99%)	75 (97%)	2 (3%)	46	71
20	1Y	86/91 (94%)	83 (96%)	3 (4%)	36	64
20	2Y	86/91 (94%)	85 (99%)	1 (1%)	71	83
21	1Z	169/179 (94%)	166 (98%)	3 (2%)	59	77
21	2Z	165/179 (92%)	161 (98%)	4 (2%)	49	72
22	10	61/67 (91%)	59 (97%)	2 (3%)	38	65
22	20	61/67 (91%)	60 (98%)	1 (2%)	62	79
23	11	79/83 (95%)	79 (100%)	0	100	100
23	21	81/83 (98%)	80 (99%)	1 (1%)	71	83
24	12	65/67 (97%)	62 (95%)	3 (5%)	27	57
24	22	66/67 (98%)	63 (96%)	3 (4%)	27	58
25	13	51/52 (98%)	48 (94%)	3 (6%)	19	50
25	23	50/52 (96%)	48 (96%)	2 (4%)	31	61
26	14	58/63 (92%)	54 (93%)	4 (7%)	15	43
26	24	54/63 (86%)	51 (94%)	3 (6%)	21	52
27	15	51/52 (98%)	49 (96%)	2 (4%)	32	61
27	25	50/52 (96%)	48 (96%)	2 (4%)	31	61
28	16	51/52 (98%)	48 (94%)	3 (6%)	19	50
28	26	50/52 (96%)	48 (96%)	2 (4%)	31	61
29	17	41/42 (98%)	39 (95%)	2 (5%)	25	55
29	27	41/42 (98%)	40 (98%)	1 (2%)	49	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	18	54/55 (98%)	52 (96%)	2 (4%)	34	62
30	28	54/55 (98%)	53 (98%)	1 (2%)	57	76
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	68
33	1b	191/220 (87%)	184 (96%)	7 (4%)	34	62
33	2b	187/220 (85%)	180 (96%)	7 (4%)	34	62
34	1c	144/188 (77%)	142 (99%)	2 (1%)	67	81
34	2c	140/188 (74%)	138 (99%)	2 (1%)	67	81
35	1d	171/181 (94%)	166 (97%)	5 (3%)	42	68
35	2d	172/181 (95%)	166 (96%)	6 (4%)	36	64
36	1e	114/123 (93%)	112 (98%)	2 (2%)	59	77
36	2e	114/123 (93%)	111 (97%)	3 (3%)	46	71
37	1f	85/90 (94%)	85 (100%)	0	100	100
37	2f	85/90 (94%)	83 (98%)	2 (2%)	49	72
38	1g	120/127 (94%)	119 (99%)	1 (1%)	81	89
38	2g	119/127 (94%)	116 (98%)	3 (2%)	47	71
39	1h	116/119 (98%)	112 (97%)	4 (3%)	37	64
39	2h	114/119 (96%)	110 (96%)	4 (4%)	36	64
40	1i	91/99 (92%)	91 (100%)	0	100	100
40	2i	88/99 (89%)	84 (96%)	4 (4%)	27	58
41	1j	68/92 (74%)	68 (100%)	0	100	100
41	2j	68/92 (74%)	67 (98%)	1 (2%)	65	80
42	1k	83/99 (84%)	81 (98%)	2 (2%)	49	72
42	2k	83/99 (84%)	82 (99%)	1 (1%)	71	83
43	1l	96/110 (87%)	94 (98%)	2 (2%)	53	75
43	2l	96/110 (87%)	93 (97%)	3 (3%)	40	67
44	1m	90/101 (89%)	88 (98%)	2 (2%)	52	74
44	2m	87/101 (86%)	87 (100%)	0	100	100
45	1n	49/50 (98%)	47 (96%)	2 (4%)	30	60
45	2n	49/50 (98%)	48 (98%)	1 (2%)	55	76
46	1o	78/80 (98%)	76 (97%)	2 (3%)	46	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	2o	78/80 (98%)	77 (99%)	1 (1%)	69	82
47	1p	69/74 (93%)	66 (96%)	3 (4%)	29	59
47	2p	68/74 (92%)	64 (94%)	4 (6%)	19	50
48	1r	59/77 (77%)	58 (98%)	1 (2%)	60	78
48	2r	59/77 (77%)	58 (98%)	1 (2%)	60	78
49	1s	68/80 (85%)	66 (97%)	2 (3%)	42	68
49	2s	67/80 (84%)	67 (100%)	0	100	100
50	1t	71/82 (87%)	69 (97%)	2 (3%)	43	69
50	2t	70/82 (85%)	67 (96%)	3 (4%)	29	59
51	1u	18/22 (82%)	18 (100%)	0	100	100
51	2u	18/22 (82%)	18 (100%)	0	100	100
52	1y	82/98 (84%)	81 (99%)	1 (1%)	71	83
52	2y	79/98 (81%)	75 (95%)	4 (5%)	24	54
All	All	9338/10072 (93%)	9038 (97%)	300 (3%)	39	66

All (300) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	61	LEU
3	1D	94	LEU
3	1D	104	TYR
3	1D	106	ILE
3	1D	111	LEU
3	1D	113	VAL
3	1D	138	VAL
3	1D	142	VAL
3	1D	193	VAL
3	1D	211	ARG
3	1D	212	SER
3	1D	221	VAL
3	1D	229	VAL
3	1D	253	GLN
4	1E	9	VAL
4	1E	12	THR
4	1E	49	LEU
4	1E	75	VAL
4	1E	101	ARG

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Mol	Chain	Res	Type
4	1E	116	VAL
4	1E	119	ARG
4	1E	144	ARG
4	1E	169	ASN
4	1E	181	LEU
4	1E	183	LEU
4	1E	184	VAL
5	1F	57	VAL
5	1F	74	ARG
5	1F	88	VAL
5	1F	110	LEU
5	1F	170	LEU
5	1F	183	VAL
5	1F	195	ASP
6	1G	7	LEU
6	1G	43	LEU
6	1G	52	ILE
6	1G	82	LEU
7	1H	45	VAL
7	1H	69	ARG
8	1I	38	LEU
8	1I	43	ASN
8	1I	47	LEU
8	1I	92	VAL
8	1I	127	VAL
8	1I	140	LEU
9	1N	33	LEU
9	1N	34	LEU
9	1N	67	LEU
9	1N	73	THR
9	1N	87	LEU
9	1N	99	LEU
9	1N	115	ARG
9	1N	121	LYS
11	1P	57	THR
11	1P	59	LEU
11	1P	112	LEU
12	1Q	6	ARG
12	1Q	55	VAL
12	1Q	109	VAL
13	1R	6	SER
13	1R	29	LEU

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Mol	Chain	Res	Type
13	1R	36	THR
13	1R	44	LEU
13	1R	47	PHE
13	1R	65	LEU
13	1R	75	LEU
13	1R	96	ARG
14	1S	25	ARG
14	1S	110	LEU
15	1T	96	ARG
16	1U	8	VAL
16	1U	30	LYS
16	1U	52	ARG
16	1U	60	LEU
16	1U	74	LEU
16	1U	104	GLN
17	1V	61	VAL
17	1V	79	VAL
17	1V	82	ARG
18	1W	17	VAL
18	1W	67	ASP
18	1W	96	ILE
18	1W	100	THR
18	1W	107	LEU
19	1X	23	GLU
20	1Y	14	LEU
20	1Y	43	ASN
20	1Y	72	VAL
21	1Z	86	VAL
21	1Z	87	ASP
21	1Z	150	LEU
22	10	9	SER
22	10	39	ARG
24	12	3	LEU
24	12	53	LEU
24	12	64	LEU
25	13	6	VAL
25	13	8	LEU
25	13	54	VAL
26	14	34	GLU
26	14	49	PHE
26	14	50	VAL
26	14	61	ARG

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Mol	Chain	Res	Type
27	15	16	ARG
27	15	21	SER
28	16	6	ARG
28	16	23	THR
28	16	48	VAL
29	17	34	ARG
29	17	43	THR
30	18	31	HIS
30	18	34	TRP
33	1b	19	HIS
33	1b	44	LEU
33	1b	111	ARG
33	1b	122	PHE
33	1b	178	ARG
33	1b	187	LEU
33	1b	196	LEU
34	1c	36	ASP
34	1c	105	GLU
35	1d	31	CYS
35	1d	135	LEU
35	1d	155	LEU
35	1d	178	VAL
35	1d	188	LEU
36	1e	41	VAL
36	1e	120	THR
38	1g	144	MET
39	1h	25	ASP
39	1h	26	VAL
39	1h	51	VAL
39	1h	63	LEU
42	1k	14	VAL
42	1k	117	ASN
43	1l	27	LEU
43	1l	33	ARG
44	1m	70	LEU
44	1m	86	CYS
45	1n	18	VAL
45	1n	33	VAL
46	1o	3	ILE
46	1o	39	LEU
47	1p	29	ASP
47	1p	45	THR

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Mol	Chain	Res	Type
47	1p	62	VAL
48	1r	76	LEU
49	1s	28	LYS
49	1s	41	VAL
50	1t	84	LEU
50	1t	100	ILE
52	1y	42	SER
3	2D	3	VAL
3	2D	69	ARG
3	2D	94	LEU
3	2D	103	ARG
3	2D	111	LEU
3	2D	113	VAL
3	2D	138	VAL
3	2D	211	ARG
3	2D	221	VAL
3	2D	237	GLU
3	2D	242	ARG
4	2E	1	MET
4	2E	7	VAL
4	2E	9	VAL
4	2E	52	LEU
4	2E	75	VAL
4	2E	93	VAL
4	2E	116	VAL
4	2E	132	HIS
4	2E	144	ARG
4	2E	154	LYS
4	2E	169	ASN
4	2E	175	VAL
5	2F	20	LEU
5	2F	33	LEU
5	2F	57	VAL
5	2F	88	VAL
5	2F	183	VAL
5	2F	192	LEU
6	2G	3	LEU
6	2G	7	LEU
6	2G	49	ASP
6	2G	138	GLN
6	2G	159	VAL
7	2H	71	LEU

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Mol	Chain	Res	Type
7	2H	81	GLU
7	2H	136	ILE
8	2I	38	LEU
8	2I	92	VAL
8	2I	116	LEU
9	2N	5	VAL
9	2N	33	LEU
9	2N	34	LEU
9	2N	43	THR
9	2N	62	VAL
9	2N	68	GLU
9	2N	73	THR
9	2N	87	LEU
9	2N	99	LEU
10	2O	10	VAL
10	2O	80	ASP
11	2P	56	SER
11	2P	112	LEU
12	2Q	109	VAL
12	2Q	112	GLU
13	2R	18	LEU
13	2R	44	LEU
13	2R	75	LEU
13	2R	79	LEU
13	2R	96	ARG
13	2R	100	LEU
14	2S	25	ARG
15	2T	49	VAL
15	2T	78	LEU
15	2T	96	ARG
15	2T	107	ASP
16	2U	8	VAL
16	2U	31	SER
16	2U	60	LEU
16	2U	74	LEU
17	2V	46	VAL
17	2V	72	VAL
17	2V	79	VAL
18	2W	23	LEU
19	2X	41	ASN
19	2X	57	LEU
20	2Y	72	VAL

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Mol	Chain	Res	Type
21	2Z	107	THR
21	2Z	126	VAL
21	2Z	150	LEU
21	2Z	193	GLU
22	20	39	ARG
23	21	4	VAL
24	22	32	LEU
24	22	45	SER
24	22	53	LEU
25	23	23	LEU
25	23	54	VAL
26	24	36	CYS
26	24	44	THR
26	24	53	GLU
27	25	6	VAL
27	25	23	HIS
28	26	14	THR
28	26	40	CYS
29	27	43	THR
30	28	31	HIS
31	29	12	ASP
33	2b	16	HIS
33	2b	24	TRP
33	2b	55	PHE
33	2b	76	GLN
33	2b	187	LEU
33	2b	189	ASP
33	2b	224	GLN
34	2c	52	LEU
34	2c	105	GLU
35	2d	8	VAL
35	2d	12	CYS
35	2d	31	CYS
35	2d	34	GLU
35	2d	135	LEU
35	2d	155	LEU
36	2e	31	LEU
36	2e	34	VAL
36	2e	41	VAL
37	2f	22	GLU
37	2f	72	VAL
38	2g	75	VAL

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Mol	Chain	Res	Type
38	2g	113	GLU
38	2g	115	ARG
39	2h	29	SER
39	2h	63	LEU
39	2h	112	LEU
39	2h	133	LEU
40	2i	17	VAL
40	2i	92	TYR
40	2i	102	LEU
40	2i	108	VAL
41	2j	34	VAL
42	2k	103	LEU
43	2l	24	VAL
43	2l	27	LEU
43	2l	112	ASP
45	2n	18	VAL
46	2o	39	LEU
47	2p	20	VAL
47	2p	42	ARG
47	2p	54	GLU
47	2p	62	VAL
48	2r	76	LEU
50	2t	24	LEU
50	2t	84	LEU
50	2t	100	ILE
52	2y	16	ILE
52	2y	46	GLN
52	2y	56	THR
52	2y	62	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
49	1s	56	GLN
33	2b	78	GLN
34	2c	6	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2856/2894 (98%)	390 (13%)	17 (0%)
1	2A	2849/2894 (98%)	429 (15%)	25 (0%)
2	1B	117/120 (97%)	8 (6%)	0
2	2B	117/120 (97%)	10 (8%)	0
32	1a	1494/1522 (98%)	213 (14%)	0
32	2a	1498/1522 (98%)	223 (14%)	0
All	All	8931/9072 (98%)	1273 (14%)	42 (0%)

All (1273) 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	118	A
1	1A	119	A
1	1A	120	U
1	1A	181	A
1	1A	182	A
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	271(I)	G
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	272(A)	U
1	1A	272(B)	G
1	1A	272(H)	C
1	1A	272(J)	C
1	1A	275	G

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Mol	Chain	Res	Type
1	1A	279	C
1	1A	311	A
1	1A	324	A
1	1A	330	A
1	1A	333	G
1	1A	345	A
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	372	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	428	A
1	1A	443	A
1	1A	448	U
1	1A	454	A
1	1A	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	518	G
1	1A	528	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	556	G
1	1A	563	G
1	1A	573	G
1	1A	574	C
1	1A	575	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G

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Mol	Chain	Res	Type
1	1A	627	A
1	1A	634	C
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	653	C
1	1A	654	U
1	1A	656	G
1	1A	668	G
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	762	U
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	811	U
1	1A	812	C
1	1A	821	A
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	880	G
1	1A	886	C
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	896	A
1	1A	910	A
1	1A	915	C
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	958	U

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Mol	Chain	Res	Type
1	1A	959	A
1	1A	961	C
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	1025	G
1	1A	1026	U
1	1A	1033	U
1	1A	1039	G
1	1A	1042	G
1	1A	1043	C
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1060	U
1	1A	1061	U
1	1A	1062	G
1	1A	1063	G
1	1A	1065	U
1	1A	1068	G
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1078	U
1	1A	1083	U
1	1A	1088	A
1	1A	1090	U
1	1A	1096	A
1	1A	1097	U
1	1A	1109	C
1	1A	1112	G
1	1A	1130	U
1	1A	1132	A
1	1A	1135	C

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Mol	Chain	Res	Type
1	1A	1136	G
1	1A	1139	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	1187	G
1	1A	1206	G
1	1A	1211	U
1	1A	1220	A
1	1A	1236	G
1	1A	1248	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	1345	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1370	C
1	1A	1379	A
1	1A	1384	A
1	1A	1385	G
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	1452	A
1	1A	1455	G
1	1A	1467	C
1	1A	1471	A
1	1A	1482	G

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Mol	Chain	Res	Type
1	1A	1493	C
1	1A	1509	A
1	1A	1531	C
1	1A	1542	A
1	1A	1543	C
1	1A	1558	A
1	1A	1569	A
1	1A	1578	U
1	1A	1579	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1616	A
1	1A	1639	U
1	1A	1648	C
1	1A	1654	A
1	1A	1664	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1721	G
1	1A	1722	A
1	1A	1739	U
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	1848	A
1	1A	1877	A

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Mol	Chain	Res	Type
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	1936	A
1	1A	1938	A
1	1A	1939	5MU
1	1A	1940	U
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1993	U
1	1A	1997	G
1	1A	2023	G
1	1A	2031	A
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2074	U
1	1A	2093	G
1	1A	2099	U
1	1A	2103	C
1	1A	2104	G
1	1A	2107	C
1	1A	2108	C
1	1A	2112	G
1	1A	2116	G
1	1A	2117	A
1	1A	2118	U
1	1A	2119	A
1	1A	2123	G

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Mol	Chain	Res	Type
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	2142	C
1	1A	2146	C
1	1A	2147	G
1	1A	2153	G
1	1A	2158	A
1	1A	2159	G
1	1A	2173	A
1	1A	2186	G
1	1A	2187	G
1	1A	2190	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2225	A
1	1A	2234	G
1	1A	2238	G
1	1A	2239	G
1	1A	2273	A
1	1A	2278	A
1	1A	2279	G
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2312	U
1	1A	2320	A
1	1A	2325	G
1	1A	2347	C
1	1A	2350	C
1	1A	2372	G
1	1A	2383	G
1	1A	2385	C
1	1A	2391	G

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Mol	Chain	Res	Type
1	1A	2406	U
1	1A	2422	A
1	1A	2424	C
1	1A	2425	A
1	1A	2428	G
1	1A	2429	G
1	1A	2430	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2470	G
1	1A	2474	C
1	1A	2476	A
1	1A	2478	A
1	1A	2502	G
1	1A	2504	U
1	1A	2505	G
1	1A	2506	U
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2554	U
1	1A	2564	A
1	1A	2566	A
1	1A	2567	G
1	1A	2572	A
1	1A	2602	A
1	1A	2603	G
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	2662	A
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A

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Mol	Chain	Res	Type
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2758	A
1	1A	2764	A
1	1A	2765	A
1	1A	2769	C
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2802	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2872	G
1	1A	2873	A
1	1A	2876	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
2	1B	13	A
2	1B	24	G
2	1B	53	A
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	106	G
2	1B	110	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	61	G
32	1a	78	G
32	1a	79	G
32	1a	101	A
32	1a	116	A
32	1a	120	A

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Mol	Chain	Res	Type
32	1a	121	C
32	1a	122	G
32	1a	129(A)	G
32	1a	131	C
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(D)	C
32	1a	189(F)	U
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	220	G
32	1a	247	G
32	1a	250	A
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	280	C
32	1a	289	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	366	C
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	390	C
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	423	G

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Mol	Chain	Res	Type
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	G
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	532	A
32	1a	547	A
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	564	C
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	618	C
32	1a	619	U
32	1a	630	G
32	1a	632	A
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	702	A
32	1a	723	U
32	1a	731	G
32	1a	755	G
32	1a	777	A
32	1a	793	U

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Mol	Chain	Res	Type
32	1a	794	A
32	1a	816	A
32	1a	817	C
32	1a	828	A
32	1a	829	G
32	1a	839	U
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	851	G
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	965	A
32	1a	967	5MC
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	998	G
32	1a	1001(A)	G
32	1a	1006	C
32	1a	1022	G
32	1a	1023	G
32	1a	1024	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

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Mol	Chain	Res	Type
32	1a	1030(B)	C
32	1a	1032	G
32	1a	1033	G
32	1a	1034	G
32	1a	1037	C
32	1a	1042	G
32	1a	1044	A
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1124	G
32	1a	1126	U
32	1a	1130	A
32	1a	1132	C
32	1a	1136	U
32	1a	1139	G
32	1a	1140	C
32	1a	1152	A
32	1a	1159	U
32	1a	1166	G
32	1a	1168	A
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1213	A
32	1a	1224	G
32	1a	1227	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A

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Mol	Chain	Res	Type
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1320	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
32	1a	1397	C
32	1a	1400	5MC
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1487	G
32	1a	1493	A
32	1a	1497	G
32	1a	1498	UR3
32	1a	1499	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
1	2A	10	G
1	2A	12	U
1	2A	14	A
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	51	G
1	2A	71	A

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Mol	Chain	Res	Type
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	102	G
1	2A	118	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	157	U
1	2A	181	A
1	2A	182	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	229	A
1	2A	230	U
1	2A	248	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	324	A
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	370	G
1	2A	372	G
1	2A	386	G
1	2A	396	G
1	2A	411	G

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Mol	Chain	Res	Type
1	2A	412	A
1	2A	428	A
1	2A	444	C
1	2A	446	G
1	2A	456	C
1	2A	457	A
1	2A	470	A
1	2A	481	G
1	2A	494	G
1	2A	505	A
1	2A	509	C
1	2A	528	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	545	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	574	C
1	2A	575	A
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	620	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	651	G
1	2A	653	C
1	2A	654	U
1	2A	655	A
1	2A	669	G
1	2A	686	G
1	2A	730	C
1	2A	740	U
1	2A	753	C
1	2A	764	A

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Mol	Chain	Res	Type
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	788	A
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	827	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	880	G
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1006	C
1	2A	1012	U
1	2A	1013	C
1	2A	1022	G

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Mol	Chain	Res	Type
1	2A	1026	U
1	2A	1033	U
1	2A	1041	C
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1048	A
1	2A	1052	C
1	2A	1053	C
1	2A	1054	A
1	2A	1058	G
1	2A	1060	U
1	2A	1063	G
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U
1	2A	1067	A
1	2A	1068	G
1	2A	1069	A
1	2A	1070	A
1	2A	1071	G
1	2A	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1078	U
1	2A	1079	C
1	2A	1082	U
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1088	A
1	2A	1090	U
1	2A	1091	G
1	2A	1092	C
1	2A	1094	U
1	2A	1096	A
1	2A	1098	A
1	2A	1109	C
1	2A	1110	G
1	2A	1112	G
1	2A	1116	C

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Mol	Chain	Res	Type
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1142(A)	A
1	2A	1171	G
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1248	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1314	C
1	2A	1321	A
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1379	A
1	2A	1384	A
1	2A	1385	G
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1493	C
1	2A	1497	U
1	2A	1509	A

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Mol	Chain	Res	Type
1	2A	1531	C
1	2A	1542	A
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1639	U
1	2A	1640	C
1	2A	1646	C
1	2A	1648	C
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1722	A
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1835	G
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1920	OMC
1	2A	1929	G

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Mol	Chain	Res	Type
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A
1	2A	1940	U
1	2A	1955	U
1	2A	1963	U
1	2A	1964	G
1	2A	1965	C
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2030	A
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2093	G
1	2A	2096	U
1	2A	2099	U
1	2A	2103	C
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2109	U
1	2A	2110	G
1	2A	2112	G
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2121	G

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Mol	Chain	Res	Type
1	2A	2123	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	2136	C
1	2A	2138	C
1	2A	2145	C
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G
1	2A	2151	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2172	U
1	2A	2173	A
1	2A	2180	U
1	2A	2186	G
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2251	OMG
1	2A	2269	A
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2292	C
1	2A	2305	A
1	2A	2308	G

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Mol	Chain	Res	Type
1	2A	2312	U
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2335	A
1	2A	2336	A
1	2A	2343	C
1	2A	2345	G
1	2A	2347	C
1	2A	2350	C
1	2A	2383	G
1	2A	2385	C
1	2A	2391	G
1	2A	2406	U
1	2A	2410	G
1	2A	2422	A
1	2A	2425	A
1	2A	2427	C
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	2470	G
1	2A	2474	C
1	2A	2476	A
1	2A	2478	A
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2554	U
1	2A	2564	A
1	2A	2566	A
1	2A	2567	G

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Mol	Chain	Res	Type
1	2A	2576	G
1	2A	2577	A
1	2A	2578	G
1	2A	2582	G
1	2A	2585	U
1	2A	2586	C
1	2A	2602	A
1	2A	2603	G
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2663	G
1	2A	2682	U
1	2A	2689	U
1	2A	2690	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2720	U
1	2A	2726	U
1	2A	2733	A
1	2A	2744	G
1	2A	2748	A
1	2A	2757	A
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2811	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2872	G
1	2A	2875	C
1	2A	2880	C
1	2A	2894	G

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Mol	Chain	Res	Type
2	2B	8	U
2	2B	13	A
2	2B	24	G
2	2B	30	C
2	2B	33	G
2	2B	51	G
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	110	G
32	2a	5	U
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	61	G
32	2a	66	G
32	2a	101	A
32	2a	116	A
32	2a	120	A
32	2a	121	C
32	2a	122	G
32	2a	129(A)	G
32	2a	131	C
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	220	G
32	2a	245	C
32	2a	247	G

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Mol	Chain	Res	Type
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	298	A
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	356	A
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	424	G
32	2a	429	U
32	2a	439	A
32	2a	452	A
32	2a	470	G
32	2a	482	A
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	517	G
32	2a	518	C
32	2a	527	G7M
32	2a	532	A
32	2a	533	A
32	2a	547	A

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Mol	Chain	Res	Type
32	2a	559	A
32	2a	560	U
32	2a	561	U
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	630	G
32	2a	632	A
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	702	A
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	829	G
32	2a	836	G
32	2a	840	C
32	2a	841	U
32	2a	848	C
32	2a	851	G
32	2a	859	A
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G

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Mol	Chain	Res	Type
32	2a	931	C
32	2a	934	C
32	2a	960	U
32	2a	961	U
32	2a	966	M2G
32	2a	967	5MC
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	978	A
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1020	U
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(A)	G
32	2a	1030(B)	C
32	2a	1041	A
32	2a	1044	A
32	2a	1053	G
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A

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Mol	Chain	Res	Type
32	2a	1118	C
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1179	A
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1211	U
32	2a	1213	A
32	2a	1224	G
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1248	A
32	2a	1250	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1281	U
32	2a	1282	C
32	2a	1285	A
32	2a	1286	A
32	2a	1287	A
32	2a	1300	G
32	2a	1303	C
32	2a	1305	G
32	2a	1312	G
32	2a	1317	C

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Mol	Chain	Res	Type
32	2a	1320	C
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1370	G
32	2a	1397	C
32	2a	1401	G
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1492	A
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G

All (42) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	266	G
1	1A	278	A
1	1A	888	C
1	1A	895	U
1	1A	1047	G
1	1A	1065	U
1	1A	1067	A
1	1A	1176	G
1	1A	1210	A
1	1A	1300	U
1	1A	1442	G
1	1A	1508	A
1	1A	1653	G
1	1A	2126	A
1	1A	2430	A

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Mol	Chain	Res	Type
1	1A	2689	U
1	1A	2893	G
1	2A	9	U
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	752	A
1	2A	840	C
1	2A	856	C
1	2A	900	A
1	2A	1053	C
1	2A	1057	A
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A
1	2A	1210	A
1	2A	1442	G
1	2A	1491	G
1	2A	1939	5MU
1	2A	1992	G
1	2A	2126	A
1	2A	2171	A
1	2A	2172	U
1	2A	2321	G
1	2A	2602	A
1	2A	2689	U
1	2A	2756	U

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

48 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	$\# Z > 2$
32	MA6	2a	1519	32	19,26,27	1.44	4 (21%)	18,38,41	1.53	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	1A	1917	1	17,21,22	1.78	5 (29%)	20,30,33	3.48	6 (30%)
43	0TD	2l	92	43	4,9,10	1.47	0	3,11,13	1.10	0
32	PSU	2a	516	32,54	17,21,22	1.88	5 (29%)	20,30,33	2.88	6 (30%)
32	UR3	1a	1498	32	14,22,23	1.20	1 (7%)	15,32,35	0.75	0
32	4OC	2a	1402	32	16,23,24	1.45	3 (18%)	17,32,35	1.25	2 (11%)
1	OMC	1A	1920	1,54	15,22,23	1.47	3 (20%)	17,31,34	1.56	3 (17%)
32	2MG	1a	1207	32,54	19,26,27	3.18	1 (5%)	21,38,41	2.46	9 (42%)
1	PSU	2A	1911	1	17,21,22	1.94	4 (23%)	20,30,33	3.29	6 (30%)
43	0TD	1l	92	43	4,9,10	1.49	0	3,11,13	1.06	0
32	4OC	1a	1402	32	16,23,24	1.48	3 (18%)	17,32,35	1.12	2 (11%)
32	G7M	1a	527	32,54	20,26,27	1.43	2 (10%)	20,39,42	1.99	5 (25%)
1	5MC	2A	1942	1	15,22,23	1.72	2 (13%)	19,32,35	1.36	3 (15%)
1	PSU	1A	2605	1	17,21,22	1.76	5 (29%)	20,30,33	2.90	6 (30%)
1	2MA	1A	2503	1,54	17,25,26	0.73	1 (5%)	19,37,40	2.11	4 (21%)
1	OMG	1A	2251	1	18,26,27	1.63	2 (11%)	20,38,41	1.81	6 (30%)
32	5MC	2a	967	32	15,22,23	1.72	2 (13%)	19,32,35	1.44	3 (15%)
1	OMU	1A	2552	1,54	14,22,23	4.63	7 (50%)	14,31,34	0.78	0
1	5MU	1A	1939	1,54	15,22,23	1.11	2 (13%)	16,32,35	1.64	3 (18%)
1	OMC	2A	1920	1	15,22,23	1.56	3 (20%)	17,31,34	1.26	2 (11%)
32	MA6	1a	1518	32	19,26,27	1.43	4 (21%)	18,38,41	1.49	2 (11%)
1	5MU	1A	1915	1,54	15,22,23	1.04	2 (13%)	16,32,35	1.91	1 (6%)
32	MA6	1a	1519	32	19,26,27	1.42	4 (21%)	18,38,41	1.51	2 (11%)
32	MA6	2a	1518	32	19,26,27	1.51	4 (21%)	18,38,41	1.51	2 (11%)
32	5MC	2a	1400	32	15,22,23	1.73	3 (20%)	19,32,35	1.37	2 (10%)
32	2MG	2a	1207	32	19,26,27	3.11	2 (10%)	21,38,41	2.12	8 (38%)
1	5MC	1A	1942	1	15,22,23	1.71	2 (13%)	19,32,35	1.28	3 (15%)
1	PSU	1A	1911	1	17,21,22	1.75	3 (17%)	20,30,33	3.62	6 (30%)
1	5MU	2A	1939	1,54	15,22,23	1.02	2 (13%)	16,32,35	1.77	2 (12%)
32	5MC	1a	1404	32	15,22,23	1.69	2 (13%)	19,32,35	1.17	2 (10%)
32	5MC	1a	1400	32	15,22,23	1.74	2 (13%)	19,32,35	1.29	2 (10%)
32	UR3	2a	1498	32,54	14,22,23	1.26	2 (14%)	15,32,35	0.57	0
32	5MC	2a	1407	32	15,22,23	1.74	3 (20%)	19,32,35	1.45	3 (15%)
32	PSU	1a	516	32	17,21,22	1.96	5 (29%)	20,30,33	2.92	6 (30%)
1	5MC	1A	1962	1,54	15,22,23	1.72	2 (13%)	19,32,35	1.32	3 (15%)
32	5MC	1a	1407	32	15,22,23	1.76	3 (20%)	19,32,35	1.23	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MU	2A	1915	1	15,22,23	1.01	1 (6%)	16,32,35	1.96	1 (6%)
32	M2G	1a	966	32	20,27,28	1.71	2 (10%)	22,40,43	1.91	6 (27%)
1	2MA	2A	2503	1,54	17,25,26	0.73	1 (5%)	19,37,40	1.99	4 (21%)
32	G7M	2a	527	32,54	20,26,27	1.42	2 (10%)	20,39,42	2.02	5 (25%)
32	5MC	1a	967	32	15,22,23	1.74	2 (13%)	19,32,35	1.63	4 (21%)
1	OMG	2A	2251	1,54	18,26,27	1.61	2 (11%)	20,38,41	1.69	4 (20%)
1	PSU	2A	2605	1	17,21,22	1.81	4 (23%)	20,30,33	2.99	6 (30%)
32	5MC	2a	1404	32	15,22,23	1.72	2 (13%)	19,32,35	1.21	2 (10%)
32	M2G	2a	966	32,54	20,27,28	1.73	2 (10%)	22,40,43	1.99	6 (27%)
1	OMU	2A	2552	1,54	14,22,23	4.60	7 (50%)	14,31,34	0.80	0
1	PSU	2A	1917	1	17,21,22	1.84	4 (23%)	20,30,33	2.91	6 (30%)
1	5MC	2A	1962	1	15,22,23	1.72	2 (13%)	19,32,35	1.26	3 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	2a	1519	32	-	6/7/29/30	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/3/12/14	-
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	2/5/25/26	0/2/2/2
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
1	OMC	1A	1920	1,54	-	1/7/27/28	0/2/2/2
32	2MG	1a	1207	32,54	-	3/5/27/28	0/3/3/3
1	PSU	2A	1911	1	-	1/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/3/12/14	-
32	4OC	1a	1402	32	-	4/9/29/30	0/2/2/2
32	G7M	1a	527	32,54	-	3/3/25/26	0/3/3/3
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,54	-	0/3/25/26	0/3/3/3
1	OMG	1A	2251	1	-	1/5/27/28	0/3/3/3
32	5MC	2a	967	32	-	2/5/25/26	0/2/2/2
1	OMU	1A	2552	1,54	-	0/7/27/28	0/2/2/2
1	5MU	1A	1939	1,54	-	2/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	2A	1920	1	-	4/7/27/28	0/2/2/2
32	MA6	1a	1518	32	-	2/7/29/30	0/3/3/3
1	5MU	1A	1915	1,54	-	0/5/25/26	0/2/2/2
32	MA6	1a	1519	32	-	2/7/29/30	0/3/3/3
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
1	5MC	1A	1942	1	-	0/5/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,54	-	0/5/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
32	UR3	2a	1498	32,54	-	0/5/25/26	0/2/2/2
32	5MC	2a	1407	32	-	1/5/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,54	-	2/5/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	2MA	2A	2503	1,54	-	1/3/25/26	0/3/3/3
32	G7M	2a	527	32,54	-	2/3/25/26	0/3/3/3
32	5MC	1a	967	32	-	2/5/25/26	0/2/2/2
1	OMG	2A	2251	1,54	-	3/5/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
32	M2G	2a	966	32,54	-	6/7/29/30	0/3/3/3
1	OMU	2A	2552	1,54	-	0/7/27/28	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1	-	2/5/25/26	0/2/2/2

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1207	2MG	C2-N2	13.61	1.45	1.34
32	2a	1207	2MG	C2-N2	13.23	1.45	1.34
1	1A	2552	OMU	O4'-C4'	10.13	1.67	1.45
1	2A	2552	OMU	O4'-C4'	10.08	1.67	1.45
1	1A	2552	OMU	C3'-C4'	-9.67	1.28	1.53
1	2A	2552	OMU	C3'-C4'	-9.54	1.28	1.53
1	2A	2552	OMU	O4'-C1'	-8.29	1.29	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2552	OMU	O4'-C1'	-8.22	1.29	1.41
32	2a	966	M2G	C2-N2	7.09	1.46	1.34
32	1a	966	M2G	C2-N2	7.02	1.46	1.34
1	1A	2251	OMG	C2-N2	6.03	1.46	1.33
1	2A	2251	OMG	C2-N2	5.95	1.45	1.33
1	1A	1962	5MC	C4-N4	5.66	1.48	1.34
1	1A	1942	5MC	C4-N4	5.60	1.48	1.34
1	2A	1962	5MC	C4-N4	5.59	1.48	1.34
1	2A	1942	5MC	C4-N4	5.56	1.48	1.34
32	1a	1407	5MC	C4-N4	5.54	1.48	1.34
32	1a	1400	5MC	C4-N4	5.53	1.48	1.34
32	1a	967	5MC	C4-N4	5.53	1.48	1.34
32	2a	1407	5MC	C4-N4	5.52	1.48	1.34
32	1a	527	G7M	C2-N2	5.51	1.44	1.33
32	2a	1404	5MC	C4-N4	5.50	1.47	1.34
32	2a	967	5MC	C4-N4	5.49	1.47	1.34
32	1a	1404	5MC	C4-N4	5.45	1.47	1.34
32	2a	527	G7M	C2-N2	5.41	1.44	1.33
32	2a	1400	5MC	C4-N4	5.38	1.47	1.34
1	2A	1911	PSU	C5-C1'	5.28	1.56	1.52
32	1a	516	PSU	C5-C1'	5.22	1.56	1.52
32	2a	516	PSU	C5-C1'	4.96	1.56	1.52
1	1A	1911	PSU	C5-C1'	4.87	1.56	1.52
1	2A	1917	PSU	C5-C1'	4.74	1.56	1.52
1	2A	2605	PSU	C5-C1'	4.62	1.56	1.52
32	1a	1402	4OC	C4-N4	4.34	1.45	1.36
32	2a	1402	4OC	C4-N4	4.27	1.45	1.36
1	1A	2605	PSU	C5-C1'	4.10	1.55	1.52
32	2a	1518	MA6	C4-N3	-4.05	1.30	1.35
1	1A	1920	OMC	C4-N4	3.79	1.46	1.35
32	1a	1518	MA6	C4-N3	-3.71	1.30	1.35
32	2a	1519	MA6	C4-N3	-3.62	1.30	1.35
32	1a	1519	MA6	C4-N3	-3.58	1.30	1.35
1	2A	1920	OMC	C4-N4	3.50	1.45	1.35
1	1A	1917	PSU	O4'-C1'	-3.43	1.39	1.44
1	2A	1911	PSU	C2-N1	-3.43	1.31	1.38
1	1A	1911	PSU	C2-N1	-3.39	1.31	1.38
32	1a	1498	UR3	C3U-N3	3.34	1.54	1.47
1	1A	2552	OMU	O2'-C2'	-3.30	1.34	1.42
32	2a	1498	UR3	C3U-N3	3.26	1.54	1.47
32	2a	516	PSU	C2-N1	-3.25	1.31	1.38
1	2A	2552	OMU	O2'-C2'	-3.21	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1917	PSU	C2-N1	-3.21	1.31	1.38
32	1a	516	PSU	C2-N1	-3.19	1.31	1.38
32	1a	516	PSU	C2-N3	-3.19	1.31	1.38
1	2A	1917	PSU	C2-N1	-3.18	1.31	1.38
1	2A	2605	PSU	C2-N1	-3.17	1.31	1.38
1	2A	1911	PSU	C2-N3	-3.16	1.31	1.38
1	1A	2605	PSU	C2-N1	-3.11	1.32	1.38
1	2A	1917	PSU	C2-N3	-3.09	1.32	1.38
1	1A	2605	PSU	C2-N3	-3.07	1.32	1.38
1	1A	1917	PSU	C2-N3	-3.01	1.32	1.38
1	2A	2552	OMU	O3'-C3'	3.01	1.50	1.43
1	2A	1920	OMC	C2-N3	-2.97	1.32	1.38
1	2A	2605	PSU	C2-N3	-2.96	1.32	1.38
1	1A	1915	5MU	O4-C4	-2.90	1.17	1.24
1	2A	1920	OMC	C6-N1	-2.87	1.32	1.35
1	1A	1939	5MU	O4-C4	-2.86	1.17	1.24
32	2a	516	PSU	C2-N3	-2.86	1.32	1.38
1	2A	1915	5MU	O4-C4	-2.84	1.17	1.24
32	1a	1402	4OC	C2-N3	-2.82	1.32	1.38
1	1A	2552	OMU	O3'-C3'	2.81	1.49	1.43
32	2a	1518	MA6	C6-N1	-2.80	1.28	1.33
1	2A	1939	5MU	O4-C4	-2.79	1.17	1.24
32	1a	516	PSU	O4-C4	-2.76	1.17	1.24
32	2a	1400	5MC	C2-N3	-2.74	1.32	1.38
1	1A	1917	PSU	C5-C1'	2.71	1.54	1.52
1	1A	1911	PSU	C2-N3	-2.70	1.32	1.38
1	1A	2605	PSU	O4-C4	-2.68	1.17	1.24
1	1A	1917	PSU	O4-C4	-2.68	1.17	1.24
32	2a	1402	4OC	C2-N3	-2.67	1.32	1.38
1	2A	1917	PSU	O4-C4	-2.66	1.17	1.24
32	1a	1400	5MC	C2-N3	-2.66	1.32	1.38
32	2a	516	PSU	O4-C4	-2.64	1.17	1.24
1	1A	1920	OMC	C6-N1	-2.62	1.32	1.35
32	2a	1519	MA6	C6-N1	-2.61	1.29	1.33
1	2A	1942	5MC	C2-N3	-2.59	1.33	1.38
32	1a	1407	5MC	C2-N3	-2.59	1.33	1.38
1	2A	2605	PSU	O4-C4	-2.55	1.18	1.24
32	1a	1518	MA6	C6-N1	-2.53	1.29	1.33
32	2a	1519	MA6	C9-N6	2.50	1.51	1.45
1	2A	1962	5MC	C2-N3	-2.49	1.33	1.38
32	1a	1519	MA6	C6-N1	-2.49	1.29	1.33
32	2a	1404	5MC	C2-N3	-2.49	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1404	5MC	C2-N3	-2.48	1.33	1.38
32	1a	516	PSU	O4'-C1'	-2.47	1.40	1.44
1	1A	1942	5MC	C2-N3	-2.47	1.33	1.38
1	1A	1962	5MC	C2-N3	-2.45	1.33	1.38
1	1A	1920	OMC	C2-N3	-2.44	1.33	1.38
32	2a	516	PSU	O4'-C1'	-2.41	1.41	1.44
1	2A	1911	PSU	O4-C4	-2.40	1.18	1.24
32	1a	1519	MA6	C8-N7	-2.38	1.30	1.34
1	1A	1939	5MU	C2-N3	-2.37	1.33	1.38
32	1a	1402	4OC	C6-N1	-2.37	1.32	1.35
32	1a	967	5MC	C2-N3	-2.36	1.33	1.38
32	1a	1519	MA6	C9-N6	2.35	1.51	1.45
32	2a	1407	5MC	C2-N3	-2.34	1.33	1.38
32	1a	1518	MA6	C8-N7	-2.34	1.30	1.34
32	2a	967	5MC	C2-N3	-2.33	1.33	1.38
32	2a	1402	4OC	C6-N1	-2.32	1.33	1.35
1	1A	2552	OMU	C2-N3	-2.31	1.33	1.38
32	2a	1518	MA6	C9-N6	2.31	1.51	1.45
32	1a	1518	MA6	C9-N6	2.28	1.50	1.45
1	1A	2251	OMG	O6-C6	-2.27	1.18	1.24
32	2a	1498	UR3	C4-N3	-2.27	1.35	1.38
32	2a	1518	MA6	C8-N7	-2.25	1.30	1.34
32	2a	527	G7M	O6-C6	-2.23	1.19	1.24
1	2A	2251	OMG	O6-C6	-2.20	1.19	1.24
32	1a	527	G7M	O6-C6	-2.18	1.19	1.24
1	2A	1939	5MU	C2-N3	-2.18	1.33	1.38
1	2A	2552	OMU	C3'-C2'	2.18	1.57	1.52
1	2A	2503	2MA	CM2-C2	2.18	1.55	1.49
32	2a	1207	2MG	O6-C6	-2.16	1.19	1.24
32	2a	1519	MA6	C8-N7	-2.15	1.30	1.34
32	1a	966	M2G	O6-C6	-2.13	1.19	1.24
1	1A	2503	2MA	CM2-C2	2.13	1.55	1.49
1	1A	1915	5MU	C2-N3	-2.09	1.34	1.38
32	2a	1407	5MC	C4-N3	-2.06	1.32	1.35
1	2A	2552	OMU	C2-N3	-2.06	1.34	1.38
32	2a	1400	5MC	C4-N3	-2.06	1.32	1.35
32	2a	966	M2G	O6-C6	-2.06	1.19	1.24
1	1A	2605	PSU	O4'-C1'	-2.05	1.41	1.44
1	1A	2552	OMU	C6-N1	-2.03	1.33	1.35
32	1a	1407	5MC	C4-N3	-2.01	1.32	1.35

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1911	PSU	N1-C2-N3	-9.90	120.56	128.43
1	2A	1911	PSU	N1-C2-N3	-9.72	120.70	128.43
1	1A	1911	PSU	C4-N3-C2	9.55	123.21	115.14
1	1A	1917	PSU	C5-C1'-C2'	-8.80	99.63	115.32
32	1a	516	PSU	N1-C2-N3	-8.73	121.49	128.43
32	2a	516	PSU	N1-C2-N3	-8.69	121.52	128.43
1	2A	2605	PSU	N1-C2-N3	-8.64	121.56	128.43
1	2A	1917	PSU	N1-C2-N3	-8.64	121.56	128.43
1	1A	2605	PSU	N1-C2-N3	-8.29	121.84	128.43
1	1A	1917	PSU	N1-C2-N3	-8.25	121.87	128.43
1	2A	1911	PSU	C4-N3-C2	8.04	121.93	115.14
1	2A	1915	5MU	C4-N3-C2	7.32	121.32	115.14
1	1A	1915	5MU	C4-N3-C2	7.08	121.12	115.14
1	1A	2503	2MA	C2-N3-C4	6.71	120.97	115.52
1	2A	2503	2MA	C2-N3-C4	6.39	120.72	115.52
1	1A	2605	PSU	C4-N3-C2	6.30	120.46	115.14
32	2a	516	PSU	C4-N3-C2	6.20	120.38	115.14
1	2A	2605	PSU	C4-N3-C2	6.18	120.36	115.14
1	1A	1911	PSU	C5-C4-N3	-6.18	117.39	125.36
32	1a	516	PSU	C4-N3-C2	6.13	120.32	115.14
1	2A	1939	5MU	C4-N3-C2	5.93	120.15	115.14
1	2A	1917	PSU	C4-N3-C2	5.92	120.14	115.14
1	1A	1917	PSU	C4-N3-C2	5.89	120.12	115.14
32	2a	966	M2G	C2-N3-C4	5.08	121.04	115.28
1	2A	1911	PSU	C5-C4-N3	-5.04	118.87	125.36
32	2a	1207	2MG	C2-N3-C4	5.00	120.96	115.28
32	1a	966	M2G	C2-N3-C4	4.97	120.92	115.28
32	2a	1518	MA6	N3-C2-N1	-4.82	121.14	128.68
32	2a	1519	MA6	N3-C2-N1	-4.82	121.15	128.68
1	1A	2251	OMG	C2-N3-C4	4.80	120.84	115.36
32	1a	1519	MA6	N3-C2-N1	-4.80	121.18	128.68
1	1A	1939	5MU	C4-N3-C2	4.78	119.18	115.14
32	1a	1207	2MG	C2-N3-C4	4.65	120.56	115.28
32	1a	1518	MA6	N3-C2-N1	-4.62	121.46	128.68
1	1A	1917	PSU	C5-C4-N3	-4.49	119.57	125.36
1	1A	1920	OMC	C2-N3-C4	4.49	120.89	116.34
32	2a	1407	5MC	C2-N3-C4	4.43	121.37	116.02
1	1A	2605	PSU	C5-C4-N3	-4.27	119.86	125.36
32	1a	527	G7M	N3-C2-N1	-4.27	121.52	127.22
32	2a	527	G7M	N3-C2-N1	-4.23	121.58	127.22
1	2A	2605	PSU	C5-C4-N3	-4.23	119.92	125.36
32	2a	516	PSU	C5-C4-N3	-4.22	119.92	125.36
1	2A	2251	OMG	C2-N3-C4	4.22	120.18	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1207	2MG	C6-N1-C2	4.20	122.70	115.18
1	1A	1917	PSU	C5-C6-N1	-4.13	119.36	124.44
32	2a	527	G7M	C6-N1-C2	4.09	122.43	115.93
32	1a	527	G7M	C6-N1-C2	4.07	122.39	115.93
1	2A	2605	PSU	C5-C1'-C2'	-4.07	108.06	115.32
1	2A	1917	PSU	C5-C4-N3	-3.99	120.22	125.36
32	1a	1207	2MG	C5-C6-N1	-3.99	117.97	123.43
32	1a	516	PSU	C5-C4-N3	-3.99	120.22	125.36
32	2a	967	5MC	C2-N3-C4	3.98	120.83	116.02
32	1a	527	G7M	C5-C6-N1	-3.98	117.98	123.43
32	1a	967	5MC	C2-N3-C4	3.98	120.82	116.02
1	2A	1920	OMC	C2-N3-C4	3.95	120.35	116.34
1	1A	1962	5MC	C2-N3-C4	3.85	120.66	116.02
32	2a	527	G7M	C5-C6-N1	-3.83	118.19	123.43
32	2a	1402	4OC	CM4-N4-C4	-3.78	119.72	122.97
1	1A	2503	2MA	C5-C6-N1	-3.77	119.10	123.06
1	2A	1917	PSU	C5-C6-N1	-3.76	119.81	124.44
32	1a	1518	MA6	C4-C5-N7	-3.76	105.48	109.40
32	2a	1404	5MC	C2-N3-C4	3.73	120.53	116.02
32	2a	966	M2G	C6-N1-C2	3.72	120.61	116.18
32	1a	1207	2MG	C4-C5-N7	-3.70	105.54	109.40
32	1a	1207	2MG	C6-C5-C4	-3.70	117.27	120.80
32	2a	527	G7M	C6-C5-C4	-3.69	117.27	120.80
1	1A	2605	PSU	C5-C6-N1	-3.67	119.92	124.44
32	1a	966	M2G	C6-N1-C2	3.65	120.52	116.18
32	1a	1519	MA6	C4-C5-N7	-3.64	105.61	109.40
32	2a	1518	MA6	C4-C5-N7	-3.63	105.61	109.40
32	1a	516	PSU	C5-C6-N1	-3.60	120.01	124.44
1	2A	1962	5MC	C2-N3-C4	3.58	120.34	116.02
1	2A	2503	2MA	C5-C6-N1	-3.57	119.32	123.06
1	1A	2251	OMG	N3-C2-N1	-3.54	122.50	127.22
1	1A	1942	5MC	C2-N3-C4	3.50	120.25	116.02
1	2A	2251	OMG	N3-C2-N1	-3.49	122.56	127.22
32	1a	527	G7M	C2-N3-C4	3.46	119.31	115.36
32	1a	1407	5MC	C2-N3-C4	3.45	120.18	116.02
32	1a	1207	2MG	N3-C2-N1	-3.44	120.79	126.23
1	1A	1920	OMC	N4-C4-N3	3.43	121.92	116.49
32	2a	527	G7M	C2-N3-C4	3.43	119.28	115.36
1	2A	1917	PSU	C6-N1-C2	3.41	120.98	115.36
1	2A	1942	5MC	C2-N3-C4	3.40	120.12	116.02
32	1a	527	G7M	C6-C5-C4	-3.40	117.56	120.80
32	2a	1519	MA6	C4-C5-N7	-3.40	105.86	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1400	5MC	C2-N3-C4	3.39	120.11	116.02
1	2A	2605	PSU	C5-C6-N1	-3.38	120.29	124.44
32	1a	516	PSU	C6-N1-C2	3.37	120.92	115.36
1	1A	2605	PSU	C5-C1'-C2'	-3.30	109.43	115.32
1	1A	1939	5MU	C5-C6-N1	-3.28	118.66	122.19
32	2a	1400	5MC	C2-N3-C4	3.28	119.97	116.02
32	2a	516	PSU	C5-C6-N1	-3.26	120.43	124.44
32	1a	1402	4OC	CM4-N4-C4	-3.24	120.19	122.97
32	1a	1404	5MC	C2-N3-C4	3.23	119.92	116.02
32	2a	1207	2MG	CM2-N2-C2	-3.22	119.70	123.59
1	2A	1911	PSU	C6-N1-C2	3.22	120.67	115.36
1	1A	1917	PSU	C6-N1-C2	3.19	120.63	115.36
1	2A	2605	PSU	C6-N1-C2	3.18	120.61	115.36
32	2a	516	PSU	C6-N1-C2	3.15	120.56	115.36
32	2a	1207	2MG	C4-C5-N7	-3.15	106.11	109.40
1	2A	1942	5MC	C5-C6-N1	-3.13	118.82	122.19
32	1a	1207	2MG	N2-C2-N1	3.12	119.95	116.96
32	2a	1400	5MC	C5-C6-N1	-3.11	118.84	122.19
32	1a	966	M2G	C6-C5-C4	-3.06	117.87	120.80
32	2a	966	M2G	C6-C5-C4	-3.06	117.88	120.80
32	1a	967	5MC	O3'-C3'-C4'	3.04	119.84	111.05
1	1A	2605	PSU	C6-N1-C2	3.03	120.36	115.36
32	2a	966	M2G	C4-C5-N7	-3.00	106.27	109.40
32	2a	1207	2MG	C6-C5-C4	-2.99	117.94	120.80
32	2a	1207	2MG	C6-N1-C2	2.99	120.53	115.18
1	2A	2251	OMG	C5-C6-N1	-2.98	119.35	123.43
1	1A	1911	PSU	C5-C1'-C2'	-2.96	110.04	115.32
1	2A	2503	2MA	C4-C5-N7	-2.96	106.32	109.40
32	1a	1207	2MG	CM2-N2-C2	-2.90	120.09	123.59
32	2a	1207	2MG	N3-C2-N1	-2.85	121.73	126.23
1	2A	1917	PSU	C5-C1'-C2'	-2.84	110.26	115.32
32	2a	966	M2G	C5-C6-N1	-2.83	119.56	123.43
32	2a	1207	2MG	C5-C6-N1	-2.82	119.58	123.43
32	2a	1207	2MG	N2-C2-N1	2.75	119.60	116.96
1	1A	1942	5MC	C5-C6-N1	-2.74	119.24	122.19
1	2A	1911	PSU	C5-C6-N1	-2.73	121.09	124.44
1	2A	1939	5MU	C5-C6-N1	-2.72	119.27	122.19
1	1A	1962	5MC	N4-C4-N3	2.71	120.86	117.03
1	1A	1911	PSU	C6-N1-C2	2.69	119.80	115.36
32	1a	1404	5MC	C5-C6-N1	-2.67	119.32	122.19
1	1A	2251	OMG	C5-C6-N1	-2.65	119.81	123.43
1	2A	1962	5MC	C5-C6-N1	-2.65	119.34	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1400	5MC	C5-C6-N1	-2.64	119.35	122.19
32	1a	966	M2G	C5-C6-N1	-2.64	119.82	123.43
1	2A	2251	OMG	C6-N1-C2	2.62	120.09	115.93
32	1a	966	M2G	C4-C5-N7	-2.57	106.72	109.40
32	1a	967	5MC	N4-C4-N3	2.56	120.66	117.03
1	1A	2251	OMG	C4-C5-N7	-2.56	106.73	109.40
32	1a	516	PSU	O4'-C1'-C2'	2.53	108.75	104.66
32	2a	966	M2G	N1-C2-N2	2.49	119.71	117.19
1	1A	2503	2MA	C4-C5-N7	-2.49	106.81	109.40
32	2a	1407	5MC	N4-C4-N3	2.48	120.54	117.03
32	1a	1407	5MC	C5-C6-N1	-2.44	119.56	122.19
1	1A	2251	OMG	C6-N1-C2	2.44	119.80	115.93
1	1A	2251	OMG	C6-C5-C4	-2.42	118.49	120.80
1	2A	1911	PSU	C4-C5-C1'	2.40	125.65	121.12
32	1a	1207	2MG	N2-C2-N3	2.39	119.26	116.96
1	1A	1911	PSU	C5-C6-N1	-2.38	121.52	124.44
32	2a	967	5MC	O3'-C3'-C2'	2.38	119.50	111.82
1	1A	2503	2MA	N3-C2-N1	-2.34	121.41	125.72
32	2a	516	PSU	O4'-C1'-C2'	2.32	108.42	104.66
1	2A	2503	2MA	N3-C2-N1	-2.29	121.51	125.72
32	2a	1404	5MC	C5-C6-N1	-2.24	119.78	122.19
32	2a	1402	4OC	C5-C4-N3	-2.21	119.44	123.16
32	1a	966	M2G	N1-C2-N2	2.21	119.42	117.19
1	2A	1920	OMC	N4-C4-N3	2.20	119.97	116.49
32	1a	1402	4OC	C5-C4-N3	-2.18	119.48	123.16
32	2a	967	5MC	N4-C4-N3	2.18	120.11	117.03
1	2A	1962	5MC	N4-C4-N3	2.17	120.10	117.03
32	1a	967	5MC	O3'-C3'-C2'	2.15	118.78	111.82
1	1A	1962	5MC	C5-C6-N1	-2.13	119.90	122.19
1	1A	1942	5MC	N4-C4-N3	2.10	120.00	117.03
1	1A	1939	5MU	O4'-C1'-C2'	-2.06	103.92	106.93
1	2A	1942	5MC	N4-C4-N3	2.04	119.92	117.03
1	1A	1920	OMC	C5-C4-N3	-2.02	119.39	121.72
32	2a	1407	5MC	CM5-C5-C4	-2.01	119.69	121.72

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C9
32	2a	1519	MA6	C5-C6-N6-C10

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Mol	Chain	Res	Type	Atoms
43	2l	92	0TD	CG-CB-SB-CSB
32	1a	1498	UR3	O4'-C4'-C5'-O5'
32	2a	1402	4OC	N3-C4-N4-CM4
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
43	1l	92	0TD	O-C-CA-CB
43	1l	92	0TD	CG-CB-SB-CSB
32	1a	1402	4OC	N3-C4-N4-CM4
32	1a	1402	4OC	C5-C4-N4-CM4
32	1a	527	G7M	C3'-C4'-C5'-O5'
1	1A	2251	OMG	C1'-C2'-O2'-CM2
32	2a	967	5MC	O4'-C1'-N1-C6
1	1A	1939	5MU	C3'-C4'-C5'-O5'
1	1A	1939	5MU	O4'-C4'-C5'-O5'
1	2A	1920	OMC	C1'-C2'-O2'-CM2
1	2A	1920	OMC	C3'-C4'-C5'-O5'
32	1a	1518	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1518	MA6	C5-C6-N6-C10
32	2a	1400	5MC	O4'-C1'-N1-C6
32	2a	1400	5MC	C2'-C1'-N1-C6
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	2a	1407	5MC	C2'-C1'-N1-C6
1	1A	1962	5MC	O4'-C1'-N1-C6
1	1A	1962	5MC	C2'-C1'-N1-C6
32	2a	527	G7M	C3'-C4'-C5'-O5'
1	2A	2251	OMG	C1'-C2'-O2'-CM2
32	2a	966	M2G	N1-C2-N2-CM1
32	2a	966	M2G	N1-C2-N2-CM2
32	2a	966	M2G	N3-C2-N2-CM1
32	2a	966	M2G	N3-C2-N2-CM2
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1498	UR3	C3'-C4'-C5'-O5'
1	2A	1920	OMC	O4'-C4'-C5'-O5'
32	1a	1518	MA6	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	966	M2G	O4'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
32	1a	967	5MC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	N1-C6-N6-C10
32	2a	1518	MA6	N1-C6-N6-C9
32	2a	966	M2G	C3'-C4'-C5'-O5'
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
1	2A	2251	OMG	O4'-C4'-C5'-O5'
1	1A	1920	OMC	C1'-C2'-O2'-CM2
1	2A	2251	OMG	C3'-C4'-C5'-O5'
32	1a	527	G7M	C4'-C5'-O5'-P
1	2A	1920	OMC	C3'-C2'-O2'-CM2
1	2A	1911	PSU	C2'-C1'-C5-C6
32	1a	1207	2MG	O4'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	967	5MC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
1	2A	2503	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

15 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1920	OMC	1	0
1	2A	1911	PSU	2	0
1	2A	1942	5MC	1	0
1	1A	2503	2MA	3	0
1	1A	2552	OMU	2	0
1	1A	1939	5MU	1	0
1	2A	1920	OMC	2	0
1	1A	1911	PSU	3	0
1	2A	1939	5MU	1	0
1	2A	1915	5MU	1	0
1	2A	2503	2MA	1	0
1	2A	2251	OMG	1	0
1	2A	2552	OMU	3	0
1	2A	1917	PSU	1	0
1	2A	1962	5MC	1	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2199 ligands modelled in this entry, 2188 are monoatomic - leaving 11 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	$\# Z > 2$
53	MPD	1a	1601	-	7,7,7	0.30	0	9,10,10	0.35	0
53	MPD	1T	2001	-	7,7,7	0.28	0	9,10,10	0.28	0
57	SF4	1d	501	-	0,12,12	0.00	-	-		
53	MPD	2B	201	-	7,7,7	0.26	0	9,10,10	0.16	0
53	MPD	2A	3001	-	7,7,7	0.31	0	9,10,10	0.34	0
57	SF4	2d	501	-	0,12,12	0.00	-	-		
53	MPD	2A	3002	-	7,7,7	0.28	0	9,10,10	0.17	0
53	MPD	1A	3001	-	7,7,7	0.28	0	9,10,10	0.21	0
53	MPD	18	101	-	7,7,7	0.28	0	9,10,10	0.35	0

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
53	MPD	1a	1601	-	-	2/5/5/5	-
53	MPD	1T	2001	-	-	0/5/5/5	-
57	SF4	1d	501	-	-	-	0/6/5/5
53	MPD	2B	201	-	-	4/5/5/5	-
53	MPD	2A	3001	-	-	1/5/5/5	-
57	SF4	2d	501	-	-	-	0/6/5/5
53	MPD	2A	3002	-	-	4/5/5/5	-
53	MPD	1A	3001	-	-	0/5/5/5	-
53	MPD	18	101	-	-	4/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	2A	3001	MPD	O2-C2-C3-C4
53	18	101	MPD	O2-C2-C3-C4
53	2B	201	MPD	C2-C3-C4-C5
53	2A	3002	MPD	C2-C3-C4-C5
53	2B	201	MPD	C2-C3-C4-O4
53	1a	1601	MPD	C2-C3-C4-O4
53	2B	201	MPD	CM-C2-C3-C4
53	2A	3002	MPD	C1-C2-C3-C4
53	18	101	MPD	C1-C2-C3-C4
53	18	101	MPD	CM-C2-C3-C4
53	2B	201	MPD	O2-C2-C3-C4
53	2A	3002	MPD	O2-C2-C3-C4
53	1a	1601	MPD	C2-C3-C4-C5
53	18	101	MPD	C2-C3-C4-C5
53	2A	3002	MPD	C2-C3-C4-O4

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	2B	201	MPD	2	0
53	2A	3001	MPD	1	0
53	18	101	MPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2851/2894 (98%)	-0.25	87 (3%) 49 47	26, 52, 150, 184	0
1	2A	2847/2894 (98%)	-0.13	100 (3%) 44 40	46, 77, 156, 186	0
2	1B	118/120 (98%)	-0.52	0 100 100	45, 72, 90, 110	0
2	2B	118/120 (98%)	0.15	3 (2%) 57 53	86, 116, 133, 144	0
3	1D	275/276 (99%)	-0.36	1 (0%) 92 92	29, 47, 64, 93	0
3	2D	275/276 (99%)	-0.17	1 (0%) 92 92	43, 67, 83, 106	0
4	1E	204/206 (99%)	-0.19	0 100 100	29, 58, 79, 112	0
4	2E	204/206 (99%)	-0.00	1 (0%) 91 90	45, 73, 98, 109	0
5	1F	203/210 (96%)	-0.27	0 100 100	27, 55, 90, 120	0
5	2F	203/210 (96%)	-0.04	1 (0%) 91 90	44, 89, 109, 129	0
6	1G	181/182 (99%)	-0.16	3 (1%) 70 67	67, 91, 111, 134	0
6	2G	181/182 (99%)	0.77	25 (13%) 2 2	106, 127, 139, 147	0
7	1H	174/180 (96%)	-0.24	1 (0%) 89 89	45, 71, 91, 101	0
7	2H	173/180 (96%)	0.71	16 (9%) 9 10	81, 113, 130, 142	0
8	1I	147/148 (99%)	0.06	1 (0%) 87 88	61, 104, 121, 131	0
8	2I	146/148 (98%)	0.24	5 (3%) 45 42	70, 109, 126, 136	0
9	1N	140/140 (100%)	-0.22	1 (0%) 87 88	39, 52, 75, 100	0
9	2N	140/140 (100%)	0.30	3 (2%) 63 61	58, 90, 111, 122	0
10	1O	122/122 (100%)	-0.26	0 100 100	36, 57, 77, 86	0
10	2O	122/122 (100%)	-0.21	0 100 100	50, 68, 83, 92	0
11	1P	149/150 (99%)	-0.17	0 100 100	25, 63, 91, 116	0
11	2P	149/150 (99%)	0.24	2 (1%) 77 75	53, 91, 116, 128	0
12	1Q	141/141 (100%)	-0.30	0 100 100	39, 56, 70, 99	0
12	2Q	141/141 (100%)	0.04	2 (1%) 75 74	68, 87, 104, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.23	0 100 100	34, 50, 67, 83	0
13	2R	118/118 (100%)	-0.00	0 100 100	54, 68, 89, 99	0
14	1S	110/112 (98%)	-0.01	2 (1%) 68 65	52, 69, 84, 95	0
14	2S	110/112 (98%)	0.73	10 (9%) 9 10	95, 108, 118, 125	0
15	1T	131/146 (89%)	-0.17	1 (0%) 86 86	49, 63, 109, 117	0
15	2T	131/146 (89%)	-0.16	0 100 100	53, 74, 104, 123	0
16	1U	116/118 (98%)	-0.42	0 100 100	31, 45, 68, 83	0
16	2U	116/118 (98%)	-0.22	1 (0%) 84 84	59, 85, 101, 117	0
17	1V	101/101 (100%)	-0.09	1 (0%) 82 82	31, 58, 77, 87	0
17	2V	101/101 (100%)	0.12	3 (2%) 50 48	60, 100, 115, 129	0
18	1W	112/113 (99%)	-0.28	0 100 100	35, 48, 71, 91	0
18	2W	112/113 (99%)	-0.10	1 (0%) 84 84	48, 66, 96, 140	0
19	1X	95/96 (98%)	-0.13	0 100 100	39, 53, 74, 97	0
19	2X	95/96 (98%)	0.23	4 (4%) 36 33	58, 79, 106, 116	0
20	1Y	107/110 (97%)	-0.13	0 100 100	44, 66, 88, 103	0
20	2Y	107/110 (97%)	0.64	7 (6%) 18 18	75, 94, 111, 121	0
21	1Z	203/206 (98%)	-0.24	1 (0%) 91 90	57, 81, 105, 117	0
21	2Z	201/206 (97%)	0.55	18 (8%) 9 10	89, 111, 124, 141	0
22	10	77/85 (90%)	-0.10	0 100 100	40, 52, 66, 79	0
22	20	77/85 (90%)	0.66	7 (9%) 9 10	67, 86, 98, 117	0
23	11	97/98 (98%)	0.15	1 (1%) 82 82	36, 55, 88, 114	0
23	21	97/98 (98%)	0.23	2 (2%) 63 61	49, 75, 100, 112	0
24	12	70/72 (97%)	-0.12	1 (1%) 75 74	47, 66, 80, 108	0
24	22	70/72 (97%)	0.16	1 (1%) 75 74	80, 93, 103, 105	0
25	13	59/60 (98%)	0.19	0 100 100	38, 53, 87, 91	0
25	23	59/60 (98%)	0.88	6 (10%) 6 7	75, 90, 116, 126	0
26	14	69/71 (97%)	0.06	3 (4%) 35 33	83, 113, 141, 146	0
26	24	69/71 (97%)	1.02	13 (18%) 1 1	125, 144, 158, 160	0
27	15	59/60 (98%)	-0.51	0 100 100	34, 44, 79, 89	0
27	25	59/60 (98%)	-0.27	0 100 100	49, 74, 88, 100	0
28	16	53/54 (98%)	-0.31	0 100 100	45, 55, 71, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.16	1 (1%) 66 64	71, 81, 93, 103	0
29	17	48/49 (97%)	0.33	3 (6%) 20 19	37, 46, 77, 81	0
29	27	48/49 (97%)	0.30	1 (2%) 63 61	53, 62, 83, 86	0
30	18	64/65 (98%)	-0.20	0 100 100	39, 49, 61, 83	0
30	28	64/65 (98%)	0.19	0 100 100	59, 73, 85, 90	0
31	19	37/37 (100%)	-0.02	0 100 100	40, 54, 64, 72	0
31	29	37/37 (100%)	0.54	1 (2%) 54 51	80, 89, 100, 105	0
32	1a	1488/1522 (97%)	-0.08	31 (2%) 63 61	50, 99, 152, 187	0
32	2a	1492/1522 (98%)	0.04	31 (2%) 63 61	63, 108, 154, 188	0
33	1b	231/256 (90%)	0.26	10 (4%) 35 33	100, 119, 139, 151	0
33	2b	231/256 (90%)	0.65	25 (10%) 5 6	111, 134, 146, 154	0
34	1c	206/239 (86%)	0.01	3 (1%) 73 71	86, 108, 129, 139	0
34	2c	206/239 (86%)	0.55	22 (10%) 6 6	104, 131, 139, 145	0
35	1d	208/209 (99%)	0.26	9 (4%) 35 33	84, 107, 124, 131	0
35	2d	208/209 (99%)	0.02	1 (0%) 91 90	76, 95, 107, 114	0
36	1e	148/162 (91%)	-0.07	2 (1%) 75 74	71, 91, 106, 126	0
36	2e	148/162 (91%)	0.17	2 (1%) 75 74	87, 104, 117, 144	0
37	1f	100/101 (99%)	-0.26	1 (1%) 82 82	65, 88, 107, 116	0
37	2f	100/101 (99%)	-0.09	1 (1%) 82 82	79, 99, 110, 114	0
38	1g	155/156 (99%)	0.20	4 (2%) 56 52	89, 106, 117, 133	0
38	2g	155/156 (99%)	0.75	19 (12%) 4 4	112, 122, 133, 150	0
39	1h	137/138 (99%)	0.24	2 (1%) 73 71	76, 94, 104, 107	0
39	2h	137/138 (99%)	0.52	6 (4%) 34 32	96, 109, 120, 128	0
40	1i	127/128 (99%)	0.44	8 (6%) 20 19	91, 117, 133, 142	0
40	2i	126/128 (98%)	1.48	37 (29%) 0 0	116, 137, 147, 153	0
41	1j	97/105 (92%)	0.64	8 (8%) 11 11	87, 121, 140, 149	0
41	2j	96/105 (91%)	1.55	30 (31%) 0 0	113, 137, 147, 164	0
42	1k	114/129 (88%)	0.03	0 100 100	60, 83, 101, 108	0
42	2k	114/129 (88%)	0.31	5 (4%) 34 32	84, 106, 122, 131	0
43	1l	121/135 (89%)	0.09	0 100 100	64, 80, 96, 114	0
43	2l	121/135 (89%)	0.15	2 (1%) 70 67	70, 87, 105, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	116/126 (92%)	0.41	6 (5%) 27 25	90, 109, 119, 125	0
44	2m	114/126 (90%)	0.84	18 (15%) 2 2	111, 134, 141, 146	0
45	1n	60/61 (98%)	0.32	1 (1%) 70 67	95, 105, 115, 120	0
45	2n	60/61 (98%)	1.39	16 (26%) 0 0	116, 130, 138, 140	0
46	1o	88/89 (98%)	0.18	2 (2%) 60 58	67, 87, 107, 114	0
46	2o	88/89 (98%)	0.13	1 (1%) 80 80	78, 101, 120, 127	0
47	1p	82/88 (93%)	0.84	8 (9%) 7 7	83, 111, 127, 138	0
47	2p	82/88 (93%)	0.47	1 (1%) 79 77	77, 92, 110, 120	0
48	1r	68/88 (77%)	0.38	2 (2%) 51 50	69, 86, 111, 119	0
48	2r	68/88 (77%)	0.50	4 (5%) 22 21	90, 106, 120, 129	0
49	1s	83/93 (89%)	0.65	6 (7%) 15 15	89, 116, 132, 142	0
49	2s	83/93 (89%)	1.48	23 (27%) 0 0	116, 138, 146, 152	0
50	1t	96/106 (90%)	0.84	11 (11%) 4 4	95, 109, 124, 134	0
50	2t	98/106 (92%)	0.36	3 (3%) 49 47	78, 100, 117, 122	0
51	1u	23/27 (85%)	2.29	12 (52%) 0 0	101, 107, 112, 117	0
51	2u	23/27 (85%)	3.08	21 (91%) 0 0	120, 125, 130, 130	0
52	1y	97/113 (85%)	0.45	0 100 100	64, 85, 106, 116	0
52	2y	96/113 (84%)	1.54	32 (33%) 0 0	99, 115, 130, 140	0
All	All	20545/21222 (96%)	0.06	768 (3%) 41 38	25, 86, 140, 188	0

All (768) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1076	C	9.9
32	2a	1001(A)	G	7.7
1	1A	1091	G	7.6
26	24	68	ARG	7.6
32	2a	1001	A	7.1
1	1A	1087	G	7.1
32	1a	1036	G	7.0
1	1A	1064	C	6.7
40	2i	7	THR	6.7
1	2A	2802	G	6.7
41	2j	6	ILE	6.5
1	2A	1067	A	6.4
1	2A	2146	C	6.3

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Mol	Chain	Res	Type	RSRZ
1	2A	2173	A	6.3
51	2u	17	THR	6.2
1	2A	2139	C	6.0
1	2A	2154	G	6.0
1	2A	2801(A)	A	6.0
1	2A	2140	C	5.9
41	2j	34	VAL	5.9
1	2A	2169	A	5.8
1	2A	2144	U	5.8
32	2a	1030(B)	C	5.8
1	2A	2142	C	5.8
38	2g	156	TRP	5.7
1	2A	2125	G	5.7
1	2A	2137	C	5.6
1	2A	2174	C	5.6
32	2a	1030(A)	G	5.6
52	2y	7	SER	5.6
39	2h	131	GLY	5.6
42	2k	13	GLN	5.4
22	20	76	GLY	5.4
1	1A	1075	C	5.2
20	2Y	1	MET	5.2
1	2A	2147	G	5.1
1	2A	1083	U	5.1
1	2A	2141	G	5.1
1	2A	2133	G	5.0
40	2i	126	SER	4.9
32	1a	1030(B)	C	4.9
1	2A	1076	C	4.9
1	2A	1085	A	4.9
1	2A	2153	G	4.9
49	2s	79	THR	4.8
18	2W	112	GLY	4.8
6	2G	39	ILE	4.8
33	2b	139	LYS	4.8
41	1j	98	ILE	4.8
1	2A	2162	G	4.8
1	2A	2145	C	4.8
32	2a	1002	G	4.7
51	1u	18	TYR	4.7
32	2a	1036	G	4.7
45	2n	38	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	2A	2155	G	4.7
1	2A	2803	C	4.7
51	2u	16	GLY	4.6
21	2Z	191	VAL	4.6
1	2A	2152	G	4.6
1	1A	2143	C	4.6
44	2m	5	ALA	4.6
41	2j	98	ILE	4.5
14	2S	31	SER	4.5
1	1A	2142	C	4.5
34	2c	159	GLY	4.5
1	2A	1064	C	4.5
34	2c	206	GLU	4.5
21	2Z	192	ALA	4.4
44	2m	65	LYS	4.4
40	2i	19	LEU	4.4
51	1u	17	THR	4.4
41	2j	96	ILE	4.4
1	1A	1057	A	4.3
6	2G	29	TRP	4.3
49	2s	69	HIS	4.3
40	2i	37	PHE	4.3
40	2i	36	TYR	4.3
1	1A	2116	G	4.3
1	2A	2896	C	4.2
1	2A	2138	C	4.2
1	2A	2175	C	4.2
1	2A	2123	G	4.2
34	2c	160	ALA	4.2
38	2g	16	LEU	4.2
35	1d	2	GLY	4.2
1	1A	1080	C	4.2
45	2n	8	GLU	4.2
1	2A	2111	C	4.1
1	2A	2143	C	4.1
52	2y	50	ALA	4.1
1	2A	2124	G	4.1
1	2A	2148	G	4.1
45	2n	18	VAL	4.1
51	2u	2	GLY	4.1
1	1A	2139	C	4.1
22	20	9	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	1A	1103	A	4.1
1	1A	1508	A	4.0
1	1A	2132	U	4.0
1	1A	1092	C	4.0
1	2A	2602	A	4.0
1	1A	2153	G	4.0
1	1A	2804	C	4.0
1	2A	2172	U	3.9
19	2X	92	LEU	3.9
33	2b	133	LYS	3.9
1	2A	10	G	3.9
51	2u	22	ARG	3.9
52	2y	38	HIS	3.9
1	1A	2803	C	3.9
52	2y	92	GLY	3.9
40	2i	88	TYR	3.9
1	2A	2804	C	3.9
21	2Z	125	LEU	3.9
40	2i	18	PHE	3.9
40	2i	87	GLN	3.8
38	2g	33	ASP	3.8
1	2A	2121	G	3.8
1	1A	1102	C	3.8
51	2u	23	PRO	3.8
21	2Z	9	TYR	3.8
52	2y	42	SER	3.8
1	2A	2122	U	3.8
1	1A	1082	U	3.8
6	2G	158	ALA	3.8
34	2c	164	ARG	3.7
40	2i	33	PHE	3.7
6	2G	90	LEU	3.7
51	1u	5	ASP	3.7
1	2A	2897	U	3.7
41	1j	72	VAL	3.7
32	1a	1035	A	3.7
41	2j	29	ARG	3.7
41	2j	27	ALA	3.7
1	2A	2129	C	3.7
40	2i	110	GLU	3.7
1	2A	2112	G	3.7
40	2i	26	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	1A	888	C	3.7
1	1A	1086	A	3.6
1	2A	2161	C	3.6
33	1b	133	LYS	3.6
22	20	8	GLY	3.6
51	2u	9	ARG	3.6
34	2c	189	ALA	3.6
6	1G	3	LEU	3.6
1	2A	2110	G	3.6
41	2j	10	GLY	3.6
49	2s	82	GLY	3.6
32	1a	1034	G	3.6
47	1p	56	ALA	3.6
1	1A	1090	U	3.6
51	2u	3	LYS	3.6
26	14	49	PHE	3.6
41	2j	26	ALA	3.5
1	2A	1046	A	3.5
9	2N	8	GLN	3.5
25	23	6	VAL	3.5
41	2j	88	LEU	3.5
1	1A	2169	A	3.5
49	1s	66	MET	3.5
1	2A	2894	G	3.5
1	2A	2128	C	3.5
34	2c	171	GLY	3.5
1	1A	2174	C	3.5
1	1A	2141	G	3.5
8	2I	12	LEU	3.5
44	2m	4	ILE	3.5
32	1a	1002	G	3.4
40	2i	30	GLY	3.4
6	2G	92	VAL	3.4
1	1A	2117	A	3.4
32	2a	1035	A	3.4
40	1i	33	PHE	3.4
47	1p	37	GLY	3.4
1	1A	1074	G	3.4
44	2m	116	THR	3.4
1	1A	2144	U	3.4
1	2A	2805	G	3.4
35	2d	4	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
26	24	7	PRO	3.4
35	1d	138	TYR	3.4
1	2A	2170	A	3.4
50	1t	9	ASN	3.4
52	2y	65	GLY	3.4
51	2u	11	GLY	3.4
1	1A	2152	G	3.4
1	2A	2793	G	3.4
38	2g	78	ARG	3.3
1	1A	2129	C	3.3
32	1a	1037	C	3.3
1	2A	2160	G	3.3
1	2A	2176	A	3.3
7	2H	112	PRO	3.3
51	2u	18	TYR	3.3
1	1A	2161	C	3.3
26	24	46	GLN	3.3
1	1A	2108	C	3.3
41	2j	77	PRO	3.3
40	2i	70	LYS	3.3
47	1p	59	TRP	3.3
1	1A	1081	U	3.3
26	14	57	GLU	3.3
33	2b	214	ILE	3.3
38	2g	32	ARG	3.3
40	1i	7	THR	3.3
1	2A	2168	G	3.3
32	1a	1001(A)	G	3.3
40	2i	115	GLY	3.2
7	2H	159	GLU	3.2
26	24	57	GLU	3.2
33	2b	70	PHE	3.2
1	1A	1089	G	3.2
51	2u	4	GLY	3.2
51	2u	12	LYS	3.2
40	2i	3	GLN	3.2
44	2m	6	GLY	3.2
32	1a	1038	C	3.2
26	24	66	SER	3.2
34	1c	201	TYR	3.2
34	2c	196	LEU	3.2
21	2Z	200	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
45	2n	10	ALA	3.2
1	2A	11	G	3.2
1	2A	2807	G	3.2
44	2m	94	ARG	3.2
51	2u	6	ARG	3.2
32	2a	1257	U	3.2
52	2y	37	PRO	3.2
1	1A	2119	A	3.2
49	2s	74	PHE	3.2
52	2y	49	VAL	3.2
52	2y	10	MET	3.1
49	2s	65	ASN	3.1
1	1A	2801(A)	A	3.1
1	2A	1104	C	3.1
52	2y	3	MET	3.1
41	1j	8	LEU	3.1
44	2m	102	ARG	3.1
1	1A	1176	G	3.1
40	1i	126	SER	3.1
1	1A	1104	C	3.1
32	1a	1027	C	3.1
1	1A	2805	G	3.1
48	2r	43	PHE	3.1
51	2u	21	TYR	3.1
40	2i	63	ILE	3.1
33	2b	143	GLU	3.1
44	2m	92	HIS	3.1
41	2j	74	ILE	3.1
8	2l	85	GLU	3.1
26	24	67	TYR	3.1
39	2h	119	LEU	3.1
40	2i	127	LYS	3.1
32	1a	218	C	3.1
26	24	69	LYS	3.1
32	1a	202	U	3.1
1	1A	2107	C	3.1
1	1A	2172	U	3.1
1	2A	1082	U	3.1
1	2A	2132	U	3.1
49	2s	12	ASP	3.0
1	1A	1083	U	3.0
49	2s	38	SER	3.0

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Mol	Chain	Res	Type	RSRZ
52	2y	11	GLU	3.0
1	2A	2130	U	3.0
41	2j	72	VAL	3.0
33	2b	142	LEU	3.0
1	1A	2148	G	3.0
1	2A	2151	G	3.0
1	1A	2794	C	3.0
1	2A	2126	A	3.0
51	2u	5	ASP	3.0
51	1u	22	ARG	3.0
40	2i	17	VAL	3.0
38	1g	156	TRP	3.0
44	2m	7	VAL	3.0
1	1A	2173	A	3.0
41	2j	40	LEU	3.0
52	2y	39	ILE	3.0
38	2g	5	ARG	3.0
23	2l	2	SER	3.0
40	2i	29	ASN	3.0
22	20	75	LEU	3.0
32	1a	1000	U	3.0
1	1A	1072	C	3.0
1	2A	2179	C	3.0
17	2V	42	GLY	3.0
49	2s	62	ILE	3.0
33	2b	163	PHE	3.0
1	1A	1077	A	2.9
1	2A	888	C	2.9
51	2u	13	ILE	2.9
21	2Z	155	LEU	2.9
1	2A	2165	G	2.9
6	2G	75	LYS	2.9
1	2A	2136	C	2.9
1	1A	1088	A	2.9
6	2G	138	GLN	2.9
1	2A	1074	G	2.9
48	2r	58	LEU	2.9
1	2A	2118	U	2.9
45	2n	11	LYS	2.9
52	2y	8	LYS	2.9
33	1b	126	GLU	2.9
41	2j	67	THR	2.9

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Mol	Chain	Res	Type	RSRZ
38	2g	6	ARG	2.9
1	2A	2127	G	2.9
20	2Y	43	ASN	2.9
45	2n	25	VAL	2.9
33	2b	52	GLU	2.9
44	2m	88	ARG	2.9
44	2m	27	LYS	2.9
1	1A	2126	A	2.9
14	2S	40	ILE	2.9
44	1m	87	TYR	2.9
1	1A	1078	U	2.9
1	2A	2119	A	2.9
32	2a	1034	G	2.9
45	2n	2	ALA	2.9
49	2s	71	LEU	2.9
1	2A	887	A	2.8
40	2i	61	ALA	2.8
40	2i	109	VAL	2.8
40	2i	42	ARG	2.8
33	1b	139	LYS	2.8
51	1u	11	GLY	2.8
20	2Y	63	LYS	2.8
33	2b	132	LYS	2.8
34	2c	157	ILE	2.8
33	1b	131	PRO	2.8
6	2G	34	LEU	2.8
44	1m	96	LEU	2.8
52	2y	93	GLU	2.8
2	2B	11	C	2.8
40	2i	5	TYR	2.8
33	2b	101	MET	2.8
1	1A	1065	U	2.8
35	1d	3	ARG	2.8
1	1A	2151	G	2.8
1	2A	2116	G	2.8
6	2G	25	TYR	2.8
32	2a	1020	U	2.8
38	2g	2	ALA	2.8
50	1t	53	LEU	2.8
8	2I	92	VAL	2.8
1	1A	2896	C	2.8
32	2a	1031	G	2.8

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Mol	Chain	Res	Type	RSRZ
40	2i	6	GLY	2.8
1	2A	1075	C	2.8
32	1a	1030(C)	G	2.8
41	1j	25	GLU	2.8
1	1A	2178	C	2.8
51	1u	12	LYS	2.8
32	1a	204	U	2.7
52	2y	41	LEU	2.7
38	2g	81	GLY	2.7
40	2i	62	TYR	2.7
51	1u	21	TYR	2.7
7	2H	103	LEU	2.7
11	2P	1	MET	2.7
26	14	65	ASP	2.7
32	2a	1286	A	2.7
32	2a	84	U	2.7
34	2c	28	GLN	2.7
45	2n	14	PRO	2.7
14	2S	32	LEU	2.7
26	24	51	ASP	2.7
49	2s	83	HIS	2.7
51	1u	3	LYS	2.7
1	1A	1079	C	2.7
49	2s	84	GLY	2.7
33	1b	136	VAL	2.7
20	2Y	91	GLU	2.7
34	2c	162	GLN	2.7
32	2a	993	G	2.7
32	2a	1000	U	2.7
32	2a	1039	C	2.7
8	2I	77	LEU	2.7
6	2G	5	LEU	2.7
7	2H	128	PRO	2.7
49	2s	60	VAL	2.7
51	1u	19	GLY	2.7
49	2s	64	GLU	2.7
50	1t	73	HIS	2.7
44	2m	84	ILE	2.7
1	2A	229	A	2.7
32	1a	1006	C	2.7
29	17	46	VAL	2.7
32	1a	1026	G	2.7

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Mol	Chain	Res	Type	RSRZ
7	2H	116	GLU	2.6
45	2n	7	ILE	2.6
1	1A	2125	G	2.6
23	21	53	VAL	2.6
9	1N	140	VAL	2.6
32	2a	1030(C)	G	2.6
14	2S	26	LEU	2.6
1	1A	1067	A	2.6
32	2a	1270	C	2.6
41	2j	69	ASN	2.6
38	1g	120	ILE	2.6
43	2l	19	ARG	2.6
50	1t	64	ASP	2.6
7	2H	33	LEU	2.6
21	2Z	199	LYS	2.6
1	1A	1093	G	2.6
38	2g	82	GLY	2.6
49	2s	35	SER	2.6
3	2D	276	LYS	2.6
14	2S	39	ILE	2.6
33	2b	122	PHE	2.6
48	1r	29	PHE	2.6
26	24	45	GLY	2.6
44	1m	117	VAL	2.6
24	22	1	MET	2.6
20	2Y	90	LEU	2.6
21	2Z	124	ILE	2.6
6	2G	3	LEU	2.6
34	2c	188	LEU	2.6
41	1j	71	LEU	2.6
49	2s	49	ILE	2.6
38	2g	7	ALA	2.6
47	1p	32	TYR	2.6
8	1l	117	GLU	2.6
1	1A	2894	G	2.6
1	2A	2120	G	2.6
6	2G	2	PRO	2.6
1	2A	1095	A	2.6
2	2B	12	C	2.6
41	2j	73	ASP	2.6
44	1m	32	GLU	2.6
39	2h	112	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	1A	2602	A	2.6
1	2A	1087	G	2.6
32	1a	344	A	2.6
34	2c	163	ALA	2.6
4	2E	59	VAL	2.6
52	2y	20	VAL	2.6
40	2i	64	THR	2.6
32	2a	1030(D)	A	2.5
40	2i	105	ASP	2.5
9	2N	140	VAL	2.5
1	1A	2140	C	2.5
26	24	65	ASP	2.5
41	2j	62	HIS	2.5
52	2y	6	THR	2.5
40	2i	69	GLY	2.5
32	1a	1030	C	2.5
20	2Y	16	ALA	2.5
52	2y	19	HIS	2.5
1	1A	2115	G	2.5
21	2Z	161	VAL	2.5
49	2s	41	VAL	2.5
51	2u	8	THR	2.5
51	2u	24	ARG	2.5
37	1f	95	GLU	2.5
1	2A	2107	C	2.5
39	2h	54	ASP	2.5
6	2G	15	VAL	2.5
21	2Z	198	LYS	2.5
40	2i	8	GLY	2.5
49	2s	53	ASN	2.5
8	2I	107	ILE	2.5
32	1a	1001	A	2.5
42	2k	31	THR	2.5
38	2g	73	MET	2.5
49	2s	32	LYS	2.5
1	2A	34	C	2.5
1	2A	2171	A	2.5
34	1c	193	TYR	2.5
38	2g	4	ARG	2.5
44	2m	34	LEU	2.5
34	1c	149	ALA	2.5
1	2A	1086	A	2.5

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Mol	Chain	Res	Type	RSRZ
49	2s	31	ILE	2.5
1	1A	2897	U	2.5
32	2a	1531	A	2.5
1	1A	2109	U	2.5
7	2H	90	LYS	2.5
40	2i	101	PHE	2.5
32	2a	1271	G	2.5
38	2g	155	ARG	2.5
41	2j	70	ARG	2.5
14	2S	33	LYS	2.4
44	1m	85	GLY	2.4
32	2a	841	U	2.4
32	2a	1040	U	2.4
51	2u	10	ARG	2.4
14	2S	52	SER	2.4
1	2A	2159	G	2.4
47	1p	6	LEU	2.4
44	2m	78	ILE	2.4
49	2s	16	LEU	2.4
41	2j	89	ASP	2.4
34	2c	192	THR	2.4
38	1g	42	ILE	2.4
1	2A	1081	U	2.4
1	1A	2168	G	2.4
1	2A	352	G	2.4
17	2V	101	GLY	2.4
35	1d	137	SER	2.4
40	2i	122	ALA	2.4
39	1h	112	LEU	2.4
45	2n	13	THR	2.4
5	2F	23	ASP	2.4
1	1A	2147	G	2.4
52	2y	64	SER	2.4
14	2S	54	LEU	2.4
25	23	26	LEU	2.4
33	2b	187	LEU	2.4
34	2c	153	VAL	2.4
52	2y	63	ALA	2.4
39	2h	113	SER	2.4
40	2i	9	ARG	2.4
1	2A	2131	G	2.4
21	2Z	25	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
32	1a	1031	G	2.4
33	2b	136	VAL	2.4
52	2y	87	LYS	2.4
1	1A	887	A	2.4
7	2H	123	PHE	2.4
40	1i	128	ARG	2.4
7	2H	24	VAL	2.4
52	2y	9	GLN	2.4
33	2b	128	GLU	2.4
39	1h	111	ILE	2.4
46	1o	87	ILE	2.4
25	23	8	LEU	2.4
1	2A	2167	U	2.4
1	2A	2180	U	2.4
32	2a	723	U	2.4
33	1b	135	GLN	2.4
38	2g	76	ARG	2.4
51	2u	15	ARG	2.4
6	2G	142	PRO	2.4
33	2b	8	LYS	2.4
45	2n	34	TYR	2.4
50	1t	48	LYS	2.4
45	2n	39	LEU	2.4
52	2y	13	THR	2.4
6	1G	49	ASP	2.3
32	2a	1492	A	2.3
51	1u	15	ARG	2.3
51	2u	14	TRP	2.3
40	1i	6	GLY	2.3
41	2j	97	GLU	2.3
41	1j	6	ILE	2.3
49	1s	62	ILE	2.3
33	2b	140	HIS	2.3
41	2j	5	ARG	2.3
11	2P	91	PHE	2.3
32	1a	1039	C	2.3
19	2X	1	MET	2.3
22	20	71	ASP	2.3
1	2A	2808	U	2.3
38	2g	42	ILE	2.3
33	1b	190	THR	2.3
1	2A	1079	C	2.3

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Mol	Chain	Res	Type	RSRZ
33	2b	152	PHE	2.3
24	12	12	GLU	2.3
14	1S	58	LEU	2.3
1	2A	2135	A	2.3
45	2n	22	THR	2.3
34	2c	65	ALA	2.3
12	2Q	104	PHE	2.3
17	1V	63	GLY	2.3
32	1a	1024	G	2.3
32	2a	1202	G	2.3
41	2j	35	SER	2.3
31	29	28	GLU	2.3
51	1u	14	TRP	2.3
6	2G	137	GLU	2.3
47	1p	1	MET	2.3
1	1A	2124	G	2.3
6	2G	94	LEU	2.3
32	1a	1447	A	2.3
33	2b	218	ALA	2.3
28	26	11	LEU	2.3
38	2g	154	TYR	2.3
12	2Q	59	ARG	2.3
39	2h	95	VAL	2.3
52	2y	17	ARG	2.3
1	2A	1062	G	2.3
7	1H	2	SER	2.3
23	11	98	LEU	2.3
41	1j	35	SER	2.3
7	2H	107	VAL	2.3
38	1g	154	TYR	2.3
33	2b	99	GLY	2.3
6	2G	49	ASP	2.3
1	1A	2160	G	2.3
32	1a	1033	G	2.3
50	1t	20	LEU	2.3
52	2y	95	ARG	2.3
44	1m	86	CYS	2.3
21	2Z	93	ASP	2.3
41	1j	73	ASP	2.3
6	2G	140	ILE	2.3
7	2H	51	ARG	2.2
25	23	35	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
32	1a	723	U	2.2
6	1G	25	TYR	2.2
21	2Z	201	LYS	2.2
25	23	2	PRO	2.2
41	2j	23	ILE	2.2
52	2y	72	THR	2.2
21	2Z	4	ARG	2.2
33	1b	130	ARG	2.2
33	2b	138	LEU	2.2
41	2j	85	LEU	2.2
22	20	74	ARG	2.2
35	1d	122	ARG	2.2
41	2j	45	ARG	2.2
50	2t	45	GLN	2.2
29	17	47	ARG	2.2
6	2G	4	ASP	2.2
14	2S	37	ALA	2.2
29	27	27	GLY	2.2
40	2i	90	PRO	2.2
1	1A	1085	A	2.2
1	2A	2794	C	2.2
34	2c	197	GLY	2.2
41	2j	65	LEU	2.2
6	2G	102	PHE	2.2
33	2b	108	ILE	2.2
49	1s	40	ILE	2.2
33	2b	100	GLY	2.2
32	1a	345	C	2.2
40	2i	75	ASP	2.2
1	1A	1063	G	2.2
32	1a	1030(A)	G	2.2
32	2a	1131	G	2.2
45	2n	15	LYS	2.2
19	2X	83	VAL	2.2
1	1A	1026	U	2.2
40	2i	21	PRO	2.2
48	1r	32	ARG	2.2
51	2u	7	ARG	2.2
1	2A	2109	U	2.2
6	2G	82	LEU	2.2
29	17	48	LYS	2.2
45	2n	21	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
41	2j	54	PHE	2.2
7	2H	17	VAL	2.2
33	2b	9	GLU	2.2
34	2c	207	VAL	2.2
49	1s	41	VAL	2.2
21	2Z	164	ALA	2.2
6	2G	26	GLN	2.2
36	2e	45	PHE	2.2
47	2p	19	ILE	2.2
44	2m	96	LEU	2.1
46	1o	31	LEU	2.1
34	2c	161	GLU	2.1
49	2s	28	LYS	2.1
34	2c	101	LEU	2.1
52	2y	94	ALA	2.1
6	2G	159	VAL	2.1
1	1A	2167	U	2.1
47	1p	60	LEU	2.1
1	2A	2181	G	2.1
32	2a	1117	G	2.1
34	2c	66	VAL	2.1
41	2j	64	GLU	2.1
42	2k	32	ILE	2.1
50	2t	6	PRO	2.1
1	1A	2128	C	2.1
1	1A	2138	C	2.1
21	2Z	160	GLY	2.1
26	24	29	PRO	2.1
33	2b	37	ASN	2.1
40	1i	43	ALA	2.1
41	2j	68	HIS	2.1
50	1t	75	ASN	2.1
1	1A	2166	G	2.1
19	2X	67	GLY	2.1
21	2Z	83	PRO	2.1
36	1e	12	LEU	2.1
7	2H	169	VAL	2.1
37	2f	89	MET	2.1
42	2k	119	CYS	2.1
49	1s	44	MET	2.1
3	1D	275	LYS	2.1
42	2k	126	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
33	2b	31	TYR	2.1
1	2A	2106	G	2.1
50	1t	79	ARG	2.1
33	1b	123	ALA	2.1
40	2i	91	ASP	2.1
1	1A	2176	A	2.1
1	1A	2136	C	2.1
1	1A	2146	C	2.1
1	2A	1042	G	2.1
32	2a	1042	G	2.1
34	2c	87	LEU	2.1
49	2s	20	LEU	2.1
51	1u	2	GLY	2.1
52	2y	84	GLN	2.1
38	2g	120	ILE	2.1
45	2n	29	ARG	2.1
50	1t	55	ILE	2.1
52	2y	77	LEU	2.1
26	24	52	THR	2.1
38	2g	43	PHE	2.1
1	1A	2133	G	2.1
17	2V	43	GLU	2.1
35	1d	132	ARG	2.1
52	2y	16	ILE	2.1
34	2c	155	GLY	2.1
40	1i	8	GLY	2.1
52	2y	30	TRP	2.1
52	2y	70	MET	2.1
32	1a	1286	A	2.1
44	2m	30	ALA	2.1
1	2A	2163	C	2.1
1	2A	2164	C	2.1
14	2S	35	ILE	2.1
6	2G	62	LEU	2.1
40	2i	102	LEU	2.1
16	2U	89	GLU	2.1
35	1d	118	ARG	2.1
49	1s	29	ARG	2.1
9	2N	50	ASP	2.1
32	1a	1028	C	2.1
35	1d	86	LYS	2.0
1	2A	2149	G	2.0

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Mol	Chain	Res	Type	RSRZ
14	1S	37	ALA	2.0
26	24	25	TYR	2.0
44	2m	87	TYR	2.0
36	1e	118	ILE	2.0
33	1b	163	PHE	2.0
21	2Z	169	GLU	2.0
32	2a	1030	C	2.0
7	2H	164	TYR	2.0
32	1a	1257	U	2.0
32	2a	1021	G	2.0
46	2o	88	ARG	2.0
47	1p	29	ASP	2.0
50	1t	19	SER	2.0
1	1A	2170	A	2.0
32	1a	1531	A	2.0
7	2H	89	ILE	2.0
36	2e	12	LEU	2.0
7	2H	21	PRO	2.0
15	1T	38	ASN	2.0
50	2t	9	ASN	2.0
1	1A	2793	G	2.0
21	1Z	202	GLU	2.0
40	1i	66	ARG	2.0
48	2r	85	LEU	2.0
1	1A	2163	C	2.0
41	2j	63	PHE	2.0
43	2l	5	PRO	2.0
20	2Y	42	VAL	2.0
6	2G	72	ARG	2.0
25	23	15	TYR	2.0
35	1d	68	TYR	2.0
45	1n	12	ARG	2.0
1	1A	2154	G	2.0
1	1A	2181	G	2.0
2	2B	54	G	2.0
44	2m	41	PRO	2.0
1	1A	2790	A	2.0
49	2s	63	THR	2.0
22	20	70	GLN	2.0
50	1t	45	GLN	2.0
48	2r	66	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	5MC	2a	967	21/22	0.79	0.25	112,121,129,135	0
1	PSU	1A	1911	20/21	0.88	0.15	94,100,105,113	0
32	M2G	2a	966	25/26	0.88	0.23	111,117,124,126	0
1	PSU	1A	1917	20/21	0.90	0.17	91,102,109,109	0
1	5MU	2A	1915	21/22	0.90	0.14	114,125,132,139	0
1	OMC	2A	1920	21/22	0.90	0.16	91,103,111,113	0
1	PSU	2A	1917	20/21	0.91	0.13	106,117,121,124	0
1	5MC	2A	1942	21/22	0.92	0.18	69,75,78,79	0
32	5MC	2a	1407	21/22	0.92	0.18	88,96,104,106	0
32	PSU	2a	516	20/21	0.92	0.13	97,104,116,117	0
43	0TD	1l	92	10/11	0.92	0.27	85,89,94,102	0
32	2MG	2a	1207	24/25	0.92	0.21	138,142,147,153	0
32	G7M	2a	527	24/25	0.93	0.19	84,91,98,100	0
43	0TD	2l	92	10/11	0.93	0.27	80,82,89,105	0
32	2MG	1a	1207	24/25	0.93	0.15	109,112,119,126	0
32	4OC	2a	1402	22/23	0.94	0.19	81,94,100,103	0
1	OMC	1A	1920	21/22	0.94	0.18	74,83,97,101	0
32	MA6	2a	1519	24/25	0.94	0.23	78,89,96,98	0
32	PSU	1a	516	20/21	0.94	0.12	80,90,97,98	0
1	PSU	2A	1911	20/21	0.94	0.10	97,107,115,117	0
1	5MU	1A	1915	21/22	0.94	0.17	100,108,116,117	0
32	5MC	2a	1404	21/22	0.94	0.17	88,94,102,105	0
32	MA6	2a	1518	24/25	0.94	0.22	78,87,92,95	0
32	5MC	2a	1400	21/22	0.94	0.22	97,105,110,111	0
32	M2G	1a	966	25/26	0.95	0.16	83,88,97,99	0
32	5MC	1a	1407	21/22	0.95	0.17	71,77,85,86	0
32	5MC	1a	967	21/22	0.95	0.17	88,92,101,102	0
32	4OC	1a	1402	22/23	0.96	0.17	61,68,71,73	0
32	MA6	1a	1518	24/25	0.96	0.17	61,66,70,74	0
1	5MU	1A	1939	21/22	0.96	0.19	34,46,54,57	0
32	MA6	1a	1519	24/25	0.96	0.18	57,67,73,75	0
32	5MC	1a	1404	21/22	0.96	0.16	60,65,71,72	0
32	UR3	1a	1498	21/22	0.97	0.15	60,68,72,84	0
1	5MU	2A	1939	21/22	0.97	0.17	53,57,61,62	0
1	OMG	1A	2251	24/25	0.97	0.15	31,36,42,46	0
1	2MA	2A	2503	23/24	0.97	0.20	44,50,59,61	0
32	5MC	1a	1400	21/22	0.97	0.16	64,71,76,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	UR3	2a	1498	21/22	0.97	0.16	83,86,91,94	0
1	OMG	2A	2251	24/25	0.97	0.17	52,60,65,67	0
1	PSU	2A	2605	20/21	0.97	0.16	53,63,70,75	0
32	G7M	1a	527	24/25	0.97	0.14	64,79,84,88	0
1	OMU	1A	2552	21/22	0.97	0.18	43,48,52,59	0
1	5MC	1A	1962	21/22	0.97	0.17	50,56,61,63	0
1	5MC	2A	1962	21/22	0.97	0.14	54,59,69,74	0
1	5MC	1A	1942	21/22	0.98	0.12	46,55,61,63	0
1	OMU	2A	2552	21/22	0.98	0.15	49,54,59,62	0
1	2MA	1A	2503	23/24	0.98	0.18	21,35,41,44	0
1	PSU	1A	2605	20/21	0.98	0.16	37,41,47,48	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3834	1/1	0.07	0.60	90,90,90,90	0
54	MG	1A	3260	1/1	0.15	0.42	141,141,141,141	0
54	MG	2A	3565	1/1	0.20	0.59	155,155,155,155	0
54	MG	2A	3193	1/1	0.24	0.37	104,104,104,104	0
54	MG	2A	3114	1/1	0.25	0.53	68,68,68,68	0
54	MG	1a	1839	1/1	0.25	0.90	95,95,95,95	0
54	MG	2A	3087	1/1	0.26	0.53	99,99,99,99	0
54	MG	1a	1802	1/1	0.36	0.14	142,142,142,142	0
54	MG	2A	3463	1/1	0.38	0.18	90,90,90,90	0
54	MG	1A	3600	1/1	0.38	0.72	74,74,74,74	0
54	MG	2A	3597	1/1	0.38	0.15	101,101,101,101	0
54	MG	2B	204	1/1	0.43	0.42	110,110,110,110	0
54	MG	2a	1690	1/1	0.43	0.61	94,94,94,94	0
54	MG	1a	1743	1/1	0.43	0.34	103,103,103,103	0
54	MG	1A	3591	1/1	0.44	0.20	87,87,87,87	0
54	MG	2A	3488	1/1	0.45	0.41	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1b	301	1/1	0.46	0.20	116,116,116,116	0
54	MG	1A	3684	1/1	0.46	0.28	74,74,74,74	0
54	MG	1d	502	1/1	0.46	0.55	101,101,101,101	0
54	MG	1A	3629	1/1	0.47	0.34	73,73,73,73	0
54	MG	2B	203	1/1	0.50	0.26	74,74,74,74	0
54	MG	1A	3806	1/1	0.50	0.43	85,85,85,85	0
54	MG	2A	3333	1/1	0.50	0.30	57,57,57,57	0
54	MG	2a	1664	1/1	0.52	0.49	94,94,94,94	0
54	MG	2a	1663	1/1	0.52	0.51	110,110,110,110	0
54	MG	2A	3301	1/1	0.53	0.47	103,103,103,103	0
54	MG	2B	211	1/1	0.54	0.57	89,89,89,89	0
54	MG	2a	1658	1/1	0.55	0.46	102,102,102,102	0
54	MG	1a	1760	1/1	0.55	0.22	128,128,128,128	0
54	MG	1a	1850	1/1	0.55	0.31	129,129,129,129	0
54	MG	1B	1030	1/1	0.55	0.16	78,78,78,78	0
54	MG	2A	3637	1/1	0.56	0.22	64,64,64,64	0
54	MG	2a	1718	1/1	0.56	0.17	95,95,95,95	0
54	MG	2B	213	1/1	0.56	0.17	97,97,97,97	0
54	MG	2A	3557	1/1	0.56	0.14	106,106,106,106	0
54	MG	2i	201	1/1	0.57	1.34	103,103,103,103	0
54	MG	2A	3036	1/1	0.58	0.28	64,64,64,64	0
54	MG	2a	1655	1/1	0.58	1.18	114,114,114,114	0
54	MG	1a	1826	1/1	0.58	0.13	109,109,109,109	0
54	MG	2B	214	1/1	0.59	0.10	101,101,101,101	0
54	MG	2A	3118	1/1	0.59	0.40	81,81,81,81	0
53	MPD	2B	201	8/8	0.59	0.67	101,115,117,121	0
54	MG	2A	3209	1/1	0.59	0.43	59,59,59,59	0
54	MG	2A	3110	1/1	0.60	0.12	107,107,107,107	0
54	MG	2A	3302	1/1	0.60	0.20	59,59,59,59	0
54	MG	2A	3322	1/1	0.60	0.23	90,90,90,90	0
54	MG	1A	3703	1/1	0.60	0.25	41,41,41,41	0
54	MG	1a	1722	1/1	0.60	0.15	85,85,85,85	0
54	MG	1a	1712	1/1	0.60	0.14	109,109,109,109	0
54	MG	2A	3615	1/1	0.60	0.46	75,75,75,75	0
54	MG	2a	1668	1/1	0.60	0.19	90,90,90,90	0
54	MG	1a	1768	1/1	0.61	0.15	81,81,81,81	0
54	MG	2A	3543	1/1	0.61	0.20	89,89,89,89	0
54	MG	1A	3577	1/1	0.61	0.15	72,72,72,72	0
54	MG	1a	1711	1/1	0.61	0.26	82,82,82,82	0
54	MG	2A	3491	1/1	0.61	0.21	52,52,52,52	0
54	MG	2A	3392	1/1	0.61	0.21	81,81,81,81	0
54	MG	1A	3613	1/1	0.61	0.20	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3556	1/1	0.61	0.11	90,90,90,90	0
54	MG	1A	3356	1/1	0.62	0.18	88,88,88,88	0
54	MG	2A	3313	1/1	0.62	0.31	90,90,90,90	0
54	MG	2A	3061	1/1	0.63	0.28	61,61,61,61	0
54	MG	1A	3818	1/1	0.63	0.25	59,59,59,59	0
54	MG	1A	3748	1/1	0.63	0.12	92,92,92,92	0
54	MG	10	101	1/1	0.63	0.26	82,82,82,82	0
54	MG	2A	3058	1/1	0.63	0.51	70,70,70,70	0
54	MG	2A	3586	1/1	0.64	0.14	104,104,104,104	0
54	MG	1A	3111	1/1	0.64	0.10	69,69,69,69	0
54	MG	2A	3083	1/1	0.64	0.23	87,87,87,87	0
54	MG	1a	1843	1/1	0.64	0.50	81,81,81,81	0
54	MG	1a	1764	1/1	0.64	0.18	92,92,92,92	0
54	MG	2B	205	1/1	0.64	0.48	70,70,70,70	0
54	MG	2A	3197	1/1	0.64	0.22	78,78,78,78	0
54	MG	2a	1659	1/1	0.64	0.72	87,87,87,87	0
54	MG	2A	3242	1/1	0.65	0.20	77,77,77,77	0
54	MG	2A	3022	1/1	0.65	0.51	80,80,80,80	0
54	MG	1e	203	1/1	0.65	0.47	89,89,89,89	0
54	MG	2A	3356	1/1	0.66	0.29	91,91,91,91	0
54	MG	2A	3373	1/1	0.66	0.27	87,87,87,87	0
54	MG	2A	3482	1/1	0.66	0.20	106,106,106,106	0
54	MG	1a	1762	1/1	0.66	0.19	108,108,108,108	0
54	MG	1A	3481	1/1	0.66	0.24	74,74,74,74	0
54	MG	2a	1719	1/1	0.66	0.08	110,110,110,110	0
54	MG	1G	202	1/1	0.66	0.14	79,79,79,79	0
54	MG	2a	1709	1/1	0.66	0.37	83,83,83,83	0
54	MG	2A	3051	1/1	0.66	0.25	78,78,78,78	0
54	MG	2A	3230	1/1	0.67	0.56	58,58,58,58	0
54	MG	2k	201	1/1	0.67	0.13	83,83,83,83	0
54	MG	2A	3561	1/1	0.67	0.10	97,97,97,97	0
54	MG	2A	3441	1/1	0.67	0.22	88,88,88,88	0
54	MG	1A	3855	1/1	0.67	0.22	54,54,54,54	0
54	MG	1B	1018	1/1	0.67	0.33	84,84,84,84	0
54	MG	2a	1693	1/1	0.67	0.23	84,84,84,84	0
54	MG	1f	202	1/1	0.67	0.20	93,93,93,93	0
54	MG	2A	3438	1/1	0.67	0.24	80,80,80,80	0
54	MG	2A	3187	1/1	0.68	0.59	70,70,70,70	0
54	MG	1a	1761	1/1	0.68	0.24	114,114,114,114	0
54	MG	2A	3566	1/1	0.68	0.15	81,81,81,81	0
54	MG	2a	1681	1/1	0.68	0.07	94,94,94,94	0
54	MG	2a	1608	1/1	0.68	1.00	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3334	1/1	0.68	0.24	49,49,49,49	0
54	MG	1A	3241	1/1	0.68	0.17	93,93,93,93	0
54	MG	1A	3171	1/1	0.68	0.21	56,56,56,56	0
54	MG	2A	3384	1/1	0.69	0.22	76,76,76,76	0
54	MG	2A	3317	1/1	0.69	0.43	103,103,103,103	0
54	MG	2a	1737	1/1	0.69	0.26	131,131,131,131	0
54	MG	1a	1852	1/1	0.69	0.13	106,106,106,106	0
54	MG	1a	1665	1/1	0.69	0.43	86,86,86,86	0
54	MG	2A	3244	1/1	0.69	0.27	72,72,72,72	0
54	MG	2a	1615	1/1	0.69	0.19	77,77,77,77	0
54	MG	1a	1858	1/1	0.69	0.39	90,90,90,90	0
54	MG	1a	1822	1/1	0.69	0.43	101,101,101,101	0
54	MG	2A	3055	1/1	0.70	0.54	66,66,66,66	0
54	MG	1A	3852	1/1	0.70	0.21	85,85,85,85	0
54	MG	1A	3161	1/1	0.70	0.32	61,61,61,61	0
54	MG	2a	1617	1/1	0.70	0.44	73,73,73,73	0
54	MG	1A	3861	1/1	0.70	0.15	133,133,133,133	0
54	MG	1a	1694	1/1	0.70	0.43	73,73,73,73	0
54	MG	1A	3211	1/1	0.70	0.45	50,50,50,50	0
54	MG	1B	1017	1/1	0.70	0.45	65,65,65,65	0
54	MG	2A	3086	1/1	0.70	0.41	94,94,94,94	0
54	MG	1A	3880	1/1	0.70	0.20	50,50,50,50	0
54	MG	2A	3630	1/1	0.70	0.43	58,58,58,58	0
54	MG	2a	1607	1/1	0.70	0.22	94,94,94,94	0
54	MG	1A	3815	1/1	0.70	0.32	61,61,61,61	0
54	MG	1a	1668	1/1	0.70	0.43	69,69,69,69	0
54	MG	1A	3757	1/1	0.70	0.12	44,44,44,44	0
54	MG	2a	1745	1/1	0.71	0.21	85,85,85,85	0
54	MG	1a	1769	1/1	0.71	0.23	90,90,90,90	0
54	MG	1a	1789	1/1	0.71	0.66	107,107,107,107	0
54	MG	1A	3418	1/1	0.71	0.25	39,39,39,39	0
54	MG	2A	3183	1/1	0.71	0.44	84,84,84,84	0
54	MG	2A	3325	1/1	0.71	0.08	96,96,96,96	0
54	MG	1a	1603	1/1	0.71	0.13	118,118,118,118	0
54	MG	2G	201	1/1	0.71	0.23	114,114,114,114	0
54	MG	1g	203	1/1	0.71	0.24	62,62,62,62	0
54	MG	1A	3718	1/1	0.71	0.14	69,69,69,69	0
54	MG	1Q	201	1/1	0.71	0.21	51,51,51,51	0
54	MG	2O	202	1/1	0.71	0.35	94,94,94,94	0
54	MG	2a	1720	1/1	0.71	0.21	117,117,117,117	0
54	MG	2A	3045	1/1	0.71	0.44	74,74,74,74	0
54	MG	1A	3426	1/1	0.71	0.14	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3410	1/1	0.72	0.33	75,75,75,75	0
54	MG	2a	1660	1/1	0.72	0.35	79,79,79,79	0
54	MG	1a	1823	1/1	0.72	0.20	99,99,99,99	0
54	MG	2A	3105	1/1	0.72	1.12	95,95,95,95	0
54	MG	1A	3472	1/1	0.72	0.28	43,43,43,43	0
54	MG	2A	3377	1/1	0.72	0.37	57,57,57,57	0
54	MG	1t	201	1/1	0.72	0.29	110,110,110,110	0
54	MG	1A	3749	1/1	0.72	0.12	74,74,74,74	0
54	MG	2T	201	1/1	0.72	0.14	61,61,61,61	0
54	MG	23	101	1/1	0.72	0.71	81,81,81,81	0
54	MG	2A	3452	1/1	0.72	0.41	70,70,70,70	0
54	MG	21	104	1/1	0.72	0.23	95,95,95,95	0
54	MG	2A	3075	1/1	0.72	0.45	70,70,70,70	0
54	MG	2a	1701	1/1	0.73	1.03	101,101,101,101	0
54	MG	1e	202	1/1	0.73	0.50	78,78,78,78	0
54	MG	1A	3737	1/1	0.73	0.10	74,74,74,74	0
54	MG	1A	3164	1/1	0.73	0.26	49,49,49,49	0
54	MG	2a	1742	1/1	0.73	0.12	96,96,96,96	0
54	MG	2A	3403	1/1	0.73	0.13	74,74,74,74	0
54	MG	1a	1779	1/1	0.73	0.28	81,81,81,81	0
54	MG	1a	1687	1/1	0.73	0.32	72,72,72,72	0
54	MG	2a	1724	1/1	0.73	0.10	108,108,108,108	0
54	MG	1F	311	1/1	0.73	0.47	90,90,90,90	0
54	MG	2a	1731	1/1	0.73	0.16	86,86,86,86	0
54	MG	1a	1833	1/1	0.73	0.15	122,122,122,122	0
54	MG	2A	3447	1/1	0.74	0.17	69,69,69,69	0
54	MG	2A	3040	1/1	0.74	0.10	65,65,65,65	0
54	MG	1a	1719	1/1	0.74	0.34	102,102,102,102	0
54	MG	1A	3227	1/1	0.74	0.40	88,88,88,88	0
54	MG	2A	3569	1/1	0.74	0.14	87,87,87,87	0
54	MG	1A	3204	1/1	0.74	0.17	76,76,76,76	0
54	MG	1a	1778	1/1	0.74	0.29	72,72,72,72	0
54	MG	2A	3537	1/1	0.74	0.20	97,97,97,97	0
54	MG	10	106	1/1	0.74	0.49	81,81,81,81	0
54	MG	1A	3584	1/1	0.74	0.15	70,70,70,70	0
54	MG	1a	1735	1/1	0.74	0.19	83,83,83,83	0
54	MG	2B	215	1/1	0.75	0.12	112,112,112,112	0
54	MG	1A	3030	1/1	0.75	0.69	69,69,69,69	0
54	MG	1A	3678	1/1	0.75	0.31	115,115,115,115	0
54	MG	2A	3005	1/1	0.75	0.31	68,68,68,68	0
53	MPD	1a	1601	8/8	0.75	0.33	97,116,129,130	0
54	MG	1a	1792	1/1	0.75	0.31	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3720	1/1	0.75	0.70	64,64,64,64	0
54	MG	1B	1019	1/1	0.75	0.09	75,75,75,75	0
54	MG	2A	3638	1/1	0.75	0.22	55,55,55,55	0
54	MG	1A	3895	1/1	0.75	0.35	56,56,56,56	0
54	MG	2a	1764	1/1	0.75	0.39	61,61,61,61	0
54	MG	1A	3329	1/1	0.75	0.11	57,57,57,57	0
54	MG	1A	3608	1/1	0.75	0.61	56,56,56,56	0
54	MG	2A	3493	1/1	0.75	0.19	65,65,65,65	0
54	MG	1a	1821	1/1	0.75	0.45	88,88,88,88	0
54	MG	1A	3637	1/1	0.75	0.41	86,86,86,86	0
54	MG	2a	1752	1/1	0.75	0.13	103,103,103,103	0
54	MG	2A	3455	1/1	0.75	0.33	68,68,68,68	0
54	MG	2a	1683	1/1	0.75	0.17	83,83,83,83	0
54	MG	2A	3207	1/1	0.75	0.41	61,61,61,61	0
54	MG	2A	3071	1/1	0.75	0.43	51,51,51,51	0
54	MG	1A	3408	1/1	0.75	0.24	19,19,19,19	0
54	MG	2A	3151	1/1	0.75	0.47	72,72,72,72	0
54	MG	2A	3538	1/1	0.75	0.24	42,42,42,42	0
54	MG	1a	1602	1/1	0.75	0.28	63,63,63,63	0
54	MG	1A	3369	1/1	0.76	0.19	37,37,37,37	0
54	MG	1A	3545	1/1	0.76	0.13	50,50,50,50	0
54	MG	2A	3169	1/1	0.76	0.38	80,80,80,80	0
54	MG	2A	3215	1/1	0.76	0.18	65,65,65,65	0
54	MG	1A	3828	1/1	0.76	0.22	64,64,64,64	0
54	MG	1A	3086	1/1	0.76	0.32	68,68,68,68	0
54	MG	2A	3572	1/1	0.76	0.11	57,57,57,57	0
54	MG	2a	1762	1/1	0.76	0.33	105,105,105,105	0
54	MG	1n	103	1/1	0.76	0.40	100,100,100,100	0
54	MG	2A	3096	1/1	0.76	0.34	57,57,57,57	0
54	MG	1B	1009	1/1	0.76	0.38	77,77,77,77	0
54	MG	1A	3879	1/1	0.76	0.42	100,100,100,100	0
54	MG	2A	3102	1/1	0.76	0.17	95,95,95,95	0
54	MG	1a	1683	1/1	0.76	0.15	73,73,73,73	0
54	MG	2A	3408	1/1	0.76	0.20	81,81,81,81	0
54	MG	1a	1815	1/1	0.76	0.13	81,81,81,81	0
54	MG	2j	201	1/1	0.76	0.37	112,112,112,112	0
54	MG	2A	3077	1/1	0.76	0.51	67,67,67,67	0
54	MG	1a	1663	1/1	0.76	0.66	68,68,68,68	0
54	MG	1a	1748	1/1	0.76	0.37	86,86,86,86	0
54	MG	1a	1770	1/1	0.77	0.20	99,99,99,99	0
54	MG	1a	1670	1/1	0.77	0.34	91,91,91,91	0
54	MG	2A	3236	1/1	0.77	0.18	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2a	1740	1/1	0.77	0.09	98,98,98,98	0
54	MG	2a	1644	1/1	0.77	0.19	92,92,92,92	0
54	MG	1A	3850	1/1	0.77	0.41	54,54,54,54	0
54	MG	1A	3715	1/1	0.77	0.14	71,71,71,71	0
54	MG	1g	202	1/1	0.77	0.36	85,85,85,85	0
54	MG	1a	1807	1/1	0.77	0.29	87,87,87,87	0
54	MG	19	103	1/1	0.77	0.64	93,93,93,93	0
54	MG	1a	1709	1/1	0.77	0.83	99,99,99,99	0
54	MG	2A	3545	1/1	0.77	0.16	110,110,110,110	0
54	MG	1y	204	1/1	0.77	0.46	99,99,99,99	0
54	MG	2A	3553	1/1	0.77	0.13	100,100,100,100	0
54	MG	1A	3028	1/1	0.77	0.44	47,47,47,47	0
54	MG	1A	3543	1/1	0.77	0.32	42,42,42,42	0
54	MG	1a	1799	1/1	0.77	0.15	96,96,96,96	0
54	MG	1a	1634	1/1	0.77	0.22	62,62,62,62	0
54	MG	1a	1681	1/1	0.77	0.20	113,113,113,113	0
54	MG	1A	3373	1/1	0.77	0.10	67,67,67,67	0
54	MG	1a	1695	1/1	0.77	0.14	94,94,94,94	0
53	MPD	2A	3002	8/8	0.77	0.41	89,92,94,95	0
54	MG	1A	3887	1/1	0.77	0.17	40,40,40,40	0
54	MG	1A	3170	1/1	0.77	0.58	62,62,62,62	0
54	MG	1A	3017	1/1	0.77	0.36	57,57,57,57	0
54	MG	2A	3522	1/1	0.77	0.28	96,96,96,96	0
54	MG	2A	3219	1/1	0.77	0.16	70,70,70,70	0
54	MG	1A	3243	1/1	0.78	0.18	45,45,45,45	0
54	MG	1a	1679	1/1	0.78	0.25	57,57,57,57	0
54	MG	2A	3097	1/1	0.78	0.29	71,71,71,71	0
54	MG	2A	3456	1/1	0.78	0.24	71,71,71,71	0
54	MG	2a	1692	1/1	0.78	0.28	75,75,75,75	0
54	MG	2A	3533	1/1	0.78	0.20	61,61,61,61	0
54	MG	1A	3216	1/1	0.78	0.13	66,66,66,66	0
54	MG	2a	1715	1/1	0.78	0.11	88,88,88,88	0
54	MG	2A	3388	1/1	0.78	0.23	73,73,73,73	0
54	MG	2A	3304	1/1	0.78	0.19	65,65,65,65	0
54	MG	2A	3090	1/1	0.78	0.38	81,81,81,81	0
54	MG	2A	3472	1/1	0.78	0.16	69,69,69,69	0
54	MG	2A	3202	1/1	0.78	0.46	73,73,73,73	0
54	MG	1A	3743	1/1	0.78	0.31	47,47,47,47	0
54	MG	2A	3180	1/1	0.78	0.25	61,61,61,61	0
54	MG	2A	3575	1/1	0.78	0.20	52,52,52,52	0
54	MG	1d	507	1/1	0.78	0.09	116,116,116,116	0
54	MG	1a	1636	1/1	0.78	0.23	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2a	1670	1/1	0.78	0.43	57,57,57,57	0
54	MG	1a	1631	1/1	0.78	0.16	68,68,68,68	0
54	MG	1a	1857	1/1	0.78	0.14	92,92,92,92	0
54	MG	1P	205	1/1	0.78	0.42	117,117,117,117	0
54	MG	2a	1733	1/1	0.79	0.20	86,86,86,86	0
54	MG	1A	3732	1/1	0.79	0.69	60,60,60,60	0
54	MG	2R	202	1/1	0.79	0.27	70,70,70,70	0
54	MG	1A	3353	1/1	0.79	0.14	38,38,38,38	0
54	MG	1d	506	1/1	0.79	0.10	98,98,98,98	0
54	MG	1A	3619	1/1	0.79	0.33	55,55,55,55	0
54	MG	2A	3034	1/1	0.79	0.18	62,62,62,62	0
54	MG	2B	217	1/1	0.79	0.12	81,81,81,81	0
54	MG	1a	1734	1/1	0.79	0.53	130,130,130,130	0
54	MG	2A	3359	1/1	0.79	0.22	73,73,73,73	0
54	MG	2a	1675	1/1	0.79	0.42	87,87,87,87	0
54	MG	1a	1773	1/1	0.79	0.22	77,77,77,77	0
54	MG	2A	3007	1/1	0.79	0.25	63,63,63,63	0
54	MG	2A	3582	1/1	0.79	0.30	91,91,91,91	0
54	MG	2A	3342	1/1	0.79	0.18	69,69,69,69	0
54	MG	2A	3481	1/1	0.79	0.37	92,92,92,92	0
54	MG	2A	3213	1/1	0.79	0.63	73,73,73,73	0
54	MG	1A	3354	1/1	0.79	0.22	38,38,38,38	0
54	MG	1A	3220	1/1	0.79	0.32	54,54,54,54	0
54	MG	2a	1645	1/1	0.79	0.22	120,120,120,120	0
54	MG	1a	1831	1/1	0.79	0.26	96,96,96,96	0
54	MG	1a	1650	1/1	0.79	0.82	74,74,74,74	0
54	MG	1A	3578	1/1	0.79	0.19	62,62,62,62	0
54	MG	2a	1754	1/1	0.79	0.18	121,121,121,121	0
54	MG	1a	1810	1/1	0.79	0.28	82,82,82,82	0
54	MG	1a	1808	1/1	0.79	0.26	63,63,63,63	0
54	MG	1A	3694	1/1	0.79	0.22	61,61,61,61	0
54	MG	2A	3519	1/1	0.79	0.13	64,64,64,64	0
54	MG	1a	1787	1/1	0.79	0.12	74,74,74,74	0
54	MG	2A	3082	1/1	0.79	0.18	76,76,76,76	0
54	MG	1A	3303	1/1	0.79	0.13	60,60,60,60	0
54	MG	1A	3415	1/1	0.79	0.14	40,40,40,40	0
54	MG	2A	3576	1/1	0.79	0.19	63,63,63,63	0
54	MG	2a	1734	1/1	0.80	0.13	62,62,62,62	0
54	MG	10	104	1/1	0.80	0.32	54,54,54,54	0
54	MG	2A	3175	1/1	0.80	0.17	63,63,63,63	0
54	MG	1A	3230	1/1	0.80	0.23	49,49,49,49	0
54	MG	2A	3138	1/1	0.80	0.51	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2a	1708	1/1	0.80	0.15	72,72,72,72	0
54	MG	1A	3735	1/1	0.80	0.20	58,58,58,58	0
54	MG	2a	1695	1/1	0.80	0.24	95,95,95,95	0
54	MG	1a	1749	1/1	0.80	0.71	100,100,100,100	0
54	MG	2A	3292	1/1	0.80	0.36	74,74,74,74	0
54	MG	1A	3682	1/1	0.80	0.17	79,79,79,79	0
54	MG	1A	3618	1/1	0.80	0.39	68,68,68,68	0
54	MG	2A	3618	1/1	0.80	0.14	104,104,104,104	0
54	MG	1A	3410	1/1	0.80	0.20	20,20,20,20	0
54	MG	2A	3194	1/1	0.80	0.14	60,60,60,60	0
54	MG	2l	202	1/1	0.80	0.60	55,55,55,55	0
54	MG	1A	3617	1/1	0.80	0.26	100,100,100,100	0
54	MG	2a	1657	1/1	0.80	0.37	89,89,89,89	0
54	MG	2a	1711	1/1	0.80	0.10	80,80,80,80	0
54	MG	1A	3384	1/1	0.80	0.30	74,74,74,74	0
54	MG	1a	1782	1/1	0.80	0.36	86,86,86,86	0
54	MG	1d	505	1/1	0.80	0.23	56,56,56,56	0
54	MG	1a	1675	1/1	0.80	0.32	68,68,68,68	0
54	MG	2A	3498	1/1	0.80	0.23	67,67,67,67	0
54	MG	1A	3097	1/1	0.80	0.34	38,38,38,38	0
54	MG	1F	304	1/1	0.80	0.37	43,43,43,43	0
54	MG	2B	206	1/1	0.80	0.36	61,61,61,61	0
54	MG	2A	3165	1/1	0.80	0.25	72,72,72,72	0
54	MG	2A	3225	1/1	0.80	0.66	80,80,80,80	0
54	MG	1a	1754	1/1	0.80	0.16	78,78,78,78	0
54	MG	1D	312	1/1	0.80	0.62	62,62,62,62	0
54	MG	1A	3683	1/1	0.80	0.17	34,34,34,34	0
54	MG	1A	3641	1/1	0.80	0.27	33,33,33,33	0
54	MG	1A	3872	1/1	0.80	0.29	77,77,77,77	0
54	MG	2A	3307	1/1	0.80	0.19	75,75,75,75	0
54	MG	1A	3562	1/1	0.80	0.41	81,81,81,81	0
54	MG	2D	306	1/1	0.80	0.24	52,52,52,52	0
54	MG	2A	3137	1/1	0.81	0.38	67,67,67,67	0
54	MG	2A	3539	1/1	0.81	0.20	74,74,74,74	0
54	MG	2A	3489	1/1	0.81	0.10	74,74,74,74	0
54	MG	2a	1732	1/1	0.81	0.14	91,91,91,91	0
54	MG	2a	1680	1/1	0.81	0.42	121,121,121,121	0
54	MG	2a	1605	1/1	0.81	0.17	91,91,91,91	0
54	MG	2A	3462	1/1	0.81	0.17	74,74,74,74	0
54	MG	1a	1714	1/1	0.81	0.30	83,83,83,83	0
54	MG	1V	203	1/1	0.81	0.57	86,86,86,86	0
54	MG	2A	3149	1/1	0.81	0.25	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2a	1759	1/1	0.81	0.54	80,80,80,80	0
54	MG	2A	3094	1/1	0.81	0.30	74,74,74,74	0
54	MG	2A	3171	1/1	0.81	0.15	84,84,84,84	0
54	MG	2A	3610	1/1	0.81	0.16	61,61,61,61	0
54	MG	2A	3464	1/1	0.81	0.54	69,69,69,69	0
54	MG	2a	1746	1/1	0.81	0.18	119,119,119,119	0
54	MG	2A	3370	1/1	0.81	0.21	82,82,82,82	0
54	MG	2A	3346	1/1	0.81	0.17	89,89,89,89	0
54	MG	2a	1738	1/1	0.81	0.24	93,93,93,93	0
54	MG	2A	3177	1/1	0.81	0.41	60,60,60,60	0
54	MG	1A	3165	1/1	0.81	0.23	78,78,78,78	0
54	MG	2a	1697	1/1	0.81	0.17	75,75,75,75	0
54	MG	1A	3516	1/1	0.81	0.38	73,73,73,73	0
54	MG	2a	1707	1/1	0.81	0.24	84,84,84,84	0
54	MG	1A	3502	1/1	0.81	0.13	91,91,91,91	0
54	MG	2A	3128	1/1	0.81	0.38	58,58,58,58	0
54	MG	1A	3143	1/1	0.81	0.34	70,70,70,70	0
54	MG	2A	3285	1/1	0.81	0.33	68,68,68,68	0
54	MG	1h	201	1/1	0.81	0.34	64,64,64,64	0
54	MG	1A	3326	1/1	0.81	0.21	44,44,44,44	0
54	MG	2a	1673	1/1	0.81	0.36	69,69,69,69	0
54	MG	1a	1635	1/1	0.81	0.11	80,80,80,80	0
54	MG	2A	3130	1/1	0.81	0.36	62,62,62,62	0
56	ZN	14	101	1/1	0.81	0.06	135,135,135,135	0
54	MG	2A	3305	1/1	0.81	0.24	58,58,58,58	0
54	MG	2A	3153	1/1	0.81	0.46	78,78,78,78	0
54	MG	1A	3037	1/1	0.81	0.48	56,56,56,56	0
54	MG	1a	1614	1/1	0.81	0.12	94,94,94,94	0
54	MG	2A	3574	1/1	0.81	0.23	56,56,56,56	0
54	MG	2A	3181	1/1	0.82	0.30	57,57,57,57	0
54	MG	1A	3724	1/1	0.82	0.63	91,91,91,91	0
54	MG	2A	3329	1/1	0.82	0.19	93,93,93,93	0
55	ARG	1F	303	12/12	0.82	0.29	56,82,107,107	0
54	MG	1a	1811	1/1	0.82	0.61	118,118,118,118	0
54	MG	1A	3011	1/1	0.82	0.39	55,55,55,55	0
54	MG	1a	1705	1/1	0.82	0.07	93,93,93,93	0
54	MG	2A	3404	1/1	0.82	0.20	81,81,81,81	0
54	MG	2A	3469	1/1	0.82	0.21	64,64,64,64	0
54	MG	1B	1007	1/1	0.82	0.28	67,67,67,67	0
54	MG	2A	3604	1/1	0.82	0.09	66,66,66,66	0
54	MG	2a	1604	1/1	0.82	0.18	91,91,91,91	0
54	MG	2A	3093	1/1	0.82	0.12	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3063	1/1	0.82	0.44	41,41,41,41	0
54	MG	1A	3179	1/1	0.82	0.34	49,49,49,49	0
54	MG	2A	3343	1/1	0.82	0.20	47,47,47,47	0
54	MG	2a	1638	1/1	0.82	0.45	77,77,77,77	0
54	MG	2A	3232	1/1	0.82	0.31	69,69,69,69	0
54	MG	1A	3560	1/1	0.82	0.11	48,48,48,48	0
54	MG	2A	3320	1/1	0.82	0.12	72,72,72,72	0
54	MG	1a	1820	1/1	0.82	0.22	124,124,124,124	0
54	MG	2A	3601	1/1	0.82	0.15	75,75,75,75	0
54	MG	1A	3173	1/1	0.82	0.30	80,80,80,80	0
54	MG	1A	3506	1/1	0.82	0.19	65,65,65,65	0
54	MG	2A	3080	1/1	0.82	0.09	130,130,130,130	0
54	MG	2A	3081	1/1	0.82	0.35	52,52,52,52	0
54	MG	1A	3191	1/1	0.82	0.25	64,64,64,64	0
54	MG	2a	1653	1/1	0.82	0.11	86,86,86,86	0
54	MG	1A	3727	1/1	0.82	0.57	58,58,58,58	0
54	MG	1a	1819	1/1	0.82	0.20	97,97,97,97	0
54	MG	1B	1011	1/1	0.82	0.20	64,64,64,64	0
54	MG	1t	202	1/1	0.82	0.48	92,92,92,92	0
54	MG	1A	3236	1/1	0.82	0.45	52,52,52,52	0
54	MG	1A	3570	1/1	0.82	0.20	81,81,81,81	0
54	MG	2a	1647	1/1	0.82	0.33	67,67,67,67	0
54	MG	1A	3047	1/1	0.82	0.34	73,73,73,73	0
54	MG	1a	1784	1/1	0.82	0.73	82,82,82,82	0
54	MG	2A	3501	1/1	0.82	0.26	60,60,60,60	0
54	MG	2A	3113	1/1	0.82	0.20	64,64,64,64	0
54	MG	1A	3530	1/1	0.82	0.33	103,103,103,103	0
54	MG	1a	1801	1/1	0.83	0.17	107,107,107,107	0
54	MG	1A	3225	1/1	0.83	0.30	54,54,54,54	0
54	MG	2A	3374	1/1	0.83	0.18	60,60,60,60	0
54	MG	1A	3837	1/1	0.83	0.30	56,56,56,56	0
54	MG	2a	1735	1/1	0.83	0.18	76,76,76,76	0
54	MG	1A	3106	1/1	0.83	0.33	48,48,48,48	0
54	MG	1a	1827	1/1	0.83	0.22	95,95,95,95	0
54	MG	2A	3210	1/1	0.83	0.30	61,61,61,61	0
54	MG	2B	202	1/1	0.83	0.25	99,99,99,99	0
54	MG	1A	3452	1/1	0.83	0.15	52,52,52,52	0
54	MG	1a	1856	1/1	0.83	0.20	83,83,83,83	0
54	MG	1A	3848	1/1	0.83	0.18	55,55,55,55	0
54	MG	1R	203	1/1	0.83	0.45	52,52,52,52	0
54	MG	2a	1656	1/1	0.83	0.79	106,106,106,106	0
54	MG	1a	1803	1/1	0.83	0.09	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3190	1/1	0.83	0.33	76,76,76,76	0
54	MG	2a	1616	1/1	0.83	0.19	80,80,80,80	0
54	MG	2A	3135	1/1	0.83	0.17	69,69,69,69	0
54	MG	2a	1671	1/1	0.83	0.23	79,79,79,79	0
54	MG	2A	3188	1/1	0.83	0.36	67,67,67,67	0
54	MG	1A	3319	1/1	0.83	0.48	72,72,72,72	0
54	MG	1A	3504	1/1	0.83	0.25	25,25,25,25	0
54	MG	1a	1842	1/1	0.83	0.14	73,73,73,73	0
54	MG	2A	3453	1/1	0.83	0.12	43,43,43,43	0
54	MG	2a	1736	1/1	0.83	0.25	100,100,100,100	0
54	MG	2A	3251	1/1	0.83	0.16	76,76,76,76	0
54	MG	1A	3486	1/1	0.83	0.16	69,69,69,69	0
54	MG	2a	1636	1/1	0.83	0.14	99,99,99,99	0
54	MG	1A	3198	1/1	0.83	0.23	64,64,64,64	0
54	MG	2a	1684	1/1	0.83	0.12	73,73,73,73	0
54	MG	1a	1646	1/1	0.83	0.08	102,102,102,102	0
54	MG	2A	3517	1/1	0.83	0.16	57,57,57,57	0
54	MG	2a	1643	1/1	0.83	0.39	51,51,51,51	0
53	MPD	1T	2001	8/8	0.83	0.29	77,82,86,94	0
54	MG	2A	3399	1/1	0.83	0.11	68,68,68,68	0
54	MG	2A	3397	1/1	0.83	0.13	58,58,58,58	0
54	MG	1A	3555	1/1	0.83	0.14	79,79,79,79	0
54	MG	1A	3283	1/1	0.83	0.23	64,64,64,64	0
54	MG	2A	3031	1/1	0.83	0.15	75,75,75,75	0
54	MG	1A	3796	1/1	0.83	0.43	66,66,66,66	0
54	MG	2A	3587	1/1	0.83	0.13	83,83,83,83	0
54	MG	2a	1758	1/1	0.83	0.10	102,102,102,102	0
54	MG	1A	3435	1/1	0.83	0.20	51,51,51,51	0
54	MG	2a	1710	1/1	0.83	0.24	98,98,98,98	0
54	MG	1A	3250	1/1	0.83	0.29	61,61,61,61	0
54	MG	2a	1621	1/1	0.83	0.41	52,52,52,52	0
54	MG	1A	3839	1/1	0.83	0.29	61,61,61,61	0
54	MG	2A	3154	1/1	0.83	0.47	66,66,66,66	0
54	MG	2A	3613	1/1	0.83	0.22	102,102,102,102	0
54	MG	2A	3365	1/1	0.83	0.38	70,70,70,70	0
54	MG	1A	3185	1/1	0.83	0.14	61,61,61,61	0
54	MG	1A	3599	1/1	0.83	0.28	49,49,49,49	0
54	MG	1a	1700	1/1	0.83	0.33	77,77,77,77	0
54	MG	1A	3700	1/1	0.83	0.31	58,58,58,58	0
54	MG	1A	3262	1/1	0.83	0.12	45,45,45,45	0
54	MG	2A	3198	1/1	0.83	0.32	72,72,72,72	0
54	MG	1A	3592	1/1	0.84	0.26	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1F	302	1/1	0.84	0.28	57,57,57,57	0
54	MG	2a	1716	1/1	0.84	0.10	89,89,89,89	0
54	MG	1A	3730	1/1	0.84	0.26	75,75,75,75	0
54	MG	1A	3430	1/1	0.84	0.09	82,82,82,82	0
54	MG	2a	1633	1/1	0.84	0.14	92,92,92,92	0
54	MG	2A	3385	1/1	0.84	0.19	73,73,73,73	0
54	MG	2A	3143	1/1	0.84	0.27	61,61,61,61	0
54	MG	1A	3308	1/1	0.84	0.18	40,40,40,40	0
54	MG	2A	3487	1/1	0.84	0.12	75,75,75,75	0
54	MG	2A	3330	1/1	0.84	0.26	82,82,82,82	0
54	MG	1A	3565	1/1	0.84	0.55	69,69,69,69	0
54	MG	1A	3672	1/1	0.84	0.30	78,78,78,78	0
54	MG	2B	207	1/1	0.84	0.78	99,99,99,99	0
54	MG	1a	1652	1/1	0.84	0.51	74,74,74,74	0
54	MG	2A	3627	1/1	0.84	0.10	55,55,55,55	0
54	MG	2A	3042	1/1	0.84	0.23	65,65,65,65	0
54	MG	1A	3746	1/1	0.84	0.17	55,55,55,55	0
54	MG	1A	3009	1/1	0.84	0.27	59,59,59,59	0
54	MG	1a	1666	1/1	0.84	0.50	78,78,78,78	0
54	MG	1A	3389	1/1	0.84	0.18	56,56,56,56	0
54	MG	2A	3609	1/1	0.84	0.20	80,80,80,80	0
54	MG	1a	1806	1/1	0.84	0.36	85,85,85,85	0
54	MG	2a	1639	1/1	0.84	0.26	124,124,124,124	0
54	MG	2A	3050	1/1	0.84	0.71	70,70,70,70	0
54	MG	1A	3478	1/1	0.84	0.21	50,50,50,50	0
54	MG	1A	3332	1/1	0.84	0.24	36,36,36,36	0
54	MG	2A	3063	1/1	0.84	0.28	52,52,52,52	0
54	MG	1A	3413	1/1	0.84	0.18	42,42,42,42	0
54	MG	1A	3704	1/1	0.84	0.32	61,61,61,61	0
54	MG	1a	1776	1/1	0.84	0.18	91,91,91,91	0
54	MG	1T	2002	1/1	0.84	0.36	54,54,54,54	0
54	MG	1A	3355	1/1	0.84	0.17	20,20,20,20	0
54	MG	1A	3317	1/1	0.84	0.29	76,76,76,76	0
54	MG	2A	3550	1/1	0.84	0.26	105,105,105,105	0
54	MG	1A	3446	1/1	0.84	0.12	60,60,60,60	0
54	MG	2A	3580	1/1	0.84	0.38	97,97,97,97	0
54	MG	1a	1673	1/1	0.84	0.15	59,59,59,59	0
54	MG	1A	3548	1/1	0.84	0.20	63,63,63,63	0
54	MG	1A	3662	1/1	0.84	0.18	43,43,43,43	0
54	MG	2A	3337	1/1	0.84	0.18	69,69,69,69	0
54	MG	2A	3454	1/1	0.84	0.41	66,66,66,66	0
54	MG	2a	1689	1/1	0.84	0.21	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2a	1698	1/1	0.84	0.18	95,95,95,95	0
54	MG	1A	3677	1/1	0.84	0.45	71,71,71,71	0
54	MG	1A	3740	1/1	0.84	0.18	47,47,47,47	0
54	MG	15	104	1/1	0.84	0.22	72,72,72,72	0
54	MG	1a	1630	1/1	0.84	0.21	54,54,54,54	0
54	MG	1A	3674	1/1	0.84	0.11	57,57,57,57	0
54	MG	2A	3424	1/1	0.84	0.16	88,88,88,88	0
54	MG	2A	3117	1/1	0.84	0.27	45,45,45,45	0
54	MG	1A	3479	1/1	0.84	0.15	70,70,70,70	0
54	MG	2l	201	1/1	0.84	0.31	89,89,89,89	0
54	MG	1a	1745	1/1	0.85	0.24	78,78,78,78	0
54	MG	2A	3044	1/1	0.85	0.20	71,71,71,71	0
54	MG	1a	1699	1/1	0.85	0.17	90,90,90,90	0
54	MG	1a	1632	1/1	0.85	0.41	59,59,59,59	0
54	MG	2A	3451	1/1	0.85	0.23	63,63,63,63	0
54	MG	1a	1710	1/1	0.85	0.20	56,56,56,56	0
54	MG	2a	1725	1/1	0.85	0.20	73,73,73,73	0
54	MG	1a	1619	1/1	0.85	0.19	102,102,102,102	0
54	MG	2A	3173	1/1	0.85	0.31	63,63,63,63	0
54	MG	2A	3353	1/1	0.85	0.18	42,42,42,42	0
54	MG	2a	1753	1/1	0.85	0.17	73,73,73,73	0
54	MG	1a	1627	1/1	0.85	0.12	72,72,72,72	0
54	MG	1A	3423	1/1	0.85	0.47	81,81,81,81	0
54	MG	1A	3651	1/1	0.85	0.25	53,53,53,53	0
54	MG	1a	1641	1/1	0.85	0.22	60,60,60,60	0
54	MG	1a	1713	1/1	0.85	0.09	92,92,92,92	0
54	MG	2A	3228	1/1	0.85	0.21	99,99,99,99	0
54	MG	2a	1667	1/1	0.85	0.54	79,79,79,79	0
54	MG	1A	3169	1/1	0.85	0.51	56,56,56,56	0
54	MG	2A	3155	1/1	0.85	0.33	59,59,59,59	0
54	MG	1a	1691	1/1	0.85	0.21	68,68,68,68	0
54	MG	2A	3473	1/1	0.85	0.06	104,104,104,104	0
54	MG	1A	3073	1/1	0.85	0.30	75,75,75,75	0
54	MG	2A	3577	1/1	0.85	0.10	54,54,54,54	0
54	MG	1A	3117	1/1	0.85	0.46	26,26,26,26	0
54	MG	1A	3175	1/1	0.85	0.54	51,51,51,51	0
54	MG	1A	3124	1/1	0.85	0.15	67,67,67,67	0
54	MG	1A	3051	1/1	0.85	0.14	77,77,77,77	0
54	MG	1a	1703	1/1	0.85	0.09	54,54,54,54	0
54	MG	2V	201	1/1	0.85	0.32	101,101,101,101	0
54	MG	2A	3115	1/1	0.85	0.13	73,73,73,73	0
53	MPD	2A	3001	8/8	0.85	0.30	54,73,76,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3666	1/1	0.85	0.26	43,43,43,43	0
54	MG	1a	1684	1/1	0.85	0.34	56,56,56,56	0
54	MG	1a	1653	1/1	0.85	0.19	55,55,55,55	0
54	MG	2A	3486	1/1	0.85	0.25	96,96,96,96	0
54	MG	1a	1796	1/1	0.85	0.24	81,81,81,81	0
54	MG	1A	3612	1/1	0.85	0.15	45,45,45,45	0
54	MG	2A	3344	1/1	0.85	0.10	55,55,55,55	0
54	MG	2A	3021	1/1	0.85	0.29	59,59,59,59	0
54	MG	2A	3542	1/1	0.85	0.15	90,90,90,90	0
54	MG	1A	3860	1/1	0.85	0.26	65,65,65,65	0
54	MG	1A	3605	1/1	0.85	0.38	71,71,71,71	0
54	MG	2B	210	1/1	0.85	0.16	84,84,84,84	0
54	MG	1A	3476	1/1	0.85	0.76	65,65,65,65	0
54	MG	2A	3364	1/1	0.85	0.10	55,55,55,55	0
54	MG	1A	3781	1/1	0.85	0.16	55,55,55,55	0
54	MG	1A	3690	1/1	0.85	0.60	51,51,51,51	0
54	MG	1A	3242	1/1	0.85	0.10	90,90,90,90	0
54	MG	2a	1606	1/1	0.85	0.28	57,57,57,57	0
54	MG	1A	3665	1/1	0.85	0.16	59,59,59,59	0
54	MG	2A	3196	1/1	0.85	0.47	58,58,58,58	0
54	MG	2A	3073	1/1	0.85	0.20	60,60,60,60	0
54	MG	2A	3483	1/1	0.85	0.15	53,53,53,53	0
54	MG	1a	1685	1/1	0.85	0.10	74,74,74,74	0
54	MG	2A	3076	1/1	0.85	0.31	76,76,76,76	0
54	MG	2A	3620	1/1	0.85	0.32	101,101,101,101	0
54	MG	2F	301	1/1	0.85	0.22	54,54,54,54	0
54	MG	1a	1847	1/1	0.85	0.20	62,62,62,62	0
54	MG	2A	3425	1/1	0.86	0.10	78,78,78,78	0
54	MG	1a	1791	1/1	0.86	0.14	70,70,70,70	0
54	MG	1P	204	1/1	0.86	0.16	50,50,50,50	0
54	MG	17	103	1/1	0.86	0.24	62,62,62,62	0
54	MG	2A	3570	1/1	0.86	0.22	69,69,69,69	0
54	MG	2a	1646	1/1	0.86	0.13	69,69,69,69	0
54	MG	2A	3032	1/1	0.86	0.21	61,61,61,61	0
54	MG	1A	3518	1/1	0.86	0.14	56,56,56,56	0
54	MG	1F	312	1/1	0.86	0.43	52,52,52,52	0
54	MG	1A	3172	1/1	0.86	0.20	71,71,71,71	0
54	MG	1A	3537	1/1	0.86	0.27	39,39,39,39	0
54	MG	1A	3374	1/1	0.86	0.14	73,73,73,73	0
54	MG	2A	3480	1/1	0.86	0.12	61,61,61,61	0
54	MG	2A	3029	1/1	0.86	0.19	48,48,48,48	0
54	MG	2A	3234	1/1	0.86	0.21	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3083	1/1	0.86	0.74	51,51,51,51	0
54	MG	1H	202	1/1	0.86	0.29	64,64,64,64	0
54	MG	1A	3771	1/1	0.86	0.08	48,48,48,48	0
54	MG	1A	3439	1/1	0.86	0.26	114,114,114,114	0
54	MG	1A	3324	1/1	0.86	0.14	57,57,57,57	0
54	MG	2A	3111	1/1	0.86	0.14	57,57,57,57	0
54	MG	1A	3805	1/1	0.86	0.30	49,49,49,49	0
54	MG	1a	1771	1/1	0.86	0.36	89,89,89,89	0
54	MG	2A	3450	1/1	0.86	0.30	49,49,49,49	0
54	MG	2A	3078	1/1	0.86	0.64	58,58,58,58	0
54	MG	2A	3275	1/1	0.86	0.17	75,75,75,75	0
54	MG	1A	3286	1/1	0.86	0.18	32,32,32,32	0
54	MG	2A	3508	1/1	0.86	0.23	64,64,64,64	0
54	MG	2A	3529	1/1	0.86	0.17	73,73,73,73	0
54	MG	1A	3822	1/1	0.86	0.09	65,65,65,65	0
54	MG	2A	3351	1/1	0.86	0.17	74,74,74,74	0
54	MG	2A	3363	1/1	0.86	0.48	76,76,76,76	0
54	MG	1A	3422	1/1	0.86	0.11	45,45,45,45	0
54	MG	1A	3108	1/1	0.86	0.36	57,57,57,57	0
54	MG	1A	3331	1/1	0.86	0.15	40,40,40,40	0
54	MG	1A	3465	1/1	0.86	0.26	46,46,46,46	0
54	MG	1A	3614	1/1	0.86	0.27	57,57,57,57	0
54	MG	2A	3258	1/1	0.86	0.14	58,58,58,58	0
54	MG	2A	3008	1/1	0.86	0.42	61,61,61,61	0
54	MG	1A	3524	1/1	0.86	0.19	59,59,59,59	0
54	MG	1A	3420	1/1	0.86	0.17	35,35,35,35	0
54	MG	2A	3395	1/1	0.86	0.21	97,97,97,97	0
54	MG	1a	1664	1/1	0.86	0.30	80,80,80,80	0
54	MG	2A	3579	1/1	0.86	0.10	52,52,52,52	0
54	MG	1A	3129	1/1	0.86	0.54	42,42,42,42	0
54	MG	2e	201	1/1	0.86	0.18	85,85,85,85	0
54	MG	2A	3206	1/1	0.86	0.24	67,67,67,67	0
54	MG	1A	3010	1/1	0.86	0.29	46,46,46,46	0
54	MG	1A	3301	1/1	0.86	0.13	51,51,51,51	0
54	MG	1A	3445	1/1	0.86	0.31	43,43,43,43	0
54	MG	1A	3217	1/1	0.86	0.36	48,48,48,48	0
54	MG	2a	1629	1/1	0.86	0.42	110,110,110,110	0
54	MG	2a	1603	1/1	0.86	0.41	58,58,58,58	0
54	MG	1a	1605	1/1	0.86	0.31	96,96,96,96	0
54	MG	2a	1625	1/1	0.86	0.39	94,94,94,94	0
54	MG	1A	3713	1/1	0.86	0.26	60,60,60,60	0
54	MG	1A	3118	1/1	0.86	0.29	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	19	101	1/1	0.86	0.27	42,42,42,42	0
54	MG	1A	3396	1/1	0.86	0.26	25,25,25,25	0
54	MG	2A	3184	1/1	0.86	0.21	56,56,56,56	0
54	MG	1a	1763	1/1	0.86	0.21	96,96,96,96	0
54	MG	11	103	1/1	0.86	0.70	48,48,48,48	0
54	MG	1A	3780	1/1	0.86	0.12	57,57,57,57	0
54	MG	1A	3821	1/1	0.86	0.24	51,51,51,51	0
54	MG	2A	3163	1/1	0.86	0.12	67,67,67,67	0
54	MG	2A	3583	1/1	0.86	0.09	96,96,96,96	0
54	MG	1A	3183	1/1	0.86	0.13	28,28,28,28	0
54	MG	2a	1635	1/1	0.86	0.16	78,78,78,78	0
54	MG	2A	3279	1/1	0.86	0.13	74,74,74,74	0
54	MG	2A	3264	1/1	0.86	0.14	98,98,98,98	0
56	ZN	24	101	1/1	0.87	0.06	154,154,154,154	0
54	MG	1A	3714	1/1	0.87	0.19	44,44,44,44	0
54	MG	2A	3104	1/1	0.87	0.21	67,67,67,67	0
54	MG	2A	3331	1/1	0.87	0.10	98,98,98,98	0
54	MG	2A	3288	1/1	0.87	0.16	39,39,39,39	0
54	MG	1A	3137	1/1	0.87	0.30	74,74,74,74	0
54	MG	2a	1632	1/1	0.87	0.21	63,63,63,63	0
54	MG	2B	208	1/1	0.87	0.49	79,79,79,79	0
54	MG	2A	3017	1/1	0.87	0.48	76,76,76,76	0
54	MG	2a	1748	1/1	0.87	0.15	100,100,100,100	0
54	MG	1A	3357	1/1	0.87	0.17	26,26,26,26	0
54	MG	1A	3103	1/1	0.87	0.18	25,25,25,25	0
54	MG	2A	3011	1/1	0.87	0.46	44,44,44,44	0
54	MG	1A	3687	1/1	0.87	0.08	66,66,66,66	0
54	MG	1A	3079	1/1	0.87	0.32	38,38,38,38	0
54	MG	1A	3024	1/1	0.87	0.12	71,71,71,71	0
54	MG	1A	3471	1/1	0.87	0.15	62,62,62,62	0
54	MG	2A	3588	1/1	0.87	0.08	93,93,93,93	0
54	MG	2A	3567	1/1	0.87	0.07	63,63,63,63	0
54	MG	2a	1640	1/1	0.87	0.32	100,100,100,100	0
54	MG	1B	1028	1/1	0.87	0.21	75,75,75,75	0
54	MG	1A	3038	1/1	0.87	0.09	53,53,53,53	0
54	MG	1a	1795	1/1	0.87	0.13	81,81,81,81	0
54	MG	2A	3642	1/1	0.87	0.39	87,87,87,87	0
54	MG	1a	1696	1/1	0.87	0.18	80,80,80,80	0
54	MG	2A	3023	1/1	0.87	0.25	50,50,50,50	0
54	MG	1a	1828	1/1	0.87	0.21	116,116,116,116	0
54	MG	2A	3328	1/1	0.87	0.19	78,78,78,78	0
54	MG	2A	3067	1/1	0.87	0.44	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3707	1/1	0.87	0.38	91,91,91,91	0
54	MG	2A	3295	1/1	0.87	0.29	84,84,84,84	0
54	MG	1B	1012	1/1	0.87	0.08	79,79,79,79	0
54	MG	2a	1652	1/1	0.87	0.25	88,88,88,88	0
54	MG	2A	3423	1/1	0.87	0.16	94,94,94,94	0
54	MG	1A	3549	1/1	0.87	0.29	59,59,59,59	0
54	MG	1A	3360	1/1	0.87	0.11	30,30,30,30	0
54	MG	1A	3425	1/1	0.87	0.16	36,36,36,36	0
54	MG	1A	3541	1/1	0.87	0.20	66,66,66,66	0
54	MG	1A	3091	1/1	0.87	0.23	57,57,57,57	0
54	MG	1A	3538	1/1	0.87	0.18	37,37,37,37	0
54	MG	1A	3036	1/1	0.87	0.14	56,56,56,56	0
54	MG	1A	3239	1/1	0.87	0.23	50,50,50,50	0
54	MG	1A	3766	1/1	0.87	0.06	69,69,69,69	0
54	MG	1A	3596	1/1	0.87	0.10	64,64,64,64	0
54	MG	2A	3297	1/1	0.87	0.17	66,66,66,66	0
54	MG	1A	3621	1/1	0.87	0.20	67,67,67,67	0
54	MG	2A	3445	1/1	0.87	0.25	68,68,68,68	0
54	MG	2a	1642	1/1	0.87	0.42	61,61,61,61	0
54	MG	2a	1679	1/1	0.87	0.12	68,68,68,68	0
54	MG	2A	3010	1/1	0.87	0.44	62,62,62,62	0
54	MG	1A	3532	1/1	0.87	0.39	46,46,46,46	0
54	MG	1a	1783	1/1	0.87	0.24	64,64,64,64	0
54	MG	1D	309	1/1	0.87	0.33	71,71,71,71	0
54	MG	1A	3221	1/1	0.87	0.11	100,100,100,100	0
54	MG	1A	3851	1/1	0.87	0.31	75,75,75,75	0
54	MG	1a	1671	1/1	0.87	0.65	71,71,71,71	0
54	MG	1a	1731	1/1	0.87	0.09	73,73,73,73	0
54	MG	2A	3004	1/1	0.87	0.21	65,65,65,65	0
54	MG	2a	1743	1/1	0.87	0.11	84,84,84,84	0
54	MG	2A	3407	1/1	0.87	0.12	66,66,66,66	0
54	MG	2G	203	1/1	0.87	0.10	104,104,104,104	0
54	MG	1A	3750	1/1	0.87	0.15	84,84,84,84	0
54	MG	2A	3589	1/1	0.87	0.14	67,67,67,67	0
54	MG	1A	3144	1/1	0.87	0.20	56,56,56,56	0
54	MG	1A	3776	1/1	0.87	0.14	40,40,40,40	0
54	MG	1E	304	1/1	0.87	0.70	80,80,80,80	0
54	MG	1A	3075	1/1	0.88	0.63	48,48,48,48	0
54	MG	2a	1750	1/1	0.88	0.21	79,79,79,79	0
54	MG	2A	3592	1/1	0.88	0.10	63,63,63,63	0
54	MG	2A	3178	1/1	0.88	0.50	44,44,44,44	0
54	MG	1B	1023	1/1	0.88	0.17	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3152	1/1	0.88	0.20	71,71,71,71	0
54	MG	2A	3478	1/1	0.88	0.15	85,85,85,85	0
54	MG	2a	1726	1/1	0.88	0.07	83,83,83,83	0
54	MG	2Y	201	1/1	0.88	0.10	66,66,66,66	0
54	MG	1a	1637	1/1	0.88	1.17	79,79,79,79	0
54	MG	2A	3492	1/1	0.88	0.17	51,51,51,51	0
54	MG	2A	3107	1/1	0.88	0.42	85,85,85,85	0
54	MG	2A	3049	1/1	0.88	0.15	65,65,65,65	0
54	MG	2A	3509	1/1	0.88	0.10	65,65,65,65	0
54	MG	2A	3605	1/1	0.88	0.21	65,65,65,65	0
54	MG	1A	3449	1/1	0.88	0.29	72,72,72,72	0
54	MG	1A	3759	1/1	0.88	0.21	51,51,51,51	0
54	MG	1d	504	1/1	0.88	0.27	70,70,70,70	0
54	MG	2a	1744	1/1	0.88	0.06	73,73,73,73	0
54	MG	1a	1849	1/1	0.88	0.15	62,62,62,62	0
54	MG	2A	3383	1/1	0.88	0.07	81,81,81,81	0
54	MG	2A	3471	1/1	0.88	0.26	58,58,58,58	0
54	MG	1A	3316	1/1	0.88	0.23	99,99,99,99	0
54	MG	2A	3461	1/1	0.88	0.24	87,87,87,87	0
54	MG	2a	1722	1/1	0.88	0.06	109,109,109,109	0
54	MG	1A	3395	1/1	0.88	0.30	57,57,57,57	0
54	MG	1a	1781	1/1	0.88	0.12	83,83,83,83	0
54	MG	2A	3350	1/1	0.88	0.15	43,43,43,43	0
54	MG	2A	3120	1/1	0.88	0.32	82,82,82,82	0
54	MG	2A	3521	1/1	0.88	0.15	88,88,88,88	0
54	MG	2A	3474	1/1	0.88	0.11	84,84,84,84	0
54	MG	1A	3006	1/1	0.88	0.13	49,49,49,49	0
54	MG	2A	3144	1/1	0.88	0.26	46,46,46,46	0
54	MG	1a	1623	1/1	0.88	0.26	62,62,62,62	0
54	MG	2A	3186	1/1	0.88	0.26	65,65,65,65	0
54	MG	1A	3432	1/1	0.88	0.12	53,53,53,53	0
54	MG	2A	3396	1/1	0.88	0.14	82,82,82,82	0
54	MG	2A	3006	1/1	0.88	0.28	64,64,64,64	0
54	MG	2A	3091	1/1	0.88	0.37	67,67,67,67	0
54	MG	2A	3386	1/1	0.88	0.27	86,86,86,86	0
54	MG	1A	3007	1/1	0.88	0.26	35,35,35,35	0
54	MG	2A	3490	1/1	0.88	0.14	64,64,64,64	0
54	MG	1A	3048	1/1	0.88	0.26	60,60,60,60	0
54	MG	2A	3524	1/1	0.88	0.21	47,47,47,47	0
54	MG	1a	1613	1/1	0.88	0.12	69,69,69,69	0
54	MG	1A	3624	1/1	0.88	0.18	70,70,70,70	0
54	MG	2A	3124	1/1	0.88	0.27	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3745	1/1	0.88	0.26	80,80,80,80	0
54	MG	2A	3531	1/1	0.88	0.48	74,74,74,74	0
54	MG	1A	3681	1/1	0.88	0.13	99,99,99,99	0
54	MG	2a	1627	1/1	0.88	0.20	69,69,69,69	0
54	MG	1a	1651	1/1	0.88	0.11	54,54,54,54	0
54	MG	1A	3554	1/1	0.88	0.18	70,70,70,70	0
54	MG	2A	3287	1/1	0.88	0.14	53,53,53,53	0
54	MG	2A	3420	1/1	0.88	0.18	51,51,51,51	0
54	MG	1a	1832	1/1	0.88	0.13	90,90,90,90	0
54	MG	1A	3823	1/1	0.88	0.12	82,82,82,82	0
54	MG	1A	3587	1/1	0.88	0.09	64,64,64,64	0
54	MG	1A	3417	1/1	0.88	0.16	34,34,34,34	0
54	MG	2A	3593	1/1	0.88	0.07	99,99,99,99	0
54	MG	2A	3274	1/1	0.88	0.17	45,45,45,45	0
54	MG	1A	3640	1/1	0.88	0.13	48,48,48,48	0
54	MG	1A	3864	1/1	0.88	0.16	50,50,50,50	0
54	MG	1A	3874	1/1	0.88	0.21	65,65,65,65	0
54	MG	1V	201	1/1	0.88	0.31	56,56,56,56	0
54	MG	1a	1774	1/1	0.88	0.17	103,103,103,103	0
54	MG	1a	1740	1/1	0.88	0.32	77,77,77,77	0
54	MG	1A	3836	1/1	0.88	0.15	35,35,35,35	0
54	MG	2A	3568	1/1	0.88	0.09	78,78,78,78	0
54	MG	2A	3554	1/1	0.88	0.12	72,72,72,72	0
54	MG	2A	3263	1/1	0.88	0.16	85,85,85,85	0
54	MG	2A	3520	1/1	0.88	0.28	91,91,91,91	0
54	MG	1a	1701	1/1	0.88	0.24	93,93,93,93	0
54	MG	1A	3299	1/1	0.88	0.40	58,58,58,58	0
54	MG	1A	3526	1/1	0.88	0.23	83,83,83,83	0
54	MG	1A	3544	1/1	0.88	0.19	69,69,69,69	0
54	MG	1A	3517	1/1	0.88	0.33	71,71,71,71	0
54	MG	2A	3109	1/1	0.88	0.61	57,57,57,57	0
54	MG	2A	3141	1/1	0.88	0.34	78,78,78,78	0
54	MG	1A	3359	1/1	0.88	0.20	38,38,38,38	0
54	MG	2B	216	1/1	0.89	0.10	106,106,106,106	0
54	MG	1A	3885	1/1	0.89	0.22	53,53,53,53	0
54	MG	2T	202	1/1	0.89	0.32	65,65,65,65	0
54	MG	1F	313	1/1	0.89	0.19	64,64,64,64	0
54	MG	2A	3280	1/1	0.89	0.14	53,53,53,53	0
54	MG	1A	3341	1/1	0.89	0.19	30,30,30,30	0
54	MG	1a	1746	1/1	0.89	0.29	91,91,91,91	0
54	MG	1A	3825	1/1	0.89	0.40	72,72,72,72	0
54	MG	1A	3412	1/1	0.89	0.14	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3758	1/1	0.89	0.20	84,84,84,84	0
54	MG	1N	203	1/1	0.89	0.45	88,88,88,88	0
54	MG	1d	503	1/1	0.89	0.28	85,85,85,85	0
54	MG	1A	3416	1/1	0.89	0.26	41,41,41,41	0
54	MG	1A	3268	1/1	0.89	0.14	42,42,42,42	0
54	MG	1D	304	1/1	0.89	0.31	47,47,47,47	0
54	MG	2A	3060	1/1	0.89	0.18	66,66,66,66	0
54	MG	1a	1693	1/1	0.89	0.31	68,68,68,68	0
54	MG	1a	1780	1/1	0.89	0.35	83,83,83,83	0
54	MG	2A	3409	1/1	0.89	0.16	45,45,45,45	0
54	MG	2A	3309	1/1	0.89	0.18	94,94,94,94	0
54	MG	1a	1628	1/1	0.89	0.15	67,67,67,67	0
54	MG	1A	3058	1/1	0.89	0.22	51,51,51,51	0
54	MG	2A	3157	1/1	0.89	0.20	56,56,56,56	0
54	MG	2A	3415	1/1	0.89	0.15	59,59,59,59	0
54	MG	2A	3203	1/1	0.89	0.42	66,66,66,66	0
54	MG	2A	3059	1/1	0.89	0.19	54,54,54,54	0
54	MG	2a	1609	1/1	0.89	0.20	62,62,62,62	0
54	MG	2A	3598	1/1	0.89	0.20	64,64,64,64	0
54	MG	13	102	1/1	0.89	0.26	55,55,55,55	0
54	MG	1y	202	1/1	0.89	0.29	98,98,98,98	0
54	MG	1A	3497	1/1	0.89	0.25	44,44,44,44	0
54	MG	1A	3782	1/1	0.89	0.13	35,35,35,35	0
54	MG	1A	3896	1/1	0.89	0.48	51,51,51,51	0
54	MG	2a	1763	1/1	0.89	0.13	96,96,96,96	0
54	MG	1A	3831	1/1	0.89	0.42	92,92,92,92	0
54	MG	2A	3064	1/1	0.89	0.52	77,77,77,77	0
54	MG	1A	3747	1/1	0.89	0.12	54,54,54,54	0
54	MG	1a	1611	1/1	0.89	0.16	90,90,90,90	0
54	MG	1A	3131	1/1	0.89	0.18	39,39,39,39	0
54	MG	1A	3602	1/1	0.89	0.68	54,54,54,54	0
54	MG	2A	3494	1/1	0.89	0.08	71,71,71,71	0
54	MG	1A	3777	1/1	0.89	0.28	35,35,35,35	0
54	MG	2A	3069	1/1	0.89	0.16	60,60,60,60	0
54	MG	2A	3281	1/1	0.89	0.16	65,65,65,65	0
54	MG	1A	3386	1/1	0.89	0.17	67,67,67,67	0
54	MG	2A	3440	1/1	0.89	0.55	76,76,76,76	0
54	MG	2A	3220	1/1	0.89	0.26	70,70,70,70	0
54	MG	2A	3253	1/1	0.89	0.18	51,51,51,51	0
54	MG	1a	1645	1/1	0.89	0.60	73,73,73,73	0
54	MG	1A	3790	1/1	0.89	0.18	34,34,34,34	0
54	MG	1A	3270	1/1	0.89	0.48	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2I	201	1/1	0.89	0.17	87,87,87,87	0
54	MG	1A	3573	1/1	0.89	0.18	30,30,30,30	0
54	MG	2A	3278	1/1	0.89	0.22	65,65,65,65	0
54	MG	1D	307	1/1	0.89	0.26	36,36,36,36	0
54	MG	1A	3244	1/1	0.89	0.23	87,87,87,87	0
54	MG	1A	3859	1/1	0.89	0.41	74,74,74,74	0
54	MG	1A	3372	1/1	0.89	0.25	59,59,59,59	0
54	MG	1W	203	1/1	0.89	0.21	45,45,45,45	0
54	MG	1A	3474	1/1	0.89	0.15	56,56,56,56	0
54	MG	2f	201	1/1	0.89	0.15	79,79,79,79	0
54	MG	2A	3046	1/1	0.89	0.25	69,69,69,69	0
54	MG	1A	3699	1/1	0.89	0.15	39,39,39,39	0
54	MG	1A	3382	1/1	0.89	0.16	63,63,63,63	0
54	MG	1A	3113	1/1	0.89	0.22	54,54,54,54	0
54	MG	1A	3676	1/1	0.89	0.38	77,77,77,77	0
54	MG	1a	1751	1/1	0.89	0.19	80,80,80,80	0
54	MG	1A	3231	1/1	0.89	0.22	55,55,55,55	0
54	MG	1a	1747	1/1	0.89	0.38	109,109,109,109	0
54	MG	1A	3702	1/1	0.89	0.25	71,71,71,71	0
54	MG	1A	3482	1/1	0.89	0.17	52,52,52,52	0
54	MG	1A	3218	1/1	0.89	0.16	50,50,50,50	0
54	MG	2A	3052	1/1	0.89	0.33	75,75,75,75	0
54	MG	2a	1628	1/1	0.89	0.24	94,94,94,94	0
54	MG	2a	1739	1/1	0.89	0.15	98,98,98,98	0
54	MG	1B	1004	1/1	0.89	0.13	60,60,60,60	0
54	MG	2a	1624	1/1	0.89	0.25	55,55,55,55	0
54	MG	2A	3339	1/1	0.89	0.12	68,68,68,68	0
54	MG	2A	3347	1/1	0.89	0.13	45,45,45,45	0
54	MG	2a	1721	1/1	0.89	0.11	86,86,86,86	0
54	MG	1A	3350	1/1	0.89	0.14	55,55,55,55	0
54	MG	2A	3354	1/1	0.89	0.34	92,92,92,92	0
54	MG	1B	1029	1/1	0.89	0.17	80,80,80,80	0
54	MG	1A	3098	1/1	0.89	0.36	44,44,44,44	0
54	MG	2a	1685	1/1	0.89	0.59	71,71,71,71	0
54	MG	1A	3126	1/1	0.89	0.23	42,42,42,42	0
54	MG	1T	2004	1/1	0.89	0.31	69,69,69,69	0
54	MG	1A	3177	1/1	0.89	0.27	49,49,49,49	0
54	MG	2a	1650	1/1	0.89	0.29	59,59,59,59	0
54	MG	1a	1616	1/1	0.89	0.20	106,106,106,106	0
54	MG	2G	202	1/1	0.89	0.15	108,108,108,108	0
54	MG	2a	1649	1/1	0.89	0.14	40,40,40,40	0
54	MG	1A	3520	1/1	0.89	0.14	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3131	1/1	0.89	0.31	64,64,64,64	0
54	MG	1A	3180	1/1	0.89	0.25	37,37,37,37	0
54	MG	1A	3711	1/1	0.89	0.05	72,72,72,72	0
54	MG	1A	3534	1/1	0.89	0.39	57,57,57,57	0
54	MG	1A	3130	1/1	0.89	0.32	39,39,39,39	0
54	MG	1A	3012	1/1	0.89	0.21	58,58,58,58	0
54	MG	1a	1824	1/1	0.89	0.27	82,82,82,82	0
54	MG	2A	3536	1/1	0.89	0.53	71,71,71,71	0
54	MG	2A	3199	1/1	0.90	0.34	64,64,64,64	0
54	MG	2A	3416	1/1	0.90	0.09	48,48,48,48	0
54	MG	1a	1625	1/1	0.90	0.44	54,54,54,54	0
54	MG	1A	3659	1/1	0.90	0.47	62,62,62,62	0
54	MG	1a	1659	1/1	0.90	0.12	70,70,70,70	0
54	MG	1f	201	1/1	0.90	0.21	68,68,68,68	0
54	MG	2a	1620	1/1	0.90	0.27	60,60,60,60	0
54	MG	1A	3229	1/1	0.90	0.43	38,38,38,38	0
54	MG	1A	3558	1/1	0.90	0.48	81,81,81,81	0
54	MG	1A	3888	1/1	0.90	0.47	80,80,80,80	0
54	MG	2a	1761	1/1	0.90	0.20	90,90,90,90	0
54	MG	2A	3443	1/1	0.90	0.14	111,111,111,111	0
54	MG	2A	3068	1/1	0.90	0.31	51,51,51,51	0
54	MG	1A	3881	1/1	0.90	0.29	38,38,38,38	0
54	MG	2A	3122	1/1	0.90	0.25	74,74,74,74	0
54	MG	2a	1618	1/1	0.90	0.18	97,97,97,97	0
54	MG	1A	3826	1/1	0.90	0.04	90,90,90,90	0
54	MG	2a	1622	1/1	0.90	0.15	38,38,38,38	0
54	MG	1A	3089	1/1	0.90	0.42	45,45,45,45	0
54	MG	2A	3212	1/1	0.90	0.21	58,58,58,58	0
54	MG	2A	3484	1/1	0.90	0.15	64,64,64,64	0
54	MG	2A	3578	1/1	0.90	0.15	52,52,52,52	0
54	MG	2A	3515	1/1	0.90	0.14	45,45,45,45	0
54	MG	2A	3314	1/1	0.90	0.08	81,81,81,81	0
54	MG	1a	1676	1/1	0.90	0.35	85,85,85,85	0
54	MG	1A	3366	1/1	0.90	0.15	45,45,45,45	0
54	MG	1A	3298	1/1	0.90	0.08	55,55,55,55	0
54	MG	2B	212	1/1	0.90	0.16	111,111,111,111	0
54	MG	1A	3178	1/1	0.90	0.25	50,50,50,50	0
54	MG	1A	3626	1/1	0.90	0.25	58,58,58,58	0
54	MG	1a	1629	1/1	0.90	0.47	68,68,68,68	0
54	MG	1a	1841	1/1	0.90	0.32	72,72,72,72	0
54	MG	1a	1686	1/1	0.90	0.41	88,88,88,88	0
54	MG	2A	3507	1/1	0.90	0.10	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2a	1634	1/1	0.90	0.29	101,101,101,101	0
54	MG	1A	3734	1/1	0.90	0.11	82,82,82,82	0
54	MG	1l	202	1/1	0.90	0.14	51,51,51,51	0
54	MG	1a	1809	1/1	0.90	0.13	87,87,87,87	0
54	MG	1B	1015	1/1	0.90	0.16	79,79,79,79	0
54	MG	1A	3347	1/1	0.90	0.14	82,82,82,82	0
54	MG	2A	3457	1/1	0.90	0.12	79,79,79,79	0
54	MG	2A	3398	1/1	0.90	0.05	78,78,78,78	0
54	MG	1A	3604	1/1	0.90	0.78	55,55,55,55	0
54	MG	2A	3161	1/1	0.90	0.32	59,59,59,59	0
54	MG	2A	3421	1/1	0.90	0.17	68,68,68,68	0
54	MG	1B	1026	1/1	0.90	0.21	94,94,94,94	0
54	MG	2a	1674	1/1	0.90	0.28	66,66,66,66	0
54	MG	2A	3419	1/1	0.90	0.33	55,55,55,55	0
54	MG	2A	3150	1/1	0.90	0.12	135,135,135,135	0
54	MG	2a	1760	1/1	0.90	0.12	102,102,102,102	0
54	MG	2A	3261	1/1	0.90	0.44	74,74,74,74	0
54	MG	1a	1689	1/1	0.90	0.34	61,61,61,61	0
54	MG	2A	3041	1/1	0.90	0.17	81,81,81,81	0
54	MG	1B	1022	1/1	0.90	0.13	59,59,59,59	0
54	MG	2a	1687	1/1	0.90	0.16	70,70,70,70	0
54	MG	2A	3170	1/1	0.90	0.46	55,55,55,55	0
54	MG	1A	3194	1/1	0.90	0.34	50,50,50,50	0
54	MG	1a	1718	1/1	0.90	0.20	86,86,86,86	0
54	MG	1A	3654	1/1	0.90	0.07	59,59,59,59	0
54	MG	1A	3866	1/1	0.90	0.13	102,102,102,102	0
54	MG	1A	3102	1/1	0.90	0.21	42,42,42,42	0
54	MG	1A	3224	1/1	0.90	0.27	45,45,45,45	0
54	MG	2a	1623	1/1	0.90	0.20	60,60,60,60	0
54	MG	1a	1667	1/1	0.90	0.24	85,85,85,85	0
54	MG	2A	3056	1/1	0.90	0.25	31,31,31,31	0
54	MG	2A	3391	1/1	0.90	0.19	65,65,65,65	0
54	MG	1A	3052	1/1	0.90	0.09	85,85,85,85	0
54	MG	2a	1665	1/1	0.90	0.19	37,37,37,37	0
54	MG	1A	3245	1/1	0.90	0.19	56,56,56,56	0
54	MG	1A	3664	1/1	0.90	0.16	32,32,32,32	0
54	MG	1a	1643	1/1	0.90	0.22	87,87,87,87	0
54	MG	1A	3817	1/1	0.90	0.09	32,32,32,32	0
54	MG	1A	3574	1/1	0.90	0.10	69,69,69,69	0
54	MG	1a	1706	1/1	0.90	0.07	72,72,72,72	0
54	MG	1A	3252	1/1	0.90	0.17	45,45,45,45	0
54	MG	2E	302	1/1	0.90	0.48	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3012	1/1	0.90	0.23	73,73,73,73	0
54	MG	1A	3556	1/1	0.90	0.15	53,53,53,53	0
54	MG	1a	1788	1/1	0.90	0.17	106,106,106,106	0
54	MG	2A	3429	1/1	0.90	0.09	81,81,81,81	0
54	MG	1A	3789	1/1	0.90	0.07	58,58,58,58	0
54	MG	1a	1727	1/1	0.90	0.15	67,67,67,67	0
54	MG	2A	3527	1/1	0.90	0.21	55,55,55,55	0
54	MG	1a	1793	1/1	0.90	0.17	89,89,89,89	0
54	MG	1A	3160	1/1	0.90	0.44	37,37,37,37	0
54	MG	1A	3385	1/1	0.90	0.20	70,70,70,70	0
54	MG	1A	3675	1/1	0.90	0.20	53,53,53,53	0
54	MG	2a	1696	1/1	0.90	0.10	82,82,82,82	0
54	MG	1A	3292	1/1	0.90	0.08	45,45,45,45	0
54	MG	1a	1838	1/1	0.90	0.12	90,90,90,90	0
54	MG	1a	1851	1/1	0.90	0.24	76,76,76,76	0
54	MG	1A	3450	1/1	0.90	0.17	61,61,61,61	0
54	MG	2A	3375	1/1	0.90	0.11	50,50,50,50	0
54	MG	2A	3603	1/1	0.90	0.15	78,78,78,78	0
54	MG	1A	3205	1/1	0.90	0.18	58,58,58,58	0
54	MG	1a	1672	1/1	0.90	0.26	85,85,85,85	0
54	MG	1a	1660	1/1	0.90	0.23	85,85,85,85	0
54	MG	1a	1621	1/1	0.90	0.19	59,59,59,59	0
54	MG	1A	3282	1/1	0.90	0.16	64,64,64,64	0
54	MG	1a	1775	1/1	0.90	0.13	98,98,98,98	0
54	MG	2W	202	1/1	0.90	0.18	79,79,79,79	0
54	MG	2A	3602	1/1	0.90	0.21	99,99,99,99	0
54	MG	2A	3563	1/1	0.91	0.15	67,67,67,67	0
54	MG	1W	202	1/1	0.91	0.14	59,59,59,59	0
54	MG	1A	3695	1/1	0.91	0.10	57,57,57,57	0
54	MG	2A	3341	1/1	0.91	0.20	83,83,83,83	0
54	MG	2A	3458	1/1	0.91	0.33	59,59,59,59	0
54	MG	2a	1614	1/1	0.91	0.14	82,82,82,82	0
54	MG	2a	1704	1/1	0.91	0.19	84,84,84,84	0
54	MG	1a	1786	1/1	0.91	0.09	82,82,82,82	0
54	MG	1A	3581	1/1	0.91	0.12	66,66,66,66	0
54	MG	2A	3133	1/1	0.91	0.26	66,66,66,66	0
54	MG	2A	3369	1/1	0.91	0.22	53,53,53,53	0
54	MG	1A	3773	1/1	0.91	0.21	79,79,79,79	0
54	MG	1A	3311	1/1	0.91	0.17	74,74,74,74	0
54	MG	1A	3340	1/1	0.91	0.15	31,31,31,31	0
54	MG	1A	3709	1/1	0.91	0.17	58,58,58,58	0
54	MG	2A	3248	1/1	0.91	0.31	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3114	1/1	0.91	0.17	40,40,40,40	0
54	MG	1Z	301	1/1	0.91	0.12	51,51,51,51	0
54	MG	1a	1606	1/1	0.91	0.12	64,64,64,64	0
54	MG	2A	3449	1/1	0.91	0.20	65,65,65,65	0
54	MG	1A	3799	1/1	0.91	0.44	53,53,53,53	0
54	MG	1a	1837	1/1	0.91	0.07	64,64,64,64	0
54	MG	2A	3284	1/1	0.91	0.10	43,43,43,43	0
54	MG	2A	3544	1/1	0.91	0.12	86,86,86,86	0
54	MG	1A	3491	1/1	0.91	0.06	66,66,66,66	0
54	MG	1A	3539	1/1	0.91	0.11	26,26,26,26	0
54	MG	1a	1818	1/1	0.91	0.16	56,56,56,56	0
54	MG	1A	3451	1/1	0.91	0.32	72,72,72,72	0
54	MG	1A	3728	1/1	0.91	0.28	60,60,60,60	0
54	MG	1A	3457	1/1	0.91	0.12	46,46,46,46	0
54	MG	1a	1726	1/1	0.91	0.31	61,61,61,61	0
54	MG	2A	3257	1/1	0.91	0.10	89,89,89,89	0
54	MG	1A	3321	1/1	0.91	0.24	61,61,61,61	0
54	MG	1A	3867	1/1	0.91	0.35	46,46,46,46	0
54	MG	1A	3444	1/1	0.91	0.12	34,34,34,34	0
54	MG	2A	3459	1/1	0.91	0.14	64,64,64,64	0
54	MG	1A	3803	1/1	0.91	0.10	70,70,70,70	0
54	MG	2A	3336	1/1	0.91	0.23	92,92,92,92	0
54	MG	2A	3035	1/1	0.91	0.11	68,68,68,68	0
54	MG	1a	1829	1/1	0.91	0.15	76,76,76,76	0
54	MG	2a	1662	1/1	0.91	0.17	64,64,64,64	0
54	MG	1A	3528	1/1	0.91	0.12	66,66,66,66	0
54	MG	1A	3797	1/1	0.91	0.12	82,82,82,82	0
54	MG	1W	204	1/1	0.91	0.29	52,52,52,52	0
54	MG	1A	3057	1/1	0.91	0.21	56,56,56,56	0
54	MG	2A	3108	1/1	0.91	0.10	50,50,50,50	0
54	MG	2a	1713	1/1	0.91	0.11	85,85,85,85	0
54	MG	2A	3048	1/1	0.91	0.09	80,80,80,80	0
54	MG	2A	3211	1/1	0.91	0.45	69,69,69,69	0
54	MG	1B	1010	1/1	0.91	0.37	58,58,58,58	0
54	MG	1A	3021	1/1	0.91	0.20	60,60,60,60	0
54	MG	1B	1024	1/1	0.91	0.09	61,61,61,61	0
54	MG	1A	3150	1/1	0.91	0.25	41,41,41,41	0
54	MG	2A	3300	1/1	0.91	0.13	51,51,51,51	0
54	MG	1A	3469	1/1	0.91	0.14	73,73,73,73	0
54	MG	1A	3658	1/1	0.91	0.11	69,69,69,69	0
54	MG	2F	302	1/1	0.91	0.29	69,69,69,69	0
54	MG	2A	3367	1/1	0.91	0.08	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3246	1/1	0.91	0.43	88,88,88,88	0
54	MG	1A	3133	1/1	0.91	0.14	49,49,49,49	0
54	MG	1A	3424	1/1	0.91	0.19	38,38,38,38	0
54	MG	1A	3069	1/1	0.91	0.23	39,39,39,39	0
54	MG	1A	3495	1/1	0.91	0.25	65,65,65,65	0
54	MG	2A	3057	1/1	0.91	0.16	55,55,55,55	0
54	MG	1A	3062	1/1	0.91	0.54	41,41,41,41	0
54	MG	1A	3433	1/1	0.91	0.11	66,66,66,66	0
54	MG	1A	3258	1/1	0.91	0.17	81,81,81,81	0
54	MG	2A	3585	1/1	0.91	0.16	81,81,81,81	0
54	MG	2A	3460	1/1	0.91	0.08	73,73,73,73	0
54	MG	1A	3289	1/1	0.91	0.09	47,47,47,47	0
54	MG	1e	201	1/1	0.91	0.17	66,66,66,66	0
54	MG	1A	3056	1/1	0.91	0.28	42,42,42,42	0
54	MG	2a	1637	1/1	0.91	0.26	65,65,65,65	0
54	MG	1A	3402	1/1	0.91	0.24	58,58,58,58	0
54	MG	2a	1691	1/1	0.91	0.13	91,91,91,91	0
54	MG	2A	3074	1/1	0.91	0.07	80,80,80,80	0
54	MG	1a	1785	1/1	0.91	0.14	84,84,84,84	0
54	MG	1A	3026	1/1	0.91	0.18	48,48,48,48	0
54	MG	2A	3499	1/1	0.91	0.09	64,64,64,64	0
54	MG	1B	1008	1/1	0.91	0.20	64,64,64,64	0
54	MG	28	101	1/1	0.91	0.33	70,70,70,70	0
54	MG	13	101	1/1	0.91	0.48	76,76,76,76	0
54	MG	1A	3679	1/1	0.91	0.24	73,73,73,73	0
54	MG	2A	3156	1/1	0.91	0.20	57,57,57,57	0
54	MG	2A	3277	1/1	0.91	0.17	58,58,58,58	0
54	MG	1A	3849	1/1	0.91	0.18	78,78,78,78	0
54	MG	1a	1752	1/1	0.91	0.21	61,61,61,61	0
54	MG	2A	3518	1/1	0.91	0.25	65,65,65,65	0
54	MG	2P	202	1/1	0.91	0.20	90,90,90,90	0
54	MG	1n	101	1/1	0.91	0.46	85,85,85,85	0
54	MG	2A	3532	1/1	0.91	0.07	89,89,89,89	0
54	MG	1A	3127	1/1	0.91	0.22	44,44,44,44	0
54	MG	1A	3802	1/1	0.91	0.29	75,75,75,75	0
54	MG	1a	1733	1/1	0.91	0.27	76,76,76,76	0
54	MG	1a	1698	1/1	0.91	0.30	48,48,48,48	0
54	MG	1A	3785	1/1	0.91	0.23	63,63,63,63	0
54	MG	2A	3475	1/1	0.91	0.13	88,88,88,88	0
54	MG	1A	3899	1/1	0.91	0.24	54,54,54,54	0
54	MG	2A	3066	1/1	0.91	0.18	50,50,50,50	0
54	MG	1A	3305	1/1	0.91	0.22	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3533	1/1	0.91	0.76	43,43,43,43	0
54	MG	1A	3033	1/1	0.91	0.15	67,67,67,67	0
54	MG	2A	3224	1/1	0.91	0.19	51,51,51,51	0
54	MG	2a	1601	1/1	0.91	0.15	74,74,74,74	0
54	MG	1a	1758	1/1	0.91	0.12	48,48,48,48	0
54	MG	1a	1772	1/1	0.91	0.17	83,83,83,83	0
54	MG	1a	1766	1/1	0.91	0.09	83,83,83,83	0
54	MG	1G	203	1/1	0.91	0.42	91,91,91,91	0
54	MG	2A	3641	1/1	0.91	0.83	88,88,88,88	0
54	MG	1A	3125	1/1	0.91	0.18	37,37,37,37	0
54	MG	1A	3824	1/1	0.91	0.16	63,63,63,63	0
54	MG	1A	3322	1/1	0.91	0.25	58,58,58,58	0
54	MG	2A	3496	1/1	0.91	0.22	69,69,69,69	0
54	MG	1A	3492	1/1	0.91	0.20	70,70,70,70	0
54	MG	2A	3332	1/1	0.91	0.19	82,82,82,82	0
54	MG	1A	3383	1/1	0.91	0.13	80,80,80,80	0
54	MG	1A	3251	1/1	0.91	0.17	41,41,41,41	0
54	MG	1B	1002	1/1	0.91	0.12	57,57,57,57	0
54	MG	2A	3255	1/1	0.91	0.14	50,50,50,50	0
54	MG	2A	3503	1/1	0.91	0.14	69,69,69,69	0
54	MG	2A	3101	1/1	0.91	0.27	56,56,56,56	0
54	MG	2A	3233	1/1	0.92	0.10	57,57,57,57	0
54	MG	1A	3403	1/1	0.92	0.12	71,71,71,71	0
54	MG	2A	3633	1/1	0.92	0.23	46,46,46,46	0
54	MG	1A	3840	1/1	0.92	0.18	62,62,62,62	0
54	MG	1A	3398	1/1	0.92	0.18	89,89,89,89	0
54	MG	1A	3071	1/1	0.92	0.21	54,54,54,54	0
54	MG	2a	1700	1/1	0.92	0.08	106,106,106,106	0
54	MG	1D	301	1/1	0.92	0.24	22,22,22,22	0
54	MG	1A	3795	1/1	0.92	0.09	60,60,60,60	0
54	MG	1A	3278	1/1	0.92	0.11	45,45,45,45	0
54	MG	1B	1027	1/1	0.92	0.18	43,43,43,43	0
54	MG	1A	3334	1/1	0.92	0.24	40,40,40,40	0
54	MG	1X	102	1/1	0.92	0.09	62,62,62,62	0
54	MG	1a	1692	1/1	0.92	0.14	78,78,78,78	0
54	MG	1U	202	1/1	0.92	0.15	37,37,37,37	0
54	MG	1B	1006	1/1	0.92	0.15	69,69,69,69	0
54	MG	1A	3182	1/1	0.92	0.50	44,44,44,44	0
54	MG	1A	3723	1/1	0.92	0.38	59,59,59,59	0
54	MG	1A	3798	1/1	0.92	0.40	71,71,71,71	0
54	MG	2A	3039	1/1	0.92	0.52	48,48,48,48	0
54	MG	1A	3050	1/1	0.92	0.32	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1855	1/1	0.92	0.10	74,74,74,74	0
54	MG	2A	3541	1/1	0.92	0.09	85,85,85,85	0
54	MG	1A	3158	1/1	0.92	0.15	66,66,66,66	0
54	MG	1A	3843	1/1	0.92	0.39	54,54,54,54	0
54	MG	2A	3139	1/1	0.92	0.44	74,74,74,74	0
54	MG	2A	3338	1/1	0.92	0.30	64,64,64,64	0
54	MG	2A	3134	1/1	0.92	0.46	71,71,71,71	0
54	MG	2A	3516	1/1	0.92	0.41	85,85,85,85	0
54	MG	1A	3466	1/1	0.92	0.29	95,95,95,95	0
54	MG	1R	201	1/1	0.92	0.29	46,46,46,46	0
54	MG	1A	3215	1/1	0.92	0.14	29,29,29,29	0
54	MG	2A	3340	1/1	0.92	0.26	57,57,57,57	0
54	MG	2A	3265	1/1	0.92	0.40	61,61,61,61	0
54	MG	2A	3345	1/1	0.92	0.26	70,70,70,70	0
54	MG	1A	3588	1/1	0.92	0.09	82,82,82,82	0
54	MG	1A	3149	1/1	0.92	0.22	43,43,43,43	0
54	MG	2A	3204	1/1	0.92	0.18	51,51,51,51	0
54	MG	2A	3167	1/1	0.92	0.42	56,56,56,56	0
54	MG	1A	3312	1/1	0.92	0.18	62,62,62,62	0
54	MG	1A	3338	1/1	0.92	0.20	18,18,18,18	0
54	MG	1A	3856	1/1	0.92	0.25	53,53,53,53	0
54	MG	1A	3865	1/1	0.92	0.40	58,58,58,58	0
54	MG	1a	1649	1/1	0.92	0.20	95,95,95,95	0
54	MG	1A	3259	1/1	0.92	0.33	79,79,79,79	0
54	MG	1a	1725	1/1	0.92	0.18	104,104,104,104	0
54	MG	1A	3857	1/1	0.92	0.07	81,81,81,81	0
54	MG	1A	3249	1/1	0.92	0.25	45,45,45,45	0
54	MG	1F	310	1/1	0.92	0.16	32,32,32,32	0
54	MG	2A	3552	1/1	0.92	0.12	66,66,66,66	0
54	MG	2A	3622	1/1	0.92	0.17	97,97,97,97	0
54	MG	20	101	1/1	0.92	0.29	80,80,80,80	0
54	MG	2A	3273	1/1	0.92	0.07	73,73,73,73	0
54	MG	2A	3525	1/1	0.92	0.23	61,61,61,61	0
54	MG	2A	3298	1/1	0.92	0.25	82,82,82,82	0
54	MG	1a	1790	1/1	0.92	0.27	95,95,95,95	0
54	MG	1A	3841	1/1	0.92	0.10	49,49,49,49	0
54	MG	2A	3378	1/1	0.92	0.21	54,54,54,54	0
54	MG	2A	3439	1/1	0.92	0.12	65,65,65,65	0
54	MG	2A	3239	1/1	0.92	0.18	38,38,38,38	0
54	MG	1A	3399	1/1	0.92	0.08	78,78,78,78	0
54	MG	2T	203	1/1	0.92	0.29	73,73,73,73	0
54	MG	1a	1737	1/1	0.92	0.11	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3098	1/1	0.92	0.22	58,58,58,58	0
54	MG	2A	3099	1/1	0.92	0.23	42,42,42,42	0
54	MG	1E	301	1/1	0.92	0.15	25,25,25,25	0
54	MG	2A	3145	1/1	0.92	0.29	62,62,62,62	0
54	MG	2a	1730	1/1	0.92	0.26	97,97,97,97	0
54	MG	2A	3436	1/1	0.92	0.18	73,73,73,73	0
54	MG	1A	3456	1/1	0.92	0.15	84,84,84,84	0
54	MG	1l	201	1/1	0.92	0.06	65,65,65,65	0
54	MG	1A	3414	1/1	0.92	0.16	69,69,69,69	0
54	MG	2A	3247	1/1	0.92	0.23	64,64,64,64	0
54	MG	1a	1617	1/1	0.92	0.21	79,79,79,79	0
54	MG	2A	3119	1/1	0.92	0.55	76,76,76,76	0
54	MG	1A	3656	1/1	0.92	0.12	38,38,38,38	0
54	MG	2a	1626	1/1	0.92	0.29	57,57,57,57	0
54	MG	1D	311	1/1	0.92	0.23	47,47,47,47	0
54	MG	1A	3686	1/1	0.92	0.19	51,51,51,51	0
54	MG	2A	3140	1/1	0.92	0.14	61,61,61,61	0
54	MG	1A	3575	1/1	0.92	0.09	41,41,41,41	0
54	MG	1a	1756	1/1	0.92	0.30	78,78,78,78	0
54	MG	2A	3200	1/1	0.92	0.17	41,41,41,41	0
54	MG	1A	3593	1/1	0.92	0.24	84,84,84,84	0
54	MG	2A	3312	1/1	0.92	0.10	62,62,62,62	0
54	MG	2a	1610	1/1	0.92	0.39	106,106,106,106	0
54	MG	1A	3139	1/1	0.92	0.33	42,42,42,42	0
54	MG	1a	1830	1/1	0.92	0.29	62,62,62,62	0
54	MG	2A	3238	1/1	0.92	0.14	46,46,46,46	0
54	MG	2A	3412	1/1	0.92	0.24	70,70,70,70	0
54	MG	2A	3411	1/1	0.92	0.07	78,78,78,78	0
54	MG	1a	1757	1/1	0.92	0.16	62,62,62,62	0
54	MG	2a	1703	1/1	0.92	0.44	81,81,81,81	0
54	MG	1A	3890	1/1	0.92	0.77	45,45,45,45	0
54	MG	2A	3245	1/1	0.92	0.25	71,71,71,71	0
54	MG	1A	3603	1/1	0.92	0.12	51,51,51,51	0
54	MG	2A	3262	1/1	0.92	0.09	46,46,46,46	0
54	MG	2A	3405	1/1	0.92	0.34	81,81,81,81	0
54	MG	1a	1794	1/1	0.92	0.16	78,78,78,78	0
54	MG	2A	3054	1/1	0.92	0.23	38,38,38,38	0
54	MG	1o	101	1/1	0.92	0.15	42,42,42,42	0
54	MG	1A	3381	1/1	0.92	0.26	58,58,58,58	0
54	MG	1T	2006	1/1	0.92	0.21	83,83,83,83	0
54	MG	2A	3485	1/1	0.92	0.14	66,66,66,66	0
54	MG	1A	3470	1/1	0.92	0.17	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3621	1/1	0.92	0.23	73,73,73,73	0
54	MG	2R	201	1/1	0.92	0.25	58,58,58,58	0
54	MG	2A	3326	1/1	0.92	0.15	75,75,75,75	0
54	MG	1A	3054	1/1	0.92	0.15	57,57,57,57	0
54	MG	1A	3135	1/1	0.92	0.10	72,72,72,72	0
54	MG	1A	3755	1/1	0.92	0.21	78,78,78,78	0
54	MG	1a	1639	1/1	0.92	0.27	97,97,97,97	0
54	MG	1A	3901	1/1	0.92	0.27	64,64,64,64	0
54	MG	1A	3138	1/1	0.92	0.22	41,41,41,41	0
53	MPD	1A	3001	8/8	0.92	0.24	58,65,67,67	0
54	MG	1A	3320	1/1	0.92	0.13	52,52,52,52	0
54	MG	2a	1702	1/1	0.92	0.14	83,83,83,83	0
54	MG	2a	1619	1/1	0.92	0.09	81,81,81,81	0
54	MG	2A	3269	1/1	0.92	0.14	88,88,88,88	0
54	MG	1A	3580	1/1	0.92	0.10	48,48,48,48	0
54	MG	2A	3595	1/1	0.92	0.24	68,68,68,68	0
54	MG	1A	3219	1/1	0.92	0.20	34,34,34,34	0
54	MG	1E	305	1/1	0.92	0.42	59,59,59,59	0
54	MG	2A	3348	1/1	0.92	0.16	37,37,37,37	0
54	MG	1A	3442	1/1	0.92	0.20	35,35,35,35	0
54	MG	2A	3222	1/1	0.92	0.17	65,65,65,65	0
54	MG	1a	1708	1/1	0.92	0.32	64,64,64,64	0
54	MG	1A	3343	1/1	0.92	0.12	32,32,32,32	0
54	MG	1A	3739	1/1	0.92	0.27	72,72,72,72	0
54	MG	1A	3328	1/1	0.92	0.10	35,35,35,35	0
54	MG	1A	3525	1/1	0.92	0.12	62,62,62,62	0
54	MG	1A	3023	1/1	0.92	0.27	33,33,33,33	0
54	MG	1a	1622	1/1	0.93	0.16	106,106,106,106	0
54	MG	2A	3103	1/1	0.93	0.13	82,82,82,82	0
54	MG	1A	3754	1/1	0.93	0.13	29,29,29,29	0
54	MG	1a	1661	1/1	0.93	0.40	86,86,86,86	0
54	MG	2A	3540	1/1	0.93	0.12	77,77,77,77	0
54	MG	2A	3432	1/1	0.93	0.10	66,66,66,66	0
54	MG	2A	3016	1/1	0.93	0.20	71,71,71,71	0
54	MG	2A	3282	1/1	0.93	0.26	41,41,41,41	0
54	MG	1a	1707	1/1	0.93	0.10	57,57,57,57	0
54	MG	1a	1800	1/1	0.93	0.10	100,100,100,100	0
54	MG	1A	3622	1/1	0.93	0.12	51,51,51,51	0
54	MG	1a	1604	1/1	0.93	0.33	65,65,65,65	0
54	MG	1a	1655	1/1	0.93	0.23	61,61,61,61	0
54	MG	2A	3358	1/1	0.93	0.26	104,104,104,104	0
54	MG	1A	3756	1/1	0.93	0.09	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	15	103	1/1	0.93	0.15	67,67,67,67	0
54	MG	2A	3433	1/1	0.93	0.09	43,43,43,43	0
54	MG	2A	3511	1/1	0.93	0.13	89,89,89,89	0
54	MG	1A	3787	1/1	0.93	0.26	82,82,82,82	0
54	MG	2a	1631	1/1	0.93	0.28	60,60,60,60	0
54	MG	1A	3523	1/1	0.93	0.34	67,67,67,67	0
54	MG	1a	1612	1/1	0.93	0.24	32,32,32,32	0
54	MG	1a	1674	1/1	0.93	0.20	52,52,52,52	0
54	MG	1A	3484	1/1	0.93	0.25	64,64,64,64	0
54	MG	2A	3376	1/1	0.93	0.14	64,64,64,64	0
54	MG	1B	1003	1/1	0.93	0.23	60,60,60,60	0
54	MG	2A	3241	1/1	0.93	0.07	86,86,86,86	0
54	MG	2a	1706	1/1	0.93	0.27	82,82,82,82	0
54	MG	2p	101	1/1	0.93	0.18	55,55,55,55	0
54	MG	2a	1747	1/1	0.93	0.42	129,129,129,129	0
54	MG	2a	1699	1/1	0.93	0.11	70,70,70,70	0
54	MG	2A	3286	1/1	0.93	0.18	53,53,53,53	0
54	MG	1A	3267	1/1	0.93	0.18	58,58,58,58	0
54	MG	1A	3406	1/1	0.93	0.13	67,67,67,67	0
54	MG	1A	3496	1/1	0.93	0.16	35,35,35,35	0
54	MG	2a	1669	1/1	0.93	0.22	61,61,61,61	0
54	MG	2A	3426	1/1	0.93	0.14	55,55,55,55	0
54	MG	2A	3024	1/1	0.93	0.39	68,68,68,68	0
54	MG	2A	3418	1/1	0.93	0.16	71,71,71,71	0
54	MG	1A	3705	1/1	0.93	0.16	46,46,46,46	0
54	MG	1A	3475	1/1	0.93	0.22	44,44,44,44	0
54	MG	1A	3490	1/1	0.93	0.17	60,60,60,60	0
54	MG	1a	1844	1/1	0.93	0.20	76,76,76,76	0
54	MG	2a	1602	1/1	0.93	0.18	62,62,62,62	0
54	MG	1A	3309	1/1	0.93	0.26	59,59,59,59	0
54	MG	2A	3352	1/1	0.93	0.28	51,51,51,51	0
54	MG	2A	3355	1/1	0.93	0.13	54,54,54,54	0
54	MG	2A	3201	1/1	0.93	0.29	51,51,51,51	0
54	MG	2A	3382	1/1	0.93	0.10	59,59,59,59	0
54	MG	1A	3005	1/1	0.93	0.23	56,56,56,56	0
54	MG	1A	3783	1/1	0.93	0.24	51,51,51,51	0
54	MG	2A	3324	1/1	0.93	0.21	46,46,46,46	0
54	MG	1A	3376	1/1	0.93	0.22	30,30,30,30	0
54	MG	2A	3413	1/1	0.93	0.20	77,77,77,77	0
54	MG	10	103	1/1	0.93	0.31	56,56,56,56	0
54	MG	1A	3731	1/1	0.93	0.14	75,75,75,75	0
54	MG	1A	3784	1/1	0.93	0.14	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3072	1/1	0.93	0.14	51,51,51,51	0
54	MG	2A	3223	1/1	0.93	0.13	48,48,48,48	0
54	MG	1a	1753	1/1	0.93	0.26	84,84,84,84	0
54	MG	2a	1651	1/1	0.93	0.24	68,68,68,68	0
54	MG	1D	308	1/1	0.93	0.14	55,55,55,55	0
54	MG	2A	3158	1/1	0.93	0.10	68,68,68,68	0
54	MG	2A	3243	1/1	0.93	0.07	67,67,67,67	0
54	MG	2A	3025	1/1	0.93	0.18	50,50,50,50	0
54	MG	2A	3534	1/1	0.93	0.18	68,68,68,68	0
54	MG	2A	3164	1/1	0.93	0.25	62,62,62,62	0
54	MG	2A	3506	1/1	0.93	0.18	64,64,64,64	0
54	MG	1W	201	1/1	0.93	0.21	92,92,92,92	0
54	MG	1A	3093	1/1	0.93	0.23	43,43,43,43	0
54	MG	2a	1682	1/1	0.93	0.21	71,71,71,71	0
54	MG	1A	3489	1/1	0.93	0.20	64,64,64,64	0
54	MG	2A	3607	1/1	0.93	0.26	52,52,52,52	0
54	MG	2A	3584	1/1	0.93	0.10	60,60,60,60	0
54	MG	1B	1020	1/1	0.93	0.12	50,50,50,50	0
54	MG	1A	3042	1/1	0.93	0.12	63,63,63,63	0
54	MG	1A	3832	1/1	0.93	0.50	60,60,60,60	0
54	MG	1a	1798	1/1	0.93	0.14	107,107,107,107	0
54	MG	2A	3428	1/1	0.93	0.08	61,61,61,61	0
54	MG	1A	3779	1/1	0.93	0.10	68,68,68,68	0
54	MG	2A	3231	1/1	0.93	0.13	72,72,72,72	0
54	MG	1A	3623	1/1	0.93	0.09	65,65,65,65	0
54	MG	1a	1682	1/1	0.93	0.10	69,69,69,69	0
54	MG	2A	3323	1/1	0.93	0.13	65,65,65,65	0
54	MG	2A	3308	1/1	0.93	0.33	52,52,52,52	0
54	MG	2A	3606	1/1	0.93	0.13	63,63,63,63	0
54	MG	1A	3753	1/1	0.93	0.12	43,43,43,43	0
54	MG	1A	3411	1/1	0.93	0.12	54,54,54,54	0
54	MG	2a	1688	1/1	0.93	0.20	64,64,64,64	0
54	MG	1A	3123	1/1	0.93	0.17	49,49,49,49	0
54	MG	1A	3811	1/1	0.93	0.51	58,58,58,58	0
54	MG	2A	3514	1/1	0.93	0.08	69,69,69,69	0
54	MG	2A	3619	1/1	0.93	0.09	65,65,65,65	0
54	MG	1A	3583	1/1	0.93	0.23	60,60,60,60	0
54	MG	1A	3793	1/1	0.93	0.13	67,67,67,67	0
54	MG	2A	3127	1/1	0.93	0.13	49,49,49,49	0
54	MG	1A	3809	1/1	0.93	0.28	57,57,57,57	0
54	MG	1a	1835	1/1	0.93	0.06	80,80,80,80	0
54	MG	1A	3673	1/1	0.93	0.17	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3176	1/1	0.93	0.27	54,54,54,54	0
54	MG	1A	3760	1/1	0.93	0.08	71,71,71,71	0
54	MG	1B	1016	1/1	0.93	0.17	55,55,55,55	0
54	MG	2A	3214	1/1	0.93	0.34	48,48,48,48	0
54	MG	1a	1633	1/1	0.93	0.09	85,85,85,85	0
54	MG	2A	3221	1/1	0.93	0.21	65,65,65,65	0
54	MG	1a	1730	1/1	0.93	0.21	53,53,53,53	0
54	MG	1X	101	1/1	0.93	0.16	66,66,66,66	0
54	MG	2A	3335	1/1	0.93	0.13	61,61,61,61	0
54	MG	1A	3265	1/1	0.93	0.13	86,86,86,86	0
54	MG	1A	3819	1/1	0.93	0.20	71,71,71,71	0
54	MG	1A	3729	1/1	0.93	0.20	46,46,46,46	0
55	ARG	1B	1001	12/12	0.93	0.24	49,55,69,72	0
54	MG	2a	1630	1/1	0.93	0.36	55,55,55,55	0
54	MG	1G	201	1/1	0.93	0.14	92,92,92,92	0
54	MG	1A	3871	1/1	0.93	0.20	83,83,83,83	0
54	MG	1A	3487	1/1	0.93	0.12	56,56,56,56	0
54	MG	1A	3792	1/1	0.93	0.11	67,67,67,67	0
54	MG	2a	1686	1/1	0.93	0.05	67,67,67,67	0
54	MG	1A	3527	1/1	0.93	0.23	56,56,56,56	0
54	MG	1A	3594	1/1	0.93	0.30	31,31,31,31	0
54	MG	1A	3234	1/1	0.93	0.38	59,59,59,59	0
54	MG	2a	1723	1/1	0.93	0.09	79,79,79,79	0
54	MG	1a	1657	1/1	0.93	0.17	95,95,95,95	0
54	MG	2A	3573	1/1	0.93	0.13	52,52,52,52	0
54	MG	1A	3535	1/1	0.93	0.11	53,53,53,53	0
54	MG	2A	3444	1/1	0.93	0.13	68,68,68,68	0
54	MG	1A	3697	1/1	0.93	0.21	72,72,72,72	0
54	MG	1A	3044	1/1	0.93	0.16	41,41,41,41	0
54	MG	1A	3650	1/1	0.93	0.22	61,61,61,61	0
54	MG	2A	3013	1/1	0.93	0.16	59,59,59,59	0
54	MG	1A	3858	1/1	0.93	0.16	77,77,77,77	0
54	MG	1A	3498	1/1	0.93	0.11	55,55,55,55	0
54	MG	2A	3311	1/1	0.93	0.27	66,66,66,66	0
54	MG	1A	3653	1/1	0.93	0.14	52,52,52,52	0
54	MG	1A	3744	1/1	0.93	0.19	55,55,55,55	0
54	MG	2A	3121	1/1	0.93	0.23	82,82,82,82	0
54	MG	2A	3640	1/1	0.93	0.24	58,58,58,58	0
54	MG	1a	1812	1/1	0.93	0.16	90,90,90,90	0
54	MG	1A	3595	1/1	0.93	0.22	50,50,50,50	0
54	MG	2A	3030	1/1	0.93	0.21	64,64,64,64	0
56	ZN	2n	101	1/1	0.93	0.09	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3195	1/1	0.93	0.34	66,66,66,66	0
54	MG	1A	3680	1/1	0.93	0.10	64,64,64,64	0
54	MG	1A	3582	1/1	0.93	0.23	84,84,84,84	0
54	MG	1A	3296	1/1	0.93	0.27	38,38,38,38	0
54	MG	2A	3401	1/1	0.93	0.21	75,75,75,75	0
54	MG	1A	3628	1/1	0.93	0.30	47,47,47,47	0
54	MG	2A	3084	1/1	0.93	0.14	71,71,71,71	0
54	MG	1g	201	1/1	0.93	0.59	87,87,87,87	0
54	MG	2A	3272	1/1	0.93	0.13	64,64,64,64	0
54	MG	1a	1848	1/1	0.93	0.07	90,90,90,90	0
54	MG	1A	3892	1/1	0.93	0.29	35,35,35,35	0
54	MG	1A	3392	1/1	0.93	0.15	80,80,80,80	0
54	MG	2A	3624	1/1	0.93	0.25	39,39,39,39	0
54	MG	2A	3106	1/1	0.93	0.15	51,51,51,51	0
54	MG	1A	3668	1/1	0.93	0.18	41,41,41,41	0
54	MG	2A	3125	1/1	0.93	0.16	73,73,73,73	0
54	MG	1A	3203	1/1	0.93	0.08	60,60,60,60	0
54	MG	2a	1611	1/1	0.93	0.11	76,76,76,76	0
54	MG	1y	201	1/1	0.93	0.21	91,91,91,91	0
54	MG	2a	1728	1/1	0.93	0.05	87,87,87,87	0
54	MG	1A	3261	1/1	0.93	0.16	30,30,30,30	0
54	MG	2A	3018	1/1	0.93	0.55	45,45,45,45	0
54	MG	1T	2003	1/1	0.94	0.35	83,83,83,83	0
54	MG	2A	3505	1/1	0.94	0.12	73,73,73,73	0
54	MG	1A	3253	1/1	0.94	0.24	61,61,61,61	0
54	MG	2A	3549	1/1	0.94	0.39	60,60,60,60	0
54	MG	1A	3835	1/1	0.94	0.33	50,50,50,50	0
54	MG	2O	201	1/1	0.94	0.16	69,69,69,69	0
54	MG	2D	302	1/1	0.94	0.17	56,56,56,56	0
54	MG	1a	1729	1/1	0.94	0.21	92,92,92,92	0
54	MG	2A	3614	1/1	0.94	0.32	64,64,64,64	0
54	MG	1a	1697	1/1	0.94	0.25	63,63,63,63	0
54	MG	2A	3437	1/1	0.94	0.22	48,48,48,48	0
54	MG	1A	3437	1/1	0.94	0.12	53,53,53,53	0
54	MG	10	105	1/1	0.94	0.10	57,57,57,57	0
54	MG	2A	3435	1/1	0.94	0.19	81,81,81,81	0
54	MG	1a	1669	1/1	0.94	0.17	110,110,110,110	0
54	MG	2A	3053	1/1	0.94	0.22	56,56,56,56	0
54	MG	2A	3088	1/1	0.94	0.27	52,52,52,52	0
54	MG	2A	3254	1/1	0.94	0.15	69,69,69,69	0
54	MG	1A	3585	1/1	0.94	0.13	62,62,62,62	0
54	MG	1a	1720	1/1	0.94	0.27	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3160	1/1	0.94	0.15	37,37,37,37	0
54	MG	2A	3299	1/1	0.94	0.13	53,53,53,53	0
54	MG	1A	3148	1/1	0.94	0.13	54,54,54,54	0
54	MG	1A	3598	1/1	0.94	0.35	82,82,82,82	0
54	MG	1B	1021	1/1	0.94	0.09	54,54,54,54	0
54	MG	1A	3514	1/1	0.94	0.29	58,58,58,58	0
54	MG	1A	3657	1/1	0.94	0.09	64,64,64,64	0
54	MG	2A	3126	1/1	0.94	0.22	53,53,53,53	0
54	MG	1F	307	1/1	0.94	0.60	38,38,38,38	0
54	MG	2A	3089	1/1	0.94	0.13	61,61,61,61	0
54	MG	2A	3136	1/1	0.94	0.29	62,62,62,62	0
54	MG	2A	3535	1/1	0.94	0.10	88,88,88,88	0
54	MG	2A	3632	1/1	0.94	0.09	75,75,75,75	0
54	MG	2A	3623	1/1	0.94	0.25	76,76,76,76	0
54	MG	2a	1749	1/1	0.94	0.14	79,79,79,79	0
54	MG	2A	3562	1/1	0.94	0.12	64,64,64,64	0
54	MG	1A	3725	1/1	0.94	0.12	76,76,76,76	0
54	MG	2A	3360	1/1	0.94	0.14	47,47,47,47	0
54	MG	1A	3280	1/1	0.94	0.12	46,46,46,46	0
54	MG	1A	3493	1/1	0.94	0.15	68,68,68,68	0
54	MG	1A	3738	1/1	0.94	0.13	43,43,43,43	0
54	MG	1A	3364	1/1	0.94	0.25	24,24,24,24	0
54	MG	1a	1739	1/1	0.94	0.55	81,81,81,81	0
54	MG	1A	3607	1/1	0.94	0.17	50,50,50,50	0
54	MG	1A	3643	1/1	0.94	0.25	65,65,65,65	0
54	MG	1A	3212	1/1	0.94	0.17	43,43,43,43	0
54	MG	1A	3878	1/1	0.94	0.33	50,50,50,50	0
54	MG	2A	3062	1/1	0.94	0.19	51,51,51,51	0
54	MG	1A	3742	1/1	0.94	0.13	59,59,59,59	0
54	MG	1D	303	1/1	0.94	0.17	47,47,47,47	0
54	MG	1a	1765	1/1	0.94	0.09	103,103,103,103	0
54	MG	2A	3608	1/1	0.94	0.34	86,86,86,86	0
54	MG	2A	3431	1/1	0.94	0.27	46,46,46,46	0
54	MG	2A	3321	1/1	0.94	0.14	77,77,77,77	0
54	MG	2A	3306	1/1	0.94	0.15	34,34,34,34	0
54	MG	1A	3547	1/1	0.94	0.17	60,60,60,60	0
54	MG	1a	1759	1/1	0.94	0.45	101,101,101,101	0
54	MG	1T	2005	1/1	0.94	0.29	53,53,53,53	0
54	MG	2A	3146	1/1	0.94	0.14	70,70,70,70	0
54	MG	2A	3414	1/1	0.94	0.26	74,74,74,74	0
54	MG	2A	3174	1/1	0.94	0.10	72,72,72,72	0
54	MG	1A	3080	1/1	0.94	0.43	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3283	1/1	0.94	0.22	50,50,50,50	0
54	MG	2A	3430	1/1	0.94	0.13	64,64,64,64	0
54	MG	1A	3801	1/1	0.94	0.12	58,58,58,58	0
54	MG	1A	3104	1/1	0.94	0.30	33,33,33,33	0
54	MG	1A	3778	1/1	0.94	0.13	44,44,44,44	0
54	MG	1a	1817	1/1	0.94	0.15	57,57,57,57	0
54	MG	1A	3362	1/1	0.94	0.18	48,48,48,48	0
54	MG	2A	3643	1/1	0.94	0.10	62,62,62,62	0
54	MG	2A	3189	1/1	0.94	0.34	83,83,83,83	0
54	MG	2A	3252	1/1	0.94	0.11	49,49,49,49	0
54	MG	1A	3401	1/1	0.94	0.05	53,53,53,53	0
54	MG	2A	3442	1/1	0.94	0.36	74,74,74,74	0
54	MG	2A	3381	1/1	0.94	0.39	99,99,99,99	0
54	MG	1A	3691	1/1	0.94	0.41	61,61,61,61	0
54	MG	2a	1757	1/1	0.94	0.23	92,92,92,92	0
54	MG	1A	3375	1/1	0.94	0.18	45,45,45,45	0
54	MG	1A	3586	1/1	0.94	0.21	81,81,81,81	0
54	MG	2A	3361	1/1	0.94	0.16	53,53,53,53	0
54	MG	2a	1727	1/1	0.94	0.09	88,88,88,88	0
54	MG	1A	3167	1/1	0.94	0.47	42,42,42,42	0
54	MG	1a	1690	1/1	0.94	0.09	62,62,62,62	0
54	MG	2A	3027	1/1	0.94	0.12	47,47,47,47	0
54	MG	1A	3348	1/1	0.94	0.13	37,37,37,37	0
54	MG	2A	3191	1/1	0.94	0.13	40,40,40,40	0
54	MG	1l	102	1/1	0.94	0.15	44,44,44,44	0
54	MG	1A	3649	1/1	0.94	0.17	52,52,52,52	0
54	MG	2A	3148	1/1	0.94	0.19	42,42,42,42	0
54	MG	1A	3870	1/1	0.94	0.25	55,55,55,55	0
54	MG	1a	1750	1/1	0.94	0.22	89,89,89,89	0
54	MG	1A	3775	1/1	0.94	0.15	72,72,72,72	0
54	MG	15	101	1/1	0.94	0.26	44,44,44,44	0
54	MG	1A	3428	1/1	0.94	0.20	67,67,67,67	0
54	MG	1A	3147	1/1	0.94	0.17	35,35,35,35	0
54	MG	2A	3267	1/1	0.94	0.21	58,58,58,58	0
54	MG	1U	203	1/1	0.94	0.52	58,58,58,58	0
54	MG	1A	3190	1/1	0.94	0.10	84,84,84,84	0
54	MG	2A	3266	1/1	0.94	0.20	59,59,59,59	0
54	MG	2A	3372	1/1	0.94	0.15	63,63,63,63	0
54	MG	1a	1845	1/1	0.94	0.17	63,63,63,63	0
54	MG	1Q	202	1/1	0.94	0.20	48,48,48,48	0
54	MG	1a	1662	1/1	0.94	0.20	69,69,69,69	0
54	MG	1a	1816	1/1	0.94	0.10	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3636	1/1	0.94	0.14	81,81,81,81	0
54	MG	1A	3886	1/1	0.94	0.23	46,46,46,46	0
54	MG	1A	3663	1/1	0.94	0.15	51,51,51,51	0
54	MG	1A	3468	1/1	0.94	0.26	62,62,62,62	0
54	MG	2A	3014	1/1	0.94	0.26	66,66,66,66	0
54	MG	1a	1724	1/1	0.94	0.06	72,72,72,72	0
54	MG	1A	3421	1/1	0.94	0.10	29,29,29,29	0
54	MG	1B	1025	1/1	0.94	0.15	70,70,70,70	0
54	MG	1A	3557	1/1	0.94	0.79	41,41,41,41	0
54	MG	1A	3162	1/1	0.94	0.42	43,43,43,43	0
54	MG	1A	3072	1/1	0.94	0.26	60,60,60,60	0
54	MG	2A	3389	1/1	0.94	0.16	69,69,69,69	0
54	MG	1A	3274	1/1	0.94	0.22	22,22,22,22	0
54	MG	1a	1777	1/1	0.94	0.07	99,99,99,99	0
54	MG	1A	3027	1/1	0.94	0.23	49,49,49,49	0
54	MG	1A	3049	1/1	0.94	0.22	69,69,69,69	0
54	MG	1A	3807	1/1	0.94	0.19	64,64,64,64	0
54	MG	1A	3327	1/1	0.94	0.11	26,26,26,26	0
54	MG	1A	3712	1/1	0.94	0.13	46,46,46,46	0
54	MG	1A	3210	1/1	0.94	0.23	37,37,37,37	0
54	MG	1A	3222	1/1	0.94	0.20	52,52,52,52	0
54	MG	1A	3397	1/1	0.94	0.23	67,67,67,67	0
54	MG	2Q	201	1/1	0.94	0.27	83,83,83,83	0
54	MG	2A	3357	1/1	0.94	0.15	53,53,53,53	0
54	MG	1H	201	1/1	0.94	0.21	64,64,64,64	0
54	MG	2A	3629	1/1	0.94	0.13	67,67,67,67	0
54	MG	2A	3047	1/1	0.94	0.17	61,61,61,61	0
54	MG	1D	305	1/1	0.94	0.41	55,55,55,55	0
54	MG	1A	3510	1/1	0.94	0.18	57,57,57,57	0
54	MG	1A	3195	1/1	0.94	0.28	58,58,58,58	0
54	MG	2A	3079	1/1	0.94	0.32	67,67,67,67	0
54	MG	2A	3168	1/1	0.94	0.17	51,51,51,51	0
54	MG	2A	3132	1/1	0.94	0.26	54,54,54,54	0
54	MG	1A	3814	1/1	0.94	0.15	51,51,51,51	0
54	MG	1A	3200	1/1	0.94	0.28	40,40,40,40	0
54	MG	1a	1677	1/1	0.94	0.21	66,66,66,66	0
54	MG	2A	3371	1/1	0.94	0.18	48,48,48,48	0
54	MG	1A	3266	1/1	0.94	0.16	46,46,46,46	0
54	MG	2a	1677	1/1	0.94	0.08	98,98,98,98	0
54	MG	2A	3256	1/1	0.94	0.17	54,54,54,54	0
54	MG	1A	3291	1/1	0.94	0.14	57,57,57,57	0
54	MG	1a	1755	1/1	0.94	0.15	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2X	101	1/1	0.94	0.12	84,84,84,84	0
54	MG	1a	1609	1/1	0.94	0.25	120,120,120,120	0
54	MG	2I	101	1/1	0.94	0.15	54,54,54,54	0
54	MG	1A	3569	1/1	0.94	0.28	46,46,46,46	0
54	MG	1A	3394	1/1	0.94	0.11	78,78,78,78	0
54	MG	2A	3555	1/1	0.94	0.11	71,71,71,71	0
54	MG	2a	1714	1/1	0.94	0.08	84,84,84,84	0
54	MG	1A	3166	1/1	0.94	0.51	45,45,45,45	0
54	MG	1A	3136	1/1	0.94	0.10	43,43,43,43	0
54	MG	1A	3363	1/1	0.94	0.10	52,52,52,52	0
54	MG	2A	3448	1/1	0.94	0.12	69,69,69,69	0
54	MG	2A	3003	1/1	0.94	0.37	49,49,49,49	0
54	MG	2A	3009	1/1	0.94	0.33	63,63,63,63	0
54	MG	2A	3467	1/1	0.95	0.04	83,83,83,83	0
54	MG	1A	3564	1/1	0.95	0.63	65,65,65,65	0
54	MG	1A	3346	1/1	0.95	0.29	48,48,48,48	0
54	MG	2A	3380	1/1	0.95	0.15	48,48,48,48	0
54	MG	1a	1608	1/1	0.95	0.12	78,78,78,78	0
54	MG	1A	3119	1/1	0.95	0.50	44,44,44,44	0
54	MG	2a	1756	1/1	0.95	0.10	73,73,73,73	0
54	MG	1A	3568	1/1	0.95	0.25	51,51,51,51	0
54	MG	2a	1741	1/1	0.95	0.26	97,97,97,97	0
54	MG	1R	207	1/1	0.95	0.17	35,35,35,35	0
54	MG	1A	3508	1/1	0.95	0.08	51,51,51,51	0
54	MG	1A	3597	1/1	0.95	0.34	57,57,57,57	0
54	MG	1a	1742	1/1	0.95	0.33	95,95,95,95	0
54	MG	1A	3140	1/1	0.95	0.52	46,46,46,46	0
54	MG	1A	3159	1/1	0.95	0.46	46,46,46,46	0
54	MG	2A	3528	1/1	0.95	0.09	60,60,60,60	0
54	MG	2a	1755	1/1	0.95	0.17	79,79,79,79	0
54	MG	2A	3259	1/1	0.95	0.28	59,59,59,59	0
54	MG	1A	3764	1/1	0.95	0.33	62,62,62,62	0
54	MG	1A	3804	1/1	0.95	0.15	81,81,81,81	0
54	MG	1A	3082	1/1	0.95	0.61	47,47,47,47	0
54	MG	1G	204	1/1	0.95	0.10	73,73,73,73	0
54	MG	1A	3648	1/1	0.95	0.10	47,47,47,47	0
54	MG	2P	201	1/1	0.95	0.18	83,83,83,83	0
54	MG	1A	3733	1/1	0.95	0.17	35,35,35,35	0
54	MG	1A	3085	1/1	0.95	0.19	22,22,22,22	0
54	MG	1a	1738	1/1	0.95	0.36	78,78,78,78	0
54	MG	2A	3162	1/1	0.95	0.10	101,101,101,101	0
54	MG	1a	1854	1/1	0.95	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1R	202	1/1	0.95	0.45	41,41,41,41	0
54	MG	2A	3172	1/1	0.95	0.36	80,80,80,80	0
54	MG	1A	3891	1/1	0.95	0.19	48,48,48,48	0
54	MG	1A	3199	1/1	0.95	0.34	58,58,58,58	0
54	MG	1A	3794	1/1	0.95	0.45	67,67,67,67	0
54	MG	1a	1647	1/1	0.95	0.40	62,62,62,62	0
54	MG	1A	3615	1/1	0.95	0.18	57,57,57,57	0
54	MG	1A	3710	1/1	0.95	0.13	61,61,61,61	0
54	MG	2A	3271	1/1	0.95	0.16	67,67,67,67	0
54	MG	1A	3016	1/1	0.95	0.16	33,33,33,33	0
54	MG	1A	3447	1/1	0.95	0.52	70,70,70,70	0
54	MG	1A	3128	1/1	0.95	0.49	44,44,44,44	0
54	MG	2A	3362	1/1	0.95	0.23	75,75,75,75	0
54	MG	1A	3876	1/1	0.95	0.10	29,29,29,29	0
54	MG	1O	201	1/1	0.95	0.11	58,58,58,58	0
54	MG	1A	3238	1/1	0.95	0.19	31,31,31,31	0
54	MG	1A	3810	1/1	0.95	0.07	59,59,59,59	0
54	MG	1a	1836	1/1	0.95	0.16	85,85,85,85	0
54	MG	1A	3361	1/1	0.95	0.14	49,49,49,49	0
54	MG	1A	3455	1/1	0.95	0.11	38,38,38,38	0
54	MG	2a	1641	1/1	0.95	0.19	71,71,71,71	0
54	MG	2A	3319	1/1	0.95	0.22	60,60,60,60	0
54	MG	1A	3031	1/1	0.95	0.12	31,31,31,31	0
54	MG	2A	3268	1/1	0.95	0.17	58,58,58,58	0
54	MG	1A	3454	1/1	0.95	0.15	67,67,67,67	0
54	MG	2A	3427	1/1	0.95	0.14	68,68,68,68	0
54	MG	1A	3059	1/1	0.95	0.15	24,24,24,24	0
54	MG	1y	203	1/1	0.95	0.13	57,57,57,57	0
54	MG	1P	202	1/1	0.95	0.27	34,34,34,34	0
54	MG	2t	201	1/1	0.95	0.37	71,71,71,71	0
54	MG	1A	3515	1/1	0.95	0.13	57,57,57,57	0
54	MG	1A	3898	1/1	0.95	0.09	34,34,34,34	0
54	MG	1A	3306	1/1	0.95	0.20	57,57,57,57	0
54	MG	1A	3531	1/1	0.95	0.12	45,45,45,45	0
54	MG	2A	3026	1/1	0.95	0.27	42,42,42,42	0
54	MG	2B	209	1/1	0.95	0.22	64,64,64,64	0
54	MG	2A	3504	1/1	0.95	0.16	71,71,71,71	0
54	MG	1A	3207	1/1	0.95	0.39	37,37,37,37	0
54	MG	1A	3639	1/1	0.95	0.13	58,58,58,58	0
54	MG	2T	204	1/1	0.95	0.35	71,71,71,71	0
54	MG	2A	3422	1/1	0.95	0.07	65,65,65,65	0
54	MG	1a	1656	1/1	0.95	0.23	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3600	1/1	0.95	0.25	66,66,66,66	0
54	MG	2A	3065	1/1	0.95	0.42	67,67,67,67	0
54	MG	1A	3039	1/1	0.95	0.24	38,38,38,38	0
54	MG	1a	1797	1/1	0.95	0.17	68,68,68,68	0
54	MG	1F	308	1/1	0.95	0.09	32,32,32,32	0
54	MG	1A	3304	1/1	0.95	0.12	30,30,30,30	0
54	MG	1P	203	1/1	0.95	0.12	52,52,52,52	0
54	MG	1A	3463	1/1	0.95	0.16	54,54,54,54	0
54	MG	1A	3269	1/1	0.95	0.23	30,30,30,30	0
54	MG	1A	3566	1/1	0.95	0.31	69,69,69,69	0
54	MG	2D	301	1/1	0.95	0.56	63,63,63,63	0
54	MG	2A	3628	1/1	0.95	0.24	60,60,60,60	0
54	MG	1A	3277	1/1	0.95	0.12	89,89,89,89	0
54	MG	1A	3642	1/1	0.95	0.23	50,50,50,50	0
54	MG	1A	3213	1/1	0.95	0.23	60,60,60,60	0
54	MG	1A	3536	1/1	0.95	0.09	42,42,42,42	0
54	MG	2A	3020	1/1	0.95	0.09	60,60,60,60	0
54	MG	1a	1620	1/1	0.95	0.20	89,89,89,89	0
54	MG	1A	3688	1/1	0.95	0.14	47,47,47,47	0
54	MG	1a	1658	1/1	0.95	0.26	55,55,55,55	0
54	MG	1A	3116	1/1	0.95	0.21	28,28,28,28	0
54	MG	1A	3669	1/1	0.95	0.16	34,34,34,34	0
54	MG	1A	3018	1/1	0.95	0.37	40,40,40,40	0
54	MG	1A	3345	1/1	0.95	0.13	60,60,60,60	0
54	MG	1A	3134	1/1	0.95	0.12	38,38,38,38	0
54	MG	1A	3257	1/1	0.95	0.19	47,47,47,47	0
54	MG	2A	3349	1/1	0.95	0.19	54,54,54,54	0
54	MG	1A	3827	1/1	0.95	0.14	57,57,57,57	0
54	MG	1A	3521	1/1	0.95	0.10	60,60,60,60	0
54	MG	1A	3741	1/1	0.95	0.46	51,51,51,51	0
54	MG	1A	3473	1/1	0.95	0.16	45,45,45,45	0
54	MG	2A	3159	1/1	0.95	0.16	50,50,50,50	0
54	MG	1a	1853	1/1	0.95	0.17	65,65,65,65	0
54	MG	1A	3540	1/1	0.95	0.23	36,36,36,36	0
54	MG	1A	3313	1/1	0.95	0.10	31,31,31,31	0
54	MG	1A	3440	1/1	0.95	0.16	59,59,59,59	0
54	MG	1A	3589	1/1	0.95	0.17	43,43,43,43	0
54	MG	2A	3502	1/1	0.95	0.13	57,57,57,57	0
54	MG	1A	3716	1/1	0.95	0.13	50,50,50,50	0
54	MG	2R	203	1/1	0.95	0.23	53,53,53,53	0
54	MG	1A	3020	1/1	0.95	0.15	50,50,50,50	0
54	MG	1A	3436	1/1	0.95	0.12	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3035	1/1	0.95	0.43	57,57,57,57	0
54	MG	2A	3303	1/1	0.95	0.08	75,75,75,75	0
54	MG	1A	3808	1/1	0.95	0.10	63,63,63,63	0
54	MG	2a	1612	1/1	0.95	0.09	96,96,96,96	0
54	MG	1A	3391	1/1	0.95	0.12	53,53,53,53	0
54	MG	1A	3263	1/1	0.95	0.17	44,44,44,44	0
54	MG	1A	3434	1/1	0.95	0.07	67,67,67,67	0
54	MG	2A	3327	1/1	0.95	0.10	77,77,77,77	0
54	MG	2A	3400	1/1	0.95	0.13	55,55,55,55	0
54	MG	2A	3085	1/1	0.95	0.16	73,73,73,73	0
54	MG	1A	3192	1/1	0.95	0.21	65,65,65,65	0
54	MG	2A	3513	1/1	0.95	0.06	81,81,81,81	0
54	MG	1A	3427	1/1	0.95	0.16	46,46,46,46	0
54	MG	1A	3365	1/1	0.95	0.16	22,22,22,22	0
54	MG	1A	3279	1/1	0.95	0.12	67,67,67,67	0
54	MG	1A	3609	1/1	0.95	0.18	52,52,52,52	0
54	MG	1A	3606	1/1	0.95	0.23	55,55,55,55	0
54	MG	2I	103	1/1	0.95	0.15	60,60,60,60	0
54	MG	2A	3500	1/1	0.95	0.11	89,89,89,89	0
54	MG	1A	3726	1/1	0.95	0.40	52,52,52,52	0
54	MG	1A	3762	1/1	0.95	0.25	49,49,49,49	0
54	MG	2a	1729	1/1	0.95	0.12	93,93,93,93	0
54	MG	1A	3646	1/1	0.95	0.18	71,71,71,71	0
54	MG	1A	3689	1/1	0.95	0.12	99,99,99,99	0
54	MG	2A	3497	1/1	0.95	0.10	67,67,67,67	0
54	MG	1A	3337	1/1	0.95	0.06	70,70,70,70	0
54	MG	1A	3571	1/1	0.95	0.10	42,42,42,42	0
54	MG	2A	3636	1/1	0.95	0.12	51,51,51,51	0
54	MG	1a	1716	1/1	0.95	0.11	77,77,77,77	0
54	MG	1A	3120	1/1	0.95	0.34	39,39,39,39	0
54	MG	2A	3318	1/1	0.95	0.16	38,38,38,38	0
54	MG	1a	1624	1/1	0.95	0.34	85,85,85,85	0
54	MG	2a	1694	1/1	0.95	0.30	95,95,95,95	0
54	MG	1A	3567	1/1	0.95	0.23	71,71,71,71	0
54	MG	1A	3344	1/1	0.95	0.13	45,45,45,45	0
54	MG	1A	3441	1/1	0.96	0.09	64,64,64,64	0
54	MG	1A	3157	1/1	0.96	0.18	42,42,42,42	0
54	MG	1D	302	1/1	0.96	0.16	55,55,55,55	0
54	MG	1R	204	1/1	0.96	0.27	53,53,53,53	0
54	MG	1A	3110	1/1	0.96	0.08	64,64,64,64	0
54	MG	1A	3875	1/1	0.96	0.16	78,78,78,78	0
54	MG	2A	3617	1/1	0.96	0.14	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1615	1/1	0.96	0.17	39,39,39,39	0
54	MG	1A	3163	1/1	0.96	0.14	50,50,50,50	0
54	MG	2A	3205	1/1	0.96	0.16	53,53,53,53	0
54	MG	1A	3829	1/1	0.96	0.13	73,73,73,73	0
54	MG	1A	3112	1/1	0.96	0.06	53,53,53,53	0
54	MG	1A	3077	1/1	0.96	0.06	64,64,64,64	0
54	MG	1A	3512	1/1	0.96	0.17	63,63,63,63	0
54	MG	1A	3141	1/1	0.96	0.67	45,45,45,45	0
54	MG	1A	3155	1/1	0.96	0.23	53,53,53,53	0
54	MG	2T	205	1/1	0.96	0.15	43,43,43,43	0
54	MG	1A	3812	1/1	0.96	0.10	55,55,55,55	0
54	MG	2A	3393	1/1	0.96	0.13	77,77,77,77	0
54	MG	1A	3616	1/1	0.96	0.13	61,61,61,61	0
54	MG	1A	3409	1/1	0.96	0.09	50,50,50,50	0
54	MG	2A	3476	1/1	0.96	0.21	78,78,78,78	0
54	MG	1A	3022	1/1	0.96	0.23	43,43,43,43	0
54	MG	1A	3371	1/1	0.96	0.10	52,52,52,52	0
54	MG	2A	3530	1/1	0.96	0.21	62,62,62,62	0
54	MG	2A	3468	1/1	0.96	0.18	45,45,45,45	0
54	MG	1A	3333	1/1	0.96	0.17	21,21,21,21	0
54	MG	1a	1825	1/1	0.96	0.21	61,61,61,61	0
54	MG	1A	3767	1/1	0.96	0.06	53,53,53,53	0
54	MG	1a	1814	1/1	0.96	0.21	65,65,65,65	0
54	MG	1A	3342	1/1	0.96	0.10	28,28,28,28	0
54	MG	1A	3667	1/1	0.96	0.11	32,32,32,32	0
54	MG	2A	3179	1/1	0.96	0.35	70,70,70,70	0
54	MG	1A	3769	1/1	0.96	0.05	69,69,69,69	0
54	MG	2a	1654	1/1	0.96	0.24	100,100,100,100	0
54	MG	2A	3510	1/1	0.96	0.06	45,45,45,45	0
54	MG	1A	3542	1/1	0.96	0.12	49,49,49,49	0
54	MG	1V	202	1/1	0.96	0.28	67,67,67,67	0
54	MG	11	104	1/1	0.96	0.41	61,61,61,61	0
53	MPD	18	101	8/8	0.96	0.28	47,49,54,59	0
54	MG	1A	3438	1/1	0.96	0.16	27,27,27,27	0
54	MG	1A	3685	1/1	0.96	0.10	51,51,51,51	0
54	MG	2A	3270	1/1	0.96	0.15	56,56,56,56	0
54	MG	1A	3847	1/1	0.96	0.15	38,38,38,38	0
54	MG	1A	3285	1/1	0.96	0.20	67,67,67,67	0
54	MG	1A	3156	1/1	0.96	0.29	39,39,39,39	0
54	MG	1A	3107	1/1	0.96	0.22	47,47,47,47	0
54	MG	1A	3272	1/1	0.96	0.12	23,23,23,23	0
54	MG	2A	3237	1/1	0.96	0.17	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3708	1/1	0.96	0.51	49,49,49,49	0
54	MG	1A	3094	1/1	0.96	0.09	58,58,58,58	0
54	MG	1A	3146	1/1	0.96	0.16	46,46,46,46	0
54	MG	1A	3209	1/1	0.96	0.16	35,35,35,35	0
54	MG	1Q	203	1/1	0.96	0.18	51,51,51,51	0
54	MG	1A	3873	1/1	0.96	0.15	56,56,56,56	0
54	MG	2A	3591	1/1	0.96	0.07	85,85,85,85	0
54	MG	1a	1640	1/1	0.96	0.17	75,75,75,75	0
54	MG	2A	3402	1/1	0.96	0.12	70,70,70,70	0
54	MG	1N	202	1/1	0.96	0.61	66,66,66,66	0
54	MG	1A	3002	1/1	0.96	0.15	46,46,46,46	0
54	MG	1A	3307	1/1	0.96	0.06	41,41,41,41	0
54	MG	2A	3315	1/1	0.96	0.10	50,50,50,50	0
54	MG	1a	1610	1/1	0.96	0.15	85,85,85,85	0
54	MG	1A	3206	1/1	0.96	0.46	40,40,40,40	0
54	MG	1N	201	1/1	0.96	0.33	49,49,49,49	0
54	MG	1A	3228	1/1	0.96	0.18	62,62,62,62	0
54	MG	17	101	1/1	0.96	0.96	44,44,44,44	0
54	MG	1A	3633	1/1	0.96	0.20	60,60,60,60	0
54	MG	1a	1688	1/1	0.96	0.42	36,36,36,36	0
54	MG	2A	3235	1/1	0.96	0.08	84,84,84,84	0
54	MG	1A	3553	1/1	0.96	0.43	57,57,57,57	0
54	MG	1A	3563	1/1	0.96	0.24	66,66,66,66	0
54	MG	1a	1736	1/1	0.96	0.04	76,76,76,76	0
54	MG	1A	3246	1/1	0.96	0.12	41,41,41,41	0
54	MG	1A	3761	1/1	0.96	0.17	38,38,38,38	0
54	MG	1A	3893	1/1	0.96	0.29	44,44,44,44	0
54	MG	1A	3889	1/1	0.96	0.28	50,50,50,50	0
54	MG	2A	3466	1/1	0.96	0.10	70,70,70,70	0
54	MG	2a	1648	1/1	0.96	0.35	64,64,64,64	0
54	MG	1A	3336	1/1	0.96	0.13	44,44,44,44	0
54	MG	1a	1834	1/1	0.96	0.18	74,74,74,74	0
54	MG	1A	3293	1/1	0.96	0.12	36,36,36,36	0
54	MG	2A	3611	1/1	0.96	0.12	63,63,63,63	0
54	MG	1A	3611	1/1	0.96	0.14	59,59,59,59	0
54	MG	1A	3105	1/1	0.96	0.19	52,52,52,52	0
54	MG	1A	3087	1/1	0.96	0.16	32,32,32,32	0
54	MG	1A	3467	1/1	0.96	0.14	67,67,67,67	0
54	MG	2A	3123	1/1	0.96	0.28	47,47,47,47	0
54	MG	2A	3558	1/1	0.96	0.11	70,70,70,70	0
54	MG	1a	1607	1/1	0.96	0.07	108,108,108,108	0
54	MG	1E	303	1/1	0.96	0.23	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3390	1/1	0.96	0.11	65,65,65,65	0
54	MG	1A	3884	1/1	0.96	0.07	37,37,37,37	0
54	MG	1A	3065	1/1	0.96	0.16	49,49,49,49	0
54	MG	1A	3419	1/1	0.96	0.14	64,64,64,64	0
54	MG	1A	3845	1/1	0.96	0.23	50,50,50,50	0
54	MG	2A	3465	1/1	0.96	0.12	69,69,69,69	0
54	MG	1A	3505	1/1	0.96	0.14	49,49,49,49	0
54	MG	1U	201	1/1	0.96	0.11	29,29,29,29	0
54	MG	2A	3260	1/1	0.96	0.14	48,48,48,48	0
54	MG	1A	3352	1/1	0.96	0.14	62,62,62,62	0
54	MG	1A	3295	1/1	0.96	0.17	26,26,26,26	0
54	MG	2A	3249	1/1	0.96	0.19	74,74,74,74	0
54	MG	1A	3844	1/1	0.96	0.10	63,63,63,63	0
54	MG	2D	305	1/1	0.96	0.15	48,48,48,48	0
54	MG	2A	3495	1/1	0.96	0.15	36,36,36,36	0
54	MG	1A	3631	1/1	0.96	0.14	47,47,47,47	0
54	MG	1A	3109	1/1	0.96	0.41	46,46,46,46	0
54	MG	1a	1618	1/1	0.96	0.22	81,81,81,81	0
54	MG	1A	3788	1/1	0.96	0.50	58,58,58,58	0
54	MG	1A	3572	1/1	0.96	0.14	61,61,61,61	0
54	MG	1A	3630	1/1	0.96	0.10	50,50,50,50	0
54	MG	2A	3296	1/1	0.96	0.17	47,47,47,47	0
54	MG	1A	3900	1/1	0.96	0.19	54,54,54,54	0
54	MG	2A	3406	1/1	0.96	0.09	72,72,72,72	0
54	MG	2A	3526	1/1	0.96	0.18	77,77,77,77	0
54	MG	2A	3631	1/1	0.96	0.19	82,82,82,82	0
54	MG	1a	1813	1/1	0.96	0.19	76,76,76,76	0
54	MG	2A	3616	1/1	0.96	0.11	67,67,67,67	0
54	MG	1a	1741	1/1	0.96	0.55	89,89,89,89	0
54	MG	1A	3226	1/1	0.96	0.08	53,53,53,53	0
54	MG	1A	3290	1/1	0.96	0.13	37,37,37,37	0
54	MG	1A	3400	1/1	0.96	0.12	50,50,50,50	0
54	MG	2a	1613	1/1	0.96	0.13	71,71,71,71	0
54	MG	1A	3271	1/1	0.96	0.14	39,39,39,39	0
54	MG	2A	3240	1/1	0.96	0.14	39,39,39,39	0
54	MG	1A	3752	1/1	0.96	0.08	37,37,37,37	0
54	MG	1a	1804	1/1	0.96	0.57	71,71,71,71	0
54	MG	1A	3459	1/1	0.96	0.17	58,58,58,58	0
54	MG	1a	1638	1/1	0.96	0.25	42,42,42,42	0
54	MG	1A	3854	1/1	0.96	0.19	34,34,34,34	0
54	MG	1A	3201	1/1	0.96	0.57	49,49,49,49	0
54	MG	1F	305	1/1	0.96	0.36	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3008	1/1	0.96	0.18	39,39,39,39	0
54	MG	1A	3187	1/1	0.96	0.08	51,51,51,51	0
54	MG	2A	3216	1/1	0.96	0.34	42,42,42,42	0
54	MG	2A	3387	1/1	0.96	0.08	63,63,63,63	0
54	MG	1A	3635	1/1	0.96	0.10	62,62,62,62	0
54	MG	2A	3294	1/1	0.96	0.11	60,60,60,60	0
54	MG	1A	3153	1/1	0.96	0.09	56,56,56,56	0
54	MG	1a	1642	1/1	0.96	0.20	84,84,84,84	0
54	MG	1A	3429	1/1	0.96	0.17	41,41,41,41	0
54	MG	1A	3335	1/1	0.96	0.23	38,38,38,38	0
54	MG	1A	3868	1/1	0.96	0.16	34,34,34,34	0
54	MG	1A	3101	1/1	0.96	0.37	46,46,46,46	0
54	MG	2A	3581	1/1	0.96	0.32	77,77,77,77	0
54	MG	1A	3590	1/1	0.96	0.08	61,61,61,61	0
54	MG	2A	3523	1/1	0.96	0.17	50,50,50,50	0
54	MG	1A	3325	1/1	0.96	0.12	57,57,57,57	0
54	MG	2A	3147	1/1	0.96	0.51	69,69,69,69	0
54	MG	1A	3055	1/1	0.96	0.21	40,40,40,40	0
54	MG	2a	1717	1/1	0.96	0.14	83,83,83,83	0
54	MG	1A	3004	1/1	0.97	0.43	48,48,48,48	0
54	MG	2A	3394	1/1	0.97	0.35	48,48,48,48	0
54	MG	1A	3632	1/1	0.97	0.14	57,57,57,57	0
54	MG	2A	3368	1/1	0.97	0.29	57,57,57,57	0
54	MG	1F	306	1/1	0.97	0.38	41,41,41,41	0
54	MG	1A	3284	1/1	0.97	0.22	60,60,60,60	0
54	MG	1a	1704	1/1	0.97	0.12	45,45,45,45	0
54	MG	2A	3594	1/1	0.97	0.15	88,88,88,88	0
54	MG	2A	3038	1/1	0.97	0.17	71,71,71,71	0
54	MG	2A	3547	1/1	0.97	0.16	72,72,72,72	0
54	MG	1A	3721	1/1	0.97	0.09	43,43,43,43	0
54	MG	2a	1676	1/1	0.97	0.15	93,93,93,93	0
54	MG	2A	3316	1/1	0.97	0.13	58,58,58,58	0
54	MG	2A	3470	1/1	0.97	0.06	46,46,46,46	0
54	MG	1a	1840	1/1	0.97	0.10	61,61,61,61	0
54	MG	1A	3458	1/1	0.97	0.08	41,41,41,41	0
54	MG	2A	3564	1/1	0.97	0.12	53,53,53,53	0
54	MG	1A	3084	1/1	0.97	0.16	40,40,40,40	0
54	MG	2A	3390	1/1	0.97	0.08	71,71,71,71	0
54	MG	1A	3644	1/1	0.97	0.24	45,45,45,45	0
54	MG	1A	3232	1/1	0.97	0.15	68,68,68,68	0
54	MG	1A	3692	1/1	0.97	0.26	41,41,41,41	0
54	MG	11	101	1/1	0.97	0.34	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1a	1721	1/1	0.97	0.08	53,53,53,53	0
54	MG	1R	205	1/1	0.97	0.16	49,49,49,49	0
54	MG	1A	3145	1/1	0.97	0.38	45,45,45,45	0
54	MG	2A	3217	1/1	0.97	0.44	60,60,60,60	0
54	MG	1D	310	1/1	0.97	0.13	53,53,53,53	0
54	MG	1A	3281	1/1	0.97	0.08	26,26,26,26	0
54	MG	1A	3315	1/1	0.97	0.17	48,48,48,48	0
54	MG	1A	3551	1/1	0.97	0.18	46,46,46,46	0
54	MG	1A	3189	1/1	0.97	0.26	43,43,43,43	0
54	MG	1A	3894	1/1	0.97	0.16	46,46,46,46	0
54	MG	1B	1005	1/1	0.97	0.13	71,71,71,71	0
54	MG	1A	3853	1/1	0.97	0.10	33,33,33,33	0
54	MG	1A	3254	1/1	0.97	0.50	62,62,62,62	0
54	MG	1A	3877	1/1	0.97	0.14	46,46,46,46	0
54	MG	1A	3367	1/1	0.97	0.13	46,46,46,46	0
54	MG	1A	3152	1/1	0.97	0.07	52,52,52,52	0
54	MG	1A	3503	1/1	0.97	0.06	66,66,66,66	0
54	MG	1A	3477	1/1	0.97	0.09	48,48,48,48	0
54	MG	1A	3483	1/1	0.97	0.14	39,39,39,39	0
54	MG	1A	3638	1/1	0.97	0.08	68,68,68,68	0
54	MG	2A	3551	1/1	0.97	0.23	86,86,86,86	0
54	MG	1A	3786	1/1	0.97	0.09	45,45,45,45	0
54	MG	1A	3647	1/1	0.97	0.31	58,58,58,58	0
54	MG	1A	3275	1/1	0.97	0.08	50,50,50,50	0
54	MG	1A	3768	1/1	0.97	0.12	51,51,51,51	0
54	MG	2A	3639	1/1	0.97	0.26	67,67,67,67	0
54	MG	2A	3310	1/1	0.97	0.17	55,55,55,55	0
54	MG	1a	1732	1/1	0.97	0.33	70,70,70,70	0
54	MG	1A	3552	1/1	0.97	0.29	36,36,36,36	0
54	MG	1A	3833	1/1	0.97	0.08	53,53,53,53	0
54	MG	1A	3121	1/1	0.97	0.47	43,43,43,43	0
54	MG	1A	3193	1/1	0.97	0.59	61,61,61,61	0
54	MG	2Q	202	1/1	0.97	0.14	70,70,70,70	0
54	MG	1A	3276	1/1	0.97	0.13	46,46,46,46	0
54	MG	1A	3765	1/1	0.97	0.06	38,38,38,38	0
54	MG	1A	3706	1/1	0.97	0.12	50,50,50,50	0
54	MG	2W	201	1/1	0.97	0.46	65,65,65,65	0
54	MG	2A	3037	1/1	0.97	0.31	52,52,52,52	0
54	MG	2A	3596	1/1	0.97	0.08	52,52,52,52	0
54	MG	2A	3434	1/1	0.97	0.16	47,47,47,47	0
54	MG	2A	3250	1/1	0.97	0.10	60,60,60,60	0
54	MG	1A	3014	1/1	0.97	0.18	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3092	1/1	0.97	0.12	29,29,29,29	0
54	MG	2A	3185	1/1	0.97	0.20	39,39,39,39	0
54	MG	1A	3693	1/1	0.97	0.42	56,56,56,56	0
54	MG	2a	1666	1/1	0.97	0.12	79,79,79,79	0
54	MG	1A	3488	1/1	0.97	0.12	49,49,49,49	0
54	MG	1a	1744	1/1	0.97	0.09	63,63,63,63	0
54	MG	1a	1644	1/1	0.97	0.26	55,55,55,55	0
54	MG	1A	3869	1/1	0.97	0.38	58,58,58,58	0
54	MG	1A	3046	1/1	0.97	0.34	46,46,46,46	0
54	MG	17	102	1/1	0.97	0.37	53,53,53,53	0
54	MG	2a	1661	1/1	0.97	0.22	84,84,84,84	0
54	MG	2A	3560	1/1	0.97	0.09	51,51,51,51	0
54	MG	1A	3223	1/1	0.97	0.17	55,55,55,55	0
54	MG	1A	3529	1/1	0.97	0.23	52,52,52,52	0
54	MG	2A	3218	1/1	0.97	0.19	73,73,73,73	0
54	MG	1A	3043	1/1	0.97	0.12	50,50,50,50	0
54	MG	2A	3116	1/1	0.97	0.17	45,45,45,45	0
54	MG	2A	3112	1/1	0.97	0.13	54,54,54,54	0
54	MG	1A	3579	1/1	0.97	0.12	49,49,49,49	0
54	MG	1A	3772	1/1	0.97	0.08	57,57,57,57	0
54	MG	1A	3099	1/1	0.97	0.48	51,51,51,51	0
54	MG	1A	3300	1/1	0.97	0.13	75,75,75,75	0
54	MG	1A	3368	1/1	0.97	0.19	54,54,54,54	0
54	MG	1A	3297	1/1	0.97	0.22	51,51,51,51	0
54	MG	2a	1678	1/1	0.97	0.20	53,53,53,53	0
54	MG	2A	3166	1/1	0.97	0.32	52,52,52,52	0
54	MG	2a	1672	1/1	0.97	0.47	55,55,55,55	0
54	MG	2A	3612	1/1	0.97	0.39	72,72,72,72	0
54	MG	1A	3151	1/1	0.97	0.16	46,46,46,46	0
54	MG	1A	3443	1/1	0.97	0.13	36,36,36,36	0
54	MG	1A	3378	1/1	0.97	0.13	71,71,71,71	0
54	MG	1A	3053	1/1	0.97	0.19	30,30,30,30	0
54	MG	1A	3701	1/1	0.97	0.17	47,47,47,47	0
54	MG	1A	3897	1/1	0.97	0.34	48,48,48,48	0
54	MG	2A	3293	1/1	0.97	0.09	44,44,44,44	0
54	MG	1A	3273	1/1	0.97	0.09	52,52,52,52	0
54	MG	2a	1751	1/1	0.97	0.16	60,60,60,60	0
54	MG	1A	3330	1/1	0.97	0.15	45,45,45,45	0
54	MG	1A	3431	1/1	0.97	0.12	36,36,36,36	0
54	MG	1A	3627	1/1	0.97	0.09	67,67,67,67	0
54	MG	1a	1680	1/1	0.97	0.19	105,105,105,105	0
54	MG	2A	3289	1/1	0.97	0.20	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3477	1/1	0.97	0.12	83,83,83,83	0
54	MG	1A	3013	1/1	0.97	0.22	36,36,36,36	0
54	MG	1A	3003	1/1	0.97	0.07	58,58,58,58	0
54	MG	1A	3288	1/1	0.97	0.07	39,39,39,39	0
54	MG	1A	3088	1/1	0.97	0.17	52,52,52,52	0
54	MG	2A	3590	1/1	0.97	0.08	52,52,52,52	0
54	MG	2a	1705	1/1	0.97	0.21	93,93,93,93	0
54	MG	1A	3774	1/1	0.97	0.10	65,65,65,65	0
54	MG	1A	3816	1/1	0.97	0.20	34,34,34,34	0
54	MG	2A	3291	1/1	0.97	0.20	64,64,64,64	0
54	MG	1A	3620	1/1	0.97	0.17	47,47,47,47	0
54	MG	1a	1728	1/1	0.97	0.08	65,65,65,65	0
54	MG	1A	3078	1/1	0.97	0.26	51,51,51,51	0
54	MG	2A	3229	1/1	0.97	0.21	56,56,56,56	0
54	MG	1A	3655	1/1	0.97	0.15	67,67,67,67	0
54	MG	1A	3235	1/1	0.97	0.20	53,53,53,53	0
54	MG	2E	301	1/1	0.97	0.09	39,39,39,39	0
54	MG	1A	3122	1/1	0.97	0.18	59,59,59,59	0
54	MG	2A	3226	1/1	0.97	0.26	52,52,52,52	0
54	MG	1D	306	1/1	0.97	0.14	53,53,53,53	0
54	MG	1a	1678	1/1	0.97	0.20	57,57,57,57	0
54	MG	1A	3830	1/1	0.97	0.21	59,59,59,59	0
54	MG	1A	3248	1/1	0.97	0.15	42,42,42,42	0
54	MG	1A	3791	1/1	0.97	0.10	48,48,48,48	0
54	MG	2A	3033	1/1	0.97	0.23	76,76,76,76	0
54	MG	1A	3448	1/1	0.97	0.24	24,24,24,24	0
54	MG	1A	3634	1/1	0.97	0.14	43,43,43,43	0
54	MG	1A	3377	1/1	0.97	0.33	55,55,55,55	0
54	MG	1A	3500	1/1	0.97	0.13	73,73,73,73	0
54	MG	1A	3294	1/1	0.97	0.18	31,31,31,31	0
54	MG	1F	301	1/1	0.97	0.09	43,43,43,43	0
54	MG	1A	3507	1/1	0.97	0.15	50,50,50,50	0
54	MG	1A	3813	1/1	0.97	0.28	75,75,75,75	0
54	MG	1A	3501	1/1	0.97	0.13	32,32,32,32	0
54	MG	16	102	1/1	0.97	0.04	54,54,54,54	0
54	MG	1A	3034	1/1	0.97	0.15	60,60,60,60	0
54	MG	1A	3351	1/1	0.97	0.05	66,66,66,66	0
54	MG	1A	3066	1/1	0.97	0.28	66,66,66,66	0
54	MG	1A	3882	1/1	0.97	0.29	42,42,42,42	0
54	MG	2A	3192	1/1	0.97	0.13	45,45,45,45	0
54	MG	1A	3464	1/1	0.97	0.08	53,53,53,53	0
54	MG	2A	3366	1/1	0.98	0.24	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3379	1/1	0.98	0.24	73,73,73,73	0
54	MG	1a	1717	1/1	0.98	0.10	46,46,46,46	0
54	MG	1A	3339	1/1	0.98	0.22	34,34,34,34	0
56	ZN	2Y	202	1/1	0.98	0.06	95,95,95,95	0
54	MG	1A	3846	1/1	0.98	0.08	43,43,43,43	0
54	MG	2A	3015	1/1	0.98	0.13	53,53,53,53	0
54	MG	1A	3176	1/1	0.98	0.18	42,42,42,42	0
54	MG	1A	3197	1/1	0.98	0.16	49,49,49,49	0
54	MG	1A	3237	1/1	0.98	0.13	61,61,61,61	0
54	MG	1A	3546	1/1	0.98	0.11	43,43,43,43	0
54	MG	1A	3652	1/1	0.98	0.06	54,54,54,54	0
54	MG	2I	102	1/1	0.98	0.07	63,63,63,63	0
54	MG	1A	3576	1/1	0.98	0.07	71,71,71,71	0
54	MG	1A	3610	1/1	0.98	0.08	42,42,42,42	0
54	MG	2A	3227	1/1	0.98	0.16	72,72,72,72	0
54	MG	1A	3453	1/1	0.98	0.20	39,39,39,39	0
54	MG	2A	3208	1/1	0.98	0.17	68,68,68,68	0
54	MG	1A	3287	1/1	0.98	0.21	47,47,47,47	0
54	MG	1A	3060	1/1	0.98	0.18	34,34,34,34	0
54	MG	2D	304	1/1	0.98	0.42	51,51,51,51	0
54	MG	1A	3379	1/1	0.98	0.06	55,55,55,55	0
54	MG	1P	201	1/1	0.98	0.13	83,83,83,83	0
56	ZN	29	101	1/1	0.98	0.07	101,101,101,101	0
54	MG	1A	3460	1/1	0.98	0.15	46,46,46,46	0
54	MG	1E	302	1/1	0.98	0.17	24,24,24,24	0
54	MG	1A	3100	1/1	0.98	0.31	49,49,49,49	0
56	ZN	25	101	1/1	0.98	0.07	83,83,83,83	0
54	MG	10	102	1/1	0.98	0.07	76,76,76,76	0
54	MG	2A	3559	1/1	0.98	0.21	50,50,50,50	0
54	MG	1A	3660	1/1	0.98	0.07	52,52,52,52	0
54	MG	1A	3349	1/1	0.98	0.15	62,62,62,62	0
54	MG	1A	3462	1/1	0.98	0.14	33,33,33,33	0
54	MG	2a	1712	1/1	0.98	0.15	75,75,75,75	0
54	MG	1A	3800	1/1	0.98	0.25	61,61,61,61	0
54	MG	2A	3626	1/1	0.98	0.17	44,44,44,44	0
54	MG	1A	3323	1/1	0.98	0.12	67,67,67,67	0
54	MG	1A	3717	1/1	0.98	0.05	44,44,44,44	0
54	MG	1A	3090	1/1	0.98	0.26	36,36,36,36	0
54	MG	1A	3184	1/1	0.98	0.26	65,65,65,65	0
54	MG	1A	3233	1/1	0.98	0.17	66,66,66,66	0
54	MG	1A	3202	1/1	0.98	0.24	33,33,33,33	0
54	MG	1F	309	1/1	0.98	0.17	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3302	1/1	0.98	0.08	43,43,43,43	0
54	MG	1A	3240	1/1	0.98	0.16	46,46,46,46	0
54	MG	1A	3064	1/1	0.98	0.21	43,43,43,43	0
54	MG	1A	3174	1/1	0.98	0.25	53,53,53,53	0
54	MG	1B	1014	1/1	0.98	0.05	50,50,50,50	0
54	MG	1A	3404	1/1	0.98	0.07	55,55,55,55	0
54	MG	2A	3417	1/1	0.98	0.30	60,60,60,60	0
54	MG	1a	1654	1/1	0.98	0.23	80,80,80,80	0
54	MG	1B	1013	1/1	0.98	0.11	49,49,49,49	0
54	MG	1a	1805	1/1	0.98	0.16	53,53,53,53	0
54	MG	1A	3142	1/1	0.98	0.23	36,36,36,36	0
54	MG	1A	3519	1/1	0.98	0.22	39,39,39,39	0
54	MG	1A	3081	1/1	0.98	0.08	61,61,61,61	0
54	MG	1A	3214	1/1	0.98	0.23	40,40,40,40	0
54	MG	1A	3645	1/1	0.98	0.15	52,52,52,52	0
54	MG	1A	3763	1/1	0.98	0.37	46,46,46,46	0
54	MG	2A	3479	1/1	0.98	0.16	52,52,52,52	0
54	MG	1A	3041	1/1	0.98	0.12	32,32,32,32	0
54	MG	1A	3358	1/1	0.98	0.05	54,54,54,54	0
54	MG	1a	1723	1/1	0.98	0.21	75,75,75,75	0
54	MG	2A	3028	1/1	0.98	0.31	44,44,44,44	0
54	MG	1A	3842	1/1	0.98	0.06	35,35,35,35	0
54	MG	1a	1648	1/1	0.98	0.30	56,56,56,56	0
54	MG	1A	3494	1/1	0.98	0.07	53,53,53,53	0
54	MG	1A	3393	1/1	0.98	0.10	60,60,60,60	0
54	MG	2A	3070	1/1	0.98	0.16	59,59,59,59	0
54	MG	1A	3698	1/1	0.98	0.13	69,69,69,69	0
56	ZN	26	101	1/1	0.98	0.12	72,72,72,72	0
54	MG	2A	3625	1/1	0.98	0.26	56,56,56,56	0
54	MG	2A	3548	1/1	0.98	0.12	62,62,62,62	0
54	MG	2A	3446	1/1	0.98	0.16	53,53,53,53	0
54	MG	2A	3095	1/1	0.98	0.16	58,58,58,58	0
54	MG	1A	3370	1/1	0.98	0.12	25,25,25,25	0
54	MG	2A	3512	1/1	0.98	0.09	67,67,67,67	0
54	MG	1A	3168	1/1	0.98	0.19	58,58,58,58	0
54	MG	2A	3092	1/1	0.98	0.10	53,53,53,53	0
56	ZN	1n	102	1/1	0.98	0.11	94,94,94,94	0
54	MG	1A	3040	1/1	0.98	0.31	32,32,32,32	0
54	MG	2A	3276	1/1	0.98	0.10	47,47,47,47	0
54	MG	1A	3670	1/1	0.98	0.18	56,56,56,56	0
54	MG	1A	3511	1/1	0.98	0.09	52,52,52,52	0
54	MG	1A	3696	1/1	0.98	0.10	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	1A	3074	1/1	0.98	0.22	47,47,47,47	0
54	MG	1A	3661	1/1	0.98	0.06	32,32,32,32	0
54	MG	2A	3182	1/1	0.98	0.15	53,53,53,53	0
54	MG	1A	3736	1/1	0.98	0.14	37,37,37,37	0
54	MG	1a	1626	1/1	0.98	0.33	70,70,70,70	0
54	MG	1A	3485	1/1	0.98	0.07	54,54,54,54	0
54	MG	1A	3029	1/1	0.98	0.22	44,44,44,44	0
54	MG	1A	3310	1/1	0.98	0.14	44,44,44,44	0
54	MG	1A	3561	1/1	0.98	0.59	70,70,70,70	0
54	MG	1A	3247	1/1	0.98	0.23	27,27,27,27	0
54	MG	1A	3513	1/1	0.98	0.24	63,63,63,63	0
54	MG	1a	1846	1/1	0.98	0.06	43,43,43,43	0
54	MG	1A	3264	1/1	0.98	0.09	47,47,47,47	0
54	MG	1A	3625	1/1	0.98	0.21	54,54,54,54	0
54	MG	1a	1715	1/1	0.98	0.06	54,54,54,54	0
54	MG	2A	3546	1/1	0.98	0.10	69,69,69,69	0
54	MG	2A	3634	1/1	0.98	0.14	56,56,56,56	0
54	MG	2A	3100	1/1	0.98	0.42	69,69,69,69	0
54	MG	2A	3043	1/1	0.98	0.12	60,60,60,60	0
54	MG	1A	3154	1/1	0.98	0.10	35,35,35,35	0
54	MG	1A	3208	1/1	0.98	0.12	40,40,40,40	0
54	MG	2A	3019	1/1	0.98	0.20	80,80,80,80	0
54	MG	2D	303	1/1	0.98	0.17	52,52,52,52	0
54	MG	1A	3314	1/1	0.98	0.11	35,35,35,35	0
54	MG	1A	3132	1/1	0.98	0.14	39,39,39,39	0
54	MG	1a	1702	1/1	0.98	0.11	47,47,47,47	0
54	MG	1A	3671	1/1	0.98	0.18	39,39,39,39	0
54	MG	1A	3115	1/1	0.98	0.24	42,42,42,42	0
54	MG	1A	3188	1/1	0.98	0.11	38,38,38,38	0
54	MG	1R	206	1/1	0.98	0.12	33,33,33,33	0
54	MG	1A	3509	1/1	0.98	0.14	52,52,52,52	0
54	MG	1A	3067	1/1	0.98	0.16	46,46,46,46	0
54	MG	1A	3407	1/1	0.98	0.21	41,41,41,41	0
54	MG	1A	3405	1/1	0.98	0.21	54,54,54,54	0
54	MG	1A	3522	1/1	0.98	0.14	59,59,59,59	0
54	MG	1A	3076	1/1	0.98	0.16	46,46,46,46	0
54	MG	1A	3499	1/1	0.98	0.13	53,53,53,53	0
54	MG	1A	3032	1/1	0.99	0.09	45,45,45,45	0
54	MG	1A	3461	1/1	0.99	0.12	42,42,42,42	0
54	MG	1A	3318	1/1	0.99	0.15	32,32,32,32	0
54	MG	1A	3061	1/1	0.99	0.23	48,48,48,48	0
54	MG	1A	3070	1/1	0.99	0.16	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	MG	2A	3129	1/1	0.99	0.18	37,37,37,37	0
54	MG	1A	3181	1/1	0.99	0.39	46,46,46,46	0
54	MG	2A	3290	1/1	0.99	0.11	57,57,57,57	0
54	MG	1A	3196	1/1	0.99	0.12	37,37,37,37	0
54	MG	1A	3068	1/1	0.99	0.21	36,36,36,36	0
54	MG	1A	3559	1/1	0.99	0.20	61,61,61,61	0
54	MG	1A	3380	1/1	0.99	0.08	23,23,23,23	0
54	MG	1A	3863	1/1	0.99	0.09	50,50,50,50	0
54	MG	1A	3019	1/1	0.99	0.17	45,45,45,45	0
54	MG	1A	3883	1/1	0.99	0.45	51,51,51,51	0
54	MG	1A	3601	1/1	0.99	0.18	39,39,39,39	0
54	MG	1A	3480	1/1	0.99	0.45	50,50,50,50	0
54	MG	1A	3719	1/1	0.99	0.08	51,51,51,51	0
54	MG	1A	3025	1/1	0.99	0.24	38,38,38,38	0
57	SF4	1d	501	8/8	0.99	0.17	77,92,105,112	0
56	ZN	15	102	1/1	0.99	0.07	53,53,53,53	0
54	MG	1A	3015	1/1	0.99	0.28	36,36,36,36	0
57	SF4	2d	501	8/8	0.99	0.15	71,89,97,104	0
54	MG	1a	1767	1/1	0.99	0.05	46,46,46,46	0
54	MG	1A	3770	1/1	0.99	0.06	37,37,37,37	0
54	MG	1A	3862	1/1	0.99	0.08	35,35,35,35	0
54	MG	1A	3550	1/1	0.99	0.07	46,46,46,46	0
54	MG	1A	3186	1/1	0.99	0.34	60,60,60,60	0
54	MG	2A	3599	1/1	0.99	0.11	48,48,48,48	0
54	MG	2A	3635	1/1	0.99	0.27	64,64,64,64	0
54	MG	1A	3751	1/1	0.99	0.04	47,47,47,47	0
54	MG	2A	3571	1/1	0.99	0.06	68,68,68,68	0
56	ZN	1Y	201	1/1	0.99	0.10	83,83,83,83	0
54	MG	1A	3045	1/1	0.99	0.13	41,41,41,41	0
54	MG	1A	3838	1/1	0.99	0.22	42,42,42,42	0
54	MG	2A	3142	1/1	0.99	0.33	28,28,28,28	0
54	MG	1A	3256	1/1	0.99	0.09	48,48,48,48	0
54	MG	1A	3095	1/1	0.99	0.24	41,41,41,41	0
54	MG	1A	3722	1/1	0.99	0.07	35,35,35,35	0
54	MG	1A	3255	1/1	0.99	0.12	42,42,42,42	0
54	MG	1A	3820	1/1	0.99	0.30	59,59,59,59	0
56	ZN	19	102	1/1	0.99	0.11	50,50,50,50	0
54	MG	1A	3387	1/1	0.99	0.12	33,33,33,33	0
54	MG	1A	3096	1/1	1.00	0.18	47,47,47,47	0
56	ZN	16	101	1/1	1.00	0.10	52,52,52,52	0
54	MG	1A	3388	1/1	1.00	0.11	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.