



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:49 pm BST

PDB ID : 5J4C
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with cisplatin (soaked) and bound to mRNA and A-, P- and E-site tRNAs at 2.8Å resolution
Authors : Melnikov, S.V.; Soll, D.; Steitz, T.A.; Polikanov, Y.S.
Deposited on : 2016-03-31
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

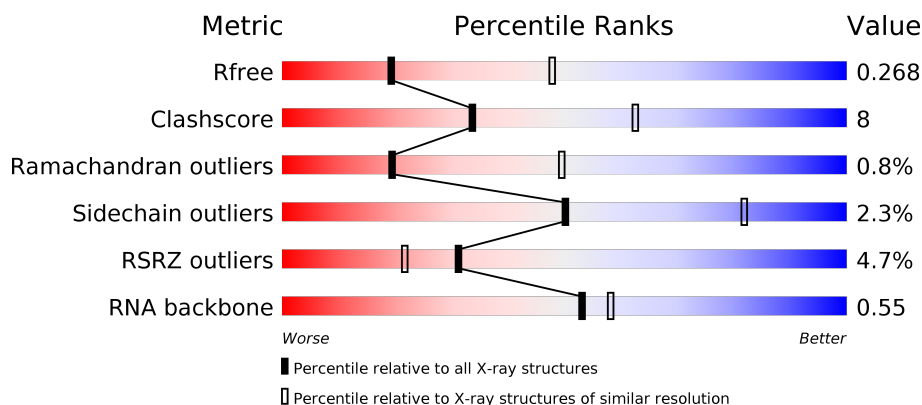
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



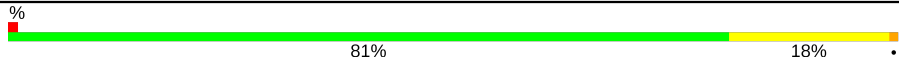

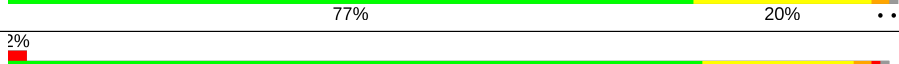
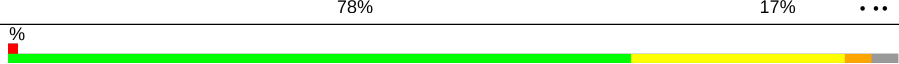
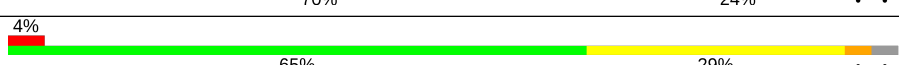


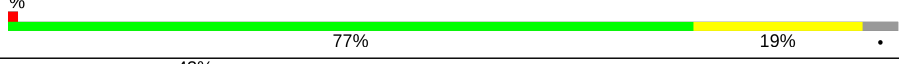



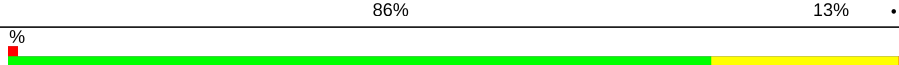

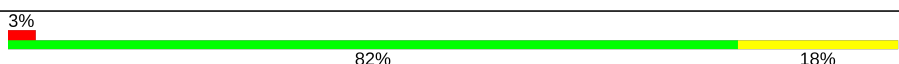
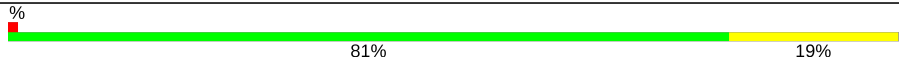

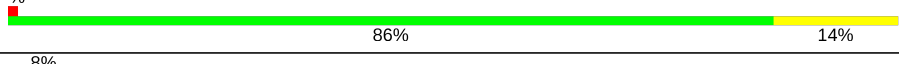



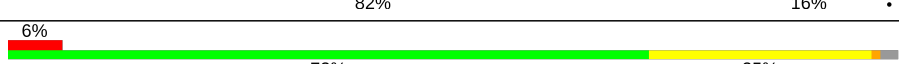
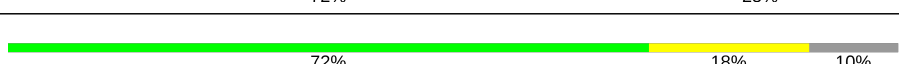



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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

Mol	Chain	Length	Quality of chain
1	1A	2915	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>28%</div> <div>6%</div> </div> </div>
1	2A	2915	<div> <div>%</div> <div> <div></div> <div>53%</div> <div>36%</div> <div>7%</div> </div> </div>
2	1B	121	<div> <div></div> <div> <div></div> <div>66%</div> <div>31%</div> </div> </div>
2	2B	121	<div> <div>%</div> <div> <div></div> <div>49%</div> <div>40%</div> <div>11%</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	















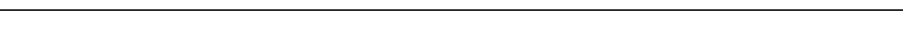
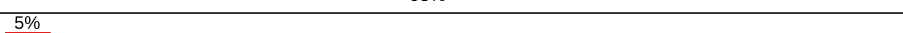
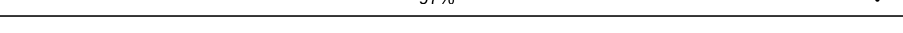


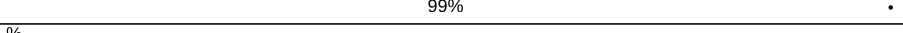
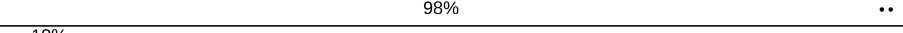
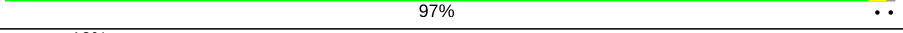
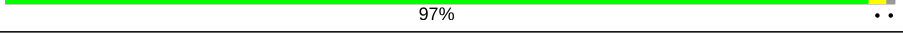
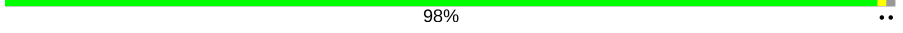
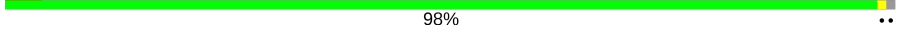
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Mol	Chain	Length	Quality of chain
15	2T	146	<div> <div>3%</div> <div>74%</div> <div>16%</div> <div>10%</div> </div>
16	1U	118	<div> <div>%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
16	2U	118	<div> <div>2%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>
17	1V	101	<div> <div>82%</div> <div>16%</div> <div>..</div> </div>
17	2V	101	<div> <div>6%</div> <div>76%</div> <div>21%</div> <div>..</div> </div>
18	1W	113	<div> <div>2%</div> <div>84%</div> <div>14%</div> <div>..</div> </div>
18	2W	113	<div> <div>%</div> <div>84%</div> <div>12%</div> <div>..</div> </div>
19	1X	96	<div> <div>79%</div> <div>20%</div> <div>.</div> </div>
19	2X	96	<div> <div>5%</div> <div>80%</div> <div>18%</div> <div>..</div> </div>
20	1Y	110	<div> <div>%</div> <div>75%</div> <div>21%</div> <div>..</div> </div>
20	2Y	110	<div> <div>3%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>
21	1Z	206	<div> <div>3%</div> <div>60%</div> <div>14%</div> <div>25%</div> </div>
21	2Z	206	<div> <div>12%</div> <div>52%</div> <div>24%</div> <div>22%</div> </div>
22	10	85	<div> <div>%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
22	20	85	<div> <div>%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>
23	11	98	<div> <div>3%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
23	21	98	<div> <div>4%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
24	12	72	<div> <div>78%</div> <div>19%</div> <div>.</div> </div>
24	22	72	<div> <div>4%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
25	13	60	<div> <div>2%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
25	23	60	<div> <div>8%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
26	14	71	<div> <div>18%</div> <div>62%</div> <div>28%</div> <div>7%</div> <div>.</div> </div>
26	24	71	<div> <div>21%</div> <div>63%</div> <div>27%</div> <div>7%</div> <div>.</div> </div>
27	15	60	<div> <div>2%</div> <div>83%</div> <div>12%</div> <div>..</div> </div>
27	25	60	<div> <div>78%</div> <div>17%</div> <div>..</div> </div>

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

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

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	10	102	-	-	-	X
56	MG	15	102	-	-	-	X
56	MG	16	102	-	-	-	X
56	MG	1A	3091	-	-	-	X
56	MG	1A	3112	-	-	-	X
56	MG	1A	3151	-	-	-	X
56	MG	1A	3222	-	-	-	X
56	MG	1A	3251	-	-	-	X
56	MG	1A	3312	-	-	-	X
56	MG	1A	3351	-	-	-	X
56	MG	1A	3366	-	-	-	X
56	MG	1A	3367	-	-	-	X
56	MG	1A	3369	-	-	-	X
56	MG	1A	3370	-	-	-	X
56	MG	1A	3375	-	-	-	X
56	MG	1A	3383	-	-	-	X
56	MG	1A	3392	-	-	-	X
56	MG	1A	3417	-	-	-	X
56	MG	1A	3560	-	-	-	X
56	MG	1A	3575	-	-	-	X
56	MG	1A	3688	-	-	-	X
56	MG	1A	4066	-	-	-	X
56	MG	1A	4114	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
56	MG	1A	4146	-	-	-	X
56	MG	1A	4186	-	-	-	X
56	MG	1B	227	-	-	-	X
56	MG	1a	1602	-	-	-	X
56	MG	1a	1615	-	-	-	X
56	MG	1a	1723	-	-	-	X
56	MG	1w	103	-	-	-	X
56	MG	1x	102	-	-	-	X
56	MG	23	3001	-	-	-	X
56	MG	2A	3057	-	-	-	X
56	MG	2A	3092	-	-	-	X
56	MG	2A	3195	-	-	-	X
56	MG	2A	3214	-	-	-	X
56	MG	2A	3248	-	-	-	X
56	MG	2A	3251	-	-	-	X
56	MG	2A	3270	-	-	-	X
56	MG	2A	3301	-	-	-	X
56	MG	2A	3343	-	-	-	X
56	MG	2A	3377	-	-	-	X
56	MG	2A	3382	-	-	-	X
56	MG	2A	3387	-	-	-	X
56	MG	2A	3394	-	-	-	X
56	MG	2A	3411	-	-	-	X
56	MG	2A	3456	-	-	-	X
56	MG	2A	3479	-	-	-	X
56	MG	2A	3495	-	-	-	X
56	MG	2A	3792	-	-	-	X
56	MG	2A	3823	-	-	-	X
56	MG	2B	3011	-	-	-	X
56	MG	2a	3026	-	-	-	X
56	MG	2a	3029	-	-	-	X
56	MG	2a	3031	-	-	-	X
56	MG	2a	3034	-	-	-	X
56	MG	2a	3057	-	-	-	X
56	MG	2a	3060	-	-	-	X
56	MG	2a	3064	-	-	-	X
56	MG	2a	3086	-	-	-	X
56	MG	2a	3222	-	-	-	X
56	MG	2l	3001	-	-	-	X
56	MG	2v	102	-	-	-	X
56	MG	2v	103	-	-	-	X
56	MG	2w	103	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	CPT	1a	1930	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 301288 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	173	Total	C	N	O	S	0	0	0
			1321	839	246	235	1			
7	2H	173	Total	C	N	O	S	0	0	0
			1321	839	246	235	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0
			1592	713	285	518	74	2		
54	1y	74	Total	C	N	O	P	S	0	0
			1585	707	285	518	74	1		
54	2w	72	Total	C	N	O	P	S	0	0
			1544	690	278	502	72	2		
54	2y	73	Total	C	N	O	P	S	0	0
			1565	698	283	510	73	1		

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		
55	2x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2E	8	Total	Mg	0	0
			8	8		
56	17	4	Total	Mg	0	0
			4	4		
56	2d	1	Total	Mg	0	0
			1	1		
56	1T	2	Total	Mg	0	0
			2	2		
56	1N	7	Total	Mg	0	0
			7	7		
56	20	3	Total	Mg	0	0
			3	3		
56	18	3	Total	Mg	0	0
			3	3		
56	2W	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1Y	2	Total Mg 2 2	0	0
56	13	2	Total Mg 2 2	0	0
56	1f	2	Total Mg 2 2	0	0
56	1P	3	Total Mg 3 3	0	0
56	2B	21	Total Mg 21 21	0	0
56	2w	7	Total Mg 7 7	0	0
56	2a	236	Total Mg 236 236	0	0
56	1E	13	Total Mg 13 13	0	0
56	1b	2	Total Mg 2 2	0	0
56	2l	4	Total Mg 4 4	0	0
56	2F	4	Total Mg 4 4	0	0
56	16	2	Total Mg 2 2	0	0
56	28	3	Total Mg 3 3	0	0
56	2e	1	Total Mg 1 1	0	0
56	1W	6	Total Mg 6 6	0	0
56	1A	1254	Total Mg 1254 1254	0	0
56	1t	1	Total Mg 1 1	0	0
56	2p	1	Total Mg 1 1	0	0
56	1n	1	Total Mg 1 1	0	0
56	2P	2	Total Mg 2 2	0	0
56	1X	6	Total Mg 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	12	2	Total Mg 2 2	0	0
56	1y	5	Total Mg 5 5	0	0
56	1S	3	Total Mg 3 3	0	0
56	25	4	Total Mg 4 4	0	0
56	2T	1	Total Mg 1 1	0	0
56	1D	12	Total Mg 12 12	0	0
56	2N	1	Total Mg 1 1	0	0
56	1e	2	Total Mg 2 2	0	0
56	2G	1	Total Mg 1 1	0	0
56	1I	1	Total Mg 1 1	0	0
56	2f	2	Total Mg 2 2	0	0
56	1V	2	Total Mg 2 2	0	0
56	2X	2	Total Mg 2 2	0	0
56	1w	11	Total Mg 11 11	0	0
56	1a	330	Total Mg 330 330	0	0
56	2Q	3	Total Mg 3 3	0	0
56	15	4	Total Mg 4 4	0	0
56	1x	18	Total Mg 18 18	0	0
56	2j	2	Total Mg 2 2	0	0
56	1R	3	Total Mg 3 3	0	0
56	1s	1	Total Mg 1 1	0	0

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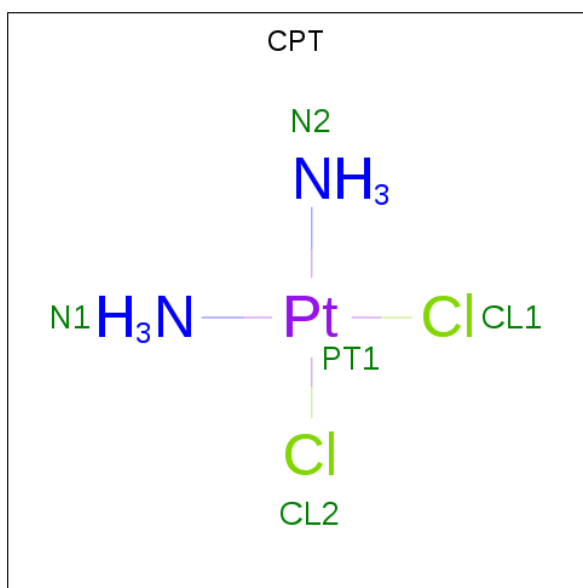
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1m	1	Total Mg 1 1	0	0
56	2U	6	Total Mg 6 6	0	0
56	1G	5	Total Mg 5 5	0	0
56	2O	1	Total Mg 1 1	0	0
56	1l	3	Total Mg 3 3	0	0
56	1d	1	Total Mg 1 1	0	0
56	2n	1	Total Mg 1 1	0	0
56	1H	1	Total Mg 1 1	0	0
56	2g	1	Total Mg 1 1	0	0
56	1v	1	Total Mg 1 1	0	0
56	2x	6	Total Mg 6 6	0	0
56	2R	2	Total Mg 2 2	0	0
56	1Z	3	Total Mg 3 3	0	0
56	2D	3	Total Mg 3 3	0	0
56	2q	4	Total Mg 4 4	0	0
56	1U	6	Total Mg 6 6	0	0
56	2r	1	Total Mg 1 1	0	0
56	1O	5	Total Mg 5 5	0	0
56	27	1	Total Mg 1 1	0	0
56	19	2	Total Mg 2 2	0	0
56	1l	4	Total Mg 4 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2V	1	Total Mg 1 1	0	0
56	1F	10	Total Mg 10 10	0	0
56	10	7	Total Mg 7 7	0	0
56	2t	1	Total Mg 1 1	0	0
56	1Q	5	Total Mg 5 5	0	0
56	2A	919	Total Mg 919 919	0	0
56	23	3	Total Mg 3 3	0	0
56	2Z	1	Total Mg 1 1	0	0
56	1B	36	Total Mg 36 36	0	0
56	2y	7	Total Mg 7 7	0	0
56	1c	2	Total Mg 2 2	0	0
56	2v	6	Total Mg 6 6	0	0

- Molecule 57 is Cisplatin (three-letter code: CPT) (formula: $\text{Cl}_2\text{H}_6\text{N}_2\text{Pt}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	1A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	1A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	1I	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	1a	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	2A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	2A	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	2I	1	Total	Cl	N	Pt	0	0
			4	1	2	1		
57	2a	1	Total	Cl	N	Pt	0	0
			4	1	2	1		

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

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

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

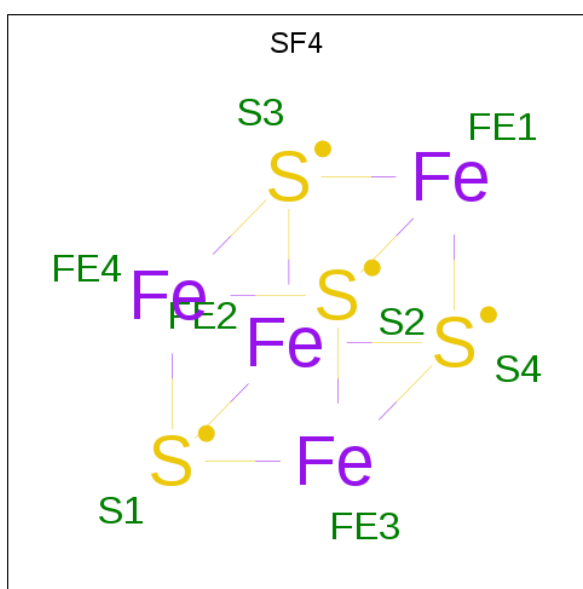
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	29	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	24	1	Total	Zn	0	0
			1	1		
59	2n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	1d	1	Total	Fe	S	0	0
			8	4	4		
60	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2273	Total	O	0	0
			2273	2273		
61	1B	70	Total	O	0	0
			70	70		
61	1D	28	Total	O	0	0
			28	28		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1E	27	Total 27	O 27	0	0
61	1F	15	Total 15	O 15	0	0
61	1G	7	Total 7	O 7	0	0
61	1H	1	Total 1	O 1	0	0
61	1I	1	Total 1	O 1	0	0
61	1N	3	Total 3	O 3	0	0
61	1O	6	Total 6	O 6	0	0
61	1P	23	Total 23	O 23	0	0
61	1Q	12	Total 12	O 12	0	0
61	1R	15	Total 15	O 15	0	0
61	1S	5	Total 5	O 5	0	0
61	1T	10	Total 10	O 10	0	0
61	1U	16	Total 16	O 16	0	0
61	1V	11	Total 11	O 11	0	0
61	1W	13	Total 13	O 13	0	0
61	1X	6	Total 6	O 6	0	0
61	1Y	5	Total 5	O 5	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	12	Total 12	O 12	0	0
61	11	14	Total 14	O 14	0	0
61	12	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	13	5	Total 5	O 5	0	0
61	14	1	Total 1	O 1	0	0
61	15	7	Total 7	O 7	0	0
61	16	2	Total 2	O 2	0	0
61	17	7	Total 7	O 7	0	0
61	18	10	Total 10	O 10	0	0
61	1a	520	Total 520	O 520	0	0
61	1b	1	Total 1	O 1	0	0
61	1d	2	Total 2	O 2	0	0
61	1e	1	Total 1	O 1	0	0
61	1g	2	Total 2	O 2	0	0
61	1i	1	Total 1	O 1	0	0
61	1l	10	Total 10	O 10	0	0
61	1m	2	Total 2	O 2	0	0
61	1n	1	Total 1	O 1	0	0
61	1o	2	Total 2	O 2	0	0
61	1p	2	Total 2	O 2	0	0
61	1q	3	Total 3	O 3	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	5	Total 5	O 5	0	0
61	1w	19	Total 19	O 19	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1x	15	Total 15	O 15	0	0
61	1y	2	Total 2	O 2	0	0
61	2A	1393	Total 1393	O 1393	0	0
61	2B	28	Total 28	O 28	0	0
61	2D	29	Total 29	O 29	0	0
61	2E	18	Total 18	O 18	0	0
61	2F	17	Total 17	O 17	0	0
61	2I	4	Total 4	O 4	0	0
61	2N	1	Total 1	O 1	0	0
61	2O	1	Total 1	O 1	0	0
61	2P	16	Total 16	O 16	0	0
61	2Q	2	Total 2	O 2	0	0
61	2R	2	Total 2	O 2	0	0
61	2T	7	Total 7	O 7	0	0
61	2U	3	Total 3	O 3	0	0
61	2V	2	Total 2	O 2	0	0
61	2W	4	Total 4	O 4	0	0
61	2X	2	Total 2	O 2	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	2	Total 2	O 2	0	0
61	20	4	Total 4	O 4	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	21	11	Total 11	O 11	0	0
61	22	1	Total 1	O 1	0	0
61	23	1	Total 1	O 1	0	0
61	25	3	Total 3	O 3	0	0
61	27	3	Total 3	O 3	0	0
61	28	4	Total 4	O 4	0	0
61	29	1	Total 1	O 1	0	0
61	2a	373	Total 373	O 373	0	0
61	2d	2	Total 2	O 2	0	0
61	2e	2	Total 2	O 2	0	0
61	2g	1	Total 1	O 1	0	0
61	2i	1	Total 1	O 1	0	0
61	2j	4	Total 4	O 4	0	0
61	2l	6	Total 6	O 6	0	0
61	2p	1	Total 1	O 1	0	0
61	2q	1	Total 1	O 1	0	0
61	2r	1	Total 1	O 1	0	0
61	2t	4	Total 4	O 4	0	0
61	2v	2	Total 2	O 2	0	0
61	2w	3	Total 3	O 3	0	0
61	2x	9	Total 9	O 9	0	0

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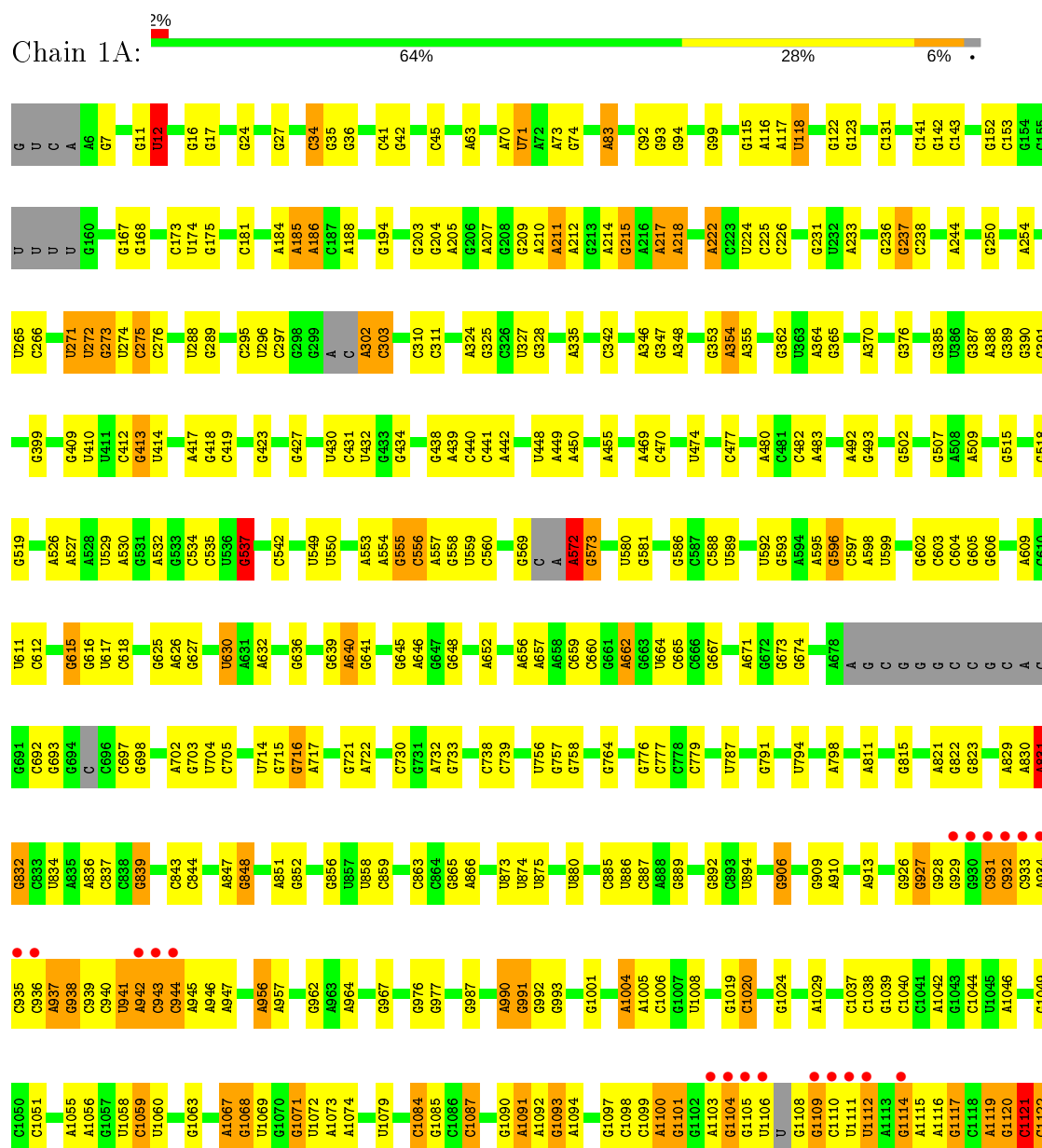
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2y	20	Total	O	0	0
			20	20		

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.

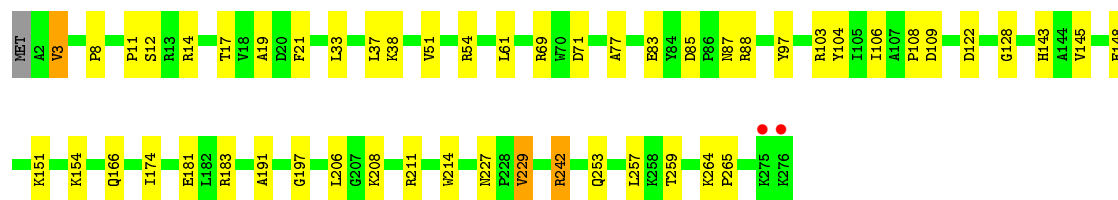
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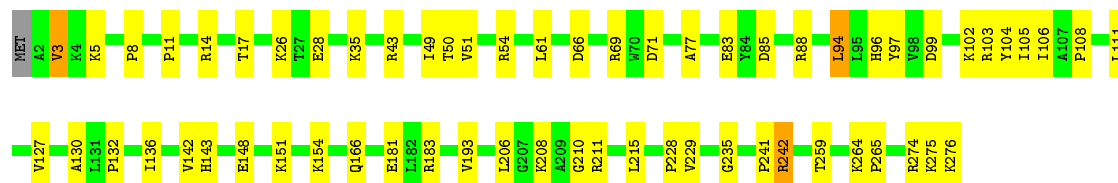
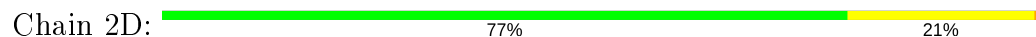
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G2615	C2486	A2347	U2256	G2177	G2091	A1974	C1831	A1711	A1579	U1442	G1206	U1124
U2616	C2487	A2348	G2263	G2178	G2095	A1975	G1832	G1715	C1579	U1451	G1210	C1125
G2617	C2488	C2359	C2273	A2180	G2096	U1976	A1833	A1716	U	U1452	U1211	C1126
U2618	C2489	C2362	U2274	G2181	U2097	U1977	A1834	C1717	G	C1453	C1212	U1127
U2621	A2490	G2366	G2275	C2182	U2098	C1980	G1842	G1730	A	G1462	U1213	U1128
C2622	C2495	C2367	G2276	G2183	U2099	G1981	G1845	G1721	C	C1463	G1214	U1129
C2624	C2496	C2368	U2121	G2184	U2122	C1984	A1846	G1730	G1588	G1464	G1215	A1130
C2629	U2504	A2372	A2280	G2186	U2124	U1985	G1847	C1731	C1594	U1346	G1216	A1131
G2630	U2505	A2373	A2281	C2187	G2125	C1989	A1848	U1735	A1605	A1347	G1217	G1133
C2631	G2507	G2376	G2282	G2188	G2126	G1990	G1849	U1740	A1613	A1348	G1218	G1135
G2635	C2510	G2377	U2283	G2189	G2127	U1991	U1849	G1744	A1614	G1349	G1219	U1136
A2641	C2511	C2378	C2284	A2193	G2128	A1992	G1857	G1745	A1615	G1357	G1221	G1137
G2642	C2514	A2388	G2287	U2194	G2129	A1993	G1858	A1746	G1616	U1358	G1222	G1138
G2650	G2517	A2389	G2288	A2195	C2130	A1994	G1859	G1747	G1617	U1359	C1224	G1139
A2651	U2518	A2390	G2289	C2196	U2131	A2003	G1860	A1748	A1627	C1360	G1225	A1141
G2652	G2520	G2395	A2290	C2197	G2132	C2005	A1871	G1748	A1626	C1361	G1226	A1142
		G2396	G2291	A2198	G2133	C2006	G1872	G1749	A1627	U1362	C1230	A1143
		C2397	G2292	C2199	G2134		G1873	A1749	A1627	A1363	G1231	G1144
				C2200	U2135	A2008	C1874			G1378	G1232	G1145
					A2136		C1875			G1378	G1232	U1147
					G2137		G1876			G1385	U1233	C1148
					G2138		A1877			A1239		A1149
					A2141		A1878			A1388		C1150
					G2142		A1879			C1246		U1151
					G2143		U1882			U1398		G1152
					U2144		C1883			A1255		G1153
					G2145		G1896			U1256		U1154
					G2146		A1899			G1402		C1155
					G2147		G1900			U1403		A1156
					A2148		C1901			G1404		A1157
					G2149		A2036			A1405		G1158
					G2150		A2037			A1406		U1159
					C2151		A2041			G1410		G1160
					U2152		A2041			A1411		G1161
					G2153		A1911			A1412		C1162
					U2154		A1912			A1413		G1163
					G2155		C1915			G1296		
					A2156		U1809			G1416		G1171
					A2157		U1810			G1417		
					G2158		A1811			U1418		A1174
					C2162		A1922			A1299		A1175
					G2163		A1928			C1422		U1176
					C2164		G1928			G1302		G1177
					G2165		A1938			G1305		
					C2166		U1839			A1425		G1180
					G2167		A1940			G1427		G1181
					C2168		A1941			G1310		
					G2169		A1822			A1311		U1186
					G2170		A1822			U1312		U1187
					G2171		G1951			U1313		A1188
					U2172		G1952			A1554		
					G2173		G1952			C1555		C1189
					G2174		A1959			A1556		G1200
							A1960			U1430		A1201
							A1960			C1432		U1318
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							A1961			U1436		G1200
							A1961			U1440		A1202



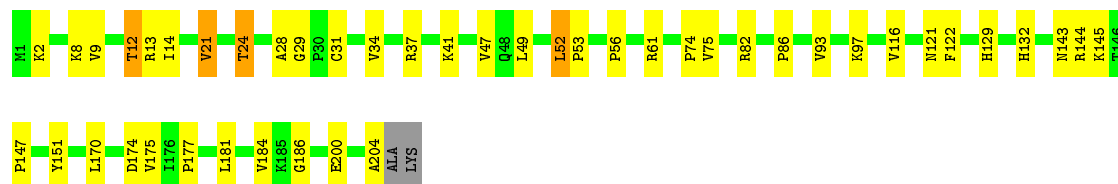
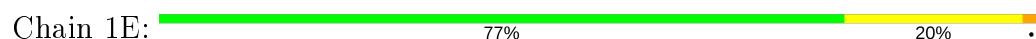
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U2180	G2181	G2120	A2031	G1921	G1696	C1584	U1405	A1486	U1188	U1113	C	C991
G2181	G2181	G2121	A2032	G1922	G1697	A1586	U1406	G1487	A1189	G1114	A	G992
C2182	U2034	U2122	G2035	A1927	A1698	C1588	C1407	A1286	G1190	G1115	G	G993
C2184	C2036	G2123	G2036	A1928	G1699	A1590	C1408	U1292	G1191	G1116	G	C994
C2185	C2040	G2124	C2040	A1929	A1700	G1593	G1409	C1293	G1192	G1117	A	C995
	U2041	G2125	U2041	A1928	A1701	G1594	G1410	G1297	G1193	G1118	G	A996
U2189	A2042	A2126	A2042	A1929	G1702	C1599	C1411	C1297	A1194	C1119	U	G997
C2190	C2043	C2128	A2043	U1931	G1703	A1603	G1416	G1298	C1200	G1120	U	A1000
G2191	C2044	U2130	C2044	A1932	C1711	C1604	G1417	G1299	C1211	C1121	G	A1001
G2192		G2131		G1933	C1712		G1418	U1300	A1204	G1122	G	G1002
							A1419	A1301	U1205	G1123	C	G1003
A2198	G2048		G2048	A1936			U1420	U1302		G1125	U	C1004
U2203	G2049	U2133	G2049	A1937	G1721	C1607	U1421	U1303	A1210	A1126	U	C1005
C2205	C2050	A2134	A2051	A1938	A1722	A1608	G1422	C1314	U1211		A	C1006
G2206	A2051	A2135		U1939	U1739	A1609	G1427	U1306	G1212	U1130	G	G1007
G2207	C2055	C2136	C2055	U1940	G1746	A1509B	A1427	G1319	A1213	G1131	A	C1008
A2208	G2056		G2056	C1941		G1613	G1428	C1320	C1217	A1132	A	A1009
U2218	A2059	C2137	A2059	U1955	G1756	A1614	G1429	G1324	C1218	U1133	G	A1010
	G2061	C2138	G2061		C1761		G1430	U1326	G1219	C1135	C	G1011
A2225	A2060	C2140	A2060	U1958	G1762	G1619	U1431	U1326	A1220	G1136	A	U1012
U2232	A2062	C2141	G2062	U1963	G1763		A1434	A1331	G1221	G1138	C	U1014
G2238	C2065	C2142	C2065	G1964	G1764	U1629	G1435	G1332	C1221A	G1139	C	G1015
G2239	C2066	U2145	C2066	C1965		A1632	C1437	C1333	C1224	G1140	A	G1016
G2242	G2067	C2146	G2067	C1967	G1769	G1633	G1441	G1346	A1226	U1142	U	G1017
U2243	U2068	G2147	U2068	G1968	G1772		G1442	U1352	G1229	G1144	U	A1020
A2247	G2069	G2148	G2069	A1969	G1773	G1636	G1445	A1353	G1230	C1147	A	G1022
U2249	A2070	C2149	A2070	A1970	C1774	A1637	U1448	G1355	G1231	A1148	A	U1023
G2250	A2071	U2150	A2071	A1972	U1775	C1638	A1449	G1356	A1237	G1149	A	G1025
	U2074	G2152	U2074	G1973	U1778	G1639	G1450	U1359	G1238	G1151	A	A1027
	U2075	G2153	U2075	C1974	U1779	C1640	U1453	A1360	G1239	C1152	G	A1028
		U2154			A1780		G1455	G1364	U1240	G1153	U	A1029
U2285	G2094	G2156	G2094	U1991	C1781	G1647	U1461	A1366	A1247	G1154	G	G1031
	C2095	G2157	C2095	G1992	C1782	C1648	G1462	A1367	A1253	U1165	A	U1033
A2288	U2096	A2158	U2096	U1993	A1783		C1463	A1368	A1254	C1166	A	G1036
C2274	C2097	G2160	C2097	C1996	A1784	G1651	G1465	G1369	U1255	G1169	A	G1037
C2275	U2098	C2161	U2098	G1997	A1785	A1652	G1466	G1370	G1256	G1170	U	C1038
G2276	U2099	G2162	U2099	G1998	A1786	A1654	G1467	G1371	C1257	G1171	A	G1039
G2277	G2100	C2163	G2100	C1999			C1468	U1372	U1263	A	C	G1040
A2278	G2104		G2104	G2010	C1790	G1660		A1373	G1264	U	U	C1041
C2283	C2105	G2165	C2105	U2011	A1791	G1661		A1378	A1265	G	C	G1042
C2284	G2106	G2166	G2106	G2012	U1794	A1664		A1379	A1266	A	A	C1043
C2285	C2107	U2167	C2107	A2013	U1796	A1665		G1380	U1267	C1178	C	G
C2286	C2108	G2168	C2108	A2014	U1797	A1668		G1385	U1268	C1179	U	A
A2287	U2109	A2169	U2109	G1906	U1798	A1669		A1384	A1269	G1180	G	G
A2288	G2110	A2170	G2110	A1913	G1799	A1670		C1386	G1270		U	A
G2289	C2111	A2171	C2111	U1914	C1800	U1671			G1271	G1183	C	A
G2290	G2112	U2172	G2112	U1915	A1801	A1569			U1272	G1184	C	A
	U2113	A2173	U2113	U1916	A1802	G1674			U1273	G1185	G	A
U2291	A2114	C2174	A2114	A1916	A1803						U	A
C2292	G2115	C2175	G2115	U1917	U1804	U1688					C	A
C2293	G2116	A2176	G2116	A1918	U1805	A1689					C	A
C2294	A2117	C2177	A2117	A1919	C1582						A	G



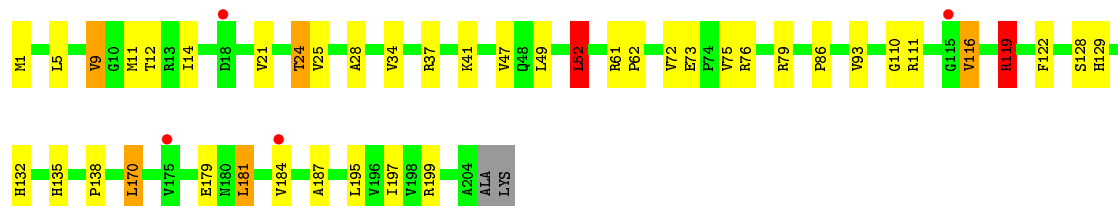
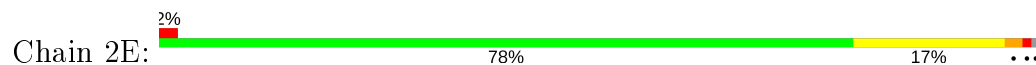
• Molecule 3: 50S ribosomal protein L2



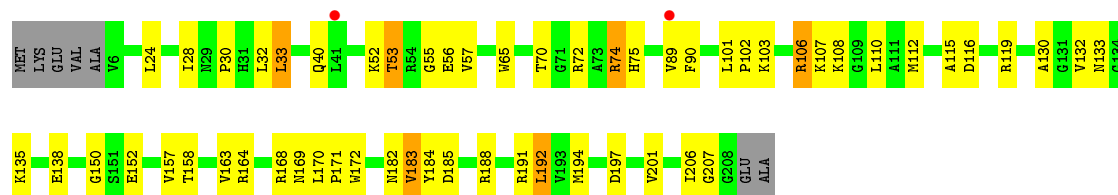
• Molecule 4: 50S ribosomal protein L3



• Molecule 4: 50S ribosomal protein L3

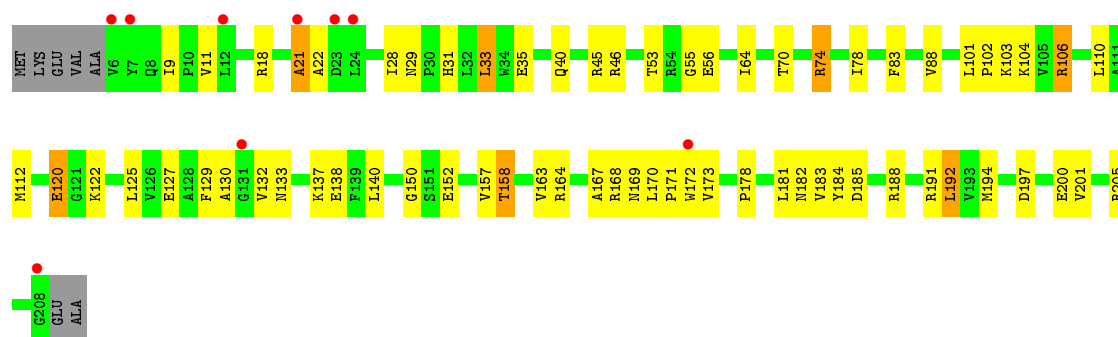


• Molecule 5: 50S ribosomal protein L4




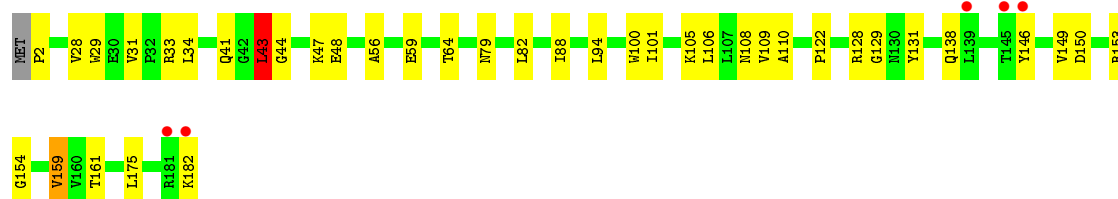
• Molecule 5: 50S ribosomal protein L4

Chain 2F: 




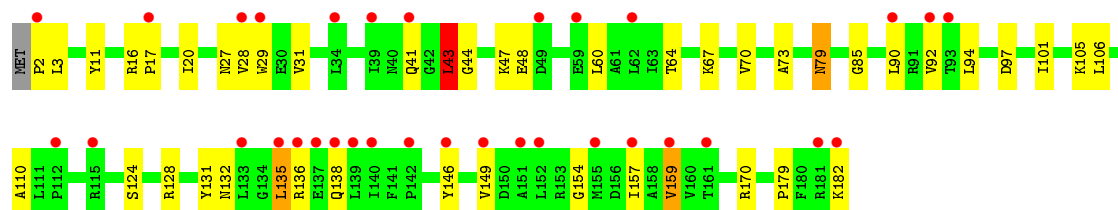
- Molecule 6: 50S ribosomal protein L5

Chain 1G: 




- Molecule 6: 50S ribosomal protein L5

Chain 2G: 




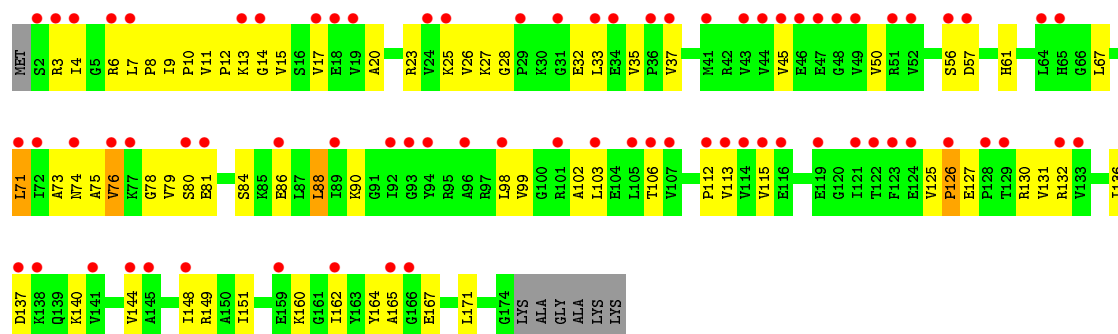
- Molecule 7: 50S ribosomal protein L6

Chain 1H: 

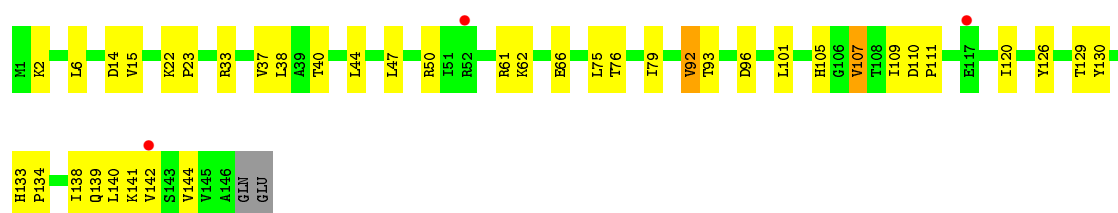
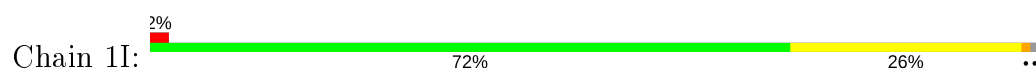


- Molecule 7: 50S ribosomal protein L6

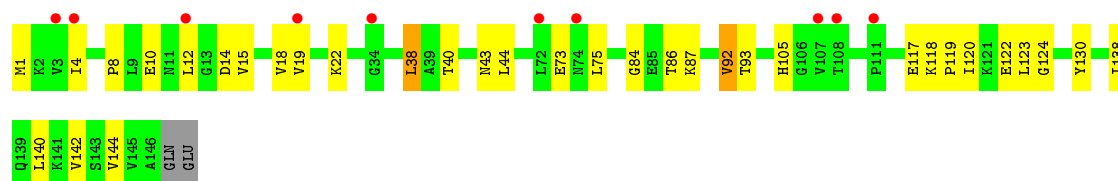
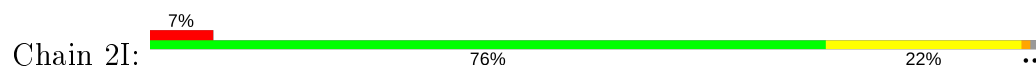
Chain 2H: 



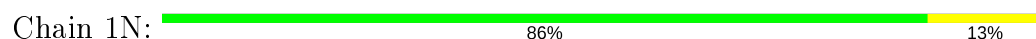
• Molecule 8: 50S ribosomal protein L9



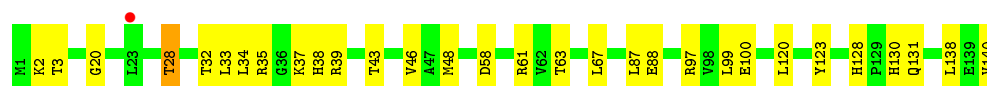
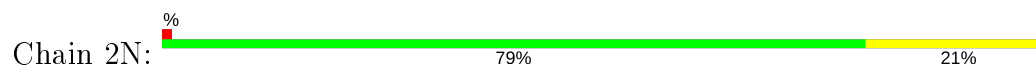
• Molecule 8: 50S ribosomal protein L9



• Molecule 9: 50S ribosomal protein L13

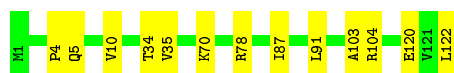


• Molecule 9: 50S ribosomal protein L13

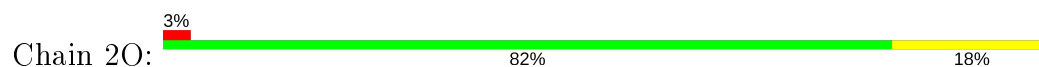


• Molecule 10: 50S ribosomal protein L14

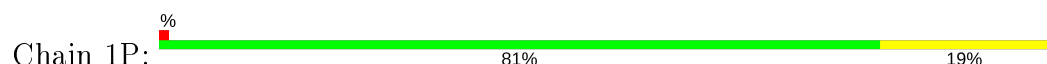




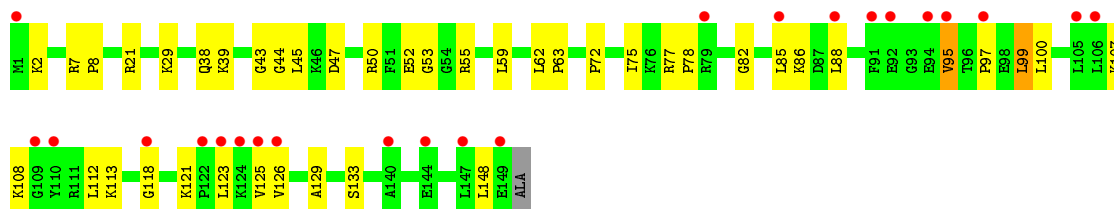
- Molecule 10: 50S ribosomal protein L14



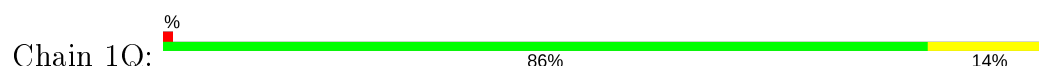
- Molecule 11: 50S ribosomal protein L15



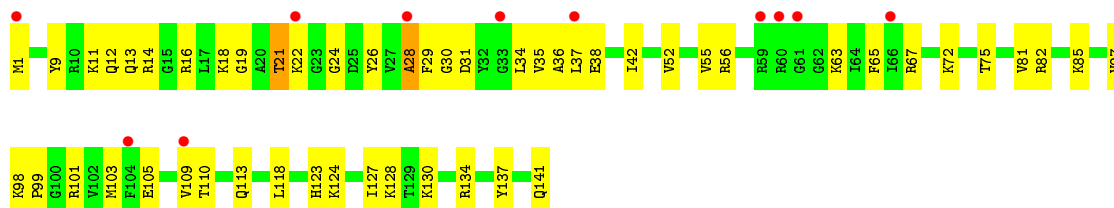
- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16




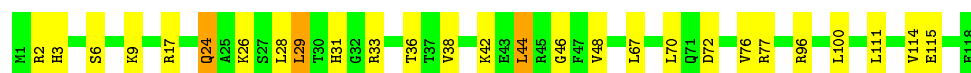
- Molecule 12: 50S ribosomal protein L16




- Molecule 13: 50S ribosomal protein L17

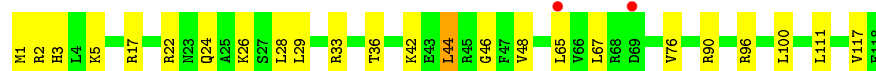


Chain 1R:  77% 20% .




- Molecule 13: 50S ribosomal protein L17

Chain 2R:  2% 80% 19% .




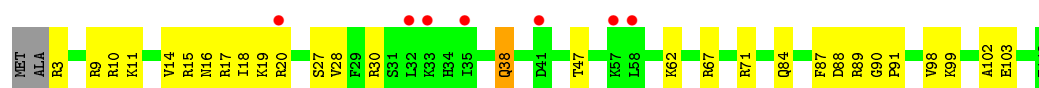
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  82% 16% .



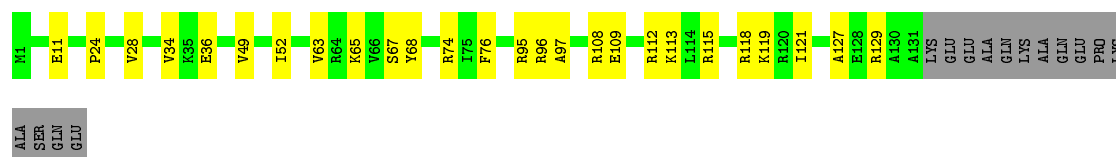
- Molecule 14: 50S ribosomal protein L18

Chain 2S:  6% 72% 25% ..



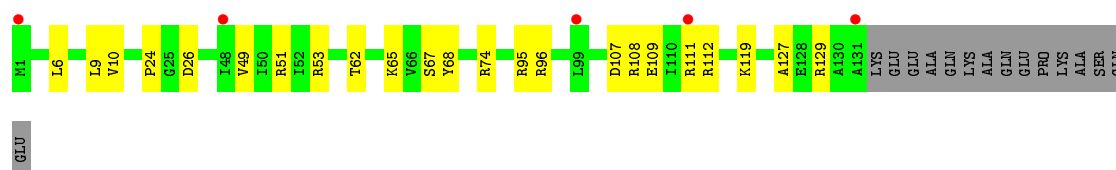
- Molecule 15: 50S ribosomal protein L19

Chain 1T:  72% 18% 10%




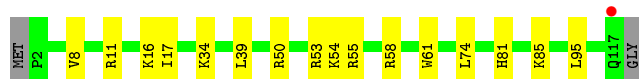
- Molecule 15: 50S ribosomal protein L19

Chain 2T:  3% 74% 16% 10%

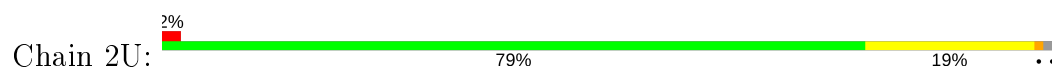


- Molecule 16: 50S ribosomal protein L20

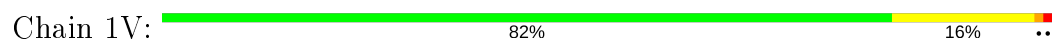
Chain 1U:  % 85% 14% .



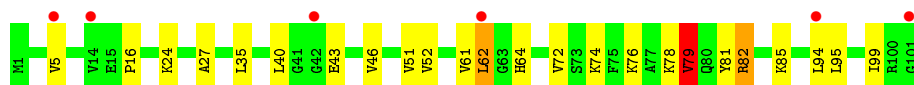
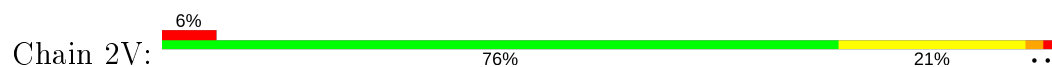
- Molecule 16: 50S ribosomal protein L20



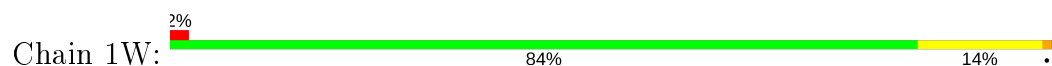
- Molecule 17: 50S ribosomal protein L21



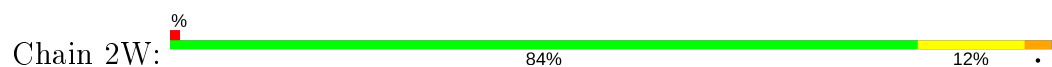
- Molecule 17: 50S ribosomal protein L21



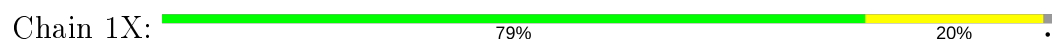
- Molecule 18: 50S ribosomal protein L22



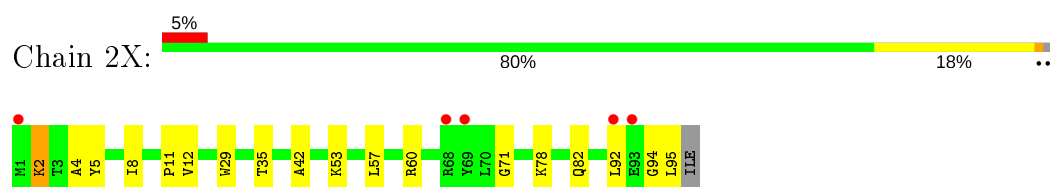
- Molecule 18: 50S ribosomal protein L22



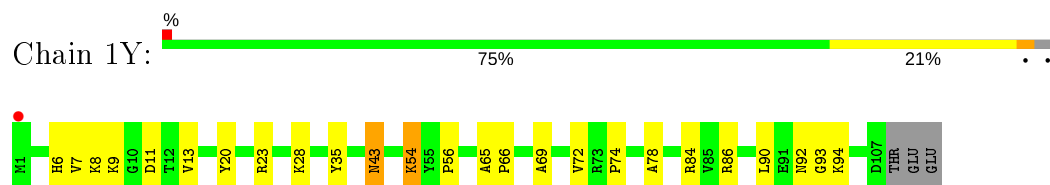
- Molecule 19: 50S ribosomal protein L23



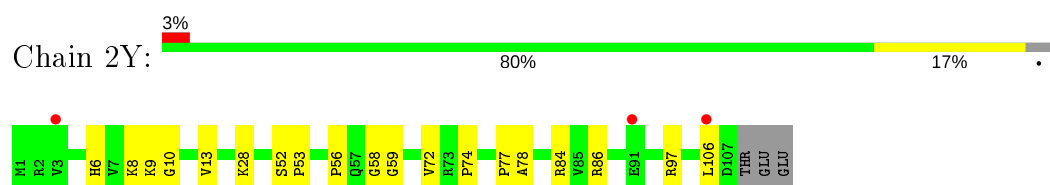
- Molecule 19: 50S ribosomal protein L23



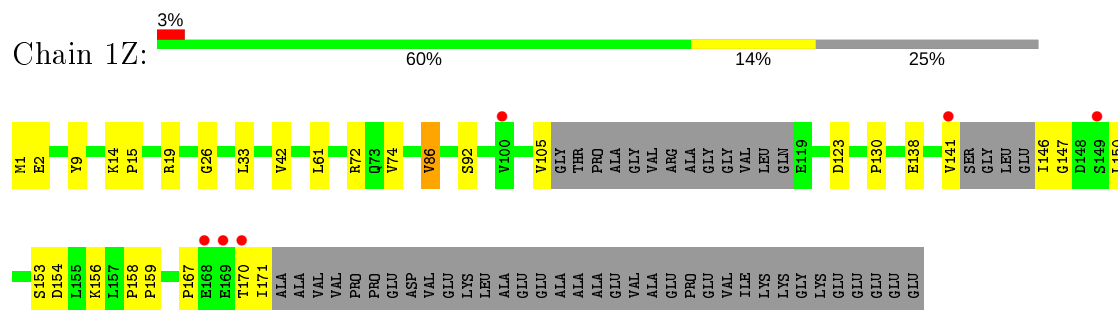
- Molecule 20: 50S ribosomal protein L24



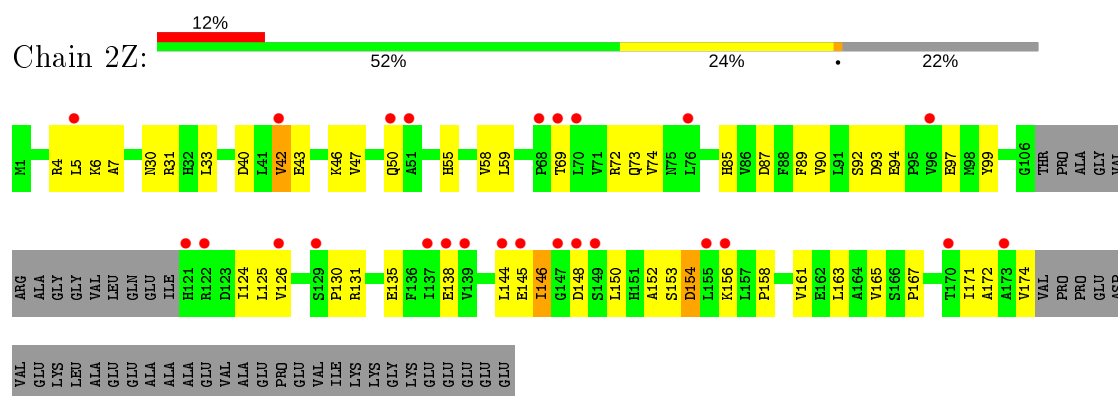
- Molecule 20: 50S ribosomal protein L24



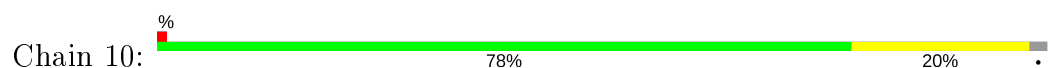
- Molecule 21: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L25

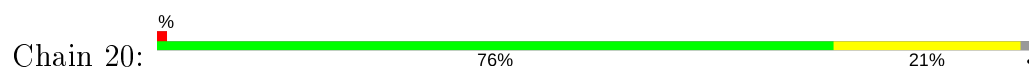


- Molecule 22: 50S ribosomal protein L27

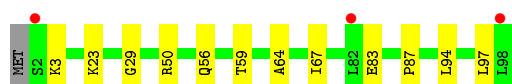
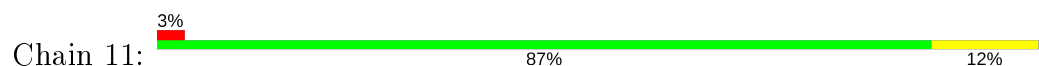




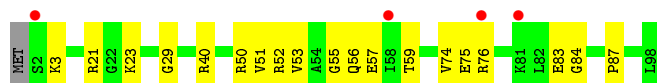
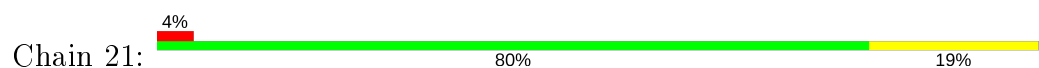
- Molecule 22: 50S ribosomal protein L27



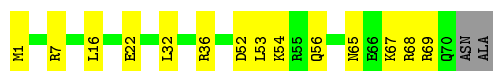
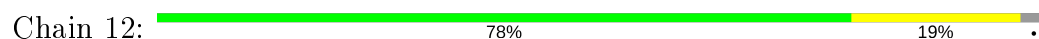
- Molecule 23: 50S ribosomal protein L28



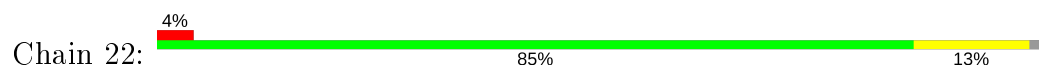
- Molecule 23: 50S ribosomal protein L28



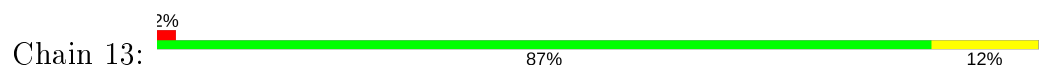
- Molecule 24: 50S ribosomal protein L29



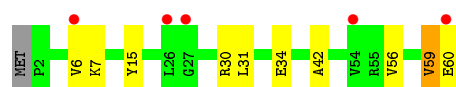
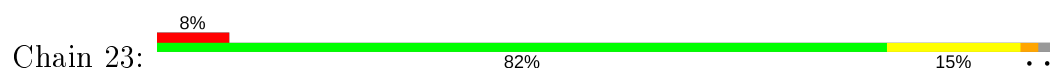
- Molecule 24: 50S ribosomal protein L29



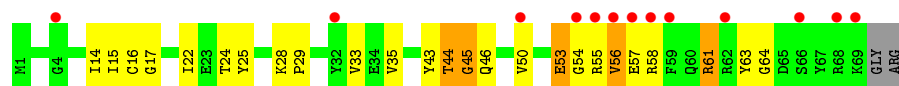
- Molecule 25: 50S ribosomal protein L30



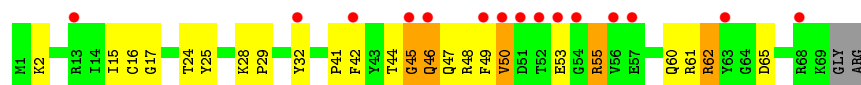
- Molecule 25: 50S ribosomal protein L30



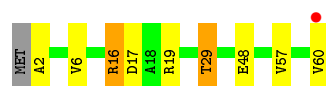
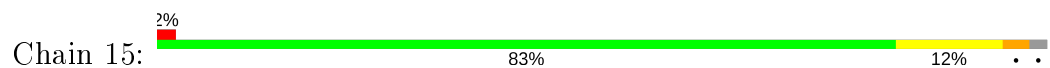
- Molecule 26: 50S ribosomal protein L31



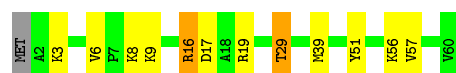
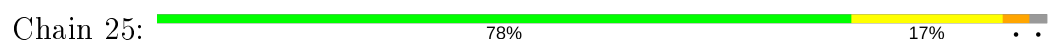
- Molecule 26: 50S ribosomal protein L31



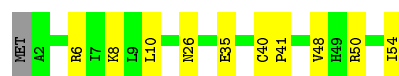
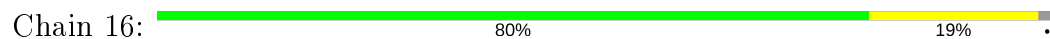
- Molecule 27: 50S ribosomal protein L32



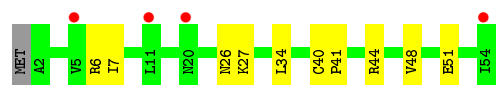
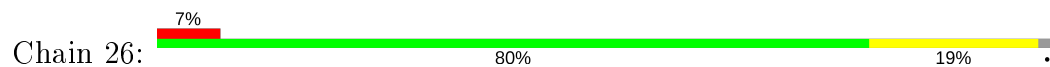
- Molecule 27: 50S ribosomal protein L32



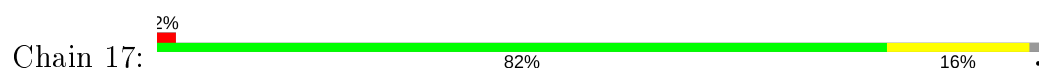
- Molecule 28: 50S ribosomal protein L33



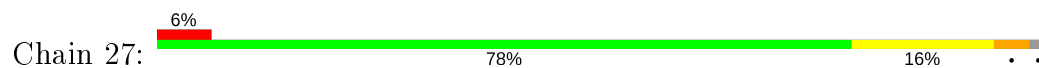
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



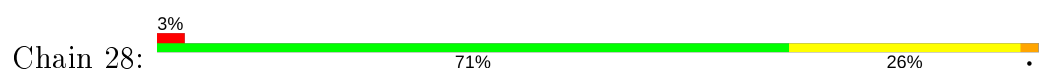
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



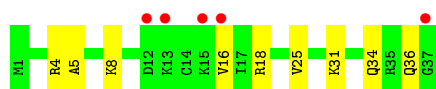
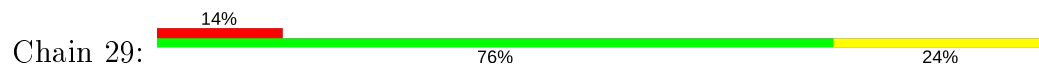
- Molecule 30: 50S ribosomal protein L35



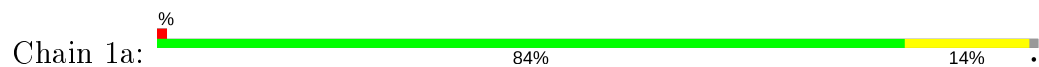
- Molecule 31: 50S ribosomal protein L36

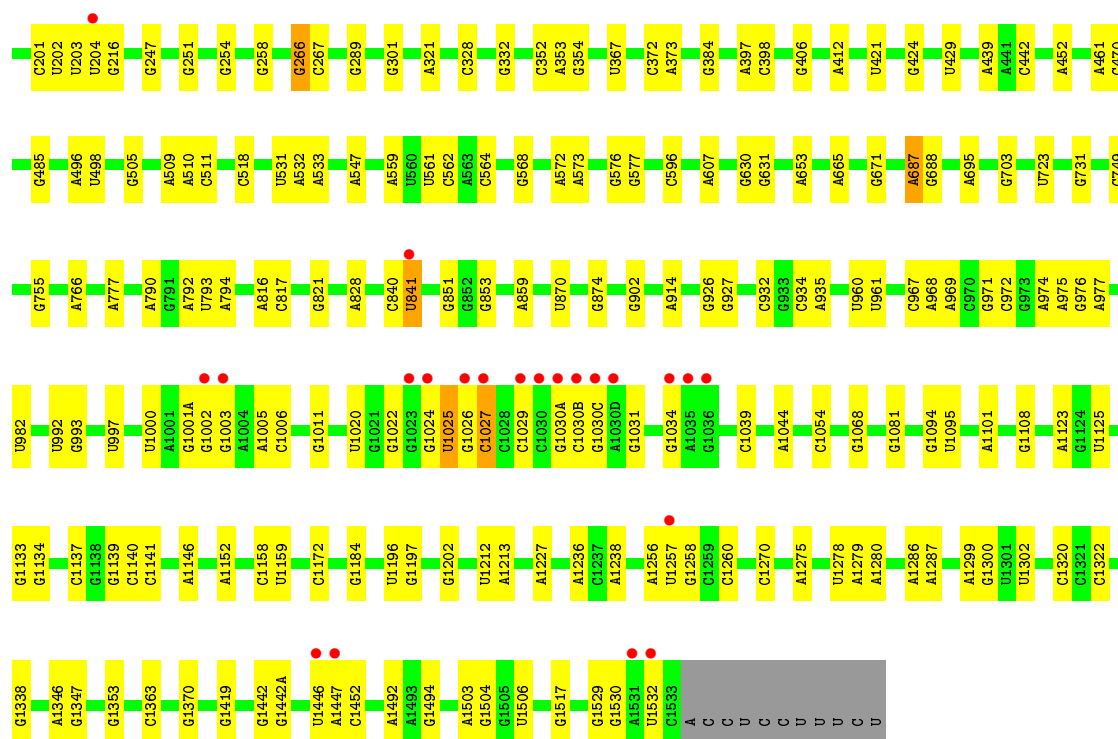


- Molecule 31: 50S ribosomal protein L36

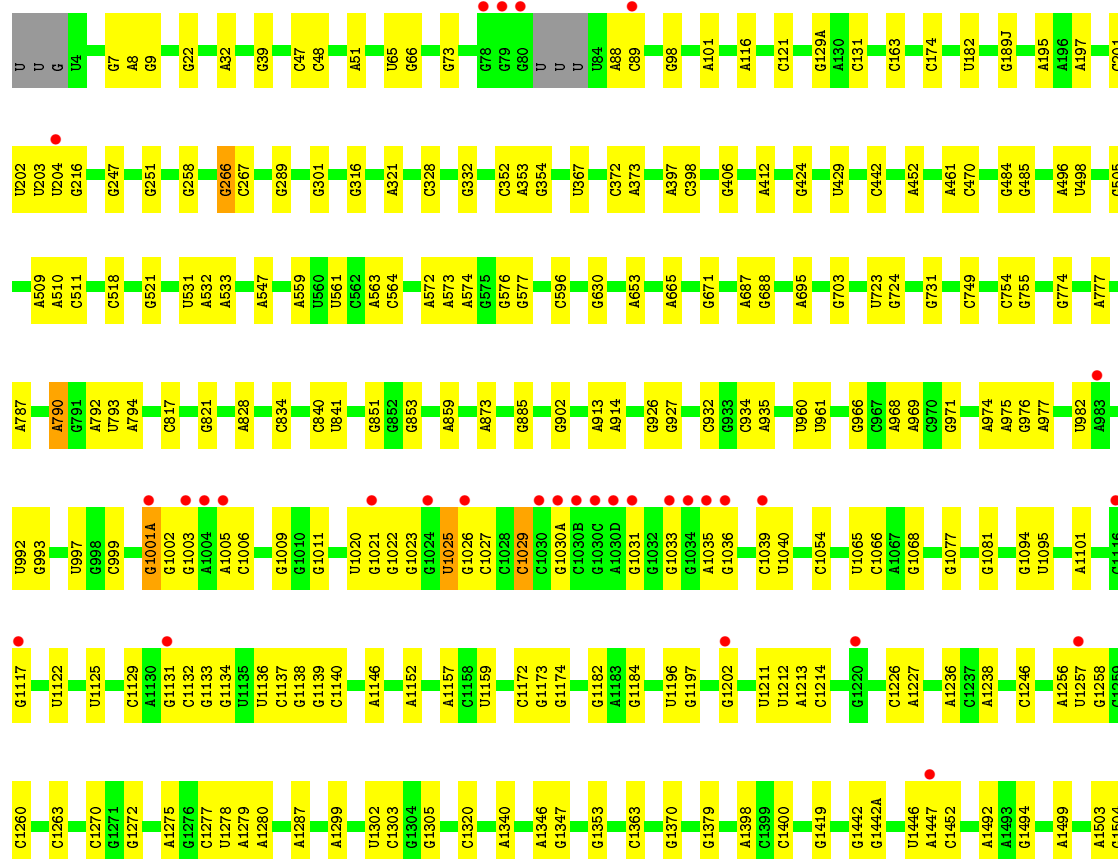


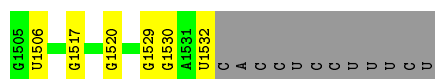
- Molecule 32: 16S ribosomal RNA



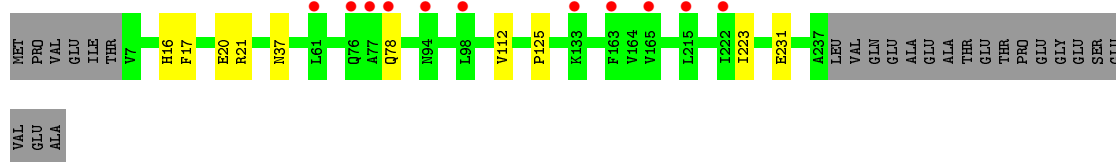
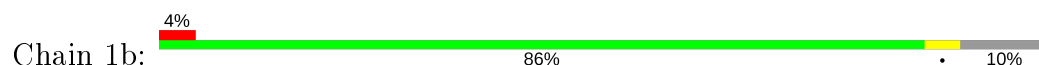


Chain 2a: 2% 83% 16%

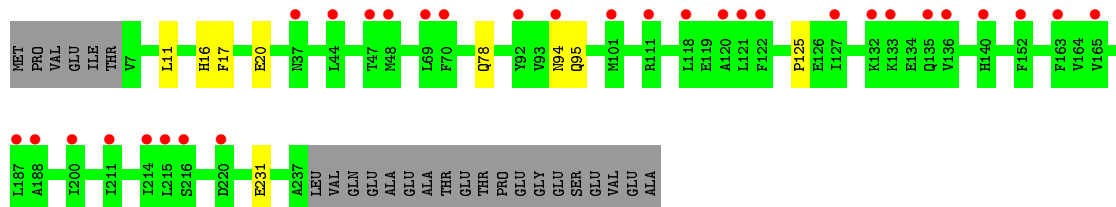
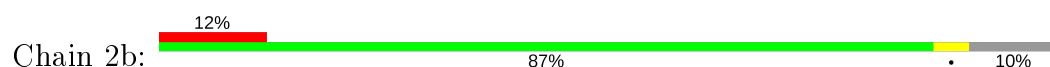




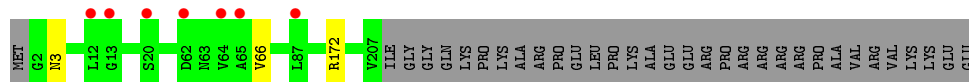
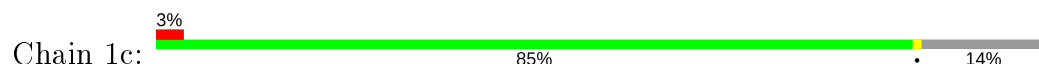
- Molecule 33: 30S ribosomal protein S2



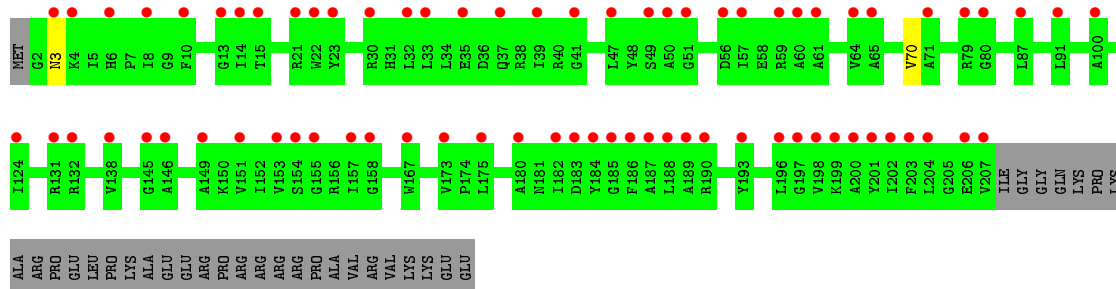
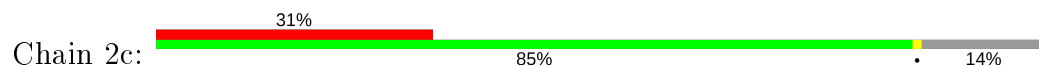
- Molecule 33: 30S ribosomal protein S2



- Molecule 34: 30S ribosomal protein S3



- Molecule 34: 30S ribosomal protein S3



- Molecule 35: 30S ribosomal protein S4

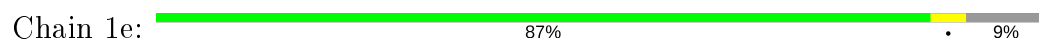




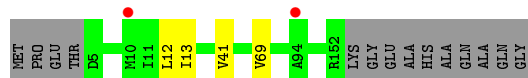
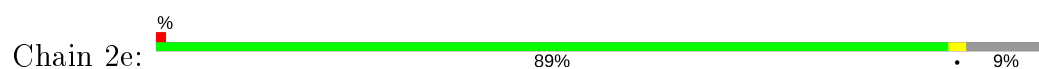
- Molecule 35: 30S ribosomal protein S4



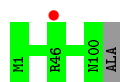
- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



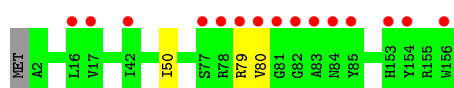
- Molecule 37: 30S ribosomal protein S6



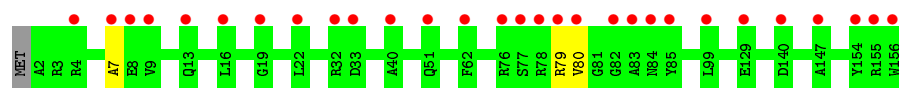
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7



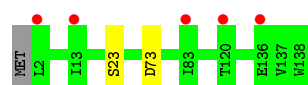
- Molecule 38: 30S ribosomal protein S7



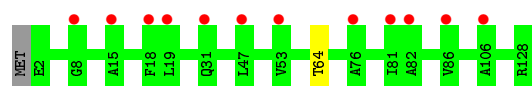
- Molecule 39: 30S ribosomal protein S8



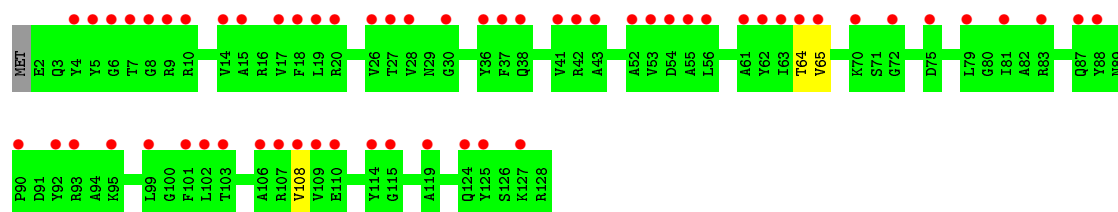
- Molecule 39: 30S ribosomal protein S8



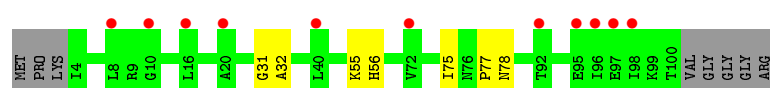
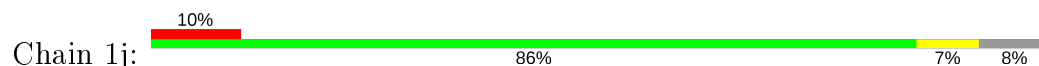
- Molecule 40: 30S ribosomal protein S9



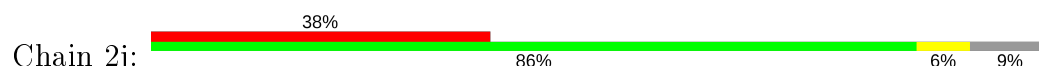
- Molecule 40: 30S ribosomal protein S9

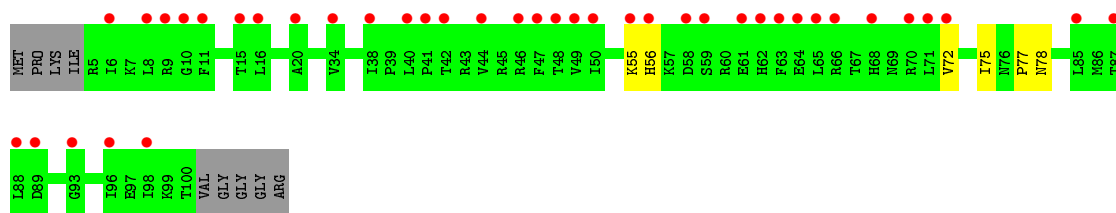


- Molecule 41: 30S ribosomal protein S10

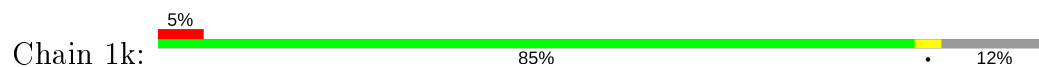


- Molecule 41: 30S ribosomal protein S10

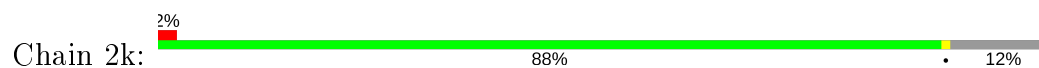




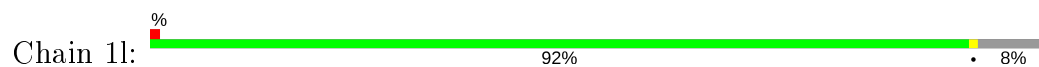
- Molecule 42: 30S ribosomal protein S11



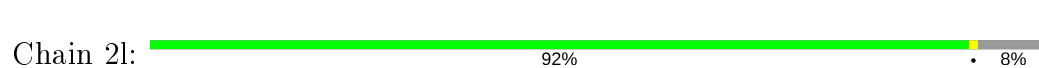
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S12



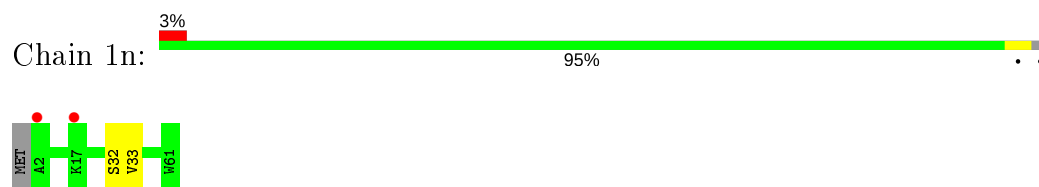
- Molecule 44: 30S ribosomal protein S13



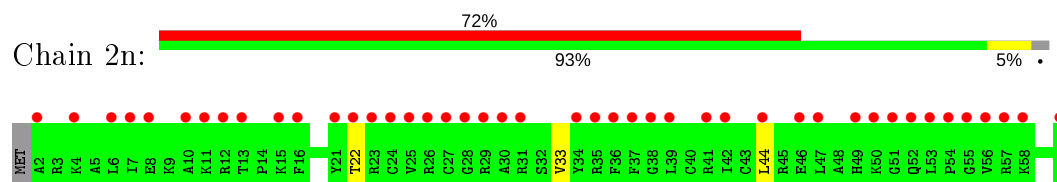
- Molecule 44: 30S ribosomal protein S13



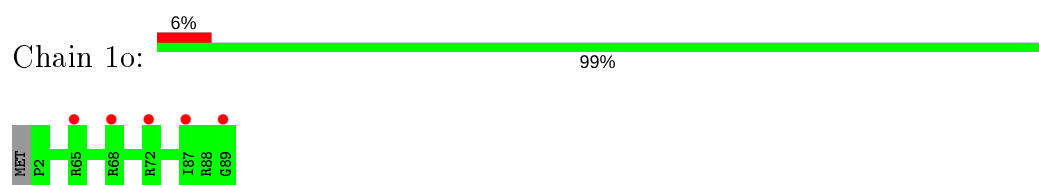
- Molecule 45: 30S ribosomal protein S14 type Z



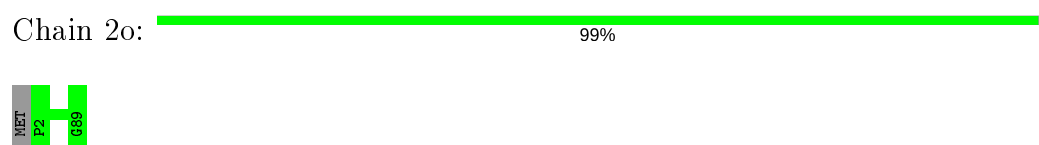
- Molecule 45: 30S ribosomal protein S14 type Z



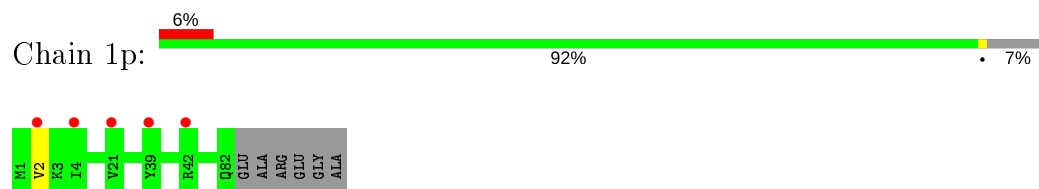
- Molecule 46: 30S ribosomal protein S15



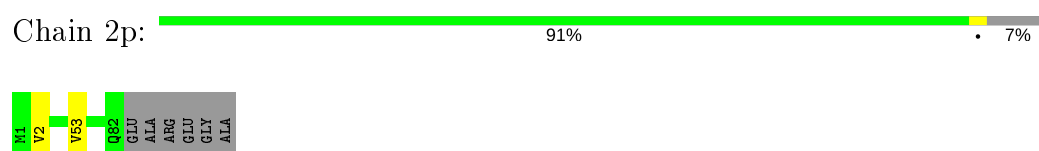
- Molecule 46: 30S ribosomal protein S15



- Molecule 47: 30S ribosomal protein S16

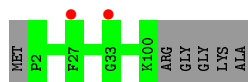


- Molecule 47: 30S ribosomal protein S16

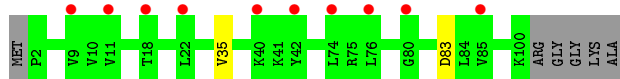


- Molecule 48: 30S ribosomal protein S17

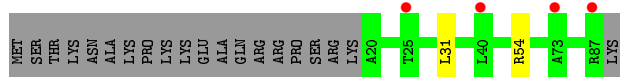
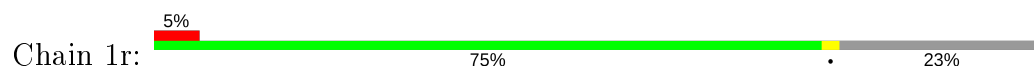




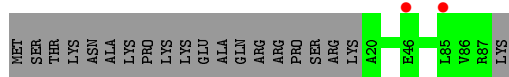
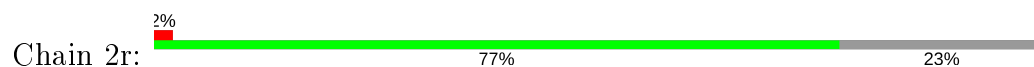
- Molecule 48: 30S ribosomal protein S17



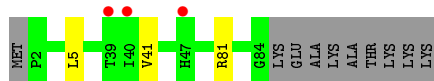
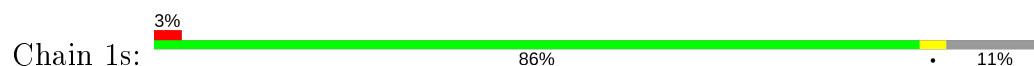
- Molecule 49: 30S ribosomal protein S18



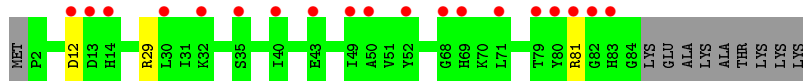
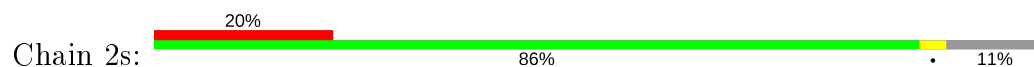
- Molecule 49: 30S ribosomal protein S18



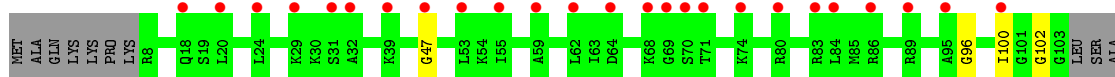
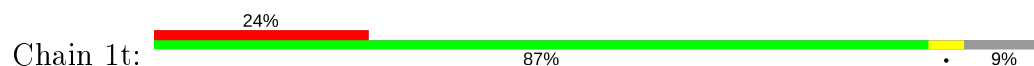
- Molecule 50: 30S ribosomal protein S19



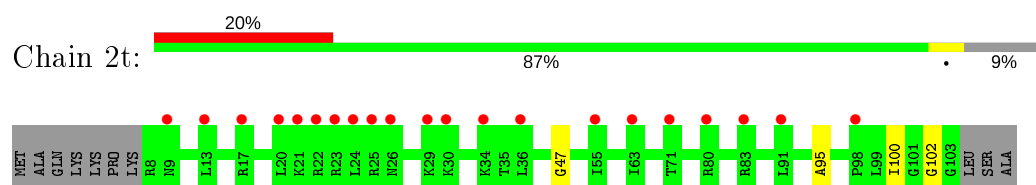
- Molecule 50: 30S ribosomal protein S19



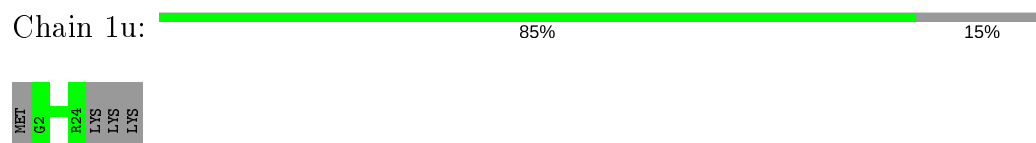
- Molecule 51: 30S ribosomal protein S20



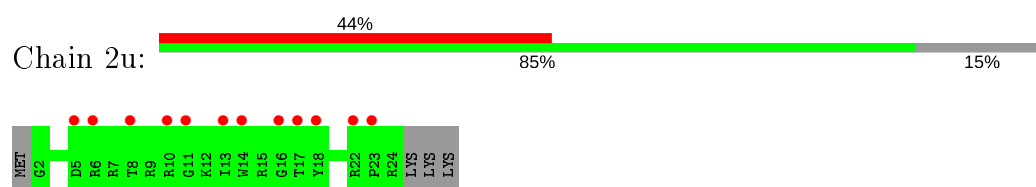
- Molecule 51: 30S ribosomal protein S20



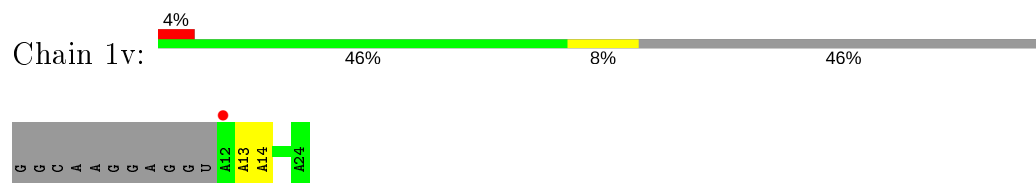
- Molecule 52: 30S ribosomal protein Thx



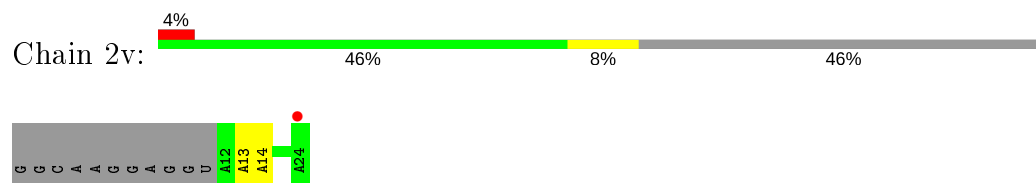
- Molecule 52: 30S ribosomal protein Thx



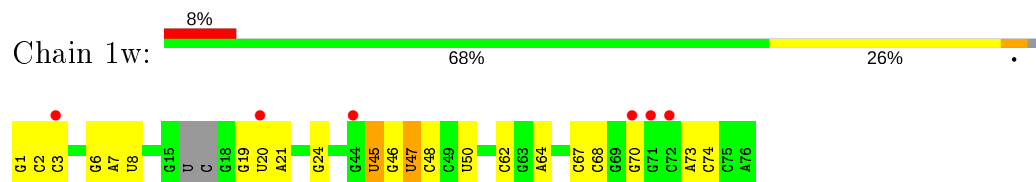
- Molecule 53: mRNA



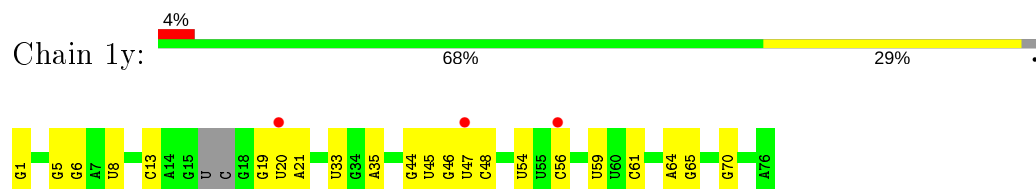
- Molecule 53: mRNA



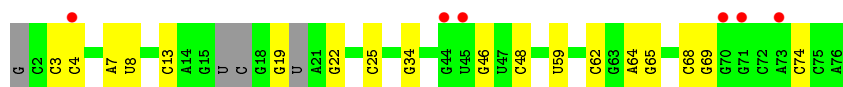
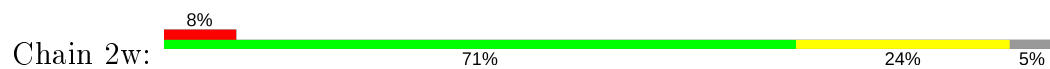
- Molecule 54: A-site and E-site tRNAs



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



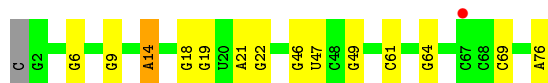
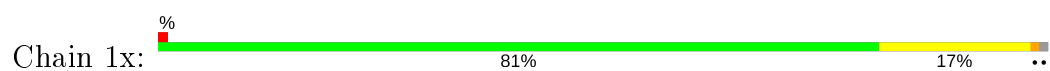
- Molecule 54: A-site and E-site tRNAs



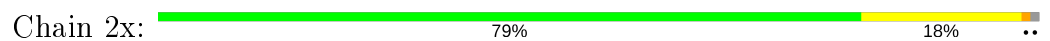
- Molecule 54: A-site and E-site tRNAs



- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.98Å 446.99Å 621.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.65 – 2.80 152.64 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (152.65-2.80) 98.3 (152.64-2.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.219 , 0.268 0.219 , 0.268	Depositor DCC
R_{free} test set	69488 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 65.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	301288	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, M2G, OMG, 2MU, MIA, CPT, SF4, 0TD, MG, 2MA, 2MG, 5MC, UR3, MA6, 4OC, 4SU, 7MG, K, PSU

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	0.51	2/69009 (0.0%)	0.91	44/107712 (0.0%)
1	2A	0.41	2/67293 (0.0%)	0.90	25/105034 (0.0%)
2	1B	0.44	1/2882 (0.0%)	0.83	0/4494
2	2B	0.49	1/2879 (0.0%)	0.92	2/4487 (0.0%)
3	1D	0.38	0/2186	0.58	0/2944
3	2D	0.33	0/2186	0.58	1/2944 (0.0%)
4	1E	0.36	0/1592	0.54	0/2149
4	2E	0.33	0/1592	0.57	1/2149 (0.0%)
5	1F	0.35	0/1619	0.52	0/2193
5	2F	0.33	0/1615	0.54	0/2188
6	1G	0.30	0/1448	0.51	0/1957
6	2G	0.31	0/1453	0.54	0/1963
7	1H	0.32	0/1347	0.51	0/1823
7	2H	0.29	0/1347	0.52	1/1823 (0.1%)
8	1I	0.29	0/1112	0.52	0/1514
8	2I	0.27	0/1079	0.50	0/1475
9	1N	0.35	0/1144	0.49	0/1543
9	2N	0.31	0/1144	0.50	0/1543
10	1O	0.37	0/943	0.53	0/1269
10	2O	0.30	0/943	0.48	0/1269
11	1P	0.35	0/1152	0.56	0/1533
11	2P	0.31	0/1152	0.58	0/1533
12	1Q	0.36	0/1143	0.50	0/1527
12	2Q	0.32	0/1143	0.55	0/1527
13	1R	0.35	0/982	0.54	0/1312
13	2R	0.31	0/982	0.53	0/1312
14	1S	0.32	0/883	0.51	0/1176
14	2S	0.32	0/880	0.51	0/1172
15	1T	0.34	0/1105	0.50	0/1477
15	2T	0.31	0/1097	0.50	0/1468
16	1U	0.39	0/977	0.52	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.32	0/977	0.50	0/1301
17	1V	0.35	0/782	0.51	0/1049
17	2V	0.32	0/782	0.52	0/1049
18	1W	0.38	0/897	0.52	0/1205
18	2W	0.33	0/897	0.52	0/1205
19	1X	0.38	0/764	0.57	0/1025
19	2X	0.31	0/764	0.49	0/1025
20	1Y	0.36	0/819	0.55	0/1095
20	2Y	0.32	0/819	0.51	0/1095
21	1Z	0.30	0/1267	0.52	0/1717
21	2Z	0.31	0/1299	0.54	0/1763
22	10	0.36	0/662	0.54	0/881
22	20	0.30	0/662	0.49	0/881
23	11	0.34	0/762	0.51	0/1014
23	21	0.31	0/762	0.52	0/1014
24	12	0.34	0/590	0.51	0/781
24	22	0.31	0/590	0.43	0/781
25	13	0.35	0/474	0.52	0/635
25	23	0.29	0/469	0.48	0/630
26	14	0.36	0/565	0.64	0/761
26	24	0.32	0/545	0.50	0/737
27	15	0.33	0/469	0.52	0/635
27	25	0.31	0/469	0.50	0/635
28	16	0.35	0/460	0.48	0/613
28	26	0.33	0/456	0.48	0/608
29	17	0.36	0/426	0.52	0/561
29	27	0.33	0/426	0.58	0/561
30	18	0.36	0/525	0.53	0/691
30	28	0.31	0/525	0.51	0/691
31	19	0.39	0/310	0.53	0/407
31	29	0.29	0/310	0.49	0/407
32	1a	0.37	1/35795 (0.0%)	0.86	23/55864 (0.0%)
32	2a	0.35	3/35886 (0.0%)	0.86	30/56005 (0.1%)
33	1b	0.29	0/1881	0.53	0/2542
33	2b	0.31	0/1860	0.52	0/2518
34	1c	0.28	0/1572	0.47	0/2126
34	2c	0.30	0/1566	0.50	0/2119
35	1d	0.30	0/1685	0.50	0/2262
35	2d	0.29	0/1704	0.50	0/2284
36	1e	0.31	0/1145	0.52	0/1543
36	2e	0.31	0/1149	0.54	0/1548
37	1f	0.30	0/823	0.50	0/1115
37	2f	0.30	0/829	0.45	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.29	0/1250	0.47	0/1679
38	2g	0.28	0/1254	0.49	0/1683
39	1h	0.28	0/1108	0.49	0/1494
39	2h	0.27	0/1108	0.50	0/1494
40	1i	0.29	0/1002	0.52	0/1346
40	2i	0.28	0/997	0.50	0/1343
41	1j	0.27	0/722	0.53	0/982
41	2j	0.30	0/727	0.53	0/988
42	1k	0.28	0/844	0.49	0/1145
42	2k	0.29	0/848	0.49	0/1149
43	1l	0.32	0/937	0.53	0/1260
43	2l	0.28	0/937	0.57	1/1260 (0.1%)
44	1m	0.29	0/969	0.53	0/1302
44	2m	0.29	0/961	0.56	0/1291
45	1n	0.32	0/501	0.54	0/664
45	2n	0.29	0/501	0.52	0/664
46	1o	0.28	0/739	0.46	0/985
46	2o	0.28	0/739	0.50	0/985
47	1p	0.29	0/697	0.51	0/939
47	2p	0.29	0/693	0.50	0/935
48	1q	0.30	0/836	0.49	0/1117
48	2q	0.28	0/836	0.49	0/1117
49	1r	0.30	0/560	0.53	0/746
49	2r	0.30	0/560	0.47	0/746
50	1s	0.27	0/667	0.52	0/900
50	2s	0.32	0/661	0.61	0/893
51	1t	0.27	0/730	0.49	0/965
51	2t	0.27	0/729	0.48	0/965
52	1u	0.26	0/203	0.47	0/266
52	2u	0.26	0/203	0.49	0/266
53	1v	0.35	0/310	0.82	0/480
53	2v	0.34	0/310	0.78	0/480
54	1w	0.53	1/1606 (0.1%)	1.07	5/2497 (0.2%)
54	1y	0.48	1/1606 (0.1%)	1.02	4/2497 (0.2%)
54	2w	0.44	0/1556	1.03	0/2418
54	2y	0.51	1/1583 (0.1%)	1.06	3/2459 (0.1%)
55	1x	0.54	2/1725 (0.1%)	1.14	16/2689 (0.6%)
55	2x	0.46	0/1725	1.08	16/2689 (0.6%)
All	All	0.40	15/316668 (0.0%)	0.82	172/474091 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	1	G	OP3-P	-10.24	1.48	1.61
2	2B	1	U	OP3-P	-10.23	1.48	1.61
54	1y	1	G	OP3-P	-10.13	1.49	1.61
2	1B	1	U	OP3-P	-10.08	1.49	1.61
54	1w	1	G	OP3-P	-9.91	1.49	1.61
1	2A	1848	A	C8-N7	9.09	1.38	1.31
1	1A	1879	A	C8-N7	8.93	1.37	1.31
32	2a	790	A	C8-N7	8.69	1.37	1.31
32	1a	790	A	C8-N7	8.68	1.37	1.31
1	2A	2531	A	C8-N7	8.67	1.37	1.31
1	1A	2543	A	C8-N7	8.01	1.37	1.31
32	2a	1272	G	C6-N1	-7.94	1.33	1.39
32	2a	1272	G	N1-C2	-6.71	1.32	1.37
55	1x	22	G	N7-C5	5.51	1.42	1.39
55	1x	14	A	N7-C5	-5.03	1.36	1.39

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	C5-C6-O6	16.43	138.46	128.60
32	2a	1272	G	N3-C2-N2	14.39	129.97	119.90
32	2a	1263	C	N1-C2-O2	14.28	127.47	118.90
32	2a	1272	G	N1-C2-N2	-14.21	103.41	116.20
32	2a	1272	G	N1-C6-O6	-12.06	112.66	119.90
2	2B	80	U	O4'-C1'-N1	10.54	116.63	108.20
32	2a	1263	C	N3-C2-O2	-10.00	114.90	121.90
1	1A	1121	C	N1-C2-O2	9.97	124.88	118.90
55	1x	46	G	C6-N1-C2	-9.16	119.60	125.10
32	2a	1263	C	C2-N3-C4	9.15	124.48	119.90
1	1A	1121	C	C2-N3-C4	9.15	124.47	119.90
55	1x	14	A	C4-C5-C6	8.98	121.49	117.00
55	2x	46	G	C6-N1-C2	-8.83	119.80	125.10
32	1a	1027	C	C5-C4-N4	8.69	126.29	120.20
32	1a	1027	C	N3-C4-C5	-8.51	118.50	121.90
55	1x	14	A	C5-N7-C8	8.34	108.07	103.90
32	1a	1027	C	N3-C2-O2	-8.34	116.06	121.90
1	1A	2189	U	C2-N1-C1'	8.27	127.62	117.70
32	2a	1272	G	C4-N9-C1'	8.11	137.05	126.50
1	1A	1109	G	C5-C6-O6	8.09	133.46	128.60
54	1y	33	U	C2-N1-C1'	8.08	127.40	117.70
1	2A	2473	U	C2-N1-C1'	7.91	127.19	117.70
32	1a	1027	C	C6-N1-C2	-7.79	117.19	120.30
32	2a	1272	G	C8-N9-C1'	-7.50	117.25	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2189	U	N1-C2-O2	7.44	128.01	122.80
1	1A	12	U	C2-N1-C1'	7.43	126.62	117.70
1	2A	2140	C	N1-C2-O2	7.31	123.29	118.90
1	1A	848	G	O5'-P-OP2	-7.30	99.13	105.70
1	1A	1109	G	C6-N1-C2	7.29	129.47	125.10
1	2A	2167	U	C2-N1-C1'	7.28	126.43	117.70
32	1a	1030(B)	C	C2-N1-C1'	7.26	126.78	118.80
1	2A	787	U	O5'-P-OP1	-7.25	99.18	105.70
32	1a	1030(B)	C	N1-C2-O2	7.24	123.25	118.90
1	1A	1985	U	C2-N1-C1'	7.20	126.34	117.70
1	1A	1359	U	C2-N1-C1'	7.20	126.34	117.70
32	2a	1263	C	C6-N1-C2	-7.08	117.47	120.30
1	1A	537	G	O4'-C1'-N9	7.05	113.84	108.20
55	2x	17	C	N1-C2-O2	7.03	123.12	118.90
55	2x	17	C	N3-C2-O2	-6.96	117.03	121.90
1	2A	2167	U	N1-C2-O2	6.96	127.67	122.80
55	1x	14	A	C5-C6-N1	-6.89	114.26	117.70
1	2A	2248	C	O5'-P-OP2	-6.87	99.52	105.70
55	2x	22	G	C5-N7-C8	-6.84	100.88	104.30
1	1A	2189	U	N3-C2-O2	-6.83	117.42	122.20
1	2A	2167	U	N3-C2-O2	-6.78	117.45	122.20
55	2x	46	G	N3-C2-N2	-6.78	115.16	119.90
32	1a	254	G	O5'-P-OP1	-6.73	99.64	105.70
1	1A	1985	U	N1-C2-O2	6.72	127.50	122.80
54	1w	47	U	C2-N1-C1'	6.71	125.76	117.70
1	1A	831	A	O4'-C1'-N9	6.68	113.54	108.20
55	1x	22	G	C4-C5-C6	-6.67	114.80	118.80
55	1x	22	G	N1-C6-O6	-6.63	115.92	119.90
1	1A	2701	U	P-O3'-C3'	6.60	127.62	119.70
32	1a	1030(B)	C	C6-N1-C2	-6.53	117.69	120.30
32	2a	1025	U	N1-C2-O2	6.51	127.36	122.80
1	1A	1426	G	O5'-P-OP2	-6.46	99.88	105.70
32	2a	1001(A)	G	N3-C4-N9	6.46	129.88	126.00
1	1A	215	G	O4'-C1'-N9	6.44	113.35	108.20
1	1A	1109	G	N3-C2-N2	6.26	124.28	119.90
1	2A	2128	C	C2-N3-C4	6.26	123.03	119.90
1	1A	1020	C	N1-C2-O2	-6.23	115.16	118.90
32	2a	1263	C	C5-C4-N4	6.20	124.54	120.20
55	1x	22	G	C5-N7-C8	-6.19	101.20	104.30
32	1a	1034	G	N3-C2-N2	6.19	124.23	119.90
1	2A	1992	G	P-O3'-C3'	6.15	127.08	119.70
55	2x	14	A	C5-N7-C8	6.09	106.95	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1034	G	N9-C4-C5	-6.09	102.96	105.40
1	1A	1128	U	C2-N1-C1'	6.06	124.98	117.70
55	2x	22	G	C4-C5-C6	-6.05	115.17	118.80
55	2x	17	C	C2-N1-C1'	6.04	125.44	118.80
1	2A	2061	G	O5'-P-OP2	-6.00	100.30	105.70
32	1a	1030(B)	C	N3-C2-O2	-5.97	117.72	121.90
1	1A	894	U	C2-N1-C1'	5.95	124.84	117.70
1	2A	801	G	O5'-P-OP2	-5.93	100.36	105.70
1	1A	2158	C	C5-C6-N1	5.92	123.96	121.00
32	1a	1027	C	N1-C2-O2	5.90	122.44	118.90
1	1A	2014	G	P-O3'-C3'	5.90	126.78	119.70
1	1A	834	U	O5'-P-OP1	-5.87	100.41	105.70
1	1A	2641	A	P-O3'-C3'	5.84	126.70	119.70
32	1a	266	G	P-O3'-C3'	5.83	126.69	119.70
54	1y	33	U	C6-N1-C1'	-5.82	113.06	121.20
54	1y	33	U	N1-C2-O2	5.81	126.87	122.80
32	2a	1025	U	C2-N1-C1'	5.79	124.65	117.70
32	2a	1003	G	C8-N9-C4	-5.79	104.08	106.40
1	2A	2130	U	C5-C6-N1	5.78	125.59	122.70
3	2D	94	LEU	CA-CB-CG	5.78	128.59	115.30
32	2a	1003	G	N7-C8-N9	5.74	115.97	113.10
55	1x	46	G	N9-C4-C5	5.74	107.69	105.40
55	2x	17	C	C6-N1-C2	-5.74	118.01	120.30
32	1a	1158	C	N1-C2-O2	5.72	122.33	118.90
55	1x	22	G	N3-C4-N9	-5.72	122.57	126.00
55	1x	22	G	C8-N9-C1'	5.71	134.42	127.00
32	2a	1263	C	C5-C6-N1	5.68	123.84	121.00
1	1A	2189	U	C5-C6-N1	5.67	125.54	122.70
32	2a	754	C	C2-N1-C1'	5.65	125.01	118.80
54	2y	58	A	OP1-P-O3'	5.64	117.61	105.20
1	2A	2689	U	P-O3'-C3'	5.62	126.45	119.70
55	2x	14	A	C4-C5-C6	5.60	119.80	117.00
1	1A	1219	A	OP1-P-O3'	5.59	117.51	105.20
54	1w	45	U	C2-N1-C1'	5.59	124.40	117.70
1	1A	1121	C	C5-C4-N4	5.58	124.11	120.20
32	1a	1158	C	C2-N1-C1'	5.56	124.92	118.80
32	2a	1001(A)	G	C4-N9-C1'	5.55	133.72	126.50
1	2A	748	G	C8-N9-C1'	5.55	134.21	127.00
1	2A	576	U	O5'-P-OP1	-5.54	100.71	105.70
32	2a	266	G	P-O3'-C3'	5.54	126.34	119.70
32	2a	1029	C	N1-C2-O2	5.53	122.22	118.90
32	1a	1025	U	N1-C2-O2	5.52	126.67	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	46	G	C5-C6-N1	5.52	114.26	111.50
32	2a	1272	G	C6-N1-C2	5.51	128.41	125.10
1	1A	1219	A	P-O3'-C3'	5.50	126.30	119.70
1	1A	892	G	O4'-C1'-N9	5.49	112.59	108.20
32	2a	754	C	N1-C2-O2	5.49	122.19	118.90
54	1w	45	U	N1-C2-O2	5.47	126.63	122.80
1	2A	2140	C	C2-N1-C1'	5.46	124.80	118.80
55	2x	22	G	N1-C6-O6	-5.45	116.63	119.90
1	2A	748	G	C4-N9-C1'	-5.44	119.43	126.50
55	2x	14	A	C5-C6-N1	-5.43	114.98	117.70
55	1x	22	G	C6-C5-N7	5.40	133.64	130.40
54	1y	33	U	C5-C6-N1	5.39	125.40	122.70
55	1x	46	G	C4-C5-N7	-5.36	108.66	110.80
32	2a	1272	G	C2-N3-C4	-5.36	109.22	111.90
55	2x	22	G	C8-N9-C1'	5.36	133.96	127.00
1	1A	2802	C	C2-N1-C1'	-5.34	112.92	118.80
32	1a	1027	C	C2-N3-C4	5.33	122.56	119.90
1	1A	1405	A	N1-C2-N3	5.32	131.96	129.30
55	1x	46	G	C5-C6-N1	5.31	114.16	111.50
55	2x	22	G	C5-C6-N1	5.30	114.15	111.50
4	2E	119	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	1A	572	A	P-O3'-C3'	5.27	126.02	119.70
1	1A	2165	C	C2-N3-C4	5.27	122.53	119.90
1	1A	1121	C	N3-C2-O2	-5.26	118.22	121.90
1	1A	599	U	O5'-P-OP1	-5.26	100.96	105.70
32	2a	1272	G	C5-C6-N1	-5.25	108.88	111.50
32	2a	65	U	P-O3'-C3'	5.24	125.99	119.70
54	1w	47	U	N1-C2-O2	5.24	126.47	122.80
1	2A	528	A	OP1-P-O3'	5.23	116.70	105.20
54	1w	47	U	C5-C6-N1	5.23	125.31	122.70
32	1a	1002	G	C4-N9-C1'	5.22	133.28	126.50
1	1A	1901	C	C6-N1-C2	-5.21	118.22	120.30
32	2a	266	G	N3-C4-C5	-5.20	126.00	128.60
32	1a	687	A	P-O3'-C3'	5.20	125.94	119.70
1	2A	2345	G	C8-N9-C4	-5.20	104.32	106.40
1	2A	2473	U	C6-N1-C1'	-5.19	113.93	121.20
2	2B	1	U	C2-N1-C1'	5.18	123.92	117.70
55	1x	14	A	C4-N9-C1'	5.17	135.61	126.30
32	2a	913	A	P-O3'-C3'	5.17	125.90	119.70
55	1x	14	A	C8-N9-C1'	-5.16	118.41	127.70
1	1A	12	U	N1-C2-O2	5.15	126.40	122.80
54	2y	58	A	P-O3'-C3'	5.15	125.88	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1027	C	C6-N1-C1'	5.13	126.96	120.80
1	2A	228	A	P-O3'-C3'	5.13	125.86	119.70
1	1A	12	U	N3-C2-O2	-5.12	118.62	122.20
32	1a	841	U	C5-C6-N1	5.12	125.26	122.70
32	1a	1034	G	C6-N1-C2	5.12	128.17	125.10
1	1A	1177	G	O4'-C1'-N9	5.11	112.28	108.20
1	1A	2189	U	C6-N1-C1'	-5.09	114.07	121.20
32	2a	1025	U	C6-N1-C1'	-5.09	114.07	121.20
1	1A	2621	U	N1-C2-O2	-5.09	119.23	122.80
54	2y	60	U	N3-C2-O2	-5.09	118.64	122.20
43	2l	29	GLY	N-CA-C	-5.08	100.39	113.10
55	1x	22	G	C5-C6-N1	5.08	114.04	111.50
1	2A	897	C	C5-C6-N1	5.08	123.54	121.00
1	2A	1779	U	O4'-C1'-N1	5.07	112.26	108.20
1	1A	2701	U	N3-C2-O2	-5.07	118.65	122.20
7	2H	171	LEU	CA-CB-CG	5.05	126.93	115.30
1	2A	1204	A	O4'-C1'-N9	5.05	112.24	108.20
55	2x	46	G	N9-C4-C5	5.05	107.42	105.40
1	2A	2174	C	N1-C2-O2	5.05	121.93	118.90
32	1a	1030(B)	C	C5-C6-N1	5.04	123.52	121.00
1	1A	1985	U	N3-C2-O2	-5.03	118.68	122.20
32	2a	563	A	O4'-C1'-N9	5.00	112.20	108.20

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	61852	0	31191	646	0
1	2A	60322	0	30423	856	0
2	1B	2577	0	1305	22	0
2	2B	2575	0	1303	45	0
3	1D	2136	0	2218	47	0
3	2D	2136	0	2218	55	0
4	1E	1559	0	1618	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	2E	1559	0	1618	31	0
5	1F	1584	0	1625	41	0
5	2F	1580	0	1619	49	0
6	1G	1423	0	1436	28	0
6	2G	1428	0	1438	36	0
7	1H	1321	0	1394	22	0
7	2H	1321	0	1394	41	0
8	1I	1097	0	1140	26	0
8	2I	1064	0	1082	21	0
9	1N	1117	0	1184	13	0
9	2N	1117	0	1184	22	0
10	1O	933	0	996	11	0
10	2O	933	0	996	15	0
11	1P	1135	0	1212	24	0
11	2P	1135	0	1212	39	0
12	1Q	1122	0	1179	16	0
12	2Q	1122	0	1179	41	0
13	1R	968	0	1033	20	0
13	2R	968	0	1033	17	0
14	1S	873	0	927	17	0
14	2S	870	0	923	22	0
15	1T	1091	0	1151	18	0
15	2T	1083	0	1136	14	0
16	1U	959	0	1019	13	0
16	2U	959	0	1018	18	0
17	1V	771	0	830	10	0
17	2V	771	0	830	17	0
18	1W	886	0	940	14	0
18	2W	886	0	940	11	0
19	1X	750	0	814	12	0
19	2X	750	0	814	15	0
20	1Y	806	0	881	16	0
20	2Y	806	0	881	13	0
21	1Z	1240	0	1240	16	0
21	2Z	1271	0	1273	35	0
22	10	653	0	674	22	0
22	20	653	0	674	16	0
23	11	755	0	826	11	0
23	21	755	0	826	17	0
24	12	588	0	643	11	0
24	22	588	0	643	8	0
25	13	469	0	518	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	23	464	0	514	8	0
26	14	552	0	533	18	0
26	24	532	0	503	20	0
27	15	455	0	465	7	0
27	25	455	0	465	10	0
28	16	453	0	473	6	0
28	26	449	0	469	6	0
29	17	418	0	467	5	0
29	27	418	0	467	13	0
30	18	517	0	582	19	0
30	28	517	0	582	16	0
31	19	307	0	335	2	0
31	29	307	0	335	8	0
32	1a	32246	0	16296	0	0
32	2a	32327	0	16338	0	0
33	1b	1846	0	1867	0	0
33	2b	1825	0	1828	0	0
34	1c	1548	0	1535	0	0
34	2c	1542	0	1517	0	0
35	1d	1655	0	1672	0	0
35	2d	1674	0	1714	0	0
36	1e	1129	0	1185	0	0
36	2e	1133	0	1191	0	0
37	1f	810	0	804	0	0
37	2f	816	0	808	0	0
38	1g	1231	0	1238	0	0
38	2g	1235	0	1249	0	0
39	1h	1088	0	1126	0	0
39	2h	1088	0	1126	0	0
40	1i	983	0	986	0	0
40	2i	978	0	966	0	0
41	1j	709	0	650	0	0
41	2j	714	0	672	0	0
42	1k	829	0	825	0	0
42	2k	833	0	836	0	0
43	1l	932	0	981	0	0
43	2l	932	0	981	0	0
44	1m	958	0	1002	0	0
44	2m	950	0	988	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0
46	1o	728	0	760	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	677	0	686	0	0
48	1q	823	0	891	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	652	0	662	0	0
50	2s	646	0	644	0	0
51	1t	728	0	798	0	0
51	2t	727	0	796	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1v	277	0	140	0	0
53	2v	277	0	140	0	0
54	1w	1592	0	819	0	0
54	1y	1585	0	804	0	0
54	2w	1544	0	788	0	0
54	2y	1565	0	795	0	0
55	1x	1625	0	829	0	0
55	2x	1625	0	828	0	0
56	10	7	0	0	0	0
56	11	3	0	0	0	0
56	12	2	0	0	0	0
56	13	2	0	0	0	0
56	15	4	0	0	0	0
56	16	2	0	0	0	0
56	17	4	0	0	0	0
56	18	3	0	0	0	0
56	19	2	0	0	0	0
56	1A	1254	0	0	0	0
56	1B	36	0	0	0	0
56	1D	12	0	0	0	0
56	1E	13	0	0	0	0
56	1F	10	0	0	0	0
56	1G	5	0	0	0	0
56	1H	1	0	0	0	0
56	1I	1	0	0	0	0
56	1N	7	0	0	0	0
56	1O	5	0	0	0	0
56	1P	3	0	0	0	0
56	1Q	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1R	3	0	0	0	0
56	1S	3	0	0	0	0
56	1T	2	0	0	0	0
56	1U	6	0	0	0	0
56	1V	2	0	0	0	0
56	1W	6	0	0	0	0
56	1X	6	0	0	0	0
56	1Y	2	0	0	0	0
56	1Z	3	0	0	0	0
56	1a	330	0	0	0	0
56	1b	2	0	0	0	0
56	1c	2	0	0	0	0
56	1d	1	0	0	0	0
56	1e	2	0	0	0	0
56	1f	2	0	0	0	0
56	1l	4	0	0	0	0
56	1m	1	0	0	0	0
56	1n	1	0	0	0	0
56	1s	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	1	0	0	0	0
56	1w	11	0	0	0	0
56	1x	18	0	0	0	0
56	1y	5	0	0	0	0
56	20	3	0	0	0	0
56	23	3	0	0	0	0
56	25	4	0	0	0	0
56	27	1	0	0	0	0
56	28	3	0	0	0	0
56	2A	919	0	0	0	0
56	2B	21	0	0	0	0
56	2D	3	0	0	0	0
56	2E	8	0	0	0	0
56	2F	4	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	1	0	0	0	0
56	2P	2	0	0	0	0
56	2Q	3	0	0	0	0
56	2R	2	0	0	0	0
56	2T	1	0	0	0	0
56	2U	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2V	1	0	0	0	0
56	2W	4	0	0	0	0
56	2X	2	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	236	0	0	0	0
56	2d	1	0	0	0	0
56	2e	1	0	0	0	0
56	2f	2	0	0	0	0
56	2g	1	0	0	0	0
56	2j	2	0	0	0	0
56	2l	4	0	0	0	0
56	2n	1	0	0	0	0
56	2p	1	0	0	0	0
56	2q	4	0	0	0	0
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	6	0	0	0	0
56	2w	7	0	0	0	0
56	2x	6	0	0	0	0
56	2y	7	0	0	0	0
57	1A	8	0	0	1	0
57	1I	4	0	0	0	0
57	1a	4	0	0	0	0
57	2A	8	0	0	1	0
57	2I	4	0	0	1	0
57	2a	4	0	0	0	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	10	12	0	0	1	0
61	11	14	0	0	0	0
61	12	3	0	0	0	0
61	13	5	0	0	0	0
61	14	1	0	0	0	0
61	15	7	0	0	0	0
61	16	2	0	0	0	0
61	17	7	0	0	0	0
61	18	10	0	0	1	0
61	1A	2273	0	0	110	0
61	1B	70	0	0	2	0
61	1D	28	0	0	0	0
61	1E	27	0	0	5	0
61	1F	15	0	0	0	0
61	1G	7	0	0	0	0
61	1H	1	0	0	0	0
61	1I	1	0	0	0	0
61	1N	3	0	0	0	0
61	1O	6	0	0	0	0
61	1P	23	0	0	1	0
61	1Q	12	0	0	0	0
61	1R	15	0	0	1	0
61	1S	5	0	0	0	0
61	1T	10	0	0	1	0
61	1U	16	0	0	0	0
61	1V	11	0	0	0	0
61	1W	13	0	0	2	0
61	1X	6	0	0	0	0
61	1Y	5	0	0	0	0
61	1Z	1	0	0	0	0
61	1a	520	0	0	0	0
61	1b	1	0	0	0	0
61	1d	2	0	0	0	0
61	1e	1	0	0	0	0
61	1g	2	0	0	0	0
61	1i	1	0	0	0	0
61	1l	10	0	0	0	0
61	1m	2	0	0	0	0
61	1n	1	0	0	0	0
61	1o	2	0	0	0	0
61	1p	2	0	0	0	0
61	1q	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1u	1	0	0	0	0
61	1v	5	0	0	0	0
61	1w	19	0	0	0	0
61	1x	15	0	0	0	0
61	1y	2	0	0	0	0
61	20	4	0	0	0	0
61	21	11	0	0	0	0
61	22	1	0	0	0	0
61	23	1	0	0	0	0
61	25	3	0	0	0	0
61	27	3	0	0	0	0
61	28	4	0	0	0	0
61	29	1	0	0	0	0
61	2A	1393	0	0	97	0
61	2B	28	0	0	0	0
61	2D	29	0	0	0	0
61	2E	18	0	0	0	0
61	2F	17	0	0	0	0
61	2I	4	0	0	0	0
61	2N	1	0	0	0	0
61	2O	1	0	0	0	0
61	2P	16	0	0	2	0
61	2Q	2	0	0	0	0
61	2R	2	0	0	0	0
61	2T	7	0	0	0	0
61	2U	3	0	0	0	0
61	2V	2	0	0	0	0
61	2W	4	0	0	0	0
61	2X	2	0	0	0	0
61	2Y	1	0	0	0	0
61	2Z	2	0	0	0	0
61	2a	373	0	0	0	0
61	2d	2	0	0	0	0
61	2e	2	0	0	0	0
61	2g	1	0	0	0	0
61	2i	1	0	0	0	0
61	2j	4	0	0	0	0
61	2l	6	0	0	0	0
61	2p	1	0	0	0	0
61	2q	1	0	0	0	0
61	2r	1	0	0	0	0
61	2t	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2v	2	0	0	0	0
61	2w	3	0	0	0	0
61	2x	9	0	0	0	0
61	2y	20	0	0	0	0
All	All	301288	0	196660	2326	0

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

All (2326) 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)
1:2A:2138:C:N4	1:2A:2153:G:H1	1.49	1.10
1:1A:1740:U:H1'	3:1D:14:ARG:HH22	1.24	1.02
1:1A:2149:G:H1	1:1A:2183:C:N4	1.56	1.01
1:2A:79:G:H1	1:2A:90:U:H3	29.43	0.98
1:1A:2146:G:H1	1:1A:2196:C:H42	0.99	0.98
1:2A:1422:G:H5''	10:2O:48:PRO:HB3	99.87	0.97
1:2A:1002:G:H1	1:2A:1038:C:N4	42.66	0.96
1:1A:2331:G:H22	14:1S:3:ARG:HD3	1.29	0.96
1:2A:83:G:H1	1:2A:102:G:HO2'	1.11	0.96
3:2D:242:ARG:HH11	3:2D:242:ARG:HG3	1.28	0.96
1:2A:2138:C:H42	1:2A:2153:G:H1	1.00	0.95
1:1A:1105:G:H1	1:1A:1125:C:H42	1.15	0.94
1:1A:2146:G:H1	1:1A:2196:C:N4	1.66	0.94
1:1A:2121:U:H3	1:1A:2212:G:H1	1.16	0.93
1:2A:2121:G:H1	1:2A:2177:C:H42	1.09	0.93
1:1A:1128:U:H3	1:1A:1132:A:N6	1.65	0.93
1:1A:1101:G:H1	1:1A:1150:C:H42	1.11	0.93
1:2A:2129:C:H42	1:2A:2159:G:H1	1.07	0.93
1:2A:2138:C:N3	1:2A:2153:G:N2	2.16	0.92
3:1D:242:ARG:HG3	3:1D:242:ARG:HH11	1.31	0.92
1:1A:2149:G:H1	1:1A:2183:C:H42	0.93	0.92
1:1A:2439:C:OP1	61:1A:4301:HOH:O	1.86	0.92
22:10:10:THR:HG22	22:10:12:ASN:H	1.31	0.92
12:2Q:12:GLN:HE21	12:2Q:72:LYS:HG3	1.34	0.91
1:2A:2127:G:C6	1:2A:2161:C:N4	2.39	0.90
1:1A:656:A:OP1	11:1P:65:ARG:NH1	2.05	0.90
1:1A:1117:G:O6	1:1A:1146:C:N4	2.03	0.89
20:1Y:92:ASN:HB3	20:1Y:94:LYS:H	1.38	0.88
1:1A:1649:A:OP1	61:1A:4302:HOH:O	1.91	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:20:10:THR:HG22	22:20:12:ASN:H	1.38	0.88
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.56	0.88
1:1A:1128:U:O4	1:1A:1132:A:N1	2.07	0.88
30:18:6:THR:HG22	30:18:63:PRO:HD2	1.55	0.88
1:1A:2157:A:H5'	1:1A:2182:G:H4'	1.56	0.87
1:1A:839:G:O6	61:1A:4303:HOH:O	1.92	0.86
1:1A:1111:U:O2	1:1A:1119:A:N6	2.09	0.85
1:2A:1002:G:H1	1:2A:1038:C:H42	43.05	0.85
1:1A:2158:C:N3	1:1A:2177:G:N2	2.25	0.84
5:1F:188:ARG:HA	11:1P:3:LEU:HD11	1.59	0.84
1:1A:1004:A:N6	1:1A:1037:C:N3	55.38	0.84
1:1A:1108:G:H1	1:1A:1123:A:H61	1.18	0.84
1:2A:2127:G:N1	1:2A:2161:C:C4	2.45	0.84
1:1A:1357:G:O6	61:1A:4305:HOH:O	1.95	0.84
1:1A:931:C:H42	1:1A:938:G:H1	1.24	0.84
1:2A:583:G:N7	61:2A:4019:HOH:O	2.10	0.84
1:1A:1104:G:H1	1:1A:1126:C:H42	1.22	0.83
1:2A:1171:G:H1	1:2A:1178:C:H42	1.26	0.83
1:2A:1689:A:H62	1:2A:1698:A:H2	1.22	0.83
1:2A:2129:C:N4	1:2A:2159:G:H1	1.76	0.83
1:1A:2124:U:H3	1:1A:2209:G:H1	1.26	0.83
1:2A:1204:A:H2	1:2A:1241:A:H62	1.23	0.83
1:1A:537:G:N7	61:1A:4324:HOH:O	2.10	0.83
1:1A:2367:C:H1'	22:10:39:ARG:HH21	1.44	0.83
1:1A:2511:C:OP1	61:1A:4304:HOH:O	1.94	0.83
1:1A:2695:C:O2	10:1O:70:LYS:NZ	2.12	0.82
1:1A:1087:C:H42	1:1A:1160:G:H1	1.27	0.82
1:2A:2121:G:H1	1:2A:2177:C:N4	1.76	0.82
1:1A:1128:U:H3	1:1A:1132:A:H61	0.86	0.82
1:1A:873:U:OP1	61:1A:4301:HOH:O	1.96	0.82
11:1P:100:LEU:HD12	11:1P:112:LEU:HD11	1.60	0.82
11:1P:42:SER:O	61:1P:301:HOH:O	1.96	0.81
11:1P:52:GLU:OE1	11:1P:55:ARG:NH1	2.13	0.81
1:1A:1151:U:H2'	1:1A:1152:G:H8	1.43	0.81
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.25	0.81
1:1A:1378:G:OP1	61:1A:4306:HOH:O	1.99	0.81
2:2B:22:U:H3	2:2B:61:G:H1	1.29	0.81
1:2A:2099:U:H3	1:2A:2190:G:H1	1.28	0.81
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.63	0.80
1:2A:1670:C:OP1	61:2A:4002:HOH:O	1.99	0.80
1:2A:2127:G:C2	1:2A:2161:C:N3	2.50	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:568:U:O4	61:2A:4001:HOH:O	1.98	0.80
1:1A:2158:C:N4	1:1A:2177:G:N1	2.27	0.79
1:2A:2499:C:OP2	61:2A:4003:HOH:O	1.99	0.79
1:2A:792:G:O6	61:2A:4004:HOH:O	1.99	0.79
1:1A:2641:A:O2'	1:1A:2642:G:OP2	2.00	0.79
1:2A:1648:C:OP1	61:2A:4005:HOH:O	2.00	0.79
1:2A:2345:G:H4'	1:2A:2346:A:H5''	1.62	0.79
1:1A:1104:G:H1	1:1A:1126:C:N4	1.80	0.79
1:2A:1693:U:H1'	3:2D:14:ARG:HH22	1.49	0.78
1:1A:2158:C:H42	1:1A:2177:G:H1	1.28	0.78
12:2Q:85:LYS:HG2	22:20:7:LEU:HB3	1.65	0.78
1:1A:1740:U:H1'	3:1D:14:ARG:NH2	1.95	0.78
1:1A:927:G:H2'	1:1A:928:G:H8	1.49	0.78
1:2A:2114:A:H62	1:2A:2115:G:H21	1.29	0.78
5:2F:33:LEU:HD13	5:2F:112:MET:HE2	1.65	0.78
1:1A:1101:G:H1	1:1A:1150:C:N4	1.82	0.78
26:24:53:GLU:HG2	26:24:55:ARG:H	1.47	0.78
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.16	0.78
1:2A:987:G:H1	1:2A:1218:C:H42	46.45	0.77
1:2A:962:G:OP1	61:2A:4006:HOH:O	2.03	0.77
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.50	0.77
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.67	0.77
1:2A:1762:A:N1	61:2A:4056:HOH:O	2.18	0.77
1:2A:2524:G:N7	61:2A:4046:HOH:O	2.16	0.76
1:1A:2165:C:N3	1:1A:2170:G:O6	2.19	0.76
1:2A:64:A:N6	1:2A:90:U:O4	2.18	0.76
1:2A:1693:U:H1'	3:2D:14:ARG:NH2	2.00	0.76
1:1A:1105:G:H1	1:1A:1125:C:N4	1.83	0.76
1:1A:990:A:OP2	61:1A:4307:HOH:O	2.02	0.76
11:2P:52:GLU:OE1	11:2P:55:ARG:NH1	2.19	0.76
1:1A:2442:A:OP1	61:1A:4309:HOH:O	2.04	0.75
1:1A:2158:C:N4	1:1A:2177:G:H1	1.82	0.75
5:1F:70:THR:HG23	5:1F:72:ARG:H	1.49	0.75
1:1A:2817:G:N1	1:1A:2902:G:O6	2.15	0.75
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.52	0.75
1:1A:1100:A:H61	1:1A:1151:U:H3	1.35	0.75
1:1A:2149:G:N2	1:1A:2183:C:N3	2.33	0.75
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.67	0.75
1:2A:450:G:O6	61:2A:4007:HOH:O	2.04	0.75
1:1A:2015:U:OP2	61:1A:4310:HOH:O	2.05	0.75
5:2F:101:LEU:O	5:2F:106:ARG:NH1	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1069:U:OP2	61:1A:4308:HOH:O	2.03	0.74
6:2G:179:PRO:HB2	26:24:42:PHE:HE2	1.52	0.74
1:2A:1840:G:OP2	61:2A:4008:HOH:O	2.04	0.74
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.68	0.74
1:2A:2127:G:C2	1:2A:2161:C:C4	2.75	0.74
1:1A:2440:G:OP1	61:1A:4301:HOH:O	2.05	0.74
1:1A:880:U:O2	11:1P:55:ARG:NH2	2.20	0.74
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.68	0.74
13:2R:67:LEU:HD13	13:2R:76:VAL:HG21	1.70	0.74
1:1A:1740:U:O2	3:1D:14:ARG:NH2	2.20	0.74
1:1A:2286:A:OP2	61:1A:4312:HOH:O	2.06	0.74
1:2A:993:G:N7	1:2A:1213:A:N6	48.88	0.74
7:2H:7:LEU:HD12	7:2H:8:PRO:HD2	1.69	0.74
1:1A:2220:A:OP1	8:1I:33:ARG:NH2	2.21	0.74
1:2A:677:A:OP2	61:2A:4009:HOH:O	2.05	0.74
1:1A:1221:G:N2	1:1A:1223:C:OP2	2.20	0.74
1:2A:1031:G:H5''	31:29:8:LYS:HE3	1.68	0.73
1:2A:2630:G:N2	1:2A:2788:C:O2	2.19	0.73
1:2A:1356:G:OP1	61:2A:4011:HOH:O	2.06	0.73
1:1A:2288:G:N7	61:1A:4383:HOH:O	2.22	0.73
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.21	0.73
1:2A:2049:G:N7	61:2A:4070:HOH:O	2.21	0.73
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.71	0.73
1:2A:2822:G:OP2	61:2A:4012:HOH:O	2.06	0.73
1:1A:1128:U:N3	1:1A:1132:A:N6	2.27	0.73
1:1A:2807:C:H42	1:1A:2813:G:H22	1.37	0.73
1:2A:884:C:N3	1:2A:893:C:O2'	2.21	0.73
1:2A:2143:C:H42	1:2A:2148:G:H1	1.34	0.72
1:1A:1417:G:O6	61:1A:4314:HOH:O	2.07	0.72
15:1T:112:ARG:HG3	15:1T:115:ARG:HH21	1.55	0.72
23:21:50:ARG:HG2	23:21:59:THR:HG22	1.71	0.72
1:2A:1833:U:OP1	61:2A:4010:HOH:O	2.06	0.72
1:1A:2832:G:OP2	61:1A:4316:HOH:O	2.08	0.72
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.54	0.72
1:2A:2243:U:OP1	61:2A:4014:HOH:O	2.07	0.72
1:2A:1665:A:OP2	61:2A:4016:HOH:O	2.08	0.72
26:14:54:GLY:N	26:14:55:ARG:HA	2.05	0.72
1:1A:1915:C:OP1	61:1A:4317:HOH:O	2.08	0.72
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.71	0.71
1:1A:1230:C:OP2	61:1A:4311:HOH:O	2.06	0.71
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:325:G:OP2	20:1Y:84:ARG:NH2	2.23	0.71
1:2A:731:C:OP2	61:2A:4013:HOH:O	2.07	0.71
1:1A:1588:G:O6	61:1A:4313:HOH:O	2.07	0.71
1:1A:542:C:OP1	27:15:16:ARG:NH2	2.24	0.71
1:1A:1716:A:OP2	61:1A:4315:HOH:O	2.08	0.71
1:2A:963:U:OP2	61:2A:4006:HOH:O	2.08	0.71
21:2Z:153:SER:HB3	21:2Z:167:PRO:HB3	1.71	0.71
1:2A:2104:G:H1	1:2A:2185:C:H42	1.39	0.71
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.25	0.71
1:1A:2562:G:OP1	61:1A:4315:HOH:O	2.08	0.71
1:1A:1922:A:N7	61:1A:4384:HOH:O	2.22	0.71
1:2A:1973:G:OP1	61:2A:4017:HOH:O	2.09	0.71
17:2V:40:LEU:HB2	17:2V:46:VAL:HG22	1.73	0.71
1:2A:1782:C:OP1	61:2A:4015:HOH:O	2.07	0.70
1:2A:900:A:O2'	1:2A:901:A:OP1	2.09	0.70
1:1A:1431:G:O2'	1:1A:1442:U:O2	2.09	0.70
1:2A:2127:G:N2	1:2A:2161:C:C2	2.59	0.70
1:2A:2882:A:OP1	13:2R:96:ARG:NH1	2.24	0.70
1:2A:1024:G:OP2	61:2A:4020:HOH:O	2.10	0.70
1:2A:266:G:H5''	1:2A:268:C:H41	11.75	0.70
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.26	0.70
1:1A:181:C:OP1	61:1A:4320:HOH:O	2.09	0.70
1:1A:1347:A:OP1	61:1A:4318:HOH:O	2.08	0.70
1:1A:99:G:H21	24:12:7:ARG:HH22	1.39	0.70
1:1A:2143:G:H1	1:1A:2199:C:H42	1.39	0.70
1:2A:1002:G:N2	1:2A:1038:C:N3	42.22	0.70
1:2A:852:G:H2'	1:2A:853:G:H8	1.56	0.70
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.24	0.70
1:2A:880:G:H22	1:2A:898:C:H1'	1.56	0.70
1:1A:2831:A:OP2	61:1A:4316:HOH:O	2.09	0.70
23:21:51:VAL:HG11	23:21:74:VAL:HG21	1.72	0.70
1:2A:2042:A:OP1	61:2A:4022:HOH:O	2.10	0.70
1:2A:1360:A:OP2	9:2N:35:ARG:NH2	117.75	0.70
1:1A:1700:G:H3'	13:1R:2:ARG:HD3	1.74	0.70
1:2A:1604:C:OP1	61:2A:4018:HOH:O	2.09	0.70
1:2A:1566:A:OP1	3:2D:211:ARG:NH1	2.25	0.70
1:1A:1814:A:N7	61:1A:4403:HOH:O	2.25	0.69
1:1A:71:U:OP1	61:1A:4319:HOH:O	2.09	0.69
1:1A:1832:G:OP2	3:1D:154:LYS:NZ	2.25	0.69
1:1A:2495:C:N3	12:1Q:124:LYS:NZ	2.40	0.69
1:2A:863:A:H2'	1:2A:864:G:H8	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:646:A:OP2	11:1P:108:LYS:NZ	2.22	0.69
1:1A:1809:U:OP1	61:1A:4325:HOH:O	2.10	0.69
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.10	0.69
1:2A:621:A:OP2	11:2P:108:LYS:NZ	2.25	0.69
1:1A:1055:A:OP2	9:1N:37:LYS:NZ	2.23	0.69
1:1A:2604:G:OP1	61:1A:4323:HOH:O	2.10	0.69
1:2A:1346:G:OP2	61:2A:4023:HOH:O	2.10	0.69
1:1A:2146:G:N2	1:1A:2196:C:N3	2.38	0.69
1:2A:2677:G:N3	61:2A:4092:HOH:O	2.25	0.69
1:1A:1361:C:OP2	61:1A:4306:HOH:O	2.11	0.69
1:2A:2518:A:OP2	61:2A:4028:HOH:O	2.11	0.69
1:2A:2807:G:N1	1:2A:2893:G:O6	2.17	0.69
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.26	0.69
1:2A:317:G:O6	61:2A:4024:HOH:O	2.11	0.68
1:1A:1694:G:OP1	61:1A:4326:HOH:O	2.10	0.68
1:1A:2801:C:OP1	4:1E:61:ARG:NH2	2.26	0.68
1:1A:237:G:OP1	61:1A:4328:HOH:O	2.11	0.68
1:2A:1772:G:OP1	61:2A:4025:HOH:O	2.11	0.68
2:2B:105:A:OP1	21:2Z:72:ARG:NH1	2.26	0.68
1:1A:1044:C:OP1	61:1A:4321:HOH:O	2.10	0.68
4:1E:47:VAL:HG21	4:1E:86:PRO:HD2	1.76	0.68
1:2A:1532:C:H42	1:2A:1537:G:H1	1.40	0.68
1:2A:2287:A:H62	1:2A:2344:U:H3	1.41	0.68
1:2A:370:G:OP2	61:2A:4021:HOH:O	2.10	0.68
1:1A:848:G:O6	5:1F:53:THR:OG1	2.10	0.68
1:2A:2513:G:N7	61:2A:4103:HOH:O	2.27	0.68
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.58	0.68
1:1A:1115:A:H4'	1:1A:1116:A:H8	1.58	0.68
1:2A:1378:A:OP1	29:27:10:ARG:NH2	2.27	0.68
1:1A:409:G:O6	61:1A:4322:HOH:O	2.10	0.68
1:1A:1842:G:N7	61:1A:4418:HOH:O	2.27	0.68
1:1A:2460:A:OP1	61:1A:4304:HOH:O	2.12	0.68
1:1A:787:U:OP2	61:1A:4327:HOH:O	2.11	0.68
1:2A:1466:G:HO2'	1:2A:1546:C:HO2'	1.37	0.68
5:2F:140:LEU:HD11	5:2F:170:LEU:HD11	1.76	0.68
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.20	0.68
1:1A:1275:G:N7	61:1A:4409:HOH:O	2.27	0.67
1:1A:1139:G:H3'	1:1A:1140:U:H5''	1.76	0.67
1:1A:625:G:O2'	1:1A:702:A:N6	2.27	0.67
1:2A:1812:A:OP2	61:2A:4033:HOH:O	2.12	0.67
1:2A:2136:C:N3	1:2A:2155:G:N2	2.38	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:2V:72:VAL:HG13	17:2V:85:LYS:HB2	1.77	0.67
1:2A:1297:C:OP2	61:2A:4032:HOH:O	2.12	0.67
1:2A:2242:G:OP1	61:2A:4026:HOH:O	2.11	0.67
1:2A:249:C:O2	30:28:12:LYS:NZ	2.28	0.67
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.28	0.67
12:2Q:26:TYR:O	12:2Q:67:ARG:NH1	2.28	0.67
26:24:15:ILE:HB	26:24:32:TYR:HD1	1.60	0.67
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.29	0.67
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.76	0.67
1:1A:556:C:OP2	61:1A:4333:HOH:O	2.13	0.67
1:1A:692:C:H42	1:1A:698:G:H1	1.41	0.67
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	1.77	0.67
1:2A:2319:G:H22	14:2S:3:ARG:HD3	1.60	0.67
1:1A:1695:C:OP1	61:1A:4326:HOH:O	2.12	0.67
1:1A:1871:G:N7	61:1A:4415:HOH:O	2.27	0.67
1:2A:2578:G:OP1	61:2A:4030:HOH:O	2.12	0.67
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.28	0.67
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.26	0.67
1:1A:2147:G:N1	1:1A:2194:U:OP1	2.25	0.67
1:1A:303:C:H42	1:1A:385:G:H1	1.43	0.67
1:2A:2317:C:N4	1:2A:2318:G:O6	2.28	0.67
1:1A:2340:A:H2'	1:1A:2341:G:C8	2.30	0.66
1:2A:1508:A:H4'	1:2A:1509(A):A:C5	2.29	0.66
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.10	0.66
30:28:6:THR:HG22	30:28:63:PRO:HD2	1.77	0.66
1:2A:2598:A:OP2	61:2A:4034:HOH:O	2.12	0.66
2:2B:106:G:H5'	21:2Z:31:ARG:HG2	1.76	0.66
11:2P:44:GLY:O	61:2P:301:HOH:O	2.13	0.66
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.29	0.66
11:1P:59:LEU:HD21	30:18:10:ALA:HA	1.78	0.66
1:2A:1441:G:O2'	61:2A:4035:HOH:O	2.13	0.66
1:1A:667:G:OP1	61:1A:4329:HOH:O	2.11	0.66
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.76	0.66
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.78	0.66
1:2A:2785:C:OP1	4:2E:41:LYS:NZ	2.28	0.66
20:2Y:9:LYS:NZ	20:2Y:28:LYS:O	2.28	0.66
1:1A:889:G:N7	61:1A:4421:HOH:O	2.28	0.66
1:2A:2524:G:O6	61:2A:4027:HOH:O	2.11	0.66
1:1A:1681:A:OP2	61:1A:4334:HOH:O	2.13	0.66
1:2A:2625:G:O6	61:2A:4038:HOH:O	2.13	0.66
1:2A:981:A:OP1	61:2A:4036:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:34:LEU:HD11	12:1Q:129:THR:HB	1.78	0.66
1:2A:1434:A:H61	1:2A:1558:A:H62	1.43	0.66
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.12	0.66
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.31	0.66
1:1A:440:C:OP2	61:1A:4332:HOH:O	2.13	0.65
1:2A:2436:G:O6	61:2A:4031:HOH:O	2.12	0.65
1:1A:2227:G:H3'	1:1A:2228:G:C8	2.32	0.65
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.31	0.65
1:2A:1509(B):A:H2'	1:2A:1510:G:H8	1.61	0.65
1:2A:1568:G:N7	61:2A:4109:HOH:O	2.28	0.65
1:1A:739:C:O2'	3:1D:38:LYS:NZ	2.29	0.65
1:1A:1388:A:OP2	61:1A:4337:HOH:O	2.15	0.65
1:1A:2205:C:H2'	1:1A:2206:G:H8	1.62	0.65
1:1A:941:U:O2'	1:1A:942:A:OP1	2.13	0.65
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.31	0.65
1:2A:2499:C:OP1	61:2A:4039:HOH:O	2.14	0.65
1:2A:1023:U:OP2	61:2A:4020:HOH:O	2.14	0.65
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.79	0.65
1:2A:794:G:OP2	61:2A:4037:HOH:O	2.13	0.65
61:2A:4012:HOH:O	4:2E:110:GLY:O	2.15	0.65
1:1A:1745:A:OP2	61:1A:4336:HOH:O	2.14	0.65
1:1A:2162:C:N3	1:1A:2173:G:O6	2.30	0.65
1:1A:2796:G:N7	61:1A:4427:HOH:O	2.28	0.65
1:2A:1002:G:C2	1:2A:1003:G:H8	4.60	0.65
1:2A:1815:A:OP2	3:2D:54:ARG:NH2	2.30	0.65
12:2Q:109:VAL:HG22	12:2Q:113:GLN:HB3	1.77	0.65
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.29	0.65
1:1A:1873:G:OP2	61:1A:4335:HOH:O	2.14	0.65
7:1H:86:GLU:OE2	7:1H:132:ARG:NH2	2.30	0.65
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.32	0.65
1:2A:2448:A:OP1	61:2A:4039:HOH:O	2.15	0.65
1:2A:731:C:OP1	61:2A:4041:HOH:O	2.14	0.65
5:2F:28:ILE:HG23	5:2F:112:MET:HE3	1.78	0.65
1:1A:2185:C:OP1	1:1A:2187:G:N2	2.30	0.65
1:1A:2129:C:H42	1:1A:2204:G:H1	1.44	0.65
1:1A:2772:G:N7	61:1A:4441:HOH:O	2.30	0.65
8:1I:129:THR:HG22	8:1I:139:GLN:HE22	1.62	0.65
1:2A:975:C:OP1	61:2A:4042:HOH:O	2.14	0.65
1:2A:2268:A:OP1	61:2A:4040:HOH:O	2.14	0.64
22:10:11:ARG:O	22:10:14:ARG:NH2	2.30	0.64
1:1A:1793:A:N1	61:1A:4438:HOH:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:121:ASN:ND2	61:1E:402:HOH:O	2.29	0.64
1:2A:1021:A:H62	1:2A:1141:U:H3	1.45	0.64
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.62	0.64
1:1A:1615:G:H5''	3:1D:61:LEU:HD13	1.77	0.64
1:1A:118:U:OP2	61:1A:4341:HOH:O	2.15	0.64
1:2A:2531:A:H61	1:2A:2662:A:H61	1.44	0.64
6:2G:135:LEU:HD21	6:2G:157:ILE:HD12	1.79	0.64
1:1A:1317:G:OP2	61:1A:4326:HOH:O	2.14	0.64
8:1I:76:THR:HG22	8:1I:141:LYS:HE2	1.80	0.64
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.30	0.64
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.11	0.64
1:2A:2125:G:N1	1:2A:2172:U:OP1	2.29	0.64
26:24:24:THR:OG1	26:24:25:TYR:N	2.31	0.64
1:1A:2331:G:H22	14:1S:3:ARG:CD	2.09	0.64
1:2A:863:A:H2'	1:2A:864:G:C8	2.33	0.63
9:2N:123:TYR:HH	9:2N:130:HIS:HE2	1.41	0.63
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HE3	1.80	0.63
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.31	0.63
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.79	0.63
1:1A:2362:C:OP2	61:1A:4345:HOH:O	2.16	0.63
1:1A:1846:A:OP2	3:1D:54:ARG:NH2	2.30	0.63
4:1E:122:PHE:O	61:1E:401:HOH:O	2.15	0.63
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.80	0.63
1:1A:2650:G:P	4:1E:82:ARG:HH12	2.22	0.63
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	1.81	0.63
1:1A:1588:G:OP2	61:1A:4343:HOH:O	2.16	0.63
1:1A:555:G:N1	1:1A:2045:G:OP1	2.24	0.63
1:2A:2680:C:OP2	4:2E:111:ARG:NH2	2.31	0.63
5:2F:132:VAL:HG21	5:2F:163:VAL:HG22	1.80	0.63
21:2Z:171:ILE:HG13	21:2Z:172:ALA:H	1.64	0.63
1:1A:1464:G:OP2	61:1A:4347:HOH:O	2.16	0.63
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.79	0.63
1:2A:857:C:H4'	22:20:23:VAL:HG21	1.81	0.63
1:2A:287:C:H2'	1:2A:288:C:C6	2.34	0.63
21:2Z:7:ALA:HB2	21:2Z:59:LEU:HD22	1.81	0.63
1:1A:2862:G:OP2	61:1A:4338:HOH:O	2.15	0.63
1:2A:2632:A:HO2'	1:2A:2811:G:HO2'	1.42	0.63
1:2A:300:A:OP1	20:2Y:86:ARG:NH2	2.31	0.63
1:1A:2163:G:O6	1:1A:2172:U:O2	2.17	0.63
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.30	0.63
1:2A:2287:A:N6	1:2A:2344:U:H3	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:11:C:OP2	2:2B:12:C:N4	2.22	0.63
1:1A:2776:G:OP2	61:1A:4346:HOH:O	2.16	0.63
1:2A:1113:U:H2'	1:2A:1114:G:C8	2.33	0.63
1:2A:1120:G:O6	61:2A:4029:HOH:O	2.11	0.62
1:2A:1799:G:O2'	3:2D:181:GLU:OE2	2.17	0.62
25:13:39:ASP:OD1	25:13:44:ARG:NH1	2.33	0.62
1:1A:2130:C:H2'	1:1A:2131:U:H6	1.63	0.62
1:1A:2812:A:H1'	1:1A:2904:U:H1'	1.80	0.62
2:1B:117:G:N7	61:1B:303:HOH:O	2.31	0.62
1:1A:928:G:N2	1:1A:943:C:O2	2.32	0.62
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.79	0.62
1:2A:2218:U:N3	23:21:55:GLY:O	2.32	0.62
3:2D:69:ARG:HE	3:2D:130:ALA:HB2	1.64	0.62
11:2P:86:LYS:HB3	11:2P:118:GLY:HA3	1.81	0.62
1:1A:414:U:O4	61:1A:4330:HOH:O	2.12	0.62
1:2A:1920:4OC:O5'	1:2A:1920:4OC:H6	1.99	0.62
1:2A:2689:U:OP2	1:2A:2719:G:N2	2.27	0.62
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.00	0.62
1:1A:1435:G:H2'	1:1A:1436:U:C6	2.90	0.62
1:1A:1834:A:O2'	3:1D:259:THR:HG21	1.99	0.62
1:2A:1530:C:H42	1:2A:1539:G:H1	1.48	0.62
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.18	0.62
1:2A:2781:A:H5''	1:2A:2782:G:H5'	1.82	0.62
7:2H:35:VAL:HG13	7:2H:71:LEU:HD22	1.81	0.62
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.82	0.62
1:1A:1299:A:OP1	61:1A:4349:HOH:O	2.16	0.62
18:1W:31:GLU:OE1	61:1W:3101:HOH:O	2.16	0.62
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.35	0.62
1:1A:215:G:H21	1:1A:217:A:H62	1.48	0.62
1:2A:752:A:H3'	29:27:1:MET:HE2	1.80	0.62
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.64	0.62
1:2A:974:G:OP1	1:2A:1187:G:O2'	2.15	0.62
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.82	0.62
21:2Z:150:LEU:HB3	21:2Z:171:ILE:HD11	1.81	0.62
1:1A:2421:G:O2'	61:1A:4350:HOH:O	2.16	0.61
1:1A:2331:G:N2	14:1S:3:ARG:HD3	2.10	0.61
28:26:40:CYS:O	28:26:44:ARG:N	2.32	0.61
19:2X:60:ARG:HH22	29:27:47:ARG:HH12	1.47	0.61
1:2A:2136:C:N4	1:2A:2155:G:N1	2.48	0.61
2:2B:66:A:N6	2:2B:108:U:H3'	2.16	0.61
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:848:G:H2'	1:2A:849:A:C8	2.35	0.61
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.35	0.61
6:2G:131:TYR:HB3	6:2G:159:VAL:HG13	1.81	0.61
1:1A:493:G:OP1	29:17:33:ARG:NH1	2.34	0.61
1:1A:1090:G:H5'	1:1A:1091:A:OP2	2.01	0.61
1:2A:330:A:H2	1:2A:1210:A:HO2'	1.47	0.61
3:2D:242:ARG:NH1	3:2D:242:ARG:HG3	2.04	0.61
19:2X:94:GLY:H	19:2X:95:LEU:HA	1.65	0.61
1:1A:1110:C:N3	1:1A:1120:G:O6	2.34	0.61
1:1A:2148:A:N1	1:1A:2184:G:O2'	2.26	0.61
1:1A:2849:G:H5'	13:1R:46:GLY:HA2	1.83	0.61
5:1F:133:ASN:N	5:1F:138:GLU:OE1	2.34	0.61
1:2A:1569:A:H5'	3:2D:61:LEU:HD11	1.83	0.61
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.31	0.61
1:1A:1100:A:N6	1:1A:1151:U:H3	1.99	0.61
1:1A:943:C:N3	1:1A:944:C:N4	2.48	0.61
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.00	0.61
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.83	0.61
8:2I:12:LEU:HD22	8:2I:19:VAL:HG21	1.82	0.61
7:2H:45:VAL:HG12	7:2H:50:VAL:HG22	1.82	0.61
1:1A:1117:G:H1'	1:1A:1135:G:H2'	1.83	0.60
1:1A:210:A:N1	1:1A:254:A:O2'	2.34	0.60
1:1A:2348:A:H61	22:10:43:THR:HG22	1.66	0.60
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.36	0.60
1:2A:861:A:N3	2:2B:79:C:O2'	2.30	0.60
1:2A:882:G:H2'	1:2A:883:G:H8	1.66	0.60
1:2A:848:G:C4	1:2A:933:A:H8	2.19	0.60
1:2A:320:A:OP2	5:2F:137:LYS:NZ	2.31	0.60
12:2Q:52:VAL:HA	12:2Q:55:VAL:HG22	1.84	0.60
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.81	0.60
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.83	0.60
18:1W:78:GLU:OE2	18:1W:99:ARG:NH1	2.34	0.60
1:2A:2728:U:H5'	10:2O:70:LYS:HZ3	1.66	0.60
9:2N:38:HIS:CE1	9:2N:39:ARG:HG3	2.37	0.60
6:1G:129:GLY:O	6:1G:161:THR:OG1	2.20	0.60
26:24:41:PRO:HG3	26:24:49:PHE:CE2	2.36	0.60
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.36	0.60
2:1B:23:G:O6	61:1B:301:HOH:O	2.13	0.60
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.00	0.60
1:2A:2112:G:N7	1:2A:2169:A:N6	2.49	0.60
1:2A:890:A:H2'	1:2A:892:G:H8	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:958:U:OP2	12:2Q:14:ARG:NH1	2.35	0.60
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	1.82	0.60
5:1F:107:LYS:NZ	5:1F:207:GLY:O	2.26	0.60
20:1Y:54:LYS:HA	20:1Y:56:PRO:HD3	1.83	0.60
1:2A:751:A:OP1	61:2A:4045:HOH:O	2.16	0.60
1:2A:796:C:H2'	1:2A:797:C:C6	2.37	0.60
21:2Z:154:ASP:N	21:2Z:154:ASP:OD1	2.31	0.60
1:1A:1151:U:H2'	1:1A:1152:G:C8	2.31	0.60
5:2F:53:THR:HG22	5:2F:56:GLU:HG3	1.84	0.60
1:1A:615:G:O6	61:1A:4331:HOH:O	2.13	0.60
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.02	0.59
6:2G:101:ILE:HG22	6:2G:105:LYS:HE2	1.82	0.59
1:2A:2849:U:OP2	15:2T:95:ARG:NH1	2.35	0.59
24:12:32:LEU:HD11	24:12:54:LYS:HG2	1.83	0.59
1:1A:346:A:OP1	5:1F:168:ARG:HD2	2.02	0.59
1:2A:1671:U:OP2	61:2A:4002:HOH:O	2.17	0.59
1:1A:1992:A:OP1	61:1A:4348:HOH:O	2.16	0.59
1:2A:2127:G:C5	1:2A:2161:C:N4	2.69	0.59
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.84	0.59
1:1A:1219:A:H4'	1:1A:1220:U:OP1	2.00	0.59
1:1A:2013:U:H2'	1:1A:2014:G:H5''	1.85	0.59
1:2A:2387:U:O2'	22:20:19:LYS:NZ	2.35	0.59
8:2I:43:ASN:ND2	23:21:75:GLU:OE2	2.35	0.59
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.83	0.59
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.35	0.59
1:2A:361:G:O6	61:2A:4043:HOH:O	2.14	0.59
1:2A:2141:G:O6	1:2A:2150:U:O2	2.20	0.59
1:2A:625:G:N7	11:2P:107:LYS:NZ	2.44	0.59
1:2A:1865:G:N7	61:2A:4135:HOH:O	2.31	0.59
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.68	0.59
1:1A:1071:G:O2'	61:1A:4308:HOH:O	2.12	0.59
1:1A:1104:G:N2	1:1A:1126:C:N3	2.43	0.59
1:2A:2136:C:N4	1:2A:2155:G:H1	2.00	0.59
2:2B:66:A:H61	2:2B:108:U:H3'	1.68	0.59
1:1A:1760:U:H2'	1:1A:1761:G:H8	1.67	0.59
1:2A:568:U:OP2	61:2A:4047:HOH:O	2.17	0.59
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.02	0.59
19:2X:11:PRO:HB3	19:2X:92:LEU:HD11	1.85	0.59
1:1A:1140:U:H1'	1:1A:1143:U:H5	1.68	0.58
1:1A:1402:G:OP2	61:1A:4353:HOH:O	2.17	0.58
1:1A:348:A:N6	1:1A:362:G:O2'	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:29:16:VAL:HG22	31:29:25:VAL:HG22	1.85	0.58
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.34	0.58
1:2A:79:G:N2	1:2A:90:U:O2	30.65	0.58
21:2Z:4:ARG:HG2	21:2Z:58:VAL:HB	1.85	0.58
1:2A:1530:C:N4	1:2A:1539:G:H1	2.02	0.58
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.85	0.58
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.03	0.58
1:2A:392:C:H5''	1:2A:409:C:H5''	1.85	0.58
1:1A:2096:U:O4	61:1A:4339:HOH:O	2.15	0.58
6:1G:138:GLN:N	6:1G:138:GLN:OE1	2.37	0.58
1:2A:1270:C:H2'	1:2A:1271:G:C8	6.53	0.58
1:1A:1202:A:OP1	16:1U:55:ARG:NH1	2.35	0.58
1:1A:779:C:OP1	61:1A:4351:HOH:O	2.17	0.58
1:1A:847:A:OP1	1:1A:847:A:H8	1.87	0.58
1:2A:1826:G:H4'	3:2D:242:ARG:CZ	2.34	0.58
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.86	0.58
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.84	0.58
1:1A:1223:C:H2'	1:1A:1224:C:C6	2.38	0.58
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.37	0.58
1:2A:1041:C:O2	1:2A:1114:G:N2	2.28	0.58
1:2A:287:C:H2'	1:2A:288:C:H6	1.69	0.58
1:2A:307:G:N1	1:2A:310:A:OP2	2.32	0.58
1:2A:665:C:H2'	1:2A:666:G:H8	1.69	0.58
7:1H:127:GLU:OE1	7:1H:130:ARG:NE	2.31	0.58
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.37	0.58
26:14:24:THR:OG1	26:14:25:TYR:N	2.37	0.58
1:1A:1093:G:H2'	1:1A:1156:G:H22	1.68	0.58
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.38	0.58
1:2A:1462:C:H4'	1:2A:2703:C:H5'	1.86	0.58
2:2B:14:U:HO2'	2:2B:15:A:H8	1.52	0.58
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.86	0.58
1:1A:630:U:OP1	5:1F:102:PRO:HA	2.03	0.58
1:2A:2355:C:H1'	22:20:39:ARG:HH21	1.69	0.58
13:2R:33:ARG:NH2	27:25:57:VAL:O	2.32	0.58
30:28:33:ASN:HA	30:28:36:LYS:HD2	1.85	0.58
6:2G:73:ALA:HB3	6:2G:85:GLY:H	1.68	0.58
4:2E:179:GLU:HG3	15:2T:9:LEU:HD21	1.85	0.58
21:2Z:33:LEU:HD11	21:2Z:90:VAL:HG21	1.85	0.58
11:2P:100:LEU:HD12	11:2P:112:LEU:HD11	1.86	0.57
4:1E:12:THR:HG22	4:1E:13:ARG:H	1.70	0.57
7:1H:149:ARG:NH2	7:1H:167:GLU:OE2	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1X:54:VAL:HG22	19:1X:81:VAL:HG12	1.86	0.57
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.40	0.57
1:2A:2138:C:N4	1:2A:2153:G:N1	2.22	0.57
1:2A:938:G:OP2	30:28:52:LYS:NZ	2.25	0.57
16:2U:66:ASN:HD21	16:2U:70:ARG:HH21	1.51	0.57
1:1A:273:G:H21	8:1I:50:ARG:HH12	1.52	0.57
1:1A:2658:C:OP2	1:1A:2745:G:O2'	2.22	0.57
24:22:1:MET:SD	24:22:56:GLN:NE2	2.78	0.57
7:2H:28:GLY:HA3	7:2H:79:VAL:HB	1.86	0.57
1:2A:236:C:H2'	1:2A:237:C:C6	2.39	0.57
1:2A:668:G:H5'	1:2A:669:G:OP2	2.04	0.57
1:2A:76:C:H42	1:2A:93:G:H1	26.94	0.57
1:1A:1060:U:OP2	61:1A:4356:HOH:O	2.18	0.57
1:1A:1801:G:OP1	61:1A:4355:HOH:O	2.17	0.57
1:1A:553:A:O2'	1:1A:554:A:H5'	2.05	0.57
1:2A:517:C:OP1	27:25:16:ARG:NH2	2.37	0.57
1:2A:2035:G:OP1	61:2A:4052:HOH:O	2.18	0.57
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.86	0.57
3:1D:71:ASP:HB3	3:1D:103:ARG:HH12	1.68	0.57
1:2A:987:G:O2'	1:2A:1000:A:N3	2.32	0.57
2:2B:4:C:H42	2:2B:117:G:H1	1.50	0.57
8:2I:87:LYS:NZ	8:2I:122:GLU:OE2	2.34	0.57
10:2O:7:TYR:CE1	10:2O:20:MET:HB2	2.40	0.57
1:1A:1425:A:H4'	1:1A:1426:G:OP2	2.04	0.57
14:1S:15:ARG:O	14:1S:19:LYS:HG2	2.04	0.57
1:2A:2129:C:N3	1:2A:2159:G:N2	2.48	0.57
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.86	0.57
1:1A:2307:C:OP1	14:1S:10:ARG:NH1	2.38	0.57
1:2A:1418:G:N7	61:2A:4138:HOH:O	2.32	0.57
18:2W:67:ASP:N	18:2W:67:ASP:OD1	2.34	0.57
21:2Z:152:ALA:HB1	21:2Z:163:LEU:HD21	1.86	0.57
1:1A:1068:G:OP2	1:1A:1068:G:H8	6.86	0.57
1:1A:1829:U:H5'	3:1D:259:THR:HG22	1.87	0.57
1:1A:1990:G:OP1	61:1A:4323:HOH:O	2.17	0.57
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	1.87	0.57
9:2N:46:VAL:HG23	9:2N:48:MET:HB2	1.86	0.57
24:12:1:MET:SD	24:12:56:GLN:NE2	2.78	0.57
12:1Q:109:VAL:HG22	12:1Q:113:GLN:HB3	1.86	0.57
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.21	0.57
1:1A:1305:G:N2	1:1A:1331:G:H1'	40.08	0.56
1:1A:2482:G:OP1	12:1Q:56:ARG:NH2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.40	0.56
1:2A:72:U:OP1	61:2A:4050:HOH:O	2.17	0.56
12:1Q:85:LYS:HG2	22:10:7:LEU:HB3	1.87	0.56
1:2A:34:C:H2'	1:2A:35:G:H8	4.65	0.56
1:1A:1500:A:OP2	61:1A:4357:HOH:O	2.18	0.56
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.85	0.56
21:1Z:150:LEU:HB3	21:1Z:171:ILE:HD11	1.87	0.56
1:1A:11:G:H2'	1:1A:12:U:H5''	1.87	0.56
1:1A:1539:C:N4	1:1A:2227:G:O2'	2.39	0.56
1:1A:2303:U:H2'	1:1A:2304:C:C6	2.40	0.56
3:1D:83:GLU:OE1	3:1D:104:TYR:OH	2.20	0.56
1:1A:2746:A:H2	4:1E:204:ALA:H	1.53	0.56
1:2A:2143:C:N4	1:2A:2148:G:H1	2.02	0.56
1:2A:662:G:O2'	1:2A:836:G:OP1	26.28	0.56
3:2D:127:VAL:HA	3:2D:193:VAL:HG23	1.88	0.56
5:2F:150:GLY:HA2	5:2F:172:TRP:CE3	2.40	0.56
1:2A:2121:G:N2	1:2A:2177:C:N3	2.47	0.56
12:2Q:42:ILE:HD13	12:2Q:97:VAL:HB	1.87	0.56
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	1.88	0.56
1:1A:1515:C:OP1	61:1A:4354:HOH:O	2.17	0.56
1:2A:1800:C:P	3:2D:183:ARG:HH12	2.28	0.56
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.88	0.56
1:1A:611:U:H2'	1:1A:612:C:C6	2.40	0.56
1:2A:1278:A:OP1	13:2R:36:THR:HG22	2.06	0.56
5:2F:178:PRO:HB2	5:2F:201:VAL:HG21	1.86	0.56
12:2Q:12:GLN:NE2	12:2Q:72:LYS:HG3	2.14	0.56
1:1A:1037:C:H2'	1:1A:1038:C:H6	2.27	0.56
1:1A:1223:C:H2'	1:1A:1224:C:H6	1.71	0.56
1:1A:1877:G:H2'	57:1A:4209:CPT:CL1	2.43	0.56
1:1A:430:U:H4'	1:1A:431:C:H5'	1.88	0.56
24:22:35:LEU:HD12	24:22:53:LEU:HD12	1.87	0.56
11:2P:38:GLN:O	11:2P:39:LYS:HB3	2.05	0.56
1:1A:1405:A:H2	1:1A:1418:U:O4	1.89	0.56
1:2A:459:U:H5''	29:27:40:TRP:CD2	2.41	0.56
1:2A:2518:A:OP2	61:2A:4048:HOH:O	2.17	0.56
1:2A:479:A:N3	1:2A:481:G:H5''	2.21	0.56
1:2A:764:A:H5''	3:2D:210:GLY:HA2	1.88	0.56
6:2G:41:GLN:HB3	6:2G:43:LEU:HD13	1.88	0.56
1:1A:1452:U:H2'	1:1A:1453:C:C6	2.41	0.55
1:1A:2178:G:H2'	1:1A:2179:G:C2	2.41	0.55
1:1A:1810:U:H2'	61:1A:4403:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:86:GLU:OE2	7:1H:130:ARG:NH1	2.39	0.55
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.70	0.55
1:2A:578:A:OP2	61:2A:4054:HOH:O	2.18	0.55
6:2G:28:VAL:O	6:2G:31:VAL:HG12	2.06	0.55
6:1G:82:LEU:HD21	6:1G:88:ILE:HG21	1.87	0.55
2:2B:75:G:H22	21:2Z:73:GLN:HE21	1.54	0.55
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	1.87	0.55
1:2A:84:A:H5'	20:2Y:8:LYS:HG2	1.89	0.55
11:1P:47:ASP:N	11:1P:47:ASP:OD1	4.17	0.55
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.52	0.55
9:2N:32:THR:HG23	9:2N:37:LYS:HB2	1.88	0.55
1:1A:1108:G:P	1:1A:1116:A:H1'	2.47	0.55
1:1A:1310:G:OP1	27:15:19:ARG:NH2	2.29	0.55
4:1E:8:LYS:NZ	61:1E:405:HOH:O	2.39	0.55
18:1W:11:ARG:HA	18:1W:100:THR:HG22	1.87	0.55
1:2A:2336:A:H61	22:20:43:THR:HG22	1.72	0.55
28:26:34:LEU:HB2	28:26:51:GLU:HB3	1.87	0.55
1:2A:2104:G:H1	1:2A:2185:C:N4	2.03	0.55
1:2A:910:A:N1	1:2A:2277:G:H1'	2.22	0.55
1:2A:975(A):G:OP2	61:2A:4053:HOH:O	2.18	0.55
2:2B:54:G:H21	6:2G:29:TRP:HE1	1.53	0.55
1:1A:1961:5MU:OP1	1:1A:2616:U:O2'	2.23	0.55
1:1A:1831:C:P	3:1D:183:ARG:HH12	2.30	0.55
1:1A:791:G:OP1	4:1E:132:HIS:ND1	2.39	0.55
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.42	0.55
1:2A:2658:C:P	7:2H:160:LYS:HZ1	2.30	0.55
14:2S:67:ARG:O	14:2S:71:ARG:HG3	2.07	0.55
1:1A:1115:A:H4'	1:1A:1116:A:C8	2.40	0.55
5:1F:103:LYS:HA	5:1F:106:ARG:HG3	1.88	0.55
1:2A:467:G:OP2	29:27:34:ARG:HD3	2.07	0.55
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.06	0.55
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.40	0.55
11:2P:95:VAL:HA	11:2P:99:LEU:HD21	1.87	0.55
6:1G:41:GLN:HB3	6:1G:43:LEU:HD13	1.87	0.55
26:24:47:GLN:C	26:24:49:PHE:H	2.10	0.55
1:2A:1529:G:O6	1:2A:1541:G:N2	2.40	0.55
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.42	0.55
1:2A:566:U:H5''	11:2P:29:LYS:HE3	1.89	0.55
13:2R:44:LEU:HD22	13:2R:48:VAL:HG23	1.89	0.55
1:1A:1133:G:H2'	1:1A:1135:G:C8	2.42	0.55
1:1A:976:G:H5'	1:1A:1358:U:O2'	103.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1W:68:ARG:HH11	18:1W:111:HIS:HA	1.71	0.55
1:2A:1022:G:N2	1:2A:1023:U:O4	2.37	0.55
1:2A:180:G:N2	1:2A:215:G:O6	2.40	0.55
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.72	0.55
1:2A:2441:C:OP2	1:2A:2586:C:O2'	2.24	0.55
1:2A:2453:A:OP1	61:2A:4057:HOH:O	2.18	0.55
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.24	0.55
1:2A:492:A:H2'	1:2A:493:G:O4'	2.07	0.55
18:2W:71:VAL:HA	18:2W:107:LEU:HD12	1.89	0.55
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.42	0.55
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.42	0.55
1:1A:236:G:H4'	1:1A:413:G:C5	2.41	0.54
1:1A:2507:G:H5''	12:1Q:82:ARG:HG2	1.89	0.54
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.41	0.54
3:2D:274:ARG:O	3:2D:275:LYS:HD2	2.07	0.54
1:1A:1817:A:H1'	1:1A:1960:A:N6	2.22	0.54
1:1A:636:G:N2	1:1A:640:A:O2'	2.40	0.54
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.25	0.54
1:2A:639:U:H2'	1:2A:640:C:C6	2.42	0.54
1:1A:937:A:H2'	1:1A:938:G:O4'	2.08	0.54
1:2A:1442:G:N3	1:2A:1442:G:H2'	2.87	0.54
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.22	0.54
1:2A:1846:G:H2'	57:2A:3903:CPT:CL1	2.44	0.54
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.90	0.54
21:2Z:30:ASN:HA	21:2Z:89:PHE:HE1	1.71	0.54
31:19:25:VAL:HB	31:19:34:GLN:HB2	1.90	0.54
1:2A:987:G:H1	1:2A:1218:C:N4	46.18	0.54
1:2A:652(B):A:N6	1:2A:655:A:N3	2.55	0.54
1:1A:1517:G:N3	1:1A:1941:A:O2'	112.27	0.54
1:1A:2205:C:H2'	1:1A:2206:G:C8	2.41	0.54
1:1A:271:U:H4'	1:1A:272:U:OP2	2.08	0.54
17:1V:72:VAL:HG13	17:1V:85:LYS:HB3	1.89	0.54
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.42	0.54
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.43	0.54
1:1A:1896:G:N7	61:1A:4470:HOH:O	2.33	0.54
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.43	0.54
28:16:10:LEU:HG	28:16:54:ILE:HG13	1.90	0.54
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.43	0.54
1:2A:700:G:O2'	1:2A:1632:A:N3	2.37	0.54
1:2A:1779:U:OP2	61:2A:4055:HOH:O	2.18	0.54
3:2D:71:ASP:HB3	3:2D:103:ARG:HH12	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1154:U:H2'	1:1A:1155:C:O4'	2.07	0.54
1:1A:798:A:H5'	18:1W:90:ARG:HA	1.90	0.54
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.43	0.54
1:2A:531:C:OP1	1:2A:561:G:N1	2.41	0.54
5:2F:103:LYS:HA	5:2F:106:ARG:HG3	1.90	0.54
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.22	0.54
1:1A:1123:A:H2'	1:1A:1124:U:H4'	1.89	0.54
1:1A:1214:G:H1	1:1A:1226:C:H42	1.56	0.54
1:1A:1981:G:N7	61:1A:4477:HOH:O	2.34	0.54
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.08	0.54
1:1A:843:C:H2'	1:1A:844:C:C6	2.43	0.53
1:1A:347:G:C8	5:1F:171:PRO:HG3	2.43	0.53
13:1R:24:GLN:HE22	13:1R:36:THR:HG21	1.72	0.53
1:2A:978:G:HO2'	1:2A:1002:G:HO2'	1.57	0.53
1:2A:2114:A:O2'	1:2A:2167:U:H1'	2.08	0.53
9:2N:67:LEU:HA	9:2N:87:LEU:HD22	1.90	0.53
21:2Z:146:ILE:HG12	21:2Z:174:VAL:HG13	1.90	0.53
1:1A:1106:U:H3	1:1A:1134:A:H8	1.53	0.53
1:1A:1410:G:N7	23:11:3:LYS:HD2	2.24	0.53
1:1A:1312:G:O2'	1:1A:2034:G:O6	2.18	0.53
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.73	0.53
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.41	0.53
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.89	0.53
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.08	0.53
6:2G:79:ASN:OD1	6:2G:79:ASN:N	2.41	0.53
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.07	0.53
1:1A:1990:G:OP1	61:1A:4358:HOH:O	2.18	0.53
1:1A:2897:U:H2'	1:1A:2898:C:C6	2.43	0.53
1:1A:662:A:OP1	11:1P:133:SER:OG	2.22	0.53
18:1W:68:ARG:HH12	18:1W:112:GLY:H	1.56	0.53
1:2A:1002:G:N1	1:2A:1003:G:H8	4.60	0.53
1:2A:1486:A:H2'	1:2A:1487:G:H8	1.73	0.53
1:2A:2148:G:H2'	1:2A:2149:G:C8	2.44	0.53
1:2A:2443:C:H2'	1:2A:2444:G:H8	1.74	0.53
1:2A:332:A:O2'	1:2A:334:C:OP2	2.23	0.53
21:2Z:46:LYS:O	21:2Z:50:GLN:NE2	2.33	0.53
17:1V:5:VAL:HG21	17:1V:35:LEU:HD23	1.90	0.53
1:2A:1428:C:O2'	1:2A:1569:A:OP2	2.25	0.53
1:2A:2314:C:H2'	1:2A:2315:G:H8	1.73	0.53
1:2A:84:A:H5''	20:2Y:8:LYS:HE3	1.89	0.53
1:1A:535:C:OP1	61:1A:4324:HOH:O	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:140:LEU:HD22	8:1I:142:VAL:HG13	1.91	0.53
1:1A:24:G:O2'	18:1W:78:GLU:O	2.22	0.53
1:2A:247:G:H4'	1:2A:386:G:C5	2.44	0.53
1:2A:925:C:H2'	1:2A:926:A:H8	1.73	0.53
19:2X:57:LEU:HD11	19:2X:78:LYS:HE2	1.89	0.53
1:1A:1046:A:H62	1:1A:1200:G:H2'	1.74	0.53
1:1A:122:G:OP1	1:1A:1422:C:O2'	2.17	0.53
1:1A:839:G:OP2	61:1A:4359:HOH:O	2.19	0.53
1:1A:776:G:C6	3:1D:208:LYS:HB2	2.44	0.53
13:1R:72:ASP:O	13:1R:76:VAL:HG23	2.08	0.53
21:1Z:153:SER:HB3	21:1Z:167:PRO:HB3	1.90	0.53
1:2A:305:U:H2'	1:2A:306:U:C6	2.44	0.53
1:2A:731:C:H5''	61:2A:4041:HOH:O	2.07	0.53
11:2P:39:LYS:HB2	11:2P:45:LEU:HG	1.90	0.53
2:2B:103:G:H21	21:2Z:73:GLN:HE22	1.56	0.53
1:1A:153:C:H42	1:1A:168:G:H1	25.38	0.53
1:1A:2389:A:H2'	1:1A:2390:A:C8	2.44	0.53
1:1A:605:G:H2'	1:1A:606:G:C8	2.44	0.53
3:1D:85:ASP:OD2	3:1D:88:ARG:NH1	2.42	0.53
4:1E:31:CYS:HB3	4:1E:49:LEU:HG	1.90	0.53
29:27:12:ARG:NH2	29:27:44:PRO:HB3	2.24	0.53
1:2A:531:C:H4'	1:2A:532:A:H5''	1.91	0.53
26:14:58:ARG:O	26:14:61:ARG:HB2	2.09	0.53
1:1A:2402:U:P	30:18:35:GLN:HE22	2.32	0.53
1:1A:967:G:O6	61:1A:4340:HOH:O	2.15	0.53
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.90	0.53
1:2A:851:U:O2'	25:23:42:ALA:O	2.26	0.53
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.23	0.53
1:2A:1899:G:N3	1:2A:1899:G:H2'	2.24	0.53
1:2A:1971:A:OP1	61:2A:4051:HOH:O	2.17	0.53
1:2A:2589:A:OP1	61:2A:4060:HOH:O	2.19	0.53
1:2A:893:C:H2'	1:2A:894:C:C5	2.44	0.53
7:2H:98:LEU:HB2	7:2H:125:VAL:HG22	1.90	0.53
1:1A:1115:A:H1'	1:1A:1142:A:H4'	1.91	0.53
1:1A:2153:G:H5''	1:1A:2154:U:H3'	1.90	0.53
1:2A:2238:G:H5''	61:2A:4365:HOH:O	2.08	0.53
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.44	0.53
1:2A:890:A:H2'	1:2A:892:G:C8	2.43	0.53
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.39	0.53
1:1A:2315:G:O6	61:1A:4342:HOH:O	2.15	0.53
1:1A:956:A:N3	1:1A:2276:C:O2'	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:29:GLY:HA3	61:1E:406:HOH:O	2.08	0.53
1:2A:2140:C:H2'	1:2A:2141:G:H5'	1.89	0.53
1:2A:822:U:OP2	61:2A:4059:HOH:O	2.19	0.53
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.09	0.53
1:1A:1410:G:P	23:11:3:LYS:HG3	2.49	0.52
1:1A:2143:G:H1	1:1A:2199:C:N4	2.06	0.52
12:1Q:81:VAL:HB	22:10:7:LEU:HD21	1.91	0.52
1:2A:2820:A:OP1	13:2R:2:ARG:NH2	2.41	0.52
14:2S:16:ASN:O	14:2S:20:ARG:HG2	2.08	0.52
21:1Z:74:VAL:HG22	21:1Z:86:VAL:HG12	1.91	0.52
1:2A:2014:A:H4'	18:2W:92:ARG:HH22	1.74	0.52
1:2A:2171:A:N3	1:2A:2172:U:N3	2.57	0.52
1:2A:2837:G:N7	61:2A:4148:HOH:O	2.34	0.52
1:2A:800:A:OP1	1:2A:800:A:H8	1.92	0.52
2:2B:17:C:H2'	2:2B:18:G:O4'	2.08	0.52
16:2U:91:ASP:O	16:2U:95:LEU:HD12	2.09	0.52
22:10:40:GLN:O	61:10:5001:HOH:O	2.19	0.52
28:16:35:GLU:OE2	28:16:50:ARG:NH1	2.36	0.52
1:1A:1093:G:H2'	1:1A:1156:G:N2	2.25	0.52
1:1A:1634:C:H2'	1:1A:1635:C:H6	1.74	0.52
1:2A:2438:U:O2'	1:2A:2440:C:OP1	2.24	0.52
1:2A:2815:C:H5'	27:25:29:THR:HG21	1.91	0.52
1:2A:860:U:H1'	1:2A:2268:A:H5'	1.91	0.52
1:1A:939:C:H2'	1:1A:940:C:C6	2.43	0.52
20:1Y:92:ASN:N	20:1Y:93:GLY:HA2	2.23	0.52
29:27:34:ARG:HG3	29:27:34:ARG:HH11	1.74	0.52
17:2V:46:VAL:HG23	17:2V:52:VAL:HG11	1.90	0.52
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.45	0.52
30:18:33:ASN:HA	30:18:36:LYS:HD2	1.91	0.52
1:1A:1846:A:P	3:1D:54:ARG:HH22	2.33	0.52
1:1A:2169:G:H2'	1:1A:2170:G:H4'	1.91	0.52
8:1I:62:LYS:O	8:1I:66:GLU:HG2	2.09	0.52
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.92	0.52
1:2A:2818:G:OP2	13:2R:42:LYS:NZ	2.29	0.52
1:2A:911:A:N6	12:2Q:11:LYS:O	2.37	0.52
12:2Q:29:PHE:HB3	12:2Q:65:PHE:CD2	2.45	0.52
15:2T:109:GLU:HG2	15:2T:112:ARG:NH2	2.24	0.52
21:2Z:31:ARG:HH11	21:2Z:94:GLU:HG2	1.73	0.52
4:1E:56:PRO:HG3	4:1E:74:PRO:HG2	1.91	0.52
16:1U:81:HIS:CE1	16:1U:85:LYS:HD2	2.44	0.52
12:2Q:81:VAL:HB	22:20:7:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:85:ASP:OD2	3:2D:88:ARG:NH1	2.42	0.52
7:2H:103:LEU:HB3	7:2H:115:VAL:HB	1.91	0.52
1:1A:2130:C:H2'	1:1A:2131:U:C6	2.44	0.52
1:1A:560:C:O3'	16:1U:53:ARG:NH1	2.43	0.52
8:1I:101:LEU:HG	8:1I:107:VAL:HG13	1.92	0.52
1:2A:568:U:H5'	1:2A:945:A:N1	2.25	0.52
10:2O:63:VAL:HG11	10:2O:85:VAL:HG23	1.92	0.52
1:1A:1255:A:H5''	1:1A:1257:G:O4'	2.10	0.52
1:1A:2892:A:OP1	13:1R:96:ARG:NH1	2.42	0.52
6:1G:43:LEU:HD11	6:1G:153:ARG:HD2	1.92	0.52
23:21:83:GLU:N	23:21:83:GLU:OE1	2.43	0.52
30:28:23:VAL:HG11	30:28:47:LYS:HD3	1.92	0.52
1:2A:821:A:N1	61:2A:4150:HOH:O	2.34	0.52
7:2H:106:THR:HG22	7:2H:112:PRO:HB3	1.92	0.52
1:1A:1848:G:OP1	3:1D:88:ARG:NH2	2.43	0.52
1:1A:580:U:H2'	1:1A:581:G:O4'	2.83	0.52
8:1I:14:ASP:OD1	8:1I:15:VAL:N	2.43	0.52
1:2A:1324:G:O2'	1:2A:1326:U:OP2	2.22	0.52
1:2A:1693:U:O2	3:2D:14:ARG:NH2	2.42	0.52
1:2A:322:A:OP1	5:2F:168:ARG:HD2	2.10	0.52
5:2F:40:GLN:NE2	5:2F:182:ASN:HB2	2.24	0.52
1:1A:2283:G:OP1	22:10:18:ALA:HB1	2.10	0.52
1:1A:1633:A:H2'	1:1A:1634:C:C6	2.45	0.52
3:1D:69:ARG:NH1	3:1D:128:GLY:O	2.34	0.52
17:1V:43:GLU:N	17:1V:43:GLU:OE1	2.43	0.52
19:1X:9:LEU:HA	24:12:36:ARG:HH21	1.74	0.52
1:2A:361:G:O2'	1:2A:362:U:H5'	2.10	0.52
1:1A:1825:U:H2'	1:1A:1826:C:H6	1.75	0.51
1:1A:664:U:H2'	1:1A:665:C:C6	2.45	0.51
3:1D:3:VAL:HG13	3:1D:17:THR:HB	1.91	0.51
5:1F:32:LEU:HD22	5:1F:112:MET:HE1	1.91	0.51
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.28	0.51
7:2H:88:LEU:HD21	7:2H:165:ALA:HA	1.91	0.51
16:2U:104:GLN:NE2	16:2U:105:VAL:HG23	2.25	0.51
30:18:29:LYS:HE2	30:18:45:GLY:HA2	1.92	0.51
1:1A:2372:A:H2'	1:1A:2373:A:O4'	2.09	0.51
1:1A:2564:2MU:O5'	1:1A:2564:2MU:H6	2.10	0.51
1:1A:559:U:H2'	1:1A:560:C:C6	2.45	0.51
1:1A:945:A:N3	1:1A:945:A:H2'	2.25	0.51
13:1R:44:LEU:HD22	13:1R:48:VAL:HG23	1.92	0.51
13:1R:28:LEU:HD23	13:1R:48:VAL:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1270:C:H2'	1:2A:1271:G:H8	5.90	0.51
1:2A:455:C:N3	1:2A:472:A:H2'	2.25	0.51
3:2D:26:LYS:HE2	3:2D:28:GLU:O	2.09	0.51
15:2T:26:ASP:O	15:2T:49:VAL:HG22	2.10	0.51
1:1A:238:C:O2	30:18:12:LYS:NZ	2.39	0.51
11:1P:126:VAL:HG12	11:1P:148:LEU:HD23	1.91	0.51
1:2A:1141:U:OP2	9:2N:63:THR:OG1	2.18	0.51
1:2A:1286:A:C8	1:2A:1287:A:H4'	8.17	0.51
1:2A:994:C:OP2	16:2U:54:LYS:NZ	2.36	0.51
1:1A:427:G:O6	61:1A:4344:HOH:O	2.16	0.51
3:1D:242:ARG:HG3	3:1D:242:ARG:NH1	2.08	0.51
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.93	0.51
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.45	0.51
1:2A:1530:C:O2'	1:2A:1531:C:O5'	2.18	0.51
1:2A:656:G:H2'	1:2A:657:U:O4'	2.10	0.51
1:2A:1693:U:C1'	3:2D:14:ARG:HH22	2.20	0.51
5:2F:164:ARG:O	5:2F:168:ARG:HB2	2.10	0.51
6:2G:138:GLN:OE1	6:2G:138:GLN:N	2.42	0.51
1:1A:1239:A:H62	1:1A:1299:A:N6	21.12	0.51
1:1A:831:A:O4'	3:1D:227:ASN:ND2	2.43	0.51
1:1A:831:A:N6	3:1D:229:VAL:HG11	2.26	0.51
1:2A:1005:C:H2'	1:2A:1006:C:H6	1.75	0.51
1:2A:2127:G:C6	1:2A:2161:C:C4	2.94	0.51
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.45	0.51
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.40	0.51
10:2O:9:GLU:N	10:2O:9:GLU:OE1	2.43	0.51
1:1A:1074:A:N6	1:1A:1171:G:H2'	2.25	0.51
1:1A:1825:U:H2'	1:1A:1826:C:C6	2.45	0.51
1:1A:2579:G:H2'	1:1A:2580:C:C6	2.45	0.51
1:1A:715:G:H5'	1:1A:716:G:OP2	2.11	0.51
5:1F:107:LYS:HE3	5:1F:206:ILE:HA	1.93	0.51
8:1I:126:TYR:HB2	8:1I:142:VAL:HG23	1.93	0.51
1:2A:1147:C:H2'	1:2A:1148:A:H8	1.75	0.51
1:2A:2141:G:H2'	1:2A:2142:C:O4'	2.11	0.51
1:2A:2404:C:O3'	11:2P:77:ARG:NH2	2.43	0.51
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.93	0.51
1:1A:1683:C:H2'	1:1A:1684:A:C8	2.46	0.51
1:1A:1827:U:H2'	1:1A:1828:C:C6	2.46	0.51
1:1A:477:C:OP1	5:1F:52:LYS:NZ	2.44	0.51
5:1F:33:LEU:HB3	11:1P:6:LEU:HD21	1.93	0.51
18:1W:34:ASN:OD1	18:1W:37:ARG:NH2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.45	0.51
1:2A:2379:G:O2'	14:2S:17:ARG:NH2	2.43	0.51
1:2A:38:A:H2'	1:2A:39:C:C6	2.46	0.51
1:2A:903:C:H2'	1:2A:904:C:C6	2.45	0.51
1:1A:1101:G:N2	1:1A:1150:C:N3	2.47	0.51
1:1A:1487:G:H2'	1:1A:1488:G:H8	1.76	0.51
27:25:16:ARG:HG3	27:25:17:ASP:N	2.26	0.51
1:2A:34:C:H2'	1:2A:35:G:C8	5.52	0.51
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.46	0.51
2:2B:70:C:H2'	2:2B:71:C:H6	1.76	0.51
1:1A:2707:C:H2'	1:1A:2708:U:C6	2.46	0.51
1:1A:964:A:N3	2:1B:80:U:O2'	2.38	0.51
15:1T:109:GLU:O	15:1T:113:LYS:HG2	2.11	0.51
1:2A:1220:A:OP2	16:2U:19:LYS:NZ	2.40	0.51
1:2A:2126:A:H61	1:2A:2162:G:HO2'	1.58	0.51
1:2A:236:C:H2'	1:2A:237:C:H6	1.75	0.51
1:2A:434:U:H2'	1:2A:435:C:C6	6.55	0.51
2:2B:51:G:N7	14:2S:62:LYS:NZ	2.49	0.51
12:2Q:38:GLU:HA	12:2Q:99:PRO:HG3	1.93	0.51
1:1A:1544:C:OP1	61:1A:4362:HOH:O	2.19	0.51
6:1G:34:LEU:HD23	6:1G:161:THR:HG22	1.91	0.51
1:2A:1299:G:OP1	61:2A:4062:HOH:O	2.20	0.51
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.46	0.51
1:2A:2154:G:H2'	1:2A:2155:G:H5'	1.93	0.51
3:2D:11:PRO:O	3:2D:14:ARG:HG2	2.11	0.51
4:2E:14:ILE:HG13	4:2E:21:VAL:HG13	1.93	0.51
21:2Z:5:LEU:HB2	21:2Z:47:VAL:HG21	1.93	0.51
1:1A:2631:C:H4'	4:1E:151:TYR:O	2.12	0.50
7:1H:56:SER:HB3	7:1H:61:HIS:ND1	2.26	0.50
22:20:11:ARG:O	22:20:14:ARG:NH2	2.34	0.50
1:2A:1812:A:H5''	61:2A:4033:HOH:O	2.11	0.50
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.75	0.50
7:2H:3:ARG:HH12	7:2H:6:ARG:N	2.09	0.50
11:2P:43:GLY:HA3	61:2P:303:HOH:O	2.11	0.50
21:2Z:93:ASP:HA	21:2Z:131:ARG:HH22	1.75	0.50
1:1A:1821:C:H2'	1:1A:1822:A:C5	2.47	0.50
1:1A:2807:C:N4	1:1A:2813:G:H22	2.07	0.50
9:1N:21:LYS:NZ	9:1N:140:VAL:OXT	2.37	0.50
1:2A:1599:C:OP1	61:2A:4058:HOH:O	2.19	0.50
1:2A:774:A:N3	1:2A:774:A:H2'	2.26	0.50
7:2H:80:SER:OG	7:2H:81:GLU:OE1	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.44	0.50
21:1Z:138:GLU:H	21:1Z:156:LYS:NZ	2.08	0.50
1:2A:323:G:O2'	1:2A:1205:U:N3	2.36	0.50
6:2G:16:ARG:HB2	6:2G:17:PRO:HD3	1.94	0.50
1:1A:991:G:OP1	61:1A:4360:HOH:O	2.19	0.50
26:24:16:CYS:SG	26:24:17:GLY:N	2.84	0.50
1:2A:1799:G:O3'	3:2D:183:ARG:NH1	2.40	0.50
1:2A:2114:A:H62	1:2A:2115:G:N2	2.06	0.50
1:2A:286:C:H2'	1:2A:287:C:C6	2.47	0.50
1:1A:2128:G:H2'	1:1A:2129:C:C6	2.46	0.50
1:2A:1503:U:H2'	1:2A:1504:C:C6	2.45	0.50
1:2A:2061:G:H5''	1:2A:2503:2MA:C2	2.42	0.50
1:1A:1040:C:OP2	16:1U:54:LYS:NZ	2.34	0.50
1:1A:1346:U:H4'	1:1A:1347:A:H5''	1.93	0.50
1:1A:738:C:H2'	1:1A:739:C:H6	2.30	0.50
5:1F:185:ASP:OD1	5:1F:188:ARG:NH1	2.41	0.50
7:1H:3:ARG:HH11	7:1H:4:ILE:H	1.60	0.50
8:1I:79:ILE:HB	8:1I:144:VAL:HG12	1.93	0.50
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.26	0.50
1:2A:307:G:H21	1:2A:330:A:H62	1.60	0.50
1:1A:1501:U:OP1	13:1R:77:ARG:NH1	2.34	0.50
1:1A:2441:G:OP1	61:1A:4301:HOH:O	2.19	0.50
4:1E:24:THR:HG22	4:1E:186:GLY:O	2.11	0.50
26:24:41:PRO:HG3	26:24:49:PHE:CZ	2.47	0.50
1:2A:1119:C:H2'	1:2A:1120:G:H8	2.92	0.50
1:2A:817:C:N4	1:2A:1529:G:O6	111.77	0.50
1:2A:1603:A:OP1	61:2A:4061:HOH:O	2.19	0.50
1:2A:2074:U:O4	61:2A:4049:HOH:O	2.17	0.50
1:2A:212:G:H2'	1:2A:213:A:O4'	2.11	0.50
1:2A:892:G:H3'	1:2A:893:C:C5'	2.42	0.50
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.45	0.50
29:27:30:VAL:O	29:27:34:ARG:HG2	2.12	0.50
1:2A:514:A:N3	1:2A:581:C:O2'	2.40	0.50
2:2B:41:U:H5	6:2G:70:VAL:H	1.60	0.50
1:1A:2255:U:OP1	61:1A:4366:HOH:O	2.20	0.50
1:1A:439:A:O5'	1:1A:439:A:H8	1.94	0.50
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.26	0.50
6:2G:179:PRO:HB2	26:24:42:PHE:CE2	2.41	0.50
7:2H:84:SER:HB3	7:2H:132:ARG:HH11	1.77	0.50
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.27	0.50
7:2H:73:ALA:O	7:2H:76:VAL:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2289:G:OP2	22:10:10:THR:HG21	2.12	0.49
1:1A:2763:A:OP2	7:1H:62:LYS:NZ	2.37	0.49
2:1B:8:U:O3'	14:1S:25:ARG:NH2	2.45	0.49
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.11	0.49
1:2A:305:U:O5'	1:2A:305:U:H6	1.95	0.49
1:2A:586:A:N1	1:2A:809:G:O2'	2.36	0.49
7:2H:125:VAL:HG12	7:2H:131:VAL:HG22	1.94	0.49
1:1A:2899:C:H2'	1:1A:2900:G:O4'	2.12	0.49
3:1D:11:PRO:O	3:1D:14:ARG:HG2	2.12	0.49
11:1P:91:PHE:O	11:1P:121:LYS:NZ	2.31	0.49
26:24:15:ILE:HB	26:24:32:TYR:CD1	2.45	0.49
2:2B:40:U:H2'	26:24:2:LYS:HE3	1.93	0.49
11:2P:59:LEU:HD21	30:28:10:ALA:HA	1.93	0.49
1:2A:1218:C:H42	1:2A:1231:G:H1	1.57	0.49
1:2A:1271:G:OP2	61:2A:4005:HOH:O	2.18	0.49
1:2A:2466:C:H5'	31:29:5:ALA:HB3	1.94	0.49
1:2A:613:G:O2'	1:2A:614(C):A:N1	2.36	0.49
2:2B:3:C:H2'	2:2B:4:C:C6	2.47	0.49
1:1A:346:A:OP2	5:1F:169:ASN:HB2	2.12	0.49
9:1N:62:VAL:HG22	9:1N:66:LYS:HD2	1.94	0.49
1:2A:1410:G:H2'	1:2A:1411:C:H6	1.76	0.49
1:2A:2127:G:H2'	1:2A:2128:C:H6	1.77	0.49
1:2A:65:C:O2'	1:2A:456:C:N3	2.36	0.49
16:2U:97:ASP:OD1	16:2U:101:ARG:NH1	2.46	0.49
13:1R:33:ARG:NH2	27:15:57:VAL:O	2.34	0.49
1:1A:721:G:O2'	5:1F:74:ARG:HD3	2.13	0.49
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.47	0.49
1:2A:89:G:H3'	1:2A:90:U:H5''	1.95	0.49
1:2A:918:A:O2'	2:2B:97:G:N2	2.44	0.49
3:2D:8:PRO:HB3	3:2D:14:ARG:HD2	1.94	0.49
21:2Z:55:HIS:HE1	21:2Z:135:GLU:HB2	1.77	0.49
24:12:22:GLU:OE2	24:12:68:ARG:NH2	2.45	0.49
1:1A:1105:G:N2	1:1A:1125:C:N3	2.55	0.49
1:1A:2764:G:C4	7:1H:2:SER:HA	2.47	0.49
1:1A:2797:C:H1'	4:1E:37:ARG:HH12	1.78	0.49
8:1I:93:THR:H	8:1I:96:ASP:HB2	1.77	0.49
1:1A:7:G:H5''	9:1N:121:LYS:HE3	1.93	0.49
27:25:51:TYR:CE2	27:25:56:LYS:HD3	2.48	0.49
1:2A:2129:C:H5'	1:2A:2130:U:OP2	2.13	0.49
1:2A:2390:U:P	30:28:35:GLN:HE22	2.36	0.49
1:2A:2812:G:H2'	1:2A:2813:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:119:ARG:CG	4:2E:119:ARG:HH11	2.25	0.49
1:1A:16:G:N2	61:1A:4561:HOH:O	2.43	0.49
1:1A:794:U:O2	1:1A:2036:A:H1'	2.12	0.49
1:1A:2198:A:H2'	1:1A:2199:C:C6	2.48	0.49
1:1A:2129:C:N4	1:1A:2204:G:H1	2.11	0.49
1:1A:419:C:OP1	61:1A:4367:HOH:O	2.20	0.49
1:1A:863:C:OP2	61:1A:4361:HOH:O	2.19	0.49
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.93	0.49
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.48	0.49
2:2B:103:G:H21	21:2Z:73:GLN:NE2	2.11	0.49
1:1A:2297:C:OP2	28:16:6:ARG:NH1	2.46	0.49
1:1A:1140:U:H1'	1:1A:1143:U:C5	2.48	0.49
1:1A:2041:A:O4'	16:1U:34:LYS:HE3	2.13	0.49
4:1E:174:ASP:OD1	4:1E:175:VAL:N	2.44	0.49
1:2A:2025:C:OP2	61:2A:4064:HOH:O	2.20	0.49
1:2A:71:A:H5''	1:2A:73:A:C8	2.48	0.49
1:2A:783:A:OP2	61:2A:4060:HOH:O	2.19	0.49
20:2Y:6:HIS:H	20:2Y:6:HIS:CD2	2.31	0.49
26:14:53:GLU:HB2	26:14:55:ARG:HA	1.95	0.49
19:1X:61:GLY:HA3	19:1X:73:ARG:O	2.12	0.49
1:2A:1119:C:H2'	1:2A:1120:G:C8	3.66	0.49
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.38	0.49
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.13	0.49
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.52	0.49
1:1A:1477:U:H2'	1:1A:1478:C:C6	2.48	0.49
1:1A:1717:C:O2	4:1E:129:HIS:NE2	2.39	0.49
15:1T:24:PRO:HA	15:1T:49:VAL:HG23	1.95	0.49
1:2A:108:U:H2'	1:2A:109:G:H8	1.78	0.49
1:2A:1170:G:O6	1:2A:1180:C:N4	2.46	0.49
1:2A:2218:U:H1'	23:21:52:ARG:HH12	1.77	0.49
1:2A:2483:C:N3	12:2Q:124:LYS:NZ	2.57	0.49
1:1A:1159:U:H2'	1:1A:1160:G:C8	2.48	0.49
1:1A:2717:A:N3	61:1A:4491:HOH:O	2.35	0.49
1:1A:492:A:N3	1:1A:730:C:H1'	2.27	0.49
1:2A:817:C:O2'	1:2A:839:U:H5''	2.13	0.49
1:2A:2511:U:O2'	4:2E:138:PRO:O	2.26	0.49
4:2E:11:MET:HG2	4:2E:24:THR:HB	1.95	0.49
15:2T:24:PRO:HA	15:2T:49:VAL:HG23	1.94	0.49
1:1A:131:C:O2	1:1A:231:G:N2	72.09	0.48
1:1A:1566:U:H2'	1:1A:1567:G:O4'	2.12	0.48
1:1A:173:C:H2'	1:1A:174:U:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2328:C:O2'	6:1G:128:ARG:NH2	2.45	0.48
1:1A:342:C:N4	1:1A:347:G:O6	5.71	0.48
2:1B:2:C:H2'	2:1B:3:C:C6	2.48	0.48
1:2A:1031:G:N3	31:29:36:GLN:NE2	2.52	0.48
1:2A:1364:G:P	23:21:3:LYS:HG3	2.53	0.48
1:2A:17:G:H2'	1:2A:18:C:H6	1.78	0.48
1:2A:271(X):G:C2	1:2A:271(Y):U:O4	2.66	0.48
1:2A:848:G:H2'	1:2A:849:A:H8	1.76	0.48
3:2D:77:ALA:HA	3:2D:97:TYR:HA	1.95	0.48
2:2B:42:C:O2'	6:2G:67:LYS:O	2.16	0.48
7:2H:137:ASP:HB3	7:2H:140:LYS:HB3	1.94	0.48
16:2U:83:LEU:HG	16:2U:88:ILE:HB	1.95	0.48
1:1A:1473:A:H4'	1:1A:1474:C:O4'	2.13	0.48
1:1A:2442:A:H2'	1:1A:2442:A:N3	2.27	0.48
1:1A:738:C:H2'	1:1A:739:C:C6	2.93	0.48
7:1H:124:GLU:OE2	7:1H:132:ARG:HD2	2.12	0.48
1:2A:1010:A:N3	1:2A:1153:C:H1'	2.28	0.48
1:2A:1385:G:O2'	1:2A:1396:U:O2	2.29	0.48
1:2A:1472:A:H2'	1:2A:1473:G:O4'	2.14	0.48
1:2A:320:A:H4'	1:2A:322:A:N7	2.28	0.48
2:2B:13:A:O2'	2:2B:14:U:H3'	2.14	0.48
29:17:30:VAL:O	29:17:34:ARG:HG3	2.12	0.48
1:1A:2127:C:H2'	1:1A:2128:G:C8	2.48	0.48
1:1A:2162:C:O2	1:1A:2173:G:N1	2.34	0.48
1:1A:302:A:H2'	1:1A:303:C:C6	2.49	0.48
1:1A:92:C:H2'	1:1A:93:G:C8	3.45	0.48
1:1A:1829:U:H5'	3:1D:259:THR:CG2	2.43	0.48
26:24:44:THR:O	26:24:46:GLN:N	2.46	0.48
1:2A:1036:G:H1	1:2A:1119:C:H42	1.60	0.48
1:2A:2503:2MA:OP2	61:2A:4063:HOH:O	2.20	0.48
1:2A:882:G:H2'	1:2A:883:G:C8	2.45	0.48
3:2D:206:LEU:O	3:2D:211:ARG:HD3	2.13	0.48
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.95	0.48
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.95	0.48
1:1A:2157:A:H2	1:1A:2158:C:C4	2.32	0.48
1:1A:929:G:H1	1:1A:940:C:H42	1.61	0.48
29:27:34:ARG:NE	29:27:39:ARG:HG2	2.27	0.48
1:2A:1463:C:H2'	1:2A:1464:C:C6	2.48	0.48
1:2A:1503:U:H2'	1:2A:1504:C:H6	1.78	0.48
1:2A:2316:C:O2'	6:2G:128:ARG:NH2	2.44	0.48
1:2A:658:C:H2'	1:2A:659:C:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:66:A:H61	2:2B:109:C:H5''	1.77	0.48
3:2D:211:ARG:O	3:2D:215:LEU:HG	2.14	0.48
4:2E:72:VAL:HG12	4:2E:73:GLU:O	2.13	0.48
5:2F:192:LEU:HD22	5:2F:194:MET:HG3	1.95	0.48
1:1A:2761:A:H5'	7:1H:4:ILE:HD12	1.96	0.48
12:1Q:85:LYS:HD3	22:10:7:LEU:HD13	1.94	0.48
1:2A:118:A:N3	1:2A:178:G:H1'	2.29	0.48
1:2A:1999:C:H4'	1:2A:2723:C:O2	2.13	0.48
1:2A:2338:G:H2'	1:2A:2339:G:H8	1.78	0.48
1:2A:271(O):C:H2'	1:2A:271(P):C:C6	2.48	0.48
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.13	0.48
1:1A:1451:U:H2'	1:1A:1452:U:C6	2.49	0.48
2:1B:108:U:H2'	2:1B:109:C:H5''	1.95	0.48
7:1H:11:VAL:HG21	7:1H:50:VAL:HG23	1.95	0.48
1:2A:2315:G:H2'	1:2A:2316:C:H6	1.78	0.48
1:2A:2320:A:H2'	1:2A:2320:A:N3	2.29	0.48
1:2A:272(B):G:H2'	1:2A:272(C):G:C8	2.48	0.48
1:2A:320:A:H4'	1:2A:322:A:C8	2.48	0.48
3:2D:96:HIS:CD2	3:2D:102:LYS:HG2	2.48	0.48
4:2E:5:LEU:HD11	4:2E:79:ARG:HB2	1.96	0.48
7:2H:56:SER:OG	7:2H:57:ASP:N	2.46	0.48
26:14:55:ARG:N	26:14:56:VAL:O	2.42	0.48
1:1A:1699:A:C2'	1:1A:1700:G:H5'	2.44	0.48
1:1A:2008:A:OP1	61:1A:4371:HOH:O	2.20	0.48
1:1A:2145:G:H1	1:1A:2197:C:H42	1.61	0.48
1:1A:2210:C:H2'	1:1A:2211:U:O4'	2.13	0.48
1:1A:2222:C:O2'	1:1A:2239:A:N1	2.43	0.48
1:1A:2545:A:H2'	1:1A:2546:A:O4'	2.13	0.48
61:1A:4841:HOH:O	4:1E:145:LYS:HE2	2.13	0.48
1:2A:272(B):G:H2'	1:2A:272(C):G:H8	1.79	0.48
2:2B:95:C:H2'	2:2B:96:U:C6	2.48	0.48
22:10:50:ASN:HB3	22:10:63:VAL:HG22	1.96	0.48
1:1A:1136:U:N3	1:1A:1148:C:H1'	2.29	0.48
1:1A:1087:C:N4	1:1A:1160:G:H1	2.04	0.48
1:1A:1413:A:H2	1:1A:1487:G:H22	74.29	0.48
1:1A:1495:G:O2'	1:1A:1575:A:N1	2.41	0.48
13:1R:31:HIS:HD2	61:1R:315:HOH:O	1.96	0.48
19:1X:57:LEU:HD11	19:1X:78:LYS:HE2	1.95	0.48
1:2A:1183:G:H5''	25:23:30:ARG:HH22	1.79	0.48
1:2A:184:C:H2'	1:2A:185:U:C6	2.49	0.48
1:2A:2126:A:H4'	1:2A:2127:G:OP1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.49	0.48
1:2A:852:G:H2'	1:2A:853:G:C8	2.44	0.48
24:12:32:LEU:CD2	24:12:36:ARG:HH11	2.27	0.48
1:1A:1071:G:C4	1:1A:1180:C:H1'	2.49	0.48
1:1A:2476:C:H1'	61:1A:5535:HOH:O	2.13	0.48
1:1A:964:A:H5''	2:1B:98:G:O2'	2.14	0.48
5:1F:164:ARG:O	5:1F:168:ARG:HB2	2.14	0.48
23:21:83:GLU:HA	23:21:84:GLY:HA2	1.68	0.48
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.14	0.48
1:2A:1557:C:H5''	1:2A:1558:A:OP2	2.13	0.48
1:2A:266:G:H2'	1:2A:266:G:N3	3.17	0.48
1:2A:581:C:H2'	1:2A:582:G:C8	2.49	0.48
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.94	0.48
5:2F:197:ASP:O	5:2F:200:GLU:HB3	2.14	0.48
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.13	0.48
9:2N:43:THR:HB	9:2N:46:VAL:HG22	1.96	0.48
11:2P:95:VAL:HG13	11:2P:125:VAL:HA	1.96	0.48
12:2Q:31:ASP:HA	12:2Q:134:ARG:NH1	2.29	0.48
25:13:26:LEU:O	25:13:35:ARG:NE	2.46	0.48
1:1A:1115:A:H2	1:1A:1141:A:HO2'	1.60	0.48
1:1A:946:A:O2'	1:1A:1333:A:N3	124.12	0.48
1:1A:1735:U:O2	1:1A:1747:A:H5'	2.14	0.48
6:1G:146:TYR:O	6:1G:149:VAL:HG12	2.14	0.48
1:1A:957:A:H2'	12:1Q:9:TYR:OH	2.14	0.48
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.49	0.48
1:2A:324:A:N6	1:2A:338:G:O2'	2.46	0.48
1:2A:340:A:H2'	1:2A:341:G:O4'	2.13	0.48
1:2A:910:A:H62	12:2Q:12:GLN:HA	1.78	0.48
1:2A:995:C:O2	9:2N:3:THR:OG1	2.32	0.48
1:2A:606:U:OP1	5:2F:104:LYS:HD2	2.14	0.48
8:2I:14:ASP:OD1	8:2I:15:VAL:N	2.47	0.48
1:2A:445:C:OP1	16:2U:2:PRO:HA	2.14	0.48
1:1A:1105:G:H2'	1:1A:1106:U:C5	2.49	0.47
1:1A:2190:G:C6	1:1A:2193:A:C8	3.02	0.47
5:1F:65:TRP:CZ2	5:1F:75:HIS:HD2	2.32	0.47
6:1G:101:ILE:HG22	6:1G:105:LYS:HE2	1.96	0.47
7:1H:56:SER:OG	7:1H:57:ASP:N	2.47	0.47
16:1U:58:ARG:HA	16:1U:61:TRP:CE3	2.49	0.47
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.46	0.47
1:2A:848:G:C2	1:2A:933:A:H1'	2.49	0.47
1:2A:2303:G:O2'	6:2G:132:ASN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:31:ASP:HA	12:2Q:134:ARG:HH11	1.78	0.47
16:2U:76:TYR:OH	16:2U:92:ARG:NE	2.36	0.47
1:1A:1338:U:H2'	1:1A:1339:C:C6	2.49	0.47
1:1A:2177:G:H3'	1:1A:2178:G:C8	2.49	0.47
1:1A:211:A:H5''	1:1A:448:U:OP1	2.14	0.47
1:1A:606:G:N2	1:1A:632:A:N7	49.49	0.47
1:1A:756:U:H2'	1:1A:757:G:C8	2.49	0.47
3:1D:145:VAL:HG13	3:1D:191:ALA:HB2	1.96	0.47
5:1F:158:THR:O	5:1F:164:ARG:NH1	2.42	0.47
5:1F:197:ASP:O	5:1F:201:VAL:HG13	2.14	0.47
7:1H:7:LEU:HD12	7:1H:8:PRO:HD2	1.96	0.47
1:2A:752:A:H3'	29:27:1:MET:CE	2.43	0.47
1:2A:1028:A:H2'	1:2A:1029:A:C8	2.49	0.47
1:2A:2295:C:OP1	14:2S:10:ARG:NH1	2.47	0.47
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.49	0.47
1:2A:2680:C:H1'	4:2E:187:ALA:HB1	1.96	0.47
12:2Q:24:GLY:HA2	12:2Q:67:ARG:NH2	2.29	0.47
21:2Z:156:LYS:HE3	21:2Z:158:PRO:HD3	1.96	0.47
1:1A:1475:G:H2'	1:1A:1476:C:C6	2.49	0.47
1:1A:886:U:H2'	1:1A:887:C:C6	2.49	0.47
1:2A:1805:U:O2	3:2D:50:THR:HB	2.14	0.47
7:2H:75:ALA:O	7:2H:79:VAL:HG22	2.14	0.47
1:1A:1108:G:C8	1:1A:1134:A:H2'	2.49	0.47
1:1A:265:U:H2'	1:1A:266:C:C6	2.48	0.47
4:1E:97:LYS:HE2	4:1E:97:LYS:HB3	1.58	0.47
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.78	0.47
1:2A:2338:G:H2'	1:2A:2339:G:C8	2.49	0.47
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	1.97	0.47
11:2P:47:ASP:N	11:2P:47:ASP:OD1	4.14	0.47
1:1A:1049:G:O2'	1:1A:1056:A:N1	2.38	0.47
1:1A:909:G:H2'	1:1A:910:A:O4'	2.15	0.47
2:1B:29:A:O2'	2:1B:58:A:N1	2.40	0.47
1:1A:2225:U:O4'	3:1D:151:LYS:HE2	2.14	0.47
5:1F:101:LEU:O	5:1F:106:ARG:NH1	2.47	0.47
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.97	0.47
28:26:7:ILE:HD13	28:26:27:LYS:HD3	1.97	0.47
1:1A:1410:G:C8	23:11:3:LYS:HD2	2.49	0.47
3:1D:206:LEU:O	3:1D:211:ARG:HD3	2.14	0.47
18:1W:37:ARG:O	61:1W:3102:HOH:O	2.20	0.47
1:2A:143(A):C:O2'	19:2X:2:LYS:NZ	2.48	0.47
1:2A:2758:A:C4	7:2H:67:LEU:HD21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:572:A:OP2	17:2V:78:LYS:NZ	2.48	0.47
2:2B:17:C:N4	2:2B:109:C:N3	2.62	0.47
2:2B:55:U:H2'	2:2B:56:G:O4'	2.14	0.47
6:2G:60:LEU:HD21	6:2G:92:VAL:HG11	1.96	0.47
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	1.97	0.47
1:1A:1613:A:OP1	3:1D:211:ARG:NH1	2.48	0.47
1:1A:1634:C:H2'	1:1A:1635:C:C6	2.49	0.47
1:1A:704:U:H2'	1:1A:705:C:C6	2.50	0.47
1:1A:987:G:OP2	11:1P:39:LYS:HE2	2.14	0.47
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.30	0.47
1:2A:2405:G:H5'	11:2P:75:ILE:HD13	1.97	0.47
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.15	0.47
1:2A:831:G:O2'	11:2P:38:GLN:OE1	2.30	0.47
1:2A:2467:C:H4'	12:2Q:123:HIS:CD2	2.50	0.47
12:2Q:29:PHE:HB3	12:2Q:65:PHE:CE2	2.50	0.47
21:2Z:92:SER:O	21:2Z:130:PRO:HG3	2.15	0.47
1:1A:1132:A:N3	1:1A:1132:A:H5''	2.29	0.47
1:1A:2157:A:H5'	1:1A:2182:G:C4'	2.38	0.47
1:1A:225:C:H2'	1:1A:226:C:C6	2.49	0.47
1:1A:2874:G:OP1	15:1T:119:LYS:HD2	2.15	0.47
2:1B:74:U:H2'	2:1B:75:G:O4'	2.14	0.47
5:1F:53:THR:HG22	5:1F:56:GLU:HG3	1.95	0.47
6:1G:150:ASP:OD1	6:1G:150:ASP:N	2.46	0.47
9:1N:67:LEU:HA	9:1N:87:LEU:HD22	1.96	0.47
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.15	0.47
1:2A:1416:G:O2'	1:2A:1417:C:OP2	2.30	0.47
1:2A:8:A:H2'	1:2A:9:U:C6	2.50	0.47
7:2H:88:LEU:HD12	7:2H:90:LYS:HE3	1.95	0.47
1:1A:1108:G:H1	1:1A:1123:A:N6	2.00	0.47
1:1A:1314:A:H2'	1:1A:1315:A:O4'	2.15	0.47
1:1A:2156:A:O2'	1:1A:2157:A:OP1	2.31	0.47
1:1A:2044:U:O2'	1:1A:2629:C:H5'	2.15	0.47
14:1S:26:LEU:HB2	14:1S:85:VAL:HG11	1.97	0.47
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.30	0.47
1:2A:807:U:O2'	1:2A:2060:A:N1	2.41	0.47
1:2A:471:A:H2'	1:2A:472:A:O4'	2.15	0.47
7:2H:99:VAL:N	7:2H:102:ALA:O	2.47	0.47
1:1A:2152:U:H2'	1:1A:2180:A:N1	2.30	0.47
1:1A:2324:U:H5'	6:1G:88:ILE:HD11	1.96	0.47
1:1A:2724:U:O2'	1:1A:2726:A:H5'	2.15	0.47
1:2A:2375:G:O2'	1:2A:2377:A:N7	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:521:G:H2'	1:2A:522:G:H8	1.79	0.47
1:2A:588:U:H2'	1:2A:589:C:C6	2.50	0.47
6:2G:106:LEU:O	6:2G:110:ALA:HB3	2.14	0.47
1:1A:1097:G:H2'	1:1A:1098:C:O4'	2.15	0.47
1:1A:1305:G:H22	1:1A:1331:G:H1'	40.37	0.47
1:1A:142:G:H2'	1:1A:143:C:C6	2.50	0.47
1:1A:2482:G:O6	1:1A:2488:A:O2'	2.23	0.47
1:1A:2702:C:N4	1:1A:2726:A:H1'	2.30	0.47
1:1A:34:C:H5''	1:1A:35:G:OP2	2.15	0.47
6:1G:41:GLN:HG2	6:1G:154:GLY:O	2.15	0.47
8:1I:6:LEU:HD11	8:1I:37:VAL:HG23	1.97	0.47
20:1Y:13:VAL:HG12	20:1Y:74:PRO:HA	1.97	0.47
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.50	0.47
22:20:45:PHE:HE1	22:20:77:ARG:NE	2.12	0.47
1:2A:2117:A:O2'	1:2A:2118:U:H5''	2.15	0.47
1:2A:2130:U:H4'	1:2A:2133:G:H4'	1.97	0.47
1:2A:2529:G:O6	31:29:31:LYS:NZ	2.48	0.47
1:2A:2758:A:H2'	1:2A:2759:G:O4'	2.15	0.47
8:2I:8:PRO:HD3	8:2I:15:VAL:HB	1.96	0.47
14:2S:30:ARG:HH11	14:2S:30:ARG:HG2	1.80	0.47
15:2T:127:ALA:C	15:2T:129:ARG:H	2.18	0.47
1:1A:1085:G:H1	1:1A:1162:C:H42	1.62	0.46
1:1A:1324:A:OP1	13:1R:36:THR:HG22	2.15	0.46
1:1A:1938:A:H2'	1:1A:1939:PSU:O4'	2.15	0.46
1:1A:302:A:O2'	1:1A:303:C:OP1	2.22	0.46
1:1A:931:C:C4	1:1A:932:C:H1'	2.50	0.46
9:1N:26:LEU:HD23	9:1N:99:LEU:HD11	1.96	0.46
20:1Y:9:LYS:NZ	20:1Y:28:LYS:O	2.39	0.46
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.98	0.46
1:2A:974:G:C6	1:2A:1186:G:C6	3.04	0.46
1:2A:1224:C:O2	17:2V:85:LYS:NZ	2.30	0.46
1:2A:2131:G:N7	1:2A:2133:G:N2	2.63	0.46
1:2A:665:C:H2'	1:2A:666:G:C8	2.49	0.46
1:2A:7:G:H2'	1:2A:8:A:H8	1.79	0.46
4:2E:128:SER:OG	4:2E:129:HIS:N	2.48	0.46
30:18:42:ARG:HD2	61:18:5001:HOH:O	2.15	0.46
1:1A:2707:C:H2'	1:1A:2708:U:H6	1.81	0.46
14:1S:11:LYS:HG3	14:1S:91:PRO:HD3	1.97	0.46
25:23:6:VAL:HG13	25:23:56:VAL:HG22	1.97	0.46
1:2A:107:C:H2'	1:2A:108:U:C6	2.50	0.46
1:2A:1920:4OC:HM22	1:2A:1921:G:H5'	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2777:G:H8	61:2A:4416:HOH:O	1.98	0.46
1:2A:2815:C:H2'	1:2A:2816:C:H6	1.79	0.46
1:2A:463:G:N2	1:2A:466:A:OP2	2.38	0.46
1:2A:90:U:H1'	1:2A:92:A:C8	2.50	0.46
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.50	0.46
3:2D:3:VAL:HG13	3:2D:17:THR:HB	1.97	0.46
8:2I:1:MET:HA	57:2I:201:CPT:CL1	2.53	0.46
9:2N:34:LEU:HD21	9:2N:120:LEU:HB2	1.97	0.46
12:2Q:38:GLU:HG3	12:2Q:127:ILE:HG22	1.96	0.46
17:2V:5:VAL:HG21	17:2V:35:LEU:HD23	1.97	0.46
1:1A:1404:G:OP2	61:1A:4373:HOH:O	2.21	0.46
1:1A:2377:G:H4'	22:10:60:PHE:CZ	2.51	0.46
1:1A:2760:G:O6	1:1A:2768:C:H5''	2.14	0.46
1:1A:2635:G:HO2'	1:1A:2835:C:HO2'	1.63	0.46
2:1B:1:U:O2'	2:1B:2:C:OP1	2.29	0.46
15:1T:49:VAL:HG12	15:1T:63:VAL:HG22	1.96	0.46
1:2A:1761:C:H2'	1:2A:1762:A:H5''	1.97	0.46
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.51	0.46
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.51	0.46
3:2D:43:ARG:NH2	3:2D:49:ILE:HD11	2.29	0.46
7:2H:74:ASN:O	7:2H:78:GLY:N	2.48	0.46
1:1A:2549:U:H2'	1:1A:2550:C:C6	2.51	0.46
1:1A:2005:C:H4'	1:1A:2618:C:H4'	1.97	0.46
26:24:28:LYS:HA	26:24:29:PRO:HD3	1.76	0.46
1:2A:107:C:H2'	1:2A:108:U:H6	1.80	0.46
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.15	0.46
1:2A:1786:A:C4	1:2A:1938:A:C6	3.03	0.46
1:2A:2095:C:H2'	1:2A:2096:U:O4'	2.15	0.46
1:2A:2335:A:C8	1:2A:2337:G:C5	3.04	0.46
1:2A:2051:A:H5'	1:2A:2578:G:O4'	2.15	0.46
6:2G:136:ARG:HA	6:2G:154:GLY:HA3	1.97	0.46
12:2Q:21:THR:HG21	12:2Q:101:ARG:HD2	1.97	0.46
1:2A:2690:C:OP1	13:2R:17:ARG:NH2	2.48	0.46
18:2W:34:ASN:OD1	18:2W:37:ARG:NH2	2.48	0.46
1:1A:2164:C:N3	1:1A:2171:G:O6	2.48	0.46
1:1A:2418:U:H2'	1:1A:2418:U:OP2	2.15	0.46
1:1A:2802:C:O2	1:1A:2903:G:N2	2.44	0.46
1:1A:441:C:H2'	1:1A:442:A:C8	2.51	0.46
20:1Y:43:ASN:HB3	20:1Y:65:ALA:HB3	1.97	0.46
1:2A:2292:C:H2'	1:2A:2293:C:H6	1.80	0.46
1:2A:2366:A:H2'	1:2A:2367:G:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.16	0.46
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.23	0.46
1:2A:949:C:H2'	1:2A:950:G:C8	2.51	0.46
1:2A:992:C:OP1	17:2V:74:LYS:NZ	2.27	0.46
2:2B:84:C:OP1	25:23:15:TYR:OH	2.28	0.46
6:2G:11:TYR:O	6:2G:16:ARG:HG2	2.15	0.46
9:2N:38:HIS:ND1	9:2N:39:ARG:HG3	2.31	0.46
1:1A:2825:C:H5'	27:15:29:THR:HG21	1.96	0.46
1:1A:1487:G:H2'	1:1A:1488:G:C8	2.50	0.46
1:1A:2053:A:C6	1:1A:2510:C:H1'	2.50	0.46
1:1A:2658:C:H2'	1:1A:2659:U:O4'	2.16	0.46
1:1A:929:G:H1	1:1A:940:C:N4	2.13	0.46
4:1E:24:THR:HG23	4:1E:184:VAL:HG13	1.97	0.46
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.50	0.46
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.98	0.46
11:1P:126:VAL:HG12	11:1P:148:LEU:CD2	2.46	0.46
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.98	0.46
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.50	0.46
1:2A:2094:G:P	8:2I:22:LYS:HD2	2.56	0.46
1:2A:2445:G:OP1	5:2F:74:ARG:NH2	2.38	0.46
1:2A:2507:C:H5''	1:2A:2573:C:N4	2.31	0.46
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.51	0.46
1:2A:613:G:N2	1:2A:614(C):A:O2'	2.49	0.46
1:2A:830:G:H4'	1:2A:831:G:OP2	2.16	0.46
2:2B:105:A:H5'	2:2B:106:G:OP2	2.15	0.46
1:2A:2294:C:P	14:2S:89:ARG:HH22	2.38	0.46
26:14:33:VAL:HG12	26:14:35:VAL:H	1.81	0.46
1:1A:1068:G:N7	9:1N:66:LYS:HE2	2.31	0.46
1:1A:2376:C:H2'	1:1A:2377:G:O4'	2.16	0.46
6:1G:29:TRP:O	6:1G:33:ARG:NH1	2.48	0.46
8:1I:61:ARG:HA	8:1I:61:ARG:HD3	1.67	0.46
15:1T:127:ALA:C	15:1T:129:ARG:H	2.18	0.46
19:1X:44:GLU:HG2	19:1X:49:VAL:O	2.16	0.46
24:22:32:LEU:O	24:22:36:ARG:HG3	2.16	0.46
1:2A:1221(A):C:C2	1:2A:1229:G:C2	3.03	0.46
1:2A:17:G:H2'	1:2A:18:C:C6	2.51	0.46
1:2A:1922:G:H2'	1:2A:1923:U:O4'	2.16	0.46
1:2A:2127:G:H2'	1:2A:2128:C:C6	2.51	0.46
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.80	0.46
13:2R:44:LEU:HD23	13:2R:44:LEU:HA	1.78	0.46
17:2V:24:LYS:HG3	17:2V:64:HIS:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:17:24:THR:HG22	29:17:26:GLY:H	1.81	0.46
1:1A:2308:U:OP2	14:1S:9:ARG:NH2	2.43	0.46
1:1A:2348:A:H61	22:10:43:THR:CG2	2.29	0.46
1:1A:2045:G:H5'	1:1A:2629:C:H4'	1.98	0.46
1:1A:354:A:HO2'	1:1A:355:A:H8	1.59	0.46
61:1A:4316:HOH:O	13:1R:3:HIS:NE2	2.35	0.46
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.48	0.46
1:2A:128:C:H2'	1:2A:129:C:H6	1.81	0.46
1:2A:2067:G:O2'	1:2A:2069:G:H5'	2.16	0.46
1:2A:2136:C:C4	1:2A:2155:G:N1	2.74	0.46
1:2A:383:U:H2'	1:2A:385:C:H5	1.80	0.46
1:2A:622:G:H2'	1:2A:623:G:H8	1.81	0.46
23:11:83:GLU:N	23:11:83:GLU:OE1	2.48	0.46
1:1A:2880:C:H2'	1:1A:2881:C:O4'	2.16	0.46
1:1A:673:G:H2'	1:1A:674:G:C8	2.87	0.46
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.15	0.46
17:1V:74:LYS:HB2	17:1V:83:ARG:HB2	1.97	0.46
29:27:34:ARG:HE	29:27:39:ARG:HG2	1.81	0.46
1:2A:1837:C:O2'	1:2A:1927:A:N3	2.39	0.46
1:2A:2136:C:HO2'	1:2A:2137:C:H6	1.60	0.46
1:2A:864:G:H1'	1:2A:914:C:N4	2.30	0.46
8:2I:124:GLY:H	8:2I:144:VAL:HG23	1.80	0.46
14:2S:14:VAL:HG21	14:2S:90:GLY:O	2.16	0.46
27:15:16:ARG:HG3	27:15:17:ASP:N	2.30	0.46
27:15:48:GLU:O	27:15:60:VAL:HG11	2.16	0.46
1:1A:1059:C:OP2	61:1A:4356:HOH:O	2.21	0.46
1:2A:1453:U:O2'	1:2A:1455:G:N7	2.45	0.46
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.51	0.46
1:2A:2689:U:P	1:2A:2719:G:H22	2.37	0.46
1:2A:2748:A:H2'	1:2A:2749:A:C8	2.51	0.46
1:2A:444:C:N4	1:2A:491:G:O6	53.17	0.46
1:2A:616:G:H5'	5:2F:205:ARG:HD3	1.97	0.46
1:2A:1009:A:P	9:2N:37:LYS:HZ1	2.39	0.46
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.97	0.46
6:1G:108:ASN:HB3	26:14:22:ILE:HD13	1.98	0.45
1:1A:1108:G:N2	1:1A:1134:A:C6	2.84	0.45
1:1A:1402:G:O6	61:1A:4372:HOH:O	2.20	0.45
1:1A:1410:G:OP2	23:11:3:LYS:HG3	2.17	0.45
1:1A:185:A:N3	1:1A:185:A:H2'	2.31	0.45
1:1A:2388:A:H2'	1:1A:2389:A:O4'	2.16	0.45
2:1B:24:G:N7	2:1B:56:G:H2'	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:89:VAL:HG12	5:1F:90:PHE:CD2	2.51	0.45
8:1I:129:THR:HG22	8:1I:139:GLN:NE2	2.29	0.45
14:1S:19:LYS:HE2	14:1S:25:ARG:NH1	2.31	0.45
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.67	0.45
1:2A:2466:C:OP1	31:29:4:ARG:HB2	2.16	0.45
1:2A:1268:A:C2	1:2A:2013:A:C4	3.04	0.45
1:2A:7:G:H2'	1:2A:8:A:C8	2.51	0.45
1:2A:568:U:H5'	1:2A:945:A:C6	2.51	0.45
1:1A:1001:G:H5''	12:1Q:77:LYS:HD2	1.98	0.45
1:1A:1653:C:H4'	1:1A:1654:A:O5'	2.16	0.45
1:1A:2147:G:H1'	1:1A:2195:A:H61	1.80	0.45
1:1A:611:U:O4	1:1A:717:A:H1'	2.16	0.45
1:1A:659:C:H2'	1:1A:660:C:C6	2.51	0.45
4:1E:14:ILE:HG13	4:1E:21:VAL:HG13	1.97	0.45
10:1O:104:ARG:CZ	15:1T:34:VAL:HG11	2.47	0.45
10:1O:120:GLU:HB2	15:1T:68:TYR:HE2	1.81	0.45
1:2A:1512:U:H2'	1:2A:1513:C:C6	2.51	0.45
1:2A:2137:C:N3	1:2A:2155:G:C6	2.85	0.45
1:2A:2166:G:H5'	1:2A:2167:U:OP2	2.17	0.45
8:2I:4:ILE:HD11	8:2I:44:LEU:HD12	1.97	0.45
14:2S:28:VAL:HG11	14:2S:98:VAL:HG13	1.97	0.45
16:2U:52:ARG:HG3	16:2U:55:ARG:NH2	2.31	0.45
1:2A:195:A:N7	61:2A:4166:HOH:O	2.36	0.45
1:2A:2131:G:N7	1:2A:2133:G:C2	2.83	0.45
1:2A:2419:U:H2'	1:2A:2420:C:C6	2.51	0.45
1:2A:2525:G:N2	1:2A:2539:C:C2	2.84	0.45
1:2A:2740:A:C6	1:2A:2741:A:C6	3.04	0.45
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.52	0.45
1:1A:1121:C:H2'	1:1A:1122:C:H5'	1.99	0.45
1:1A:1882:U:H2'	1:1A:1883:C:O4'	2.16	0.45
1:1A:295:C:H2'	1:1A:296:U:O4'	3.16	0.45
1:1A:1845:G:H4'	3:1D:51:VAL:HG21	1.98	0.45
6:1G:43:LEU:HB3	6:1G:44:GLY:H	1.48	0.45
8:1I:110:ASP:HA	8:1I:111:PRO:HD2	1.77	0.45
8:1I:130:TYR:N	8:1I:138:ILE:O	2.44	0.45
1:2A:2065:C:H2'	1:2A:2066:C:C6	2.51	0.45
1:2A:2533:A:OP1	1:2A:2665:A:O2'	2.26	0.45
1:2A:2578:G:OP2	1:2A:2578:G:H4'	2.16	0.45
1:2A:2820:A:HO2'	1:2A:2821:A:P	2.35	0.45
1:2A:699:A:H2'	1:2A:700:G:O4'	2.17	0.45
1:2A:969:U:H2'	1:2A:970:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:86:GLU:OE2	7:2H:130:ARG:NH1	2.49	0.45
7:2H:149:ARG:HA	7:2H:162:ILE:HG21	1.98	0.45
7:2H:17:VAL:O	7:2H:45:VAL:HG11	2.16	0.45
10:2O:119:PRO:HB2	15:2T:68:TYR:CE2	2.51	0.45
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.98	0.45
26:14:44:THR:O	26:14:46:GLN:N	2.50	0.45
28:16:8:LYS:HD3	30:18:34:TRP:CD2	2.51	0.45
1:1A:1128:U:C4	1:1A:1132:A:N1	2.84	0.45
1:1A:209:G:O2'	1:1A:222:A:N3	2.42	0.45
1:1A:502:G:H4'	1:1A:527:A:N1	2.31	0.45
1:1A:992:G:OP2	61:1A:4375:HOH:O	2.21	0.45
12:1Q:43:THR:HG22	12:1Q:94:VAL:HG12	1.98	0.45
1:1A:1201:A:OP1	16:1U:55:ARG:HD2	2.17	0.45
19:2X:60:ARG:NH2	29:27:47:ARG:HH12	2.12	0.45
1:2A:1027:A:C6	1:2A:1126:A:C4	3.04	0.45
1:2A:1123:C:H1'	31:29:18:ARG:HH22	1.81	0.45
1:2A:1651:G:H2'	1:2A:1652:A:O4'	2.17	0.45
1:2A:1916:A:H2'	1:2A:1917:PSU:O4'	2.16	0.45
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.16	0.45
25:13:59:VAL:O	25:13:60:GLU:HG2	2.17	0.45
1:1A:1744:G:OP2	1:1A:1745:A:O2'	2.31	0.45
1:1A:1911:A:H2'	1:1A:1912:A:C8	2.52	0.45
1:1A:35:G:H2'	1:1A:36:G:O4'	2.17	0.45
3:1D:77:ALA:HA	3:1D:97:TYR:HA	1.97	0.45
11:1P:77:ARG:HB2	11:1P:78:PRO:HD2	1.97	0.45
1:2A:112:U:H5'	24:22:65:ASN:ND2	2.30	0.45
1:2A:1200:C:H5'	61:2A:4140:HOH:O	2.16	0.45
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.16	0.45
1:2A:2183:C:H2'	1:2A:2184:G:C8	2.50	0.45
1:2A:2841:C:H2'	1:2A:2842:G:H8	1.81	0.45
1:2A:336:C:H2'	1:2A:337:C:C6	2.77	0.45
1:2A:845:G:N2	1:2A:845:G:OP2	2.40	0.45
2:2B:90:A:C5	2:2B:91:C:H1'	2.52	0.45
1:2A:801:G:O6	5:2F:53:THR:OG1	2.34	0.45
20:2Y:56:PRO:C	20:2Y:58:GLY:H	2.20	0.45
1:1A:2165:C:N3	1:1A:2170:G:C6	2.85	0.45
1:1A:2255:U:H2'	1:1A:2256:U:C6	2.52	0.45
3:1D:19:ALA:HB3	3:1D:21:PHE:CE1	2.52	0.45
18:1W:71:VAL:HA	18:1W:107:LEU:HD12	1.99	0.45
1:2A:1019:U:HO2'	1:2A:1021:A:H2	1.62	0.45
1:2A:108:U:H2'	1:2A:109:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2059:A:C8	1:2A:2503:2MA:HM23	2.51	0.45
1:2A:2741:A:H2'	1:2A:2742:C:O4'	2.16	0.45
1:2A:855:G:H2'	1:2A:856:C:C6	2.52	0.45
1:2A:908:C:OP2	12:2Q:22:LYS:NZ	2.40	0.45
4:2E:5:LEU:HD22	4:2E:197:ILE:HG12	1.98	0.45
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.52	0.45
12:2Q:35:VAL:HG13	12:2Q:130:LYS:HB3	1.97	0.45
21:2Z:6:LYS:HE3	21:2Z:43:GLU:OE1	2.16	0.45
1:1A:2291:G:O6	22:10:14:ARG:HG3	2.16	0.45
1:1A:1005:A:OP2	1:1A:1024:G:N1	25.23	0.45
1:1A:2178:G:H8	1:1A:2178:G:OP2	1.99	0.45
1:1A:714:U:O2	30:18:2:PRO:HD2	2.17	0.45
4:1E:170:LEU:HB3	4:1E:184:VAL:CG2	2.47	0.45
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.52	0.45
14:1S:11:LYS:HE2	14:1S:15:ARG:NH1	2.32	0.45
1:2A:1002:G:C2	1:2A:1003:G:C8	4.25	0.45
1:2A:1331:A:H2'	1:2A:1333:C:H5	1.82	0.45
1:2A:570:G:H2'	1:2A:2030:A:C5	2.51	0.45
1:2A:300:A:N3	1:2A:319:C:H1'	2.32	0.45
1:2A:40:C:H2'	1:2A:41:C:C6	2.52	0.45
1:2A:526:A:N3	1:2A:2044:C:H1'	2.32	0.45
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.17	0.45
4:2E:1:MET:HE3	4:2E:199:ARG:HB3	1.99	0.45
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.17	0.45
17:2V:61:VAL:HA	17:2V:94:LEU:HD23	1.99	0.45
19:2X:94:GLY:N	19:2X:95:LEU:HA	2.29	0.45
26:14:24:THR:HG1	26:14:25:TYR:H	1.64	0.45
1:1A:1121:C:C2'	1:1A:1122:C:H5'	2.47	0.45
1:1A:1138:C:H2'	1:1A:1139:G:O4'	2.17	0.45
1:1A:2197:C:H2'	1:1A:2198:A:O4'	2.17	0.45
1:1A:273:G:N2	8:1I:50:ARG:HH12	2.15	0.45
61:1A:4816:HOH:O	19:1X:50:LYS:HE2	2.17	0.45
1:2A:1171:G:H22	1:2A:1178:C:N4	2.15	0.45
1:2A:1187:G:OP2	1:2A:1187:G:H8	2.00	0.45
1:2A:2558:C:H2'	1:2A:2559:C:O4'	2.17	0.45
1:2A:223:A:O2'	1:2A:420:C:O2	2.29	0.45
1:2A:839:U:H2'	1:2A:840:C:C6	2.52	0.45
3:2D:83:GLU:OE1	3:2D:104:TYR:OH	2.28	0.45
26:14:15:ILE:O	26:14:33:VAL:N	2.49	0.45
29:17:24:THR:HG22	29:17:26:GLY:N	2.32	0.45
1:1A:167:G:H2'	1:1A:168:G:C8	3.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2018:C:H4'	1:1A:2019:G:OP1	2.15	0.45
1:1A:2273:C:OP1	22:10:19:LYS:NZ	2.49	0.45
1:1A:2864:G:H2'	1:1A:2865:C:C6	2.52	0.45
1:1A:645:G:H2'	1:1A:645:G:N3	2.31	0.45
1:1A:99:G:H21	24:12:7:ARG:NH2	2.11	0.45
2:1B:33:G:H5'	6:1G:2:PRO:HD3	1.99	0.45
21:1Z:1:MET:HA	21:1Z:2:GLU:HA	1.72	0.45
1:2A:1429:G:H2'	1:2A:1430:C:H6	1.81	0.45
1:2A:1639:U:H2'	1:2A:1640:C:H5''	1.98	0.45
1:2A:195:A:H5''	1:2A:196:A:O5'	2.17	0.45
1:2A:2443:C:H2'	1:2A:2444:G:C8	2.51	0.45
1:2A:2538:C:H2'	1:2A:2539:C:C6	2.52	0.45
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.50	0.45
1:2A:483:A:H1'	20:2Y:59:GLY:O	2.17	0.45
1:2A:601:C:O2'	1:2A:605:C:OP1	2.34	0.45
2:2B:80:U:O2'	2:2B:81:G:H8	1.99	0.45
5:2F:152:GLU:OE1	5:2F:191:ARG:NE	2.47	0.45
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.98	0.45
8:2I:75:LEU:HD22	8:2I:105:HIS:CD2	2.52	0.45
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.50	0.45
21:2Z:138:GLU:H	21:2Z:156:LYS:HE2	1.82	0.45
24:12:52:ASP:O	24:12:56:GLN:HG3	2.18	0.44
5:1F:28:ILE:O	5:1F:30:PRO:HD3	2.17	0.44
9:1N:61:ARG:HD3	9:1N:61:ARG:HA	1.81	0.44
26:24:49:PHE:HB3	26:24:50:VAL:H	1.53	0.44
1:2A:2120:G:H2'	1:2A:2121:G:H8	1.83	0.44
1:2A:948:G:OP1	61:2A:4006:HOH:O	2.21	0.44
1:1A:1314:A:C2	1:1A:2035:A:C4	3.06	0.44
1:1A:2163:G:C4	1:1A:2164:C:H1'	2.52	0.44
1:1A:2464:C:OP2	61:1A:4379:HOH:O	2.21	0.44
1:1A:756:U:H2'	1:1A:757:G:H8	1.83	0.44
5:1F:108:LYS:HE3	5:1F:112:MET:HE2	1.99	0.44
1:2A:1721:G:N1	1:2A:1739:U:OP2	2.50	0.44
1:2A:2119:A:C5	1:2A:2170:A:C6	3.06	0.44
1:2A:2314:C:H2'	1:2A:2315:G:C8	2.51	0.44
1:2A:637:A:OP1	11:2P:133:SER:OG	2.28	0.44
1:2A:1903:G:OP1	3:2D:241:PRO:HB2	2.17	0.44
1:2A:1012:U:C5	9:2N:28:THR:HG21	2.52	0.44
9:2N:33:LEU:HD12	9:2N:38:HIS:HD2	1.82	0.44
14:2S:87:PHE:CE1	14:2S:102:ALA:HB2	2.52	0.44
1:1A:1221:G:H1'	1:1A:1222:A:H5'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1717:C:OP1	61:1A:4374:HOH:O	2.21	0.44
1:1A:2190:G:O6	1:1A:2193:A:H5''	2.16	0.44
14:1S:43:GLU:OE2	22:10:49:LYS:NZ	2.30	0.44
20:1Y:6:HIS:CD2	20:1Y:6:HIS:H	2.36	0.44
1:2A:1138:G:H5''	1:2A:1139:G:OP2	2.17	0.44
1:2A:1366:A:OP1	23:21:3:LYS:NZ	2.40	0.44
1:2A:729:G:H2'	1:2A:1775:U:H1'	1.99	0.44
1:2A:2144:U:H1'	1:2A:2148:G:N2	2.32	0.44
1:2A:2152:G:C2	1:2A:2153:G:H1'	2.52	0.44
1:2A:2232:U:P	23:21:40:ARG:HH12	2.40	0.44
1:2A:2624:G:N7	61:2A:4169:HOH:O	2.36	0.44
1:2A:824:A:H1'	1:2A:2358:G:N7	2.31	0.44
3:2D:77:ALA:HB2	3:2D:97:TYR:CD1	2.53	0.44
1:1A:1627:A:H8	1:1A:1627:A:OP2	2.00	0.44
1:1A:1821:C:H5''	1:1A:1822:A:OP1	2.17	0.44
1:1A:1921:G:H2'	1:1A:1921:G:N3	2.32	0.44
1:1A:2182:G:O6	1:1A:2183:C:N4	2.50	0.44
15:1T:118:ARG:HA	15:1T:121:ILE:HD12	1.99	0.44
1:2A:1184:G:C6	1:2A:1185:C:C4	3.06	0.44
1:2A:565:C:H4'	1:2A:1253:A:C6	2.52	0.44
1:2A:1941:C:N4	1:2A:1965:C:H5'	2.33	0.44
1:2A:2357:U:OP1	22:20:20:ARG:NE	2.42	0.44
1:2A:646:A:H2'	1:2A:647:G:O4'	2.17	0.44
1:2A:996:A:C2	1:2A:997:G:C8	3.06	0.44
7:2H:33:LEU:HD11	7:2H:136:ILE:HG22	1.98	0.44
8:2I:84:GLY:O	8:2I:86:THR:N	2.47	0.44
25:23:7:LYS:HB2	25:23:34:GLU:HG3	1.99	0.44
1:2A:1263:U:C4	1:2A:1264:G:C6	3.06	0.44
1:2A:2250:G:O2'	1:2A:2496:C:OP1	2.23	0.44
1:2A:2576:G:O2'	1:2A:2579:C:OP2	2.22	0.44
1:2A:300:A:H8	1:2A:300:A:O5'	2.99	0.44
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	2.00	0.44
10:2O:76:ALA:O	15:2T:74:ARG:HG3	2.18	0.44
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.18	0.44
21:2Z:40:ASP:OD2	21:2Z:42:VAL:HG13	2.17	0.44
1:1A:1084:C:H42	1:1A:1163:G:H1	1.65	0.44
1:1A:1211:U:H2'	1:1A:1212:C:C6	2.52	0.44
1:1A:1639:G:H2'	1:1A:1640:G:C8	2.53	0.44
18:1W:68:ARG:NH1	18:1W:111:HIS:HA	2.32	0.44
1:2A:1153:C:H2'	1:2A:1154:G:O4'	2.18	0.44
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2136:C:O2'	1:2A:2137:C:H6	2.00	0.44
1:2A:2881:C:H2'	1:2A:2882:A:O4'	2.18	0.44
1:2A:864:G:H1'	1:2A:914:C:H42	1.83	0.44
4:2E:52:LEU:HB3	4:2E:76:ARG:HD3	1.99	0.44
5:2F:18:ARG:NH1	5:2F:127:GLU:OE2	2.45	0.44
1:1A:2624:C:OP2	27:15:2:ALA:N	2.51	0.44
31:19:2:LYS:NZ	31:19:31:LYS:O	2.44	0.44
1:1A:469:A:H1'	1:1A:1246:C:O4'	2.18	0.44
1:1A:2576:A:C2	1:1A:2659:U:H4'	2.52	0.44
1:1A:906:G:O2'	1:1A:962:G:O6	2.30	0.44
12:1Q:79:LEU:HD23	12:1Q:79:LEU:HA	1.89	0.44
16:1U:16:LYS:HB3	16:1U:16:LYS:HE2	1.80	0.44
21:1Z:123:ASP:N	21:1Z:123:ASP:OD1	2.51	0.44
26:24:60:GLN:O	26:24:62:ARG:N	2.51	0.44
1:2A:1268:A:H2'	1:2A:1269:A:C8	3.40	0.44
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.17	0.44
12:2Q:30:GLY:O	12:2Q:134:ARG:HD3	2.18	0.44
1:2A:2019:A:O4'	16:2U:34:LYS:HE3	2.17	0.44
1:1A:1056:A:N3	1:1A:1199:C:H1'	2.33	0.44
1:1A:1111:U:H5''	1:1A:1112:U:OP2	2.18	0.44
1:1A:174:U:H4'	1:1A:207:A:H4'	2.00	0.44
1:1A:2156:A:OP1	1:1A:2178:G:N2	2.51	0.44
1:1A:2290:A:OP2	22:10:12:ASN:ND2	2.47	0.44
1:1A:603:C:H2'	1:1A:604:C:C6	2.52	0.44
2:1B:88:C:H2'	2:1B:89:G:O4'	2.18	0.44
6:1G:79:ASN:H	6:1G:79:ASN:HD22	1.63	0.44
1:1A:1039:G:OP1	16:1U:50:ARG:HD2	2.18	0.44
25:23:31:LEU:HA	25:23:31:LEU:HD23	1.86	0.44
26:24:45:GLY:O	26:24:47:GLN:N	2.51	0.44
26:24:62:ARG:HA	26:24:62:ARG:HD3	1.66	0.44
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.18	0.44
1:2A:1647:G:OP1	61:2A:4005:HOH:O	2.21	0.44
1:2A:2238:G:N3	1:2A:2238:G:H2'	2.33	0.44
1:2A:858:U:O2	1:2A:2268:A:H2'	2.18	0.44
1:2A:319:C:H2'	1:2A:320:A:O4'	2.18	0.44
2:2B:75:G:N3	21:2Z:85:HIS:CE1	2.86	0.44
3:2D:5:LYS:HG2	3:2D:17:THR:HG22	1.99	0.44
5:2F:110:LEU:HD11	5:2F:181:LEU:HG	1.99	0.44
14:2S:11:LYS:HG3	14:2S:91:PRO:HD3	1.99	0.44
26:14:63:TYR:HA	26:14:64:GLY:HA2	1.77	0.44
1:1A:1513:G:H2'	1:1A:1594:C:N4	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2162:C:H1'	1:1A:2174:G:H22	1.81	0.44
1:1A:2584:A:C8	4:1E:144:ARG:HD3	2.52	0.44
1:1A:1830:G:O2'	3:1D:181:GLU:OE2	2.28	0.44
7:1H:160:LYS:HB3	7:1H:160:LYS:HE2	1.81	0.44
12:1Q:38:GLU:HA	12:1Q:99:PRO:HG3	2.00	0.44
1:2A:1006:C:C2	1:2A:1138:G:N2	2.86	0.44
1:2A:1973:G:H2'	1:2A:1974:C:C6	2.53	0.44
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.53	0.44
1:2A:666:G:OP2	1:2A:725:G:N2	99.18	0.44
5:2F:133:ASN:N	5:2F:138:GLU:OE1	2.50	0.44
20:2Y:52:SER:HB2	20:2Y:53:PRO:HD2	2.00	0.44
1:1A:231:G:C8	30:18:5:LYS:HG2	2.52	0.43
1:1A:1714:G:O2'	1:1A:2013:U:O4	2.29	0.43
1:1A:2298:A:H4'	1:1A:2299:A:O4'	2.18	0.43
1:1A:324:A:OP1	20:1Y:86:ARG:NH2	2.51	0.43
1:1A:656:A:H2'	1:1A:657:A:O4'	2.17	0.43
3:1D:8:PRO:HB3	3:1D:14:ARG:HD2	1.98	0.43
8:1I:22:LYS:HA	8:1I:23:PRO:HD3	1.92	0.43
2:1B:91:C:OP1	12:1Q:16:ARG:HD2	2.18	0.43
1:2A:143:G:C2	1:2A:143(A):C:C2	3.06	0.43
1:2A:1628:G:H2'	1:2A:1629:U:H6	1.82	0.43
1:2A:1633:G:OP2	61:2A:4068:HOH:O	2.21	0.43
1:2A:884:C:H3'	1:2A:885:C:C6	2.53	0.43
1:2A:64:A:O3'	19:2X:71:GLY:HA3	2.18	0.43
1:1A:815:G:O2'	1:1A:1425:A:N1	2.39	0.43
1:1A:2227:G:OP2	1:1A:2227:G:H4'	2.18	0.43
1:1A:609:A:N1	1:1A:856:G:O2'	2.40	0.43
5:1F:135:LYS:HB2	5:1F:138:GLU:HG3	1.99	0.43
6:1G:34:LEU:HD12	6:1G:100:TRP:CZ3	2.53	0.43
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.53	0.43
15:1T:65:LYS:HE3	15:1T:67:SER:HB2	2.00	0.43
21:1Z:15:PRO:O	21:1Z:19:ARG:HG3	2.17	0.43
21:1Z:9:TYR:OH	21:1Z:61:LEU:HD23	2.17	0.43
1:2A:1286:A:H2'	1:2A:1287:A:H4'	6.40	0.43
1:2A:2319:G:H22	14:2S:3:ARG:CD	2.30	0.43
1:2A:2841:C:H2'	1:2A:2842:G:C8	2.53	0.43
5:2F:29:ASN:H	5:2F:112:MET:CE	2.31	0.43
7:2H:12:PRO:O	7:2H:15:VAL:HG12	2.18	0.43
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.52	0.43
1:2A:2406:U:C2	11:2P:72:PRO:HG2	2.53	0.43
1:1A:1232:G:H5''	17:1V:81:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1239:A:H62	1:1A:1299:A:H62	20.42	0.43
1:1A:207:A:C2	1:1A:224:U:H4'	2.53	0.43
1:1A:549:U:H2'	1:1A:550:U:C6	2.54	0.43
1:1A:92:C:H2'	1:1A:93:G:H8	2.98	0.43
16:1U:34:LYS:HD3	16:1U:34:LYS:HA	1.69	0.43
1:2A:144:C:H2'	1:2A:145:G:H8	1.83	0.43
1:2A:571:A:N6	1:2A:2499:C:O3'	2.48	0.43
1:2A:573:G:O2'	1:2A:574:C:H3'	2.18	0.43
2:2B:29:A:H2'	2:2B:30:C:C6	2.53	0.43
7:2H:35:VAL:O	7:2H:37:VAL:HG23	2.18	0.43
1:1A:1218:G:O2'	1:1A:1219:A:O4'	2.33	0.43
1:1A:1849:U:O4	3:1D:154:LYS:HD2	2.18	0.43
1:1A:2279:A:H5''	1:1A:2280:A:H5'	2.01	0.43
1:1A:2859:U:H4'	1:1A:2878:A:C2	2.54	0.43
1:1A:515:G:N7	18:1W:49:LYS:NZ	2.66	0.43
10:1O:120:GLU:HB2	15:1T:68:TYR:CE2	2.53	0.43
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.82	0.43
1:2A:1225:G:C6	1:2A:1226:A:C6	3.06	0.43
1:2A:1613:G:C2	1:2A:1619:G:C5	3.06	0.43
1:2A:1493:C:N4	1:2A:2206:G:O2'	2.45	0.43
1:2A:2287:A:O2'	1:2A:2288:A:H5''	2.18	0.43
1:2A:2386:C:H2'	1:2A:2387:U:C6	2.53	0.43
1:2A:375:C:H2'	1:2A:376:C:C6	2.53	0.43
1:2A:413:C:O5'	1:2A:413:C:H6	2.01	0.43
1:2A:567:A:OP2	11:2P:29:LYS:NZ	2.38	0.43
1:2A:757:U:H2'	1:2A:758:C:O4'	2.19	0.43
1:2A:868:U:C4	1:2A:869:G:N7	2.86	0.43
14:2S:15:ARG:O	14:2S:19:LYS:HG3	2.17	0.43
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.51	0.43
2:2B:103:G:N2	21:2Z:73:GLN:HE22	2.15	0.43
1:1A:2036:A:H2'	1:1A:2037:A:C8	2.53	0.43
1:1A:2164:C:O2	1:1A:2171:G:N1	2.50	0.43
1:1A:2826:C:O2	1:1A:2893:A:O2'	2.32	0.43
6:1G:122:PRO:HG3	6:1G:182:LYS:H	1.83	0.43
1:2A:1364:G:C8	23:21:3:LYS:HD2	2.53	0.43
1:2A:1834:U:H4'	1:2A:1969:A:C6	2.53	0.43
1:2A:2119:A:N7	1:2A:2170:A:N6	2.67	0.43
1:2A:2655:G:O2'	1:2A:2664:G:O6	2.27	0.43
1:2A:524:U:H2'	1:2A:525:U:C6	2.54	0.43
1:2A:674:G:H2'	1:2A:675:A:H8	5.18	0.43
1:2A:700:G:H2'	1:2A:701:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:242:ARG:CG	3:2D:242:ARG:HH11	2.12	0.43
5:2F:33:LEU:HA	5:2F:33:LEU:HD12	1.83	0.43
7:2H:26:VAL:O	7:2H:32:GLU:HA	2.18	0.43
10:2O:34:THR:OG1	10:2O:35:VAL:N	2.50	0.43
12:2Q:81:VAL:HG12	22:20:5:LYS:HD3	2.01	0.43
1:2A:996:A:O3'	16:2U:91:ASP:HB2	2.19	0.43
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.59	0.43
11:1P:63:PRO:HB2	30:18:30:ARG:NH2	2.34	0.43
1:1A:449:A:H2'	1:1A:450:A:C8	2.53	0.43
1:1A:836:A:OP1	61:1A:4380:HOH:O	2.21	0.43
5:1F:150:GLY:HA2	5:1F:172:TRP:CE3	2.52	0.43
6:1G:64:THR:HB	6:1G:94:LEU:HD21	2.00	0.43
7:1H:4:ILE:O	7:1H:69:ARG:HD2	2.18	0.43
8:1I:133:HIS:ND1	8:1I:134:PRO:O	2.50	0.43
1:1A:233:A:H4'	11:1P:74:GLU:HB2	2.00	0.43
15:1T:24:PRO:HD3	15:1T:52:ILE:HD12	2.00	0.43
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.26	0.43
1:2A:2127:G:N2	1:2A:2161:C:N3	2.65	0.43
1:2A:2557:G:H2'	1:2A:2558:C:C6	2.54	0.43
1:2A:459:U:H4'	29:27:40:TRP:CZ3	2.53	0.43
4:2E:181:LEU:HA	4:2E:181:LEU:HD12	1.73	0.43
6:2G:170:ARG:NH2	6:2G:182:LYS:O	2.47	0.43
11:2P:7:ARG:HG3	11:2P:8:PRO:HD2	2.00	0.43
1:2A:2319:G:N2	14:2S:3:ARG:HD3	2.32	0.43
1:1A:1221:G:H1'	1:1A:1222:A:C5'	2.48	0.43
5:1F:108:LYS:HG2	5:1F:112:MET:HE2	2.00	0.43
22:20:82:ARG:HA	22:20:83:PRO:HD3	1.71	0.43
1:2A:1359:A:C2	1:2A:1372:U:O4	2.72	0.43
1:2A:1463:C:H2'	1:2A:1464:C:H6	1.84	0.43
1:2A:2406:U:C4	11:2P:72:PRO:HD2	2.54	0.43
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.51	0.43
1:2A:828:U:C5	1:2A:2247:A:H4'	2.53	0.43
2:2B:83:G:N2	2:2B:94:C:O2	2.40	0.43
5:2F:31:HIS:NE2	5:2F:35:GLU:OE2	2.50	0.43
1:2A:442:G:H4'	5:2F:46:ARG:HG3	1.99	0.43
6:2G:97:ASP:O	6:2G:101:ILE:HG13	2.19	0.43
8:2I:73:GLU:HG3	8:2I:138:ILE:HG23	2.00	0.43
10:2O:19:ILE:HG22	10:2O:43:VAL:HA	2.01	0.43
11:2P:2:LYS:HB2	11:2P:2:LYS:HE3	1.75	0.43
16:2U:52:ARG:NH1	16:2U:55:ARG:HH22	2.16	0.43
1:1A:2504:U:H2'	1:1A:2505:U:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2856:G:H2'	1:1A:2857:U:O4'	2.18	0.43
1:1A:2879:G:H2'	1:1A:2880:C:O4'	2.18	0.43
1:1A:865:G:H4'	1:1A:885:C:O3'	2.18	0.43
10:1O:34:THR:OG1	10:1O:35:VAL:N	2.51	0.43
25:23:6:VAL:HG22	25:23:56:VAL:HG13	2.01	0.43
27:25:8:LYS:O	27:25:9:LYS:HD2	2.19	0.43
1:2A:1131:G:HO2'	1:2A:1132:A:H8	1.66	0.43
1:2A:1861:G:N2	1:2A:1881:C:O2	2.49	0.43
1:2A:829:A:N7	1:2A:2248:C:H5'	2.34	0.43
1:2A:2292:C:H2'	1:2A:2293:C:C6	2.54	0.43
1:2A:10:G:O2'	1:2A:2801(A):A:N7	2.37	0.43
1:2A:2846:G:H2'	1:2A:2847:U:O4'	2.19	0.43
1:2A:39:C:O2	5:2F:46:ARG:NH2	2.52	0.43
12:2Q:16:ARG:HG3	12:2Q:18:LYS:HG3	2.00	0.43
19:2X:5:TYR:CE2	24:22:30:ARG:HB2	2.54	0.43
1:1A:1530:G:OP1	1:1A:1530:G:H4'	4.89	0.43
1:1A:2096:U:H2'	1:1A:2097:U:C6	2.53	0.43
1:1A:63:A:O3'	19:1X:71:GLY:HA3	2.19	0.43
1:1A:993:G:H2'	1:1A:993:G:N3	2.89	0.43
2:1B:96:U:H2'	2:1B:97:G:C8	2.54	0.43
1:2A:141:A:H8	1:2A:1408:C:HO2'	1.67	0.43
1:2A:1808:U:H2'	1:2A:1809:A:O4'	2.19	0.43
1:2A:2769:C:H2'	1:2A:2770:G:O4'	2.19	0.43
1:2A:2774:C:H2'	1:2A:2775:A:O4'	2.18	0.43
1:2A:2831:G:OP1	1:2A:2834:G:H4'	2.19	0.43
9:2N:20:GLY:HA2	9:2N:61:ARG:HG3	2.00	0.43
11:2P:121:LYS:HG2	11:2P:123:LEU:HG	2.01	0.43
11:2P:50:ARG:HD3	30:28:7:HIS:HD2	1.83	0.43
12:2Q:56:ARG:HD2	12:2Q:56:ARG:HA	1.75	0.43
12:2Q:19:GLY:O	12:2Q:98:LYS:HE3	2.18	0.43
1:2A:2864:G:OP1	15:2T:119:LYS:HD2	2.19	0.43
17:2V:27:ALA:O	17:2V:64:HIS:HE1	2.01	0.43
26:14:43:TYR:O	26:14:45:GLY:N	2.52	0.43
1:1A:184:A:C8	1:1A:186:A:OP1	2.71	0.43
1:1A:83:A:C5'	20:1Y:8:LYS:HG2	2.49	0.43
5:1F:152:GLU:OE1	5:1F:191:ARG:HD2	2.19	0.43
1:1A:142:G:H1'	19:1X:37:THR:HG21	2.00	0.43
1:2A:1607:C:H4'	1:2A:1608:A:O5'	2.19	0.43
1:2A:2461:C:H2'	1:2A:2462:U:C6	2.53	0.43
1:2A:2611:U:H6	1:2A:2611:U:H5'	1.84	0.43
1:2A:828:U:H4'	1:2A:831:G:N1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:880:G:H2'	1:2A:881:G:H8	1.84	0.43
1:2A:8:A:H2'	1:2A:9:U:H6	1.84	0.43
3:2D:132:PRO:O	3:2D:136:ILE:HG13	2.19	0.43
7:2H:25:LYS:HE3	7:2H:27:LYS:NZ	2.33	0.43
10:2O:120:GLU:HG2	10:2O:122:LEU:HG	2.00	0.43
16:2U:107:ALA:O	16:2U:111:GLU:HG2	2.18	0.43
18:2W:12:ILE:O	18:2W:101:SER:OG	2.31	0.43
26:14:16:CYS:SG	26:14:17:GLY:N	2.92	0.42
1:1A:441:C:H4'	1:1A:1901:C:O2	2.18	0.42
13:1R:26:LYS:HE2	13:1R:70:LEU:O	2.18	0.42
15:1T:108:ARG:HG3	15:1T:109:GLU:N	2.34	0.42
1:2A:1420:U:HO2'	1:2A:1421:G:P	2.37	0.42
1:2A:176:G:O2'	1:2A:177:G:H5'	2.19	0.42
1:2A:196:A:N3	1:2A:196:A:H2'	2.34	0.42
1:2A:2070:G:H2'	1:2A:2071:A:C8	2.54	0.42
1:2A:2135:A:C5	1:2A:2136:C:H5	2.36	0.42
1:2A:76:C:N4	1:2A:93:G:H1	26.13	0.42
1:2A:971:C:H2'	1:2A:972:G:O4'	2.19	0.42
2:2B:24:G:N7	2:2B:56:G:H2'	2.34	0.42
7:2H:9:ILE:HA	7:2H:10:PRO:HD2	1.91	0.42
9:2N:58:ASP:N	9:2N:58:ASP:OD1	2.46	0.42
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	2.01	0.42
1:1A:1688:A:H2'	1:1A:1689:G:O4'	2.19	0.42
1:1A:2158:C:N4	1:1A:2177:G:C6	2.80	0.42
1:1A:215:G:N2	1:1A:217:A:H62	2.15	0.42
1:2A:1027:A:C2	1:2A:2488:A:H5'	2.54	0.42
1:2A:1847:A:H3'	1:2A:1848:A:H5'	2.00	0.42
1:2A:243:U:O2'	1:2A:244:A:H5'	2.19	0.42
1:2A:902:C:H2'	1:2A:903:C:H6	1.84	0.42
1:2A:992:C:H2'	1:2A:993:G:H8	1.83	0.42
24:12:16:LEU:O	24:12:67:LYS:NZ	2.52	0.42
26:14:46:GLN:HG2	26:14:46:GLN:O	2.19	0.42
1:1A:1973:U:O2	1:1A:1975:A:H8	2.02	0.42
1:1A:2138:G:N1	1:1A:2184:G:OP1	2.40	0.42
1:1A:27:G:N2	1:1A:537:G:H1'	2.35	0.42
3:1D:166:GLN:HB2	3:1D:174:ILE:HG22	2.01	0.42
1:2A:2525:G:C2	1:2A:2539:C:N3	2.88	0.42
1:2A:2582:G:N2	1:2A:2583:G:H1'	2.33	0.42
17:2V:85:LYS:HB3	17:2V:85:LYS:HE3	1.85	0.42
18:2W:80:PRO:O	18:2W:100:THR:HB	2.20	0.42
12:2Q:141:GLN:NE2	21:2Z:74:VAL:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1385:G:H5''	19:1X:16:LYS:HD3	2.01	0.42
1:1A:2343:G:O2'	22:10:43:THR:HG22	2.19	0.42
1:1A:310:C:H2'	1:1A:311:C:H6	1.84	0.42
1:1A:596:G:O2'	1:1A:597:C:H3'	2.20	0.42
3:1D:37:LEU:HD22	3:1D:87:ASN:ND2	2.35	0.42
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	2.01	0.42
1:2A:1116:C:H2'	1:2A:1117:G:H8	1.83	0.42
1:2A:315:G:H2'	1:2A:316:C:C6	2.55	0.42
1:2A:643:A:N1	1:2A:2369:A:O2'	2.49	0.42
1:2A:741:G:H2'	1:2A:742:G:O4'	2.45	0.42
1:2A:911:A:H2'	12:2Q:9:TYR:OH	2.18	0.42
2:2B:55:U:O2'	6:2G:27:ASN:ND2	2.45	0.42
6:2G:70:VAL:HA	6:2G:90:LEU:HD23	2.01	0.42
7:2H:137:ASP:HB3	7:2H:140:LYS:CB	2.49	0.42
26:14:28:LYS:HA	26:14:29:PRO:HD3	1.86	0.42
29:17:12:ARG:NH2	29:17:44:PRO:HB3	2.34	0.42
1:1A:1091:A:O2'	1:1A:1093:G:C4	2.71	0.42
1:1A:1210:G:H2'	1:1A:1211:U:C6	2.54	0.42
1:1A:1412:A:H2'	1:1A:1413:A:O4'	2.19	0.42
1:1A:1874:C:H2'	1:1A:1875:C:H6	1.83	0.42
1:1A:217:A:C8	1:1A:218:A:H5'	2.55	0.42
1:1A:572:A:H1'	1:1A:573:G:OP1	2.19	0.42
1:1A:595:A:OP2	17:1V:78:LYS:NZ	2.52	0.42
1:1A:831:A:C6	3:1D:229:VAL:HG11	2.54	0.42
1:1A:83:A:H5'	20:1Y:8:LYS:HG2	2.00	0.42
6:1G:79:ASN:ND2	6:1G:79:ASN:H	2.17	0.42
20:1Y:65:ALA:HA	20:1Y:66:PRO:HD3	1.89	0.42
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	2.02	0.42
1:2A:1217:C:H2'	1:2A:1218:C:O4'	2.71	0.42
1:2A:1354:A:H2'	1:2A:1355:G:O4'	2.19	0.42
1:2A:2070:G:H2'	1:2A:2071:A:H8	1.85	0.42
1:2A:2379:G:H2'	1:2A:2380:C:C6	2.55	0.42
1:2A:2649:U:H2'	1:2A:2650:U:C6	2.54	0.42
1:2A:276:A:H5''	1:2A:277:C:H5'	2.01	0.42
1:2A:859:G:N2	1:2A:917:A:OP2	2.48	0.42
7:2H:11:VAL:HG21	7:2H:50:VAL:HG23	2.01	0.42
14:2S:99:LYS:HE2	14:2S:103:GLU:OE2	2.19	0.42
1:1A:1660:A:P	1:1A:1660:A:H8	2.42	0.42
1:1A:1766:G:H2'	1:1A:1767:A:H2'	2.01	0.42
1:1A:1896:G:OP1	61:1A:4382:HOH:O	2.22	0.42
1:1A:593:G:H2'	1:1A:2052:A:C5	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:217:A:H8	1:1A:218:A:H5'	1.85	0.42
1:1A:2327:G:H2'	1:1A:2328:C:C6	2.55	0.42
1:1A:602:G:H2'	1:1A:603:C:C6	2.55	0.42
13:1R:44:LEU:HA	13:1R:44:LEU:HD23	1.82	0.42
1:2A:1115:G:H2'	1:2A:1116:C:O4'	2.20	0.42
1:2A:1394:U:C4	1:2A:1395:A:C5	3.07	0.42
1:2A:2182:G:C6	1:2A:2183:C:C4	3.08	0.42
1:2A:2393:A:H5''	11:2P:63:PRO:HB3	2.00	0.42
4:2E:135:HIS:H	4:2E:135:HIS:CD2	2.37	0.42
7:2H:126:PRO:HB2	7:2H:127:GLU:H	1.61	0.42
9:2N:67:LEU:O	9:2N:88:GLU:HG3	2.20	0.42
12:2Q:29:PHE:HB2	12:2Q:105:GLU:OE1	2.19	0.42
1:1A:1469:G:OP1	1:1A:1538:G:O2'	2.38	0.42
1:1A:1550:C:H2'	1:1A:1551:C:C6	2.54	0.42
1:1A:1730:C:H2'	1:1A:1731:C:C6	2.54	0.42
3:1D:264:LYS:HA	3:1D:265:PRO:HD3	1.94	0.42
7:1H:137:ASP:O	7:1H:141:VAL:HG23	2.19	0.42
14:1S:26:LEU:HB2	14:1S:85:VAL:CG1	2.50	0.42
1:2A:108:U:C2	1:2A:109:G:C8	3.07	0.42
1:2A:1121:C:H2'	1:2A:1122:G:O4'	2.20	0.42
1:2A:1193:G:H2'	1:2A:1194:A:H8	1.85	0.42
1:2A:1474:C:H42	1:2A:1517:G:H1	1.67	0.42
1:2A:1587:A:H2'	1:2A:1588:C:C6	2.55	0.42
1:2A:2155:G:C5	1:2A:2156:G:H1'	2.54	0.42
1:2A:2274:A:O2'	1:2A:2276:G:OP1	2.33	0.42
1:2A:2628:C:H1'	1:2A:2781:A:H2'	2.02	0.42
1:2A:271(R):G:OP1	23:21:76:ARG:NH1	2.53	0.42
1:2A:2854:G:C6	1:2A:2855:C:C4	3.08	0.42
1:2A:593:G:H4'	30:28:63:PRO:HB3	2.00	0.42
1:2A:713:G:OP1	3:2D:166:GLN:NE2	57.30	0.42
1:2A:839:U:H2'	1:2A:840:C:H6	1.84	0.42
1:2A:984:A:H5''	1:2A:985:C:H5	1.84	0.42
3:2D:275:LYS:HA	3:2D:276:LYS:C	2.40	0.42
5:2F:120:GLU:OE2	5:2F:122:LYS:HG3	2.19	0.42
16:2U:34:LYS:HA	16:2U:34:LYS:HD3	1.73	0.42
26:14:16:CYS:HA	26:14:33:VAL:O	2.20	0.42
28:16:40:CYS:HA	28:16:41:PRO:HD3	1.84	0.42
1:1A:1233:U:H4'	17:1V:79:VAL:HG22	2.01	0.42
1:1A:1362:U:H2'	1:1A:1363:A:C8	2.54	0.42
1:1A:1554:A:H5'	1:1A:1556:A:N7	2.33	0.42
1:1A:1974:A:C6	1:1A:1975:A:N1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:417:A:H4'	1:1A:418:G:H5'	2.02	0.42
1:1A:821:A:H2'	1:1A:821:A:N3	2.34	0.42
1:2A:1190:G:O2'	1:2A:1191:G:H5'	2.20	0.42
1:2A:1364:G:N7	23:21:3:LYS:HD2	2.34	0.42
1:2A:2048:G:OP1	61:2A:4073:HOH:O	2.22	0.42
1:2A:541:C:H2'	1:2A:542:C:H6	1.84	0.42
1:2A:760:G:H2'	1:2A:761:A:O4'	2.20	0.42
1:2A:973:A:H8	1:2A:973:A:OP1	2.02	0.42
4:2E:9:VAL:HG22	4:2E:25:VAL:HB	2.02	0.42
1:2A:1257:C:H4'	5:2F:83:PHE:CD1	2.55	0.42
1:2A:811:U:H2'	11:2P:21:ARG:HA	2.00	0.42
1:1A:1067:A:H3'	1:1A:1067:A:N3	2.35	0.42
1:1A:1685:C:O3'	1:1A:2721:G:N2	2.53	0.42
1:1A:1698:G:N2	1:1A:2029:C:C2	2.88	0.42
1:1A:2274:U:H4'	1:1A:2340:A:C2	2.55	0.42
1:1A:2846:U:H2'	1:1A:2847:G:C8	2.55	0.42
2:1B:78:A:C2	2:1B:100:A:C4	3.07	0.42
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	2.01	0.42
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.20	0.42
13:1R:33:ARG:HA	13:1R:114:VAL:O	2.19	0.42
13:1R:38:VAL:HG12	13:1R:42:LYS:HE3	2.01	0.42
21:1Z:158:PRO:HA	21:1Z:159:PRO:HD3	1.84	0.42
1:2A:1027:A:N6	1:2A:1126:A:C4	2.87	0.42
1:2A:1857:G:C6	1:2A:1858:G:N1	2.88	0.42
1:2A:1517:G:H1'	1:2A:1919:A:O3'	102.74	0.42
1:2A:2408:U:H2'	1:2A:2409:G:C8	2.54	0.42
1:2A:414:C:H2'	1:2A:415:A:C8	2.55	0.42
1:2A:802:A:C5	1:2A:803:U:C4	3.08	0.42
1:2A:80:G:OP2	1:2A:80:G:H8	3.40	0.42
1:2A:1490:A:O2'	3:2D:99:ASP:OD1	2.38	0.42
6:2G:41:GLN:HG2	6:2G:154:GLY:O	2.19	0.42
30:18:31:HIS:O	30:18:32:LEU:HB2	2.19	0.42
1:1A:1730:C:H2'	1:1A:1731:C:H6	1.84	0.42
1:1A:593:G:H2'	1:1A:2052:A:N7	2.35	0.42
1:1A:2126:G:H2'	1:1A:2127:C:C6	2.55	0.42
1:1A:233:A:C2	1:1A:244:A:C4	3.08	0.42
2:1B:31:C:H4'	6:1G:29:TRP:CZ2	2.55	0.42
4:1E:52:LEU:HA	4:1E:53:PRO:HD3	1.91	0.42
9:1N:70:LYS:HD3	9:1N:87:LEU:HD12	2.02	0.42
10:1O:120:GLU:HG2	10:1O:122:LEU:HG	2.01	0.42
10:1O:104:ARG:NH2	15:1T:36:GLU:OE2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1Y:92:ASN:HB3	20:1Y:94:LYS:N	2.20	0.42
1:2A:1356:G:OP2	61:2A:4067:HOH:O	2.21	0.42
1:2A:224:G:C2	1:2A:225:A:C4	3.08	0.42
1:2A:2354:G:H21	22:20:36:ILE:HD11	1.85	0.42
1:2A:2378:A:O5'	1:2A:2378:A:H8	2.02	0.42
1:2A:244:A:C2	1:2A:255:A:C4	3.08	0.42
1:2A:744:G:OP1	4:2E:132:HIS:ND1	2.52	0.42
1:2A:921:G:H2'	1:2A:922:U:C6	2.55	0.42
1:2A:975(A):G:C2	1:2A:990:A:C8	3.07	0.42
2:2B:15:A:OP2	2:2B:69:G:N2	2.53	0.42
6:2G:124:SER:HB2	6:2G:131:TYR:CE1	2.55	0.42
7:2H:164:TYR:HB2	7:2H:167:GLU:HB2	2.00	0.42
8:2I:38:LEU:HB2	8:2I:40:THR:HG23	2.01	0.42
1:1A:1037:C:H2'	1:1A:1038:C:C6	3.00	0.41
1:1A:152:G:H2'	1:1A:153:C:C6	2.54	0.41
1:1A:1636:U:H2'	1:1A:1637:G:C8	2.55	0.41
1:1A:2234:G:OP2	61:1A:4365:HOH:O	2.20	0.41
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	2.02	0.41
8:1I:109:ILE:HG13	8:1I:130:TYR:OH	2.20	0.41
21:1Z:14:LYS:HA	21:1Z:15:PRO:HD3	1.89	0.41
1:2A:2406:U:H6	1:2A:2406:U:H2'	1.70	0.41
1:2A:2710:C:O2'	61:2A:4066:HOH:O	2.20	0.41
1:2A:274:G:H1'	1:2A:363:G:N2	2.35	0.41
1:2A:2886:G:H2'	1:2A:2887:U:H6	1.85	0.41
1:2A:721:C:H2'	1:2A:722:A:C8	2.55	0.41
2:2B:31:C:H4'	6:2G:29:TRP:CZ2	2.55	0.41
12:2Q:63:LYS:HE2	12:2Q:65:PHE:HE1	1.85	0.41
21:2Z:126:VAL:HG13	21:2Z:161:VAL:HG23	2.02	0.41
1:1A:1271:G:OP1	17:1V:69:LYS:NZ	2.32	0.41
1:1A:212:A:N1	1:1A:434:G:O2'	2.48	0.41
1:1A:2339:A:H2'	1:1A:2340:A:C8	2.55	0.41
8:1I:75:LEU:HD13	8:1I:105:HIS:NE2	2.35	0.41
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.21	0.41
1:2A:1486:A:H2'	1:2A:1487:G:C8	2.54	0.41
1:2A:1798:U:H5'	3:2D:259:THR:HG22	2.01	0.41
1:2A:2203:U:H2'	1:2A:2205:C:C6	2.55	0.41
1:2A:271(V):G:H2'	1:2A:271(W):G:O4'	2.20	0.41
1:2A:2747:G:O6	1:2A:2755:C:H5''	2.20	0.41
1:2A:415:A:H2'	1:2A:416:C:O4'	2.20	0.41
1:2A:972:G:OP2	1:2A:973:A:O2'	2.33	0.41
3:2D:228:PRO:HD3	3:2D:235:GLY:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:9:VAL:HG13	4:2E:25:VAL:O	2.19	0.41
7:2H:20:ALA:HB3	7:2H:23:ARG:HG3	2.01	0.41
17:2V:16:PRO:HD3	17:2V:99:ILE:HD11	2.02	0.41
21:2Z:125:LEU:HB3	21:2Z:165:VAL:HG13	2.01	0.41
1:1A:1112:U:H2'	1:1A:1114:G:OP2	2.20	0.41
1:1A:1222:A:H2'	1:1A:1222:A:N3	2.35	0.41
1:1A:141:C:H2'	1:1A:142:G:O4'	2.20	0.41
1:1A:2094:G:H2'	1:1A:2095:C:O4'	2.20	0.41
1:1A:2798:C:OP1	4:1E:41:LYS:NZ	2.46	0.41
2:1B:79:C:H2'	2:1B:80:U:O4'	2.19	0.41
5:1F:184:TYR:O	5:1F:188:ARG:HG3	2.21	0.41
21:1Z:26:GLY:HA3	21:1Z:86:VAL:HG23	2.01	0.41
1:2A:819:A:C4	1:2A:1189:A:C2	3.08	0.41
1:2A:220:G:O2'	1:2A:233:A:N3	2.48	0.41
1:2A:947:G:OP2	61:2A:4069:HOH:O	2.21	0.41
3:2D:66:ASP:HB3	3:2D:105:ILE:HG22	2.03	0.41
1:2A:1814:G:H4'	3:2D:51:VAL:HG21	2.03	0.41
20:2Y:77:PRO:HD2	20:2Y:106:LEU:HD23	2.02	0.41
21:2Z:73:GLN:HB3	21:2Z:87:ASP:HB2	2.02	0.41
1:1A:1109:G:N2	1:1A:1122:C:O2'	2.53	0.41
1:1A:1405:A:C2	1:1A:1418:U:O4	2.71	0.41
1:1A:1874:C:H5'	3:1D:253:GLN:OE1	2.20	0.41
1:1A:327:U:H2'	1:1A:328:G:H8	1.85	0.41
1:1A:645:G:H5'	1:1A:645:G:N3	2.35	0.41
2:1B:4:C:H2'	2:1B:5:C:O4'	2.20	0.41
1:1A:1660:A:C2	18:1W:93:ALA:HB2	2.54	0.41
23:21:53:VAL:HG22	23:21:74:VAL:HG13	2.02	0.41
1:2A:1263:U:H2'	1:2A:1264:G:C8	2.55	0.41
1:2A:128:C:H2'	1:2A:129:C:C6	2.55	0.41
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.19	0.41
1:2A:1878:G:C6	1:2A:1879:C:C4	3.08	0.41
1:2A:1991:U:H2'	1:2A:1992:G:H5''	2.02	0.41
1:2A:2370:G:C6	1:2A:2371:G:C6	3.09	0.41
1:2A:2508:G:HO2'	1:2A:2554:U:HO2'	1.65	0.41
1:2A:407:G:H2'	1:2A:408:G:H8	1.85	0.41
1:2A:729:G:C6	3:2D:208:LYS:HB2	2.55	0.41
1:2A:974:G:C4	1:2A:989:G:C2	3.08	0.41
6:2G:43:LEU:HB3	6:2G:44:GLY:H	1.46	0.41
8:2I:140:LEU:HD22	8:2I:142:VAL:HG22	2.02	0.41
9:2N:67:LEU:HB3	9:2N:88:GLU:HG3	2.02	0.41
17:2V:81:TYR:C	17:2V:82:ARG:HG2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:12:53:LEU:HD23	24:12:53:LEU:HA	1.83	0.41
1:1A:2087:C:H4'	1:1A:2263:OMG:HM22	2.03	0.41
1:1A:296:U:H2'	1:1A:297:C:O4'	2.20	0.41
1:1A:310:C:H2'	1:1A:311:C:C6	2.56	0.41
1:1A:327:U:H2'	1:1A:328:G:C8	2.55	0.41
3:1D:33:LEU:HA	3:1D:33:LEU:HD23	1.92	0.41
6:2G:3:LEU:HD22	26:24:25:TYR:CZ	2.55	0.41
26:24:46:GLN:HG2	26:24:48:ARG:HG2	2.02	0.41
1:2A:2097:C:H2'	1:2A:2098:U:O4'	2.21	0.41
1:2A:500:G:N1	1:2A:503:A:OP2	2.53	0.41
1:2A:93:G:H2'	1:2A:94:C:C6	2.55	0.41
1:2A:947:G:N2	1:2A:971:C:C2	2.88	0.41
4:2E:170:LEU:HB3	4:2E:184:VAL:CG2	2.51	0.41
2:2B:33:G:H5'	6:2G:2:PRO:HD3	2.02	0.41
21:2Z:145:GLU:HB3	21:2Z:148:ASP:HB2	2.02	0.41
1:1A:1715:A:H4'	1:1A:1716:A:O5'	2.20	0.41
1:1A:207:A:N7	61:1A:4506:HOH:O	2.37	0.41
1:1A:2172:U:C2	1:1A:2173:G:N7	2.89	0.41
1:1A:2346:G:O6	22:10:74:ARG:NH1	2.53	0.41
1:1A:2579:G:H2'	1:1A:2580:C:H6	1.86	0.41
1:1A:2651:A:H2'	1:1A:2652:G:O4'	2.20	0.41
1:1A:2711:C:H2'	1:1A:2712:C:O4'	2.21	0.41
1:1A:275:C:H2'	1:1A:276:C:C6	2.56	0.41
1:1A:2858:G:C8	15:1T:97:ALA:HB2	2.56	0.41
1:1A:41:C:H2'	1:1A:42:G:O4'	2.21	0.41
1:1A:830:A:O2'	1:1A:832:G:OP1	2.17	0.41
1:1A:2797:C:H1'	4:1E:37:ARG:NH1	2.34	0.41
6:1G:28:VAL:O	6:1G:31:VAL:HG12	2.21	0.41
7:1H:121:ILE:HA	7:1H:121:ILE:HD13	1.91	0.41
16:1U:8:VAL:HG23	16:1U:11:ARG:HH21	1.86	0.41
16:1U:8:VAL:HG23	16:1U:11:ARG:NH2	2.35	0.41
1:2A:1012:U:O2	1:2A:1017:G:O6	14.48	0.41
1:2A:1639:U:C2'	1:2A:1640:C:H5''	2.51	0.41
1:2A:1831:G:H1'	61:2A:4701:HOH:O	2.19	0.41
1:2A:2100:G:C6	1:2A:2190:G:C6	3.09	0.41
1:2A:2109:U:H3	1:2A:2180:U:H3	1.67	0.41
1:2A:2134:A:N3	1:2A:2134:A:H2'	2.35	0.41
1:2A:601:C:O2	1:2A:605:C:H4'	2.20	0.41
1:2A:747:U:O2	1:2A:2014:A:H1'	2.20	0.41
1:2A:947:G:H2'	1:2A:948:G:C8	2.55	0.41
6:2G:146:TYR:O	6:2G:149:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:117:GLU:HG3	8:2I:118:LYS:H	1.84	0.41
9:2N:138:LEU:HD23	9:2N:138:LEU:HA	1.80	0.41
14:1S:20:ARG:NH2	22:10:51:VAL:O	2.53	0.41
1:1A:1074:A:H61	1:1A:1171:G:H2'	1.85	0.41
1:1A:2343:G:O2'	1:1A:2348:A:N1	2.49	0.41
1:1A:2367:C:H1'	22:10:39:ARG:NH2	2.24	0.41
4:1E:12:THR:HG21	15:1T:11:GLU:HG2	2.03	0.41
16:1U:17:ILE:HG23	16:1U:39:LEU:HD12	2.02	0.41
23:21:50:ARG:HD2	23:21:57:GLU:OE2	2.20	0.41
1:2A:1638:C:H4'	1:2A:2710:C:O2	2.21	0.41
1:2A:2291:U:H2'	1:2A:2292:C:H6	1.81	0.41
1:2A:647:G:H8	1:2A:647:G:O5'	2.03	0.41
1:2A:751:A:C6	1:2A:789:A:C5	3.09	0.41
1:2A:921:G:H2'	1:2A:922:U:H6	1.86	0.41
13:2R:22:ARG:O	13:2R:26:LYS:HG3	2.20	0.41
61:2A:4012:HOH:O	13:2R:3:HIS:NE2	2.37	0.41
1:1A:1137:G:O6	1:1A:1146:C:N3	2.53	0.41
1:1A:1136:U:C2	1:1A:1148:C:H1'	2.56	0.41
1:1A:1186:U:H4'	1:1A:1188:A:O4'	2.21	0.41
1:1A:2556:G:H2'	1:1A:2557:G:O4'	2.21	0.41
1:1A:2859:U:OP2	15:1T:95:ARG:NH1	2.54	0.41
1:1A:946:A:H2'	1:1A:947:A:O4'	2.19	0.41
5:1F:40:GLN:NE2	5:1F:182:ASN:HB2	2.36	0.41
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.64	0.41
22:20:10:THR:HG22	22:20:12:ASN:N	2.20	0.41
26:24:53:GLU:N	26:24:53:GLU:OE1	2.37	0.41
1:2A:1628:G:H2'	1:2A:1629:U:C6	2.56	0.41
1:2A:1660:C:H2'	1:2A:1661:G:H8	1.85	0.41
1:2A:1848:A:H2'	1:2A:1849:G:H8	1.84	0.41
1:2A:2712:U:H2'	1:2A:2714:G:H5''	2.01	0.41
1:2A:271(O):C:H2'	1:2A:271(P):C:H6	1.84	0.41
1:2A:30:G:H2'	1:2A:31:C:C6	2.56	0.41
1:2A:787:U:OP2	61:2A:4071:HOH:O	2.21	0.41
1:2A:443:A:C6	5:2F:45:ARG:HD2	2.55	0.41
12:2Q:137:TYR:O	12:2Q:141:GLN:HG2	2.20	0.41
13:2R:96:ARG:NH2	13:2R:117:VAL:HG13	2.36	0.41
1:2A:2319:G:N2	14:2S:3:ARG:HA	2.36	0.41
15:2T:65:LYS:HE3	15:2T:67:SER:HB2	2.03	0.41
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	2.03	0.41
26:14:55:ARG:H	26:14:56:VAL:C	2.24	0.41
1:1A:1099:C:H42	1:1A:1152:G:H1	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1440:U:C4	1:1A:1441:A:C6	3.09	0.41
1:1A:1800:G:O2'	1:1A:1980:C:OP1	2.27	0.41
1:1A:592:U:OP2	61:1A:4381:HOH:O	2.21	0.41
5:1F:170:LEU:HA	5:1F:171:PRO:HD3	1.90	0.41
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.21	0.41
13:1R:29:LEU:HA	13:1R:29:LEU:HD12	1.76	0.41
21:1Z:105:VAL:O	21:1Z:141:VAL:HG22	2.20	0.41
1:2A:1319:G:C6	1:2A:1320:C:N4	2.89	0.41
1:2A:1331:A:H2'	1:2A:1333:C:C5	2.56	0.41
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.55	0.41
1:2A:2164:C:C5	1:2A:2165:G:N3	2.89	0.41
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.53	0.41
1:2A:2507:C:H5''	1:2A:2573:C:C4	2.56	0.41
1:2A:425:G:N2	1:2A:426:C:C2	2.89	0.41
1:2A:600:G:N2	1:2A:605:C:O3'	2.54	0.41
1:2A:784:A:H5'	1:2A:785:G:OP1	2.21	0.41
1:2A:323:G:C8	5:2F:171:PRO:HG3	2.56	0.41
7:2H:23:ARG:HA	7:2H:37:VAL:H	1.86	0.41
1:2A:832:G:N3	11:2P:53:GLY:HA3	2.35	0.41
1:2A:300:A:P	20:2Y:86:ARG:HH21	2.43	0.41
1:1A:174:U:H2'	1:1A:175:G:H8	1.86	0.41
1:1A:1857:G:H2'	1:1A:1858:C:O4'	2.20	0.41
1:1A:2332:A:H2'	1:1A:2332:A:N3	2.36	0.41
1:1A:2402:U:O2'	1:1A:2403:G:H5'	2.21	0.41
1:1A:2430:A:OP2	30:18:29:LYS:NZ	2.54	0.41
5:1F:192:LEU:HD22	5:1F:194:MET:HG3	2.03	0.41
7:1H:40:GLU:OE1	7:1H:61:HIS:NE2	2.52	0.41
9:1N:82:LEU:HA	9:1N:82:LEU:HD12	1.89	0.41
19:1X:31:HIS:HA	19:1X:32:PRO:HD3	1.94	0.41
30:28:9:GLY:O	30:28:13:ARG:HG3	2.21	0.41
1:2A:1042:G:H2'	1:2A:1043:C:O4'	4.21	0.41
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.21	0.41
1:2A:2148:G:H2'	1:2A:2149:G:H8	1.83	0.41
1:2A:2419:U:OP1	30:28:41:ILE:HD12	2.20	0.41
1:2A:39:C:H2'	1:2A:40:C:C6	2.56	0.41
1:2A:894:C:HO2'	1:2A:895:U:H6	1.66	0.41
2:2B:55:U:H1'	6:2G:29:TRP:CD1	2.56	0.41
3:2D:96:HIS:HD2	3:2D:102:LYS:HG2	1.85	0.41
4:2E:119:ARG:HG3	4:2E:119:ARG:HH11	1.86	0.41
8:2I:123:LEU:HA	8:2I:144:VAL:HG23	2.03	0.41
9:2N:97:ARG:HA	9:2N:100:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:113:LYS:HA	11:2P:129:ALA:O	2.21	0.41
1:1A:532:A:N6	1:1A:1206:G:O2'	79.79	0.41
1:1A:1427:G:N7	61:1A:4507:HOH:O	2.37	0.41
1:1A:2142:G:C2'	1:1A:2143:G:H5'	2.51	0.41
1:1A:2417:G:O2'	1:1A:2423:A:N6	2.54	0.41
1:1A:518:G:H2'	1:1A:519:G:O4'	2.21	0.41
1:1A:757:G:H2'	1:1A:758:G:H8	1.86	0.41
1:1A:722:A:C8	1:1A:851:A:C6	3.09	0.41
3:1D:211:ARG:HG3	3:1D:214:TRP:CZ3	2.55	0.41
4:1E:143:ASN:HD22	4:1E:147:PRO:CD	2.34	0.41
10:1O:87:ILE:HD12	10:1O:91:LEU:HA	2.02	0.41
23:21:56:GLN:NE2	23:21:87:PRO:HG3	2.36	0.41
25:23:59:VAL:HB	25:23:60:GLU:H	1.68	0.41
1:2A:1478:G:HO2'	1:2A:1558:A:H2	1.67	0.41
1:2A:2495:G:H5''	12:2Q:82:ARG:HG2	2.03	0.41
1:2A:250:G:C6	1:2A:251:A:C6	3.09	0.41
2:2B:11:C:H3'	2:2B:12:C:C6	2.56	0.41
3:2D:264:LYS:HA	3:2D:265:PRO:HD3	1.94	0.41
7:2H:144:VAL:O	7:2H:148:ILE:HG13	2.20	0.41
1:2A:1665:A:H4'	10:2O:67:LYS:HB2	2.02	0.41
11:2P:62:LEU:O	30:28:13:ARG:NH1	2.53	0.41
11:2P:77:ARG:HB2	11:2P:78:PRO:HD2	2.03	0.41
12:2Q:85:LYS:N	12:2Q:85:LYS:HD2	2.36	0.41
23:11:94:LEU:O	23:11:97:LEU:HB2	2.20	0.40
1:1A:1109:G:C5	1:1A:1110:C:N4	2.90	0.40
1:1A:2329:C:H2'	1:1A:2330:G:O4'	2.21	0.40
1:1A:588:C:H2'	1:1A:589:U:O4'	2.21	0.40
1:1A:616:G:C6	1:1A:617:U:C4	3.09	0.40
1:1A:928:G:C2	1:1A:929:G:H1'	2.56	0.40
1:1A:943:C:C2	1:1A:944:C:C4	3.09	0.40
5:1F:110:LEU:HA	5:1F:183:VAL:HG12	2.02	0.40
6:1G:109:VAL:HG11	26:14:14:ILE:HG21	2.04	0.40
10:1O:78:ARG:HD2	61:1T:305:HOH:O	2.21	0.40
1:2A:1526:G:C6	1:2A:1527:G:C2	3.09	0.40
1:2A:1668:A:H4'	1:2A:1669:A:O5'	2.21	0.40
1:2A:191:A:H2'	1:2A:192:C:C6	2.56	0.40
1:2A:25:U:C4	1:2A:26:G:C6	3.09	0.40
1:2A:2784:C:H1'	4:2E:37:ARG:NH1	2.33	0.40
1:2A:784:A:H5''	61:2A:4004:HOH:O	2.21	0.40
1:2A:925:C:H2'	1:2A:926:A:C8	2.56	0.40
1:2A:974:G:N2	1:2A:989:G:H1'	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:49:LEU:N	4:2E:79:ARG:O	2.52	0.40
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.28	0.40
4:2E:111:ARG:HA	13:2R:1:MET:SD	2.62	0.40
15:2T:107:ASP:O	15:2T:111:ARG:HB2	2.22	0.40
1:2A:1614:A:C2	18:2W:93:ALA:HB2	2.56	0.40
1:1A:2412:G:O6	61:1A:4364:HOH:O	2.19	0.40
1:1A:390:G:H2'	1:1A:391:G:C8	2.56	0.40
3:1D:109:ASP:HB2	3:1D:197:GLY:HA2	2.03	0.40
3:1D:206:LEU:HD23	3:1D:206:LEU:HA	1.84	0.40
4:1E:175:VAL:O	4:1E:177:PRO:HD3	2.21	0.40
9:1N:39:ARG:HA	9:1N:40:PRO:HD3	1.95	0.40
13:1R:96:ARG:HG2	13:1R:115:GLU:HG2	2.04	0.40
18:1W:68:ARG:NH1	18:1W:112:GLY:H	2.18	0.40
20:1Y:7:VAL:HG21	20:1Y:72:VAL:HG12	2.03	0.40
19:2X:5:TYR:CZ	24:22:30:ARG:HB2	2.56	0.40
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.51	0.40
1:2A:1292:U:H2'	1:2A:1293:C:H6	1.86	0.40
1:2A:143:G:C6	1:2A:143(A):C:C4	3.09	0.40
1:2A:1913:A:H4'	1:2A:1914:C:O5'	2.21	0.40
1:2A:2287:A:C4	1:2A:2289:G:C8	3.09	0.40
1:2A:250:G:H2'	1:2A:251:A:C8	2.57	0.40
1:2A:80:G:O2'	1:2A:294:A:N1	2.34	0.40
1:2A:330:A:H2	1:2A:1210:A:O2'	2.04	0.40
2:2B:40:U:N3	2:2B:44:G:OP2	2.38	0.40
11:2P:85:LEU:HA	11:2P:88:LEU:HD12	2.04	0.40
15:2T:51:ARG:HB3	15:2T:62:THR:HB	2.02	0.40
23:11:56:GLN:HE21	23:11:87:PRO:HG3	1.86	0.40
1:1A:2705:A:H2'	1:1A:2706:G:C8	2.56	0.40
1:1A:410:U:H2'	1:1A:412:C:H5	1.87	0.40
4:1E:2:LYS:HG2	4:1E:200:GLU:HB2	2.02	0.40
5:1F:132:VAL:HG21	5:1F:163:VAL:HG22	2.02	0.40
11:1P:50:ARG:HG3	30:18:61:LEU:HD21	2.03	0.40
28:26:40:CYS:HA	28:26:41:PRO:HD3	1.86	0.40
1:2A:1360:A:OP1	1:2A:1360:A:H8	5.08	0.40
1:2A:2265:U:H4'	12:2Q:13:GLN:HE22	1.86	0.40
1:2A:2377:A:H2'	1:2A:2378:A:C8	2.56	0.40
1:2A:2483:C:H2'	1:2A:2484:G:O4'	2.21	0.40
1:2A:2872:G:O2'	1:2A:2873:A:H5'	2.22	0.40
1:2A:2889:C:H2'	1:2A:2891:G:O4'	2.21	0.40
1:2A:323:G:H1'	1:2A:1205:U:O2	2.21	0.40
1:2A:655:A:H8	1:2A:656:G:O4'	2.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:952:G:C6	1:2A:966:G:C6	3.09	0.40
2:2B:28:C:H2'	2:2B:29:A:O4'	2.22	0.40
5:2F:158:THR:O	5:2F:164:ARG:NH1	2.38	0.40
12:2Q:26:TYR:CD1	12:2Q:28:ALA:HB2	2.56	0.40
12:2Q:37:LEU:HB2	12:2Q:128:LYS:O	2.22	0.40
18:2W:34:ASN:ND2	27:25:39:MET:HG3	2.37	0.40
1:1A:1411:A:OP2	23:11:3:LYS:HG2	2.22	0.40
30:18:26:LYS:HD3	30:18:48:PHE:HB3	2.04	0.40
1:1A:592:U:C4	1:1A:593:G:C6	3.09	0.40
2:1B:44:G:C2	2:1B:48:A:C2	3.10	0.40
6:1G:56:ALA:O	6:1G:59:GLU:HG2	2.22	0.40
1:1A:581:G:OP1	9:1N:111:PRO:HD2	2.22	0.40
20:1Y:20:TYR:HB3	20:1Y:23:ARG:HG3	2.02	0.40
21:1Z:156:LYS:HE3	21:1Z:158:PRO:HD3	2.03	0.40
1:2A:1218:C:N4	1:2A:1231:G:H1	2.20	0.40
1:2A:1815:A:OP1	1:2A:1815:A:H8	2.05	0.40
1:2A:2484:G:C2	1:2A:2485:G:C8	3.09	0.40
1:2A:2857:G:N2	1:2A:2860:A:OP2	2.55	0.40
1:2A:652(B):A:H61	1:2A:655:A:H1'	1.86	0.40
3:2D:69:ARG:HH11	3:2D:69:ARG:HG2	1.87	0.40
5:2F:9:ILE:HG21	5:2F:125:LEU:HD12	2.04	0.40
10:2O:15:GLY:O	10:2O:47:ILE:HG12	2.21	0.40
11:2P:126:VAL:HG12	11:2P:148:LEU:HD23	2.02	0.40
1:1A:2368:C:O3'	22:10:20:ARG:HD3	2.22	0.40
30:18:52:LYS:N	30:18:53:PRO:HD2	2.37	0.40
1:1A:1051:C:H5''	61:1A:5052:HOH:O	2.21	0.40
1:1A:1793:A:H2'	61:1A:6101:HOH:O	2.22	0.40
1:1A:364:A:H2'	1:1A:365:G:O4'	2.22	0.40
1:1A:703:G:H2'	1:1A:704:U:O4'	2.21	0.40
3:1D:71:ASP:CB	3:1D:103:ARG:HH12	2.32	0.40
4:1E:93:VAL:HG13	61:1E:406:HOH:O	2.21	0.40
5:1F:24:LEU:HD23	5:1F:115:ALA:HA	2.02	0.40
7:1H:94:TYR:OH	7:1H:152:ARG:NH1	2.54	0.40
2:1B:91:C:OP2	12:1Q:16:ARG:NH1	2.55	0.40
13:1R:9:LYS:O	13:1R:17:ARG:HD3	2.21	0.40
1:2A:151:C:H2'	1:2A:152:G:C8	2.57	0.40
1:2A:2307:G:OP1	1:2A:2307:G:H8	2.04	0.40
1:2A:2497:A:H5''	61:2A:4122:HOH:O	2.21	0.40
1:2A:614:U:H5'	1:2A:614(C):A:N6	2.37	0.40
1:2A:855:G:C5	1:2A:856:C:C4	3.10	0.40
1:2A:992:C:OP1	16:2U:47:TYR:OH	2.26	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:19:G:H2'	2:2B:20:C:O4'	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	263 (96%)	10 (4%)	0	100	100
3	2D	273/276 (99%)	263 (96%)	9 (3%)	1 (0%)	34	66
4	1E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	61
4	2E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	61
5	1F	201/210 (96%)	198 (98%)	2 (1%)	1 (0%)	29	61
5	2F	201/210 (96%)	195 (97%)	4 (2%)	2 (1%)	15	44
6	1G	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	25	56
6	2G	179/182 (98%)	167 (93%)	11 (6%)	1 (1%)	25	56
7	1H	171/180 (95%)	161 (94%)	8 (5%)	2 (1%)	13	39
7	2H	171/180 (95%)	162 (95%)	8 (5%)	1 (1%)	25	56
8	1I	144/148 (97%)	136 (94%)	8 (6%)	0	100	100
8	2I	144/148 (97%)	133 (92%)	10 (7%)	1 (1%)	22	53
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	22	53
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	140 (95%)	7 (5%)	0	100	100
11	2P	147/150 (98%)	136 (92%)	11 (8%)	0	100	100
12	1Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	2Q	139/141 (99%)	132 (95%)	6 (4%)	1 (1%)	22	53
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
14	2S	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	17	46
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15	44
17	2V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	15	44
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	110 (100%)	0	0	100	100
19	1X	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14	41
20	1Y	105/110 (96%)	100 (95%)	3 (3%)	2 (2%)	8	26
20	2Y	105/110 (96%)	101 (96%)	3 (3%)	1 (1%)	15	44
21	1Z	148/206 (72%)	134 (90%)	14 (10%)	0	100	100
21	2Z	156/206 (76%)	139 (89%)	16 (10%)	1 (1%)	25	56
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100	100
22	20	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	13	39
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
23	21	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	68 (100%)	0	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	8	28
26	14	67/71 (94%)	55 (82%)	7 (10%)	5 (8%)	1	2
26	24	67/71 (94%)	53 (79%)	8 (12%)	6 (9%)	1	1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	51 (100%)	0	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	6	22
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	201 (88%)	20 (9%)	8 (4%)	3	12
33	2b	229/256 (90%)	202 (88%)	20 (9%)	7 (3%)	4	14
34	1c	204/239 (85%)	189 (93%)	13 (6%)	2 (1%)	15	44
34	2c	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	29	61
35	1d	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	29	61
35	2d	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	29	61
36	1e	146/162 (90%)	141 (97%)	2 (1%)	3 (2%)	7	23
36	2e	146/162 (90%)	139 (95%)	6 (4%)	1 (1%)	22	53
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	145 (95%)	6 (4%)	2 (1%)	12	36
38	2g	153/156 (98%)	142 (93%)	8 (5%)	3 (2%)	7	24
39	1h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	4 (3%)	1 (1%)	22	53
40	1i	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
40	2i	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
41	1j	95/105 (90%)	82 (86%)	6 (6%)	7 (7%)	1	2
41	2j	94/105 (90%)	84 (89%)	5 (5%)	5 (5%)	2	6
42	1k	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	8	28
42	2k	112/129 (87%)	104 (93%)	7 (6%)	1 (1%)	17	46
43	1l	119/132 (90%)	114 (96%)	5 (4%)	0	100	100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	113 (93%)	7 (6%)	1 (1%)	19	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	2m	120/126 (95%)	112 (93%)	7 (6%)	1 (1%)	19	49
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
46	1o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
46	2o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
47	1p	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
47	2p	80/88 (91%)	74 (92%)	5 (6%)	1 (1%)	12	36
48	1q	97/105 (92%)	95 (98%)	2 (2%)	0	100	100
48	2q	97/105 (92%)	96 (99%)	1 (1%)	0	100	100
49	1r	66/88 (75%)	66 (100%)	0	0	100	100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100	100
50	1s	81/93 (87%)	73 (90%)	7 (9%)	1 (1%)	13	39
50	2s	81/93 (87%)	72 (89%)	7 (9%)	2 (2%)	5	19
51	1t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2	8
51	2t	94/106 (89%)	87 (93%)	3 (3%)	4 (4%)	2	8
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11368/12128 (94%)	10766 (95%)	507 (4%)	95 (1%)	19	49

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
26	14	53	GLU
26	14	61	ARG
33	1b	17	PHE
38	1g	79	ARG
41	1j	32	ALA
50	1s	81	ARG
5	2F	21	ALA
5	2F	130	ALA
7	2H	126	PRO
8	2I	10	GLU
12	2Q	28	ALA
26	24	55	ARG
26	24	61	ARG

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Mol	Chain	Res	Type
29	27	46	VAL
33	2b	16	HIS
33	2b	17	PHE
38	2g	79	ARG
50	2s	81	ARG
6	1G	43	LEU
7	1H	126	PRO
17	1V	79	VAL
26	14	45	GLY
26	14	57	GLU
41	1j	55	LYS
41	1j	56	HIS
41	1j	75	ILE
42	1k	49	GLY
51	1t	47	GLY
51	1t	96	GLY
51	1t	100	ILE
4	2E	52	LEU
9	2N	2	LYS
17	2V	79	VAL
26	24	45	GLY
33	2b	78	GLN
41	2j	56	HIS
41	2j	75	ILE
51	2t	47	GLY
51	2t	100	ILE
4	1E	52	LEU
20	1Y	78	ALA
26	14	44	THR
33	1b	20	GLU
33	1b	21	ARG
33	1b	231	GLU
41	1j	78	ASN
3	2D	3	VAL
6	2G	43	LEU
14	2S	84	GLN
26	24	46	GLN
26	24	62	ARG
33	2b	231	GLU
38	2g	7	ALA
41	2j	55	LYS
41	2j	78	ASN

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Mol	Chain	Res	Type
42	2k	49	GLY
44	2m	4	ILE
50	2s	29	ARG
51	2t	95	ALA
20	1Y	54	LYS
33	1b	78	GLN
33	1b	125	PRO
34	1c	3	ASN
35	1d	178	VAL
36	1e	86	ALA
41	1j	31	GLY
41	1j	77	PRO
19	2X	2	LYS
20	2Y	78	ALA
21	2Z	146	ILE
22	20	4	LYS
33	2b	125	PRO
34	2c	3	ASN
36	2e	69	VAL
38	2g	80	VAL
39	2h	73	ASP
33	1b	16	HIS
33	1b	37	ASN
34	1c	66	VAL
38	1g	80	VAL
26	24	65	ASP
33	2b	20	GLU
36	1e	69	VAL
33	2b	95	GLN
41	2j	77	PRO
44	1m	6	GLY
47	2p	53	VAL
7	1H	92	ILE
42	1k	105	VAL
51	1t	102	GLY
36	1e	85	GLY
25	23	59	VAL
35	2d	5	ILE
51	2t	102	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	209 (97%)	6 (3%)	43	77
3	2D	215/218 (99%)	211 (98%)	4 (2%)	57	85
4	1E	164/166 (99%)	156 (95%)	8 (5%)	25	57
4	2E	164/166 (99%)	153 (93%)	11 (7%)	16	43
5	1F	160/166 (96%)	153 (96%)	7 (4%)	28	61
5	2F	159/166 (96%)	150 (94%)	9 (6%)	20	50
6	1G	143/156 (92%)	140 (98%)	3 (2%)	53	84
6	2G	143/156 (92%)	139 (97%)	4 (3%)	43	77
7	1H	143/148 (97%)	140 (98%)	3 (2%)	53	84
7	2H	143/148 (97%)	140 (98%)	3 (2%)	53	84
8	1I	113/124 (91%)	108 (96%)	5 (4%)	28	61
8	2I	105/124 (85%)	103 (98%)	2 (2%)	57	85
9	1N	118/119 (99%)	114 (97%)	4 (3%)	37	71
9	2N	118/119 (99%)	115 (98%)	3 (2%)	47	80
10	1O	100/100 (100%)	99 (99%)	1 (1%)	76	93
10	2O	100/100 (100%)	99 (99%)	1 (1%)	76	93
11	1P	115/116 (99%)	113 (98%)	2 (2%)	60	87
11	2P	115/116 (99%)	113 (98%)	2 (2%)	60	87
12	1Q	111/111 (100%)	110 (99%)	1 (1%)	78	94
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	35	69
13	1R	101/101 (100%)	95 (94%)	6 (6%)	19	49
13	2R	101/101 (100%)	95 (94%)	6 (6%)	19	49
14	1S	86/88 (98%)	85 (99%)	1 (1%)	71	92
14	2S	85/88 (97%)	84 (99%)	1 (1%)	71	92
15	1T	115/127 (91%)	113 (98%)	2 (2%)	60	87
15	2T	113/127 (89%)	111 (98%)	2 (2%)	59	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	91 (98%)	2 (2%)	52	83
16	2U	93/94 (99%)	91 (98%)	2 (2%)	52	83
17	1V	80/82 (98%)	74 (92%)	6 (8%)	13	37
17	2V	80/82 (98%)	76 (95%)	4 (5%)	24	56
18	1W	90/92 (98%)	87 (97%)	3 (3%)	38	72
18	2W	90/92 (98%)	85 (94%)	5 (6%)	21	51
19	1X	77/78 (99%)	77 (100%)	0	100	100
19	2X	77/78 (99%)	77 (100%)	0	100	100
20	1Y	85/91 (93%)	82 (96%)	3 (4%)	36	70
20	2Y	85/91 (93%)	83 (98%)	2 (2%)	49	81
21	1Z	135/179 (75%)	130 (96%)	5 (4%)	34	68
21	2Z	137/179 (76%)	134 (98%)	3 (2%)	52	83
22	10	65/67 (97%)	65 (100%)	0	100	100
22	20	65/67 (97%)	65 (100%)	0	100	100
23	11	80/83 (96%)	80 (100%)	0	100	100
23	21	80/83 (96%)	79 (99%)	1 (1%)	69	91
24	12	65/67 (97%)	65 (100%)	0	100	100
24	22	65/67 (97%)	65 (100%)	0	100	100
25	13	51/52 (98%)	50 (98%)	1 (2%)	55	84
25	23	50/52 (96%)	50 (100%)	0	100	100
26	14	59/63 (94%)	57 (97%)	2 (3%)	37	71
26	24	53/63 (84%)	52 (98%)	1 (2%)	57	85
27	15	50/52 (96%)	47 (94%)	3 (6%)	19	48
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	48
28	16	51/52 (98%)	50 (98%)	1 (2%)	55	84
28	26	50/52 (96%)	49 (98%)	1 (2%)	55	84
29	17	41/42 (98%)	40 (98%)	1 (2%)	49	81
29	27	41/42 (98%)	39 (95%)	2 (5%)	25	57
30	18	54/55 (98%)	52 (96%)	2 (4%)	34	68
30	28	54/55 (98%)	51 (94%)	3 (6%)	21	51
31	19	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	190 (99%)	2 (1%)	76	93
33	2b	187/220 (85%)	185 (99%)	2 (1%)	73	92
34	1c	142/188 (76%)	141 (99%)	1 (1%)	84	95
34	2c	140/188 (74%)	139 (99%)	1 (1%)	84	95
35	1d	169/181 (93%)	161 (95%)	8 (5%)	26	59
35	2d	173/181 (96%)	169 (98%)	4 (2%)	50	82
36	1e	113/123 (92%)	109 (96%)	4 (4%)	36	70
36	2e	114/123 (93%)	111 (97%)	3 (3%)	46	79
37	1f	84/90 (93%)	84 (100%)	0	100	100
37	2f	85/90 (94%)	84 (99%)	1 (1%)	71	92
38	1g	119/127 (94%)	118 (99%)	1 (1%)	81	94
38	2g	120/127 (94%)	120 (100%)	0	100	100
39	1h	114/119 (96%)	112 (98%)	2 (2%)	59	86
39	2h	114/119 (96%)	113 (99%)	1 (1%)	78	94
40	1i	90/99 (91%)	89 (99%)	1 (1%)	73	92
40	2i	89/99 (90%)	86 (97%)	3 (3%)	37	71
41	1j	66/92 (72%)	66 (100%)	0	100	100
41	2j	69/92 (75%)	68 (99%)	1 (1%)	67	90
42	1k	82/99 (83%)	80 (98%)	2 (2%)	49	81
42	2k	83/99 (84%)	83 (100%)	0	100	100
43	1l	96/108 (89%)	95 (99%)	1 (1%)	76	93
43	2l	96/108 (89%)	96 (100%)	0	100	100
44	1m	93/101 (92%)	92 (99%)	1 (1%)	73	92
44	2m	92/101 (91%)	89 (97%)	3 (3%)	38	72
45	1n	49/50 (98%)	47 (96%)	2 (4%)	30	64
45	2n	49/50 (98%)	46 (94%)	3 (6%)	18	48
46	1o	78/80 (98%)	78 (100%)	0	100	100
46	2o	78/80 (98%)	78 (100%)	0	100	100
47	1p	69/74 (93%)	68 (99%)	1 (1%)	67	90
47	2p	68/74 (92%)	67 (98%)	1 (2%)	65	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	94 (100%)	0	100	100
48	2q	94/97 (97%)	92 (98%)	2 (2%)	53	84
49	1r	59/77 (77%)	57 (97%)	2 (3%)	37	71
49	2r	59/77 (77%)	59 (100%)	0	100	100
50	1s	69/80 (86%)	67 (97%)	2 (3%)	42	76
50	2s	67/80 (84%)	66 (98%)	1 (2%)	65	89
51	1t	70/82 (85%)	70 (100%)	0	100	100
51	2t	70/82 (85%)	70 (100%)	0	100	100
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9301/10064 (92%)	9088 (98%)	213 (2%)	50	82

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	106	ILE
3	1D	122	ASP
3	1D	229	VAL
3	1D	242	ARG
3	1D	257	LEU
4	1E	9	VAL
4	1E	12	THR
4	1E	21	VAL
4	1E	24	THR
4	1E	34	VAL
4	1E	75	VAL
4	1E	116	VAL
4	1E	181	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	106	ARG
5	1F	183	VAL
5	1F	192	LEU
6	1G	43	LEU
6	1G	159	VAL

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Mol	Chain	Res	Type
6	1G	175	LEU
7	1H	18	GLU
7	1H	71	LEU
7	1H	84	SER
8	1I	2	LYS
8	1I	38	LEU
8	1I	47	LEU
8	1I	92	VAL
8	1I	107	VAL
9	1N	28	THR
9	1N	62	VAL
9	1N	83	LYS
9	1N	99	LEU
10	1O	10	VAL
11	1P	95	VAL
11	1P	125	VAL
12	1Q	75	THR
13	1R	6	SER
13	1R	24	GLN
13	1R	29	LEU
13	1R	44	LEU
13	1R	100	LEU
13	1R	111	LEU
14	1S	69	VAL
15	1T	28	VAL
15	1T	96	ARG
16	1U	74	LEU
16	1U	95	LEU
17	1V	46	VAL
17	1V	52	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	79	VAL
17	1V	82	ARG
18	1W	17	VAL
18	1W	23	LEU
18	1W	107	LEU
20	1Y	11	ASP
20	1Y	43	ASN
20	1Y	90	LEU
21	1Z	33	LEU
21	1Z	42	VAL

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Mol	Chain	Res	Type
21	1Z	86	VAL
21	1Z	154	ASP
21	1Z	170	THR
25	13	54	VAL
26	14	50	VAL
26	14	56	VAL
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
28	16	48	VAL
29	17	47	ARG
30	18	29	LYS
30	18	31	HIS
33	1b	112	VAL
33	1b	223	ILE
34	1c	172	ARG
35	1d	10	ARG
35	1d	31	CYS
35	1d	49	ARG
35	1d	59	ARG
35	1d	91	SER
35	1d	135	LEU
35	1d	158	ILE
35	1d	194	LEU
36	1e	12	LEU
36	1e	31	LEU
36	1e	41	VAL
36	1e	149	GLU
38	1g	50	ILE
39	1h	69	ARG
39	1h	112	LEU
40	1i	64	THR
42	1k	31	THR
42	1k	114	VAL
43	1l	36	VAL
44	1m	19	LEU
45	1n	32	SER
45	1n	33	VAL
47	1p	2	VAL
49	1r	31	LEU
49	1r	54	ARG
50	1s	5	LEU

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Mol	Chain	Res	Type
50	1s	41	VAL
3	2D	94	LEU
3	2D	106	ILE
3	2D	142	VAL
3	2D	242	ARG
4	2E	9	VAL
4	2E	12	THR
4	2E	24	THR
4	2E	34	VAL
4	2E	52	LEU
4	2E	75	VAL
4	2E	116	VAL
4	2E	119	ARG
4	2E	170	LEU
4	2E	181	LEU
4	2E	195	LEU
5	2F	33	LEU
5	2F	70	THR
5	2F	74	ARG
5	2F	88	VAL
5	2F	106	ARG
5	2F	120	GLU
5	2F	158	THR
5	2F	183	VAL
5	2F	192	LEU
6	2G	43	LEU
6	2G	79	ASN
6	2G	135	LEU
6	2G	159	VAL
7	2H	71	LEU
7	2H	76	VAL
7	2H	88	LEU
8	2I	38	LEU
8	2I	92	VAL
9	2N	28	THR
9	2N	99	LEU
9	2N	140	VAL
10	2O	108	GLU
11	2P	95	VAL
11	2P	99	LEU
12	2Q	1	MET
12	2Q	21	THR

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Mol	Chain	Res	Type
12	2Q	75	THR
12	2Q	110	THR
13	2R	24	GLN
13	2R	29	LEU
13	2R	44	LEU
13	2R	65	LEU
13	2R	100	LEU
13	2R	111	LEU
14	2S	38	GLN
15	2T	96	ARG
15	2T	108	ARG
16	2U	74	LEU
16	2U	95	LEU
17	2V	51	VAL
17	2V	62	LEU
17	2V	79	VAL
17	2V	82	ARG
18	2W	17	VAL
18	2W	23	LEU
18	2W	67	ASP
18	2W	100	THR
18	2W	107	LEU
20	2Y	72	VAL
20	2Y	97	ARG
21	2Z	42	VAL
21	2Z	144	LEU
21	2Z	154	ASP
23	21	21	ARG
26	24	50	VAL
27	25	6	VAL
27	25	16	ARG
27	25	29	THR
28	26	48	VAL
29	27	1	MET
29	27	39	ARG
30	28	26	LYS
30	28	31	HIS
30	28	41	ILE
33	2b	11	LEU
33	2b	94	ASN
34	2c	70	VAL
35	2d	31	CYS

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Mol	Chain	Res	Type
35	2d	59	ARG
35	2d	135	LEU
35	2d	170	VAL
36	2e	12	LEU
36	2e	13	ILE
36	2e	41	VAL
37	2f	81	ILE
39	2h	23	SER
40	2i	64	THR
40	2i	65	VAL
40	2i	108	VAL
41	2j	72	VAL
44	2m	19	LEU
44	2m	47	ASP
44	2m	110	ARG
45	2n	22	THR
45	2n	33	VAL
45	2n	44	LEU
47	2p	2	VAL
48	2q	35	VAL
48	2q	83	ASP
50	2s	12	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	166	GLN
4	1E	48	GLN
4	1E	143	ASN
5	1F	69	HIS
6	1G	79	ASN
10	1O	3	GLN
13	1R	24	GLN
13	1R	91	GLN
16	1U	81	HIS
18	1W	60	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	32	HIS
21	1Z	73	GLN
23	11	56	GLN

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Mol	Chain	Res	Type
30	18	35	GLN
33	1b	40	HIS
33	1b	212	GLN
34	1c	6	HIS
34	1c	102	ASN
34	1c	162	GLN
34	1c	176	HIS
35	1d	77	ASN
35	1d	116	GLN
35	1d	119	GLN
35	1d	123	HIS
35	1d	125	HIS
36	1e	78	HIS
37	1f	73	ASN
37	1f	100	ASN
38	1g	28	ASN
39	1h	82	HIS
40	1i	3	GLN
40	1i	58	HIS
40	1i	89	ASN
40	1i	124	GLN
43	1l	99	HIS
47	1p	13	HIS
48	1q	26	GLN
49	1r	63	GLN
50	1s	69	HIS
50	1s	83	HIS
51	1t	16	HIS
51	1t	42	GLN
5	2F	69	HIS
8	2I	11	ASN
8	2I	105	HIS
11	2P	27	HIS
12	2Q	12	GLN
12	2Q	57	HIS
12	2Q	123	HIS
14	2S	38	GLN
17	2V	64	HIS
18	2W	60	ASN
19	2X	31	HIS
19	2X	82	GLN
20	2Y	6	HIS

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Mol	Chain	Res	Type
21	2Z	55	HIS
21	2Z	73	GLN
23	21	56	GLN
30	28	35	GLN
33	2b	19	HIS
33	2b	40	HIS
33	2b	140	HIS
33	2b	212	GLN
34	2c	98	ASN
35	2d	77	ASN
35	2d	116	GLN
35	2d	125	HIS
36	2e	78	HIS
37	2f	73	ASN
37	2f	100	ASN
38	2g	28	ASN
38	2g	148	ASN
39	2h	82	HIS
40	2i	3	GLN
40	2i	58	HIS
40	2i	89	ASN
40	2i	124	GLN
42	2k	22	HIS
43	2l	99	HIS
46	2o	28	GLN
49	2r	63	GLN
50	2s	47	HIS
50	2s	69	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	427 (14%)	30 (1%)
1	2A	2788/2915 (95%)	455 (16%)	22 (0%)
2	1B	120/121 (99%)	11 (9%)	1 (0%)
2	2B	118/121 (97%)	22 (18%)	0
32	1a	1494/1521 (98%)	217 (14%)	0
32	2a	1498/1521 (98%)	239 (15%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	2 (16%)	0
54	1w	71/76 (93%)	21 (29%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	1y	71/76 (93%)	20 (28%)	0
54	2w	68/76 (89%)	18 (26%)	0
54	2y	69/76 (90%)	22 (31%)	0
55	1x	75/77 (97%)	12 (16%)	0
55	2x	75/77 (97%)	12 (16%)	0
All	All	9332/9620 (97%)	1480 (15%)	53 (0%)

All (1480) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	17	G
1	1A	34	C
1	1A	45	C
1	1A	70	A
1	1A	71	U
1	1A	73	A
1	1A	74	G
1	1A	83	A
1	1A	94	G
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	123	G
1	1A	185	A
1	1A	186	A
1	1A	188	A
1	1A	194	G
1	1A	203	G
1	1A	204	G
1	1A	205	A
1	1A	211	A
1	1A	214	A
1	1A	217	A
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	250	G
1	1A	271	U
1	1A	272	U
1	1A	273	G
1	1A	274	U

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Mol	Chain	Res	Type
1	1A	275	C
1	1A	288	U
1	1A	289	G
1	1A	303	C
1	1A	335	A
1	1A	353	G
1	1A	354	A
1	1A	370	A
1	1A	376	G
1	1A	387	G
1	1A	388	A
1	1A	389	G
1	1A	399	G
1	1A	413	G
1	1A	423	G
1	1A	432	U
1	1A	438	G
1	1A	455	A
1	1A	470	C
1	1A	474	U
1	1A	480	A
1	1A	482	C
1	1A	483	A
1	1A	507	G
1	1A	526	A
1	1A	529	U
1	1A	530	A
1	1A	534	C
1	1A	537	G
1	1A	555	G
1	1A	556	C
1	1A	557	A
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	586	G
1	1A	596	G
1	1A	598	A
1	1A	615	G
1	1A	618	C
1	1A	626	A
1	1A	627	G

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Mol	Chain	Res	Type
1	1A	630	U
1	1A	639	G
1	1A	640	A
1	1A	641	G
1	1A	648	G
1	1A	652	A
1	1A	662	A
1	1A	671	A
1	1A	693	G
1	1A	697	C
1	1A	716	G
1	1A	733	G
1	1A	764	G
1	1A	777	C
1	1A	811	A
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	831	A
1	1A	832	G
1	1A	837	C
1	1A	839	G
1	1A	852	G
1	1A	858	U
1	1A	859	C
1	1A	866	A
1	1A	874	U
1	1A	875	U
1	1A	906	G
1	1A	913	A
1	1A	926	G
1	1A	927	G
1	1A	931	C
1	1A	932	C
1	1A	933	C
1	1A	934	A
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	938	G
1	1A	941	U
1	1A	942	A

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Mol	Chain	Res	Type
1	1A	943	C
1	1A	944	C
1	1A	956	A
1	1A	977	G
1	1A	990	A
1	1A	991	G
1	1A	1004	A
1	1A	1006	C
1	1A	1008	U
1	1A	1019	G
1	1A	1020	C
1	1A	1029	A
1	1A	1042	A
1	1A	1058	U
1	1A	1059	C
1	1A	1063	G
1	1A	1068	G
1	1A	1071	G
1	1A	1072	U
1	1A	1073	A
1	1A	1079	U
1	1A	1084	C
1	1A	1087	C
1	1A	1091	A
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1100	A
1	1A	1101	G
1	1A	1103	A
1	1A	1104	G
1	1A	1112	U
1	1A	1114	G
1	1A	1117	G
1	1A	1119	A
1	1A	1120	G
1	1A	1121	C
1	1A	1122	C
1	1A	1124	U
1	1A	1125	C
1	1A	1127	U
1	1A	1130	A

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Mol	Chain	Res	Type
1	1A	1132	A
1	1A	1134	A
1	1A	1135	G
1	1A	1136	U
1	1A	1137	G
1	1A	1139	G
1	1A	1140	U
1	1A	1142	A
1	1A	1144	A
1	1A	1146	C
1	1A	1147	U
1	1A	1149	A
1	1A	1153	G
1	1A	1156	G
1	1A	1157	A
1	1A	1158	G
1	1A	1161	G
1	1A	1162	C
1	1A	1174	A
1	1A	1176	U
1	1A	1180	C
1	1A	1181	G
1	1A	1201	A
1	1A	1216	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1222	A
1	1A	1223	C
1	1A	1256	U
1	1A	1263	C
1	1A	1282	G
1	1A	1296	G
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1319	U
1	1A	1346	U
1	1A	1347	A
1	1A	1349	G

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Mol	Chain	Res	Type
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1416	C
1	1A	1426	G
1	1A	1430	A
1	1A	1431	G
1	1A	1432	C
1	1A	1462	G
1	1A	1463	C
1	1A	1465	A
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1491	A
1	1A	1497	G
1	1A	1502	G
1	1A	1514	C
1	1A	1529	G
1	1A	1539	C
1	1A	1540	A
1	1A	1555	C
1	1A	1556	A
1	1A	1605	A
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1627	A
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1655	A
1	1A	1656	A
1	1A	1694	G
1	1A	1695	C
1	1A	1701	A
1	1A	1711	A
1	1A	1721	G
1	1A	1743	G
1	1A	1747	A
1	1A	1748	A

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Mol	Chain	Res	Type
1	1A	1767	A
1	1A	1768	U
1	1A	1787	G
1	1A	1793	A
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1811	A
1	1A	1813	C
1	1A	1817	A
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1847	G
1	1A	1860	A
1	1A	1870	G
1	1A	1878	A
1	1A	1879	A
1	1A	1899	A
1	1A	1900	G
1	1A	1911	A
1	1A	1922	A
1	1A	1928	G
1	1A	1951	G
1	1A	1952	G
1	1A	1959	A
1	1A	1960	A
1	1A	1977	U
1	1A	1984	5MC
1	1A	1985	U
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2003	A
1	1A	2014	G
1	1A	2015	U
1	1A	2019	G
1	1A	2045	G
1	1A	2053	A
1	1A	2054	G
1	1A	2055	A

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Mol	Chain	Res	Type
1	1A	2061	C
1	1A	2065	C
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2084	A
1	1A	2091	G
1	1A	2132	G
1	1A	2134	G
1	1A	2135	U
1	1A	2136	A
1	1A	2141	A
1	1A	2143	G
1	1A	2148	A
1	1A	2149	G
1	1A	2151	C
1	1A	2152	U
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2157	A
1	1A	2158	C
1	1A	2162	C
1	1A	2164	C
1	1A	2165	C
1	1A	2166	U
1	1A	2168	C
1	1A	2169	G
1	1A	2170	G
1	1A	2172	U
1	1A	2173	G
1	1A	2177	G
1	1A	2178	G
1	1A	2179	G
1	1A	2180	A
1	1A	2181	G
1	1A	2184	G
1	1A	2187	G
1	1A	2188	G
1	1A	2190	G

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Mol	Chain	Res	Type
1	1A	2193	A
1	1A	2194	U
1	1A	2200	C
1	1A	2203	G
1	1A	2204	G
1	1A	2206	G
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A
1	1A	2230	U
1	1A	2237	A
1	1A	2247	G
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2285	A
1	1A	2292	G
1	1A	2295	C
1	1A	2299	A
1	1A	2317	A
1	1A	2320	G
1	1A	2332	A
1	1A	2337	G
1	1A	2346	G
1	1A	2348	A
1	1A	2359	C
1	1A	2366	G
1	1A	2373	A
1	1A	2395	G
1	1A	2397	C
1	1A	2418	U
1	1A	2437	A
1	1A	2441	G
1	1A	2442	A
1	1A	2443	U
1	1A	2446	A
1	1A	2447	A
1	1A	2451	A
1	1A	2453	C

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Mol	Chain	Res	Type
1	1A	2460	A
1	1A	2486	C
1	1A	2488	A
1	1A	2490	A
1	1A	2514	G
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2541	G
1	1A	2547	G
1	1A	2561	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2585	C
1	1A	2586	G
1	1A	2594	G
1	1A	2614	A
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2641	A
1	1A	2642	G
1	1A	2666	A
1	1A	2691	A
1	1A	2701	U
1	1A	2702	C
1	1A	2703	C
1	1A	2714	U
1	1A	2715	C
1	1A	2719	G
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2745	G
1	1A	2746	A
1	1A	2757	G
1	1A	2770	A
1	1A	2771	A
1	1A	2777	A
1	1A	2778	A

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Mol	Chain	Res	Type
1	1A	2779	G
1	1A	2791	A
1	1A	2803	A
1	1A	2804	C
1	1A	2806	G
1	1A	2813	G
1	1A	2814	C
1	1A	2818	U
1	1A	2830	A
1	1A	2831	A
1	1A	2843	G
1	1A	2845	A
1	1A	2882	G
1	1A	2890	C
1	1A	2901	A
1	1A	2903	G
1	1A	2904	U
2	1B	2	C
2	1B	9	G
2	1B	13	A
2	1B	30	C
2	1B	35	U
2	1B	42	C
2	1B	52	A
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	54	C
32	1a	61	G
32	1a	65	U
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A

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Mol	Chain	Res	Type
32	1a	116	A
32	1a	120	A
32	1a	121	C
32	1a	131	C
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(D)	C
32	1a	189(G)	G
32	1a	189(H)	G
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	421	U
32	1a	424	G
32	1a	429	U
32	1a	439	A

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Mol	Chain	Res	Type
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	531	U
32	1a	532	A
32	1a	533	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	562	C
32	1a	564	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	630	G
32	1a	631	G
32	1a	653	A
32	1a	665	A
32	1a	671	G
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	703	G
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	755	G
32	1a	766	A
32	1a	777	A

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Mol	Chain	Res	Type
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	853	G
32	1a	859	A
32	1a	870	U
32	1a	874	G
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	932	C
32	1a	934	C
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	967	5MC
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1001(A)	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1011	G

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Mol	Chain	Res	Type
32	1a	1020	U
32	1a	1022	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1029	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1039	C
32	1a	1044	A
32	1a	1054	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1123	A
32	1a	1125	U
32	1a	1133	G
32	1a	1134	G
32	1a	1137	C
32	1a	1139	G
32	1a	1140	C
32	1a	1141	C
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1172	C
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U

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Mol	Chain	Res	Type
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
53	1v	14	A
54	1w	2	C
54	1w	3	C
54	1w	6	G
54	1w	7	A
54	1w	8	4SU

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Mol	Chain	Res	Type
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	24	G
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	62	C
54	1w	64	A
54	1w	67	C
54	1w	68	C
54	1w	70	G
54	1w	73	A
54	1w	74	C
55	1x	6	G
55	1x	9	G
55	1x	14	A
55	1x	18	G
55	1x	19	G
55	1x	21	A
55	1x	47	U
55	1x	49	G
55	1x	61	C
55	1x	64	G
55	1x	69	C
55	1x	76	A
54	1y	5	G
54	1y	6	G
54	1y	8	4SU
54	1y	13	C
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	35	A
54	1y	44	G
54	1y	45	U
54	1y	46	7MG
54	1y	47	U
54	1y	48	C
54	1y	54	5MU

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Mol	Chain	Res	Type
54	1y	56	C
54	1y	59	U
54	1y	61	C
54	1y	64	A
54	1y	65	G
54	1y	70	G
1	2A	11	G
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	36	G
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	78	A
1	2A	84	A
1	2A	90	U
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	104	U
1	2A	118	A
1	2A	120	U
1	2A	154(A)	C
1	2A	157	U
1	2A	172	C
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	204	A
1	2A	205	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
1	2A	248	G
1	2A	249	C

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Mol	Chain	Res	Type
1	2A	250	G
1	2A	266	G
1	2A	267	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	274	G
1	2A	277	C
1	2A	278	A
1	2A	279	C
1	2A	294	A
1	2A	311	A
1	2A	312	G
1	2A	317	G
1	2A	323	G
1	2A	329	G
1	2A	330	A
1	2A	338	G
1	2A	342	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	396	G
1	2A	406	G
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	422	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	498	G
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C

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Mol	Chain	Res	Type
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	551	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	753	C
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	783	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U

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Mol	Chain	Res	Type
1	2A	828	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	874	G
1	2A	877	U
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	892	G
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
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	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1022	G

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Mol	Chain	Res	Type
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1113	U
1	2A	1116	C
1	2A	1119	C
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1143	A
1	2A	1144	G
1	2A	1152	C
1	2A	1169	G
1	2A	1171	G
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1237	A
1	2A	1247	A
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	1313	U
1	2A	1314	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1373	A
1	2A	1378	A
1	2A	1379	A

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Mol	Chain	Res	Type
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1411	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1436	G
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1514	U
1	2A	1531	C
1	2A	1532	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1582	C
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C

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Mol	Chain	Res	Type
1	2A	1648	C
1	2A	1654	A
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1722	A
1	2A	1746	G
1	2A	1756	G
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	1829	A
1	2A	1835	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	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1955	U
1	2A	1963	U
1	2A	1965	C
1	2A	1966	A
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1997	G

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Mol	Chain	Res	Type
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2036	C
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2096	U
1	2A	2099	U
1	2A	2107	C
1	2A	2108	C
1	2A	2110	G
1	2A	2111	C
1	2A	2116	G
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2134	A
1	2A	2135	A
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2141	G
1	2A	2143	C
1	2A	2146	C
1	2A	2150	U
1	2A	2151	G
1	2A	2153	G
1	2A	2155	G
1	2A	2156	G

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Mol	Chain	Res	Type
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2162	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2174	C
1	2A	2178	C
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A
1	2A	2312	U
1	2A	2320	A
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2346	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C

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Mol	Chain	Res	Type
1	2A	2388	A
1	2A	2402	C
1	2A	2403	C
1	2A	2406	U
1	2A	2410	G
1	2A	2424	C
1	2A	2425	A
1	2A	2428	G
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	2468	G
1	2A	2469	A
1	2A	2476	A
1	2A	2478	A
1	2A	2490	G
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2554	U
1	2A	2555	U
1	2A	2562	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2582	G
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G

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Mol	Chain	Res	Type
1	2A	2638	G
1	2A	2646	C
1	2A	2654	A
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2739	U
1	2A	2750	A
1	2A	2751	G
1	2A	2757	A
1	2A	2758	A
1	2A	2759	G
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	2803	C
1	2A	2807	G
1	2A	2808	U
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2872	G
1	2A	2879	C
1	2A	2880	C
1	2A	2889	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C

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Mol	Chain	Res	Type
2	2B	5	C
2	2B	12	C
2	2B	13	A
2	2B	19	G
2	2B	20	C
2	2B	24	G
2	2B	34	U
2	2B	42	C
2	2B	53	A
2	2B	56	G
2	2B	66	A
2	2B	67	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	91	C
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	120	A
32	2a	7	G
32	2a	8	A
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	66	G
32	2a	73	G
32	2a	88	A
32	2a	89	C
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	163	C
32	2a	174	C

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Mol	Chain	Res	Type
32	2a	182	U
32	2a	189(J)	G
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	301	G
32	2a	316	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	424	G
32	2a	429	U
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A

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Mol	Chain	Res	Type
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
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	653	A
32	2a	665	A
32	2a	671	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	703	G
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	774	G
32	2a	777	A
32	2a	787	A
32	2a	790	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	834	C
32	2a	840	C

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Mol	Chain	Res	Type
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	873	A
32	2a	885	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	932	C
32	2a	934	C
32	2a	935	A
32	2a	960	U
32	2a	961	U
32	2a	966	M2G
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	982	U
32	2a	992	U
32	2a	993	G
32	2a	997	U
32	2a	999	C
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1029	C

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Mol	Chain	Res	Type
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1033	G
32	2a	1035	A
32	2a	1036	G
32	2a	1039	C
32	2a	1040	U
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1117	G
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1131	G
32	2a	1132	C
32	2a	1133	G
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1172	C
32	2a	1173	G
32	2a	1174	G
32	2a	1182	G
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1211	U

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Mol	Chain	Res	Type
32	2a	1212	U
32	2a	1213	A
32	2a	1214	C
32	2a	1226	C
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1246	C
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1275	A
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1299	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1320	C
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1370	G
32	2a	1379	G
32	2a	1398	A
32	2a	1400	5MC
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C
32	2a	1492	A
32	2a	1494	G
32	2a	1499	A

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Mol	Chain	Res	Type
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1532	U
53	2v	13	A
53	2v	14	A
54	2w	3	C
54	2w	4	C
54	2w	7	A
54	2w	8	4SU
54	2w	13	C
54	2w	19	G
54	2w	22	G
54	2w	25	C
54	2w	34	G
54	2w	46	7MG
54	2w	48	C
54	2w	59	U
54	2w	62	C
54	2w	64	A
54	2w	65	G
54	2w	68	C
54	2w	69	G
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	20	U
55	2x	21	A
55	2x	46	G
55	2x	47	U
55	2x	48	C
55	2x	56	C
55	2x	67	C
55	2x	68	C
55	2x	76	A
54	2y	15	G
54	2y	19	G

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Mol	Chain	Res	Type
54	2y	23	A
54	2y	30	G
54	2y	34	G
54	2y	45	U
54	2y	46	7MG
54	2y	49	C
54	2y	52	G
54	2y	53	G
54	2y	55	PSU
54	2y	56	C
54	2y	57	G
54	2y	58	A
54	2y	59	U
54	2y	60	U
54	2y	61	C
54	2y	65	G
54	2y	67	C
54	2y	69	G
54	2y	70	G
54	2y	73	A

All (53) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	115	G
1	1A	185	A
1	1A	271	U
1	1A	302	A
1	1A	509	A
1	1A	572	A
1	1A	732	A
1	1A	811	A
1	1A	913	A
1	1A	941	U
1	1A	1067	A
1	1A	1093	G
1	1A	1136	U
1	1A	1143	U
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G

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Mol	Chain	Res	Type
1	1A	1255	A
1	1A	1425	A
1	1A	1554	A
1	1A	1700	G
1	1A	2014	G
1	1A	2156	A
1	1A	2203	G
1	1A	2205	C
1	1A	2442	A
1	1A	2641	A
1	1A	2701	U
1	1A	2769	U
2	1B	1	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2406	U
1	2A	2689	U
1	2A	2756	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	PSU	2y	55	54	17,21,22	1.57	2 (11%)	20,30,33	3.15	6 (30%)
54	4SU	1y	8	54	14,21,22	1.17	1 (7%)	15,30,33	1.70	2 (13%)
1	PSU	1A	1939	1	17,21,22	1.42	2 (11%)	20,30,33	3.00	6 (30%)
32	M2G	2a	966	32	20,27,28	1.38	3 (15%)	22,40,43	2.08	6 (27%)
1	5MC	2A	1942	1	15,22,23	1.33	1 (6%)	19,32,35	1.31	2 (10%)
32	UR3	1a	1498	32	14,22,23	0.83	1 (7%)	15,32,35	0.72	0
54	PSU	1w	39	54	17,21,22	1.55	3 (17%)	20,30,33	2.91	5 (25%)
1	2MA	2A	2503	1,56	17,25,26	1.21	2 (11%)	19,37,40	1.95	3 (15%)
32	4OC	2a	1402	32	16,23,24	0.70	0	17,32,35	1.40	1 (5%)
1	5MC	1A	1964	1	15,22,23	1.25	1 (6%)	19,32,35	1.45	4 (21%)
1	5MC	1A	1984	1	15,22,23	1.25	1 (6%)	19,32,35	1.35	3 (15%)
32	5MC	2a	1407	32,56	15,22,23	1.31	1 (6%)	19,32,35	1.42	3 (15%)
32	5MC	1a	1407	32	15,22,23	1.23	1 (6%)	19,32,35	1.31	3 (15%)
1	PSU	2A	1911	1	17,21,22	1.72	2 (11%)	20,30,33	3.21	6 (30%)
55	5MC	2x	32	55	15,22,23	1.24	1 (6%)	19,32,35	1.41	3 (15%)
32	7MG	2a	527	32,56	22,26,27	1.77	4 (18%)	28,39,42	2.73	9 (32%)
1	PSU	1A	1933	1	17,21,22	1.44	2 (11%)	20,30,33	3.12	5 (25%)
54	PSU	2w	39	54	17,21,22	1.36	2 (11%)	20,30,33	3.43	6 (30%)
54	5MU	1w	54	54	15,22,23	1.08	1 (6%)	16,32,35	1.97	1 (6%)
55	PSU	2x	55	55	17,21,22	1.59	2 (11%)	20,30,33	3.12	6 (30%)
32	5MC	2a	1400	32	15,22,23	1.33	1 (6%)	19,32,35	1.44	3 (15%)
32	M2G	1a	966	32	20,27,28	1.44	3 (15%)	22,40,43	2.19	5 (22%)
32	PSU	1a	516	32	17,21,22	1.65	5 (29%)	20,30,33	3.00	6 (30%)
32	MA6	2a	1519	32	19,26,27	0.98	1 (5%)	18,38,41	1.60	4 (22%)
54	PSU	1y	39	54	17,21,22	1.47	3 (17%)	20,30,33	3.24	5 (25%)
1	PSU	2A	1917	1	17,21,22	1.52	2 (11%)	20,30,33	3.17	6 (30%)
1	5MU	2A	1939	1,56	15,22,23	1.05	1 (6%)	16,32,35	1.84	2 (12%)
1	2MU	2A	2552	1,56	14,22,24	0.91	0	14,31,36	0.96	2 (14%)
1	5MU	2A	1915	1	15,22,23	1.03	1 (6%)	16,32,35	1.90	2 (12%)
55	4SU	1x	8	55	14,21,22	1.46	2 (14%)	15,30,33	2.73	2 (13%)
32	UR3	2a	1498	32	14,22,23	0.84	1 (7%)	15,32,35	0.74	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	5MU	2w	54	54	15,22,23	1.10	1 (6%)	16,32,35	1.90	2 (12%)
54	MIA	1w	37	54	24,31,32	2.27	3 (12%)	26,44,47	2.50	9 (34%)
1	2MA	1A	2515	1,56	17,25,26	1.20	2 (11%)	19,37,40	2.12	3 (15%)
32	7MG	1a	527	32	22,26,27	1.78	4 (18%)	28,39,42	2.69	10 (35%)
54	MIA	2y	37	54	18,24,32	1.16	2 (11%)	18,35,47	1.36	3 (16%)
54	4SU	2y	8	54	14,21,22	1.32	1 (7%)	15,30,33	1.34	2 (13%)
55	PSU	1x	55	55,56	17,21,22	1.51	2 (11%)	20,30,33	3.27	6 (30%)
32	5MC	1a	1404	32	15,22,23	1.39	1 (6%)	19,32,35	1.34	2 (10%)
1	4OC	2A	1920	1	15,22,24	0.66	0	17,31,35	1.44	2 (11%)
32	2MG	2a	1207	32,56	19,26,27	1.20	2 (10%)	21,38,41	2.40	8 (38%)
54	7MG	2y	46	54	22,26,27	1.85	3 (13%)	28,39,42	3.04	9 (32%)
43	0TD	1l	92	43	4,9,10	3.27	1 (25%)	3,11,13	2.64	1 (33%)
32	MA6	1a	1519	32	19,26,27	1.04	1 (5%)	18,38,41	1.63	4 (22%)
32	5MC	2a	967	32	15,22,23	1.37	1 (6%)	19,32,35	1.30	3 (15%)
54	7MG	1y	46	54	22,26,27	1.89	4 (18%)	28,39,42	3.05	11 (39%)
32	PSU	2a	516	32	17,21,22	1.48	3 (17%)	20,30,33	3.17	7 (35%)
32	5MC	1a	1400	32	15,22,23	1.24	1 (6%)	19,32,35	1.50	4 (21%)
1	5MU	1A	1937	1	15,22,23	1.09	1 (6%)	16,32,35	1.71	2 (12%)
54	4SU	2w	8	54	14,21,22	1.25	1 (7%)	15,30,33	1.23	2 (13%)
54	PSU	1w	32	54	17,21,22	1.50	2 (11%)	20,30,33	3.22	6 (30%)
54	PSU	1y	32	54	17,21,22	1.49	2 (11%)	20,30,33	3.23	6 (30%)
1	5MC	2A	1962	1,56	15,22,23	1.30	1 (6%)	19,32,35	1.43	3 (15%)
54	PSU	2w	55	54	17,21,22	1.42	2 (11%)	20,30,33	3.21	6 (30%)
1	5MU	1A	1961	1,56	15,22,23	1.01	1 (6%)	16,32,35	1.92	2 (12%)
54	MIA	1y	37	54	18,24,32	1.14	2 (11%)	18,35,47	1.26	2 (11%)
32	4OC	1a	1402	32	16,23,24	0.75	0	17,32,35	1.21	1 (5%)
54	PSU	2y	39	54	17,21,22	1.51	2 (11%)	20,30,33	3.54	6 (30%)
32	MA6	2a	1518	32	19,26,27	1.02	1 (5%)	18,38,41	1.65	4 (22%)
54	MIA	2w	37	54	20,27,32	1.78	3 (15%)	22,39,47	1.86	7 (31%)
54	4SU	1w	8	54	14,21,22	1.35	2 (14%)	15,30,33	1.44	2 (13%)
54	5MU	1y	54	54	15,22,23	1.21	2 (13%)	16,32,35	2.12	2 (12%)
54	PSU	1w	55	54	17,21,22	1.47	2 (11%)	20,30,33	3.33	6 (30%)
32	MA6	1a	1518	32	19,26,27	1.02	1 (5%)	18,38,41	1.67	5 (27%)
54	7MG	1w	46	54	22,26,27	1.76	4 (18%)	28,39,42	2.78	8 (28%)
55	4SU	2x	8	55,56	14,21,22	1.41	2 (14%)	15,30,33	2.22	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	2MG	1a	1207	32	19,26,27	1.25	2 (10%)	21,38,41	2.51	9 (42%)
54	PSU	2y	32	54	17,21,22	1.45	2 (11%)	20,30,33	3.17	6 (30%)
1	OMG	2A	2251	1,55,56	18,26,27	1.21	2 (11%)	20,38,41	1.99	6 (30%)
55	5MU	1x	54	55	15,22,23	1.11	1 (6%)	16,32,35	1.97	1 (6%)
54	7MG	2w	46	54	22,26,27	1.79	4 (18%)	28,39,42	2.75	9 (32%)
54	5MU	2y	54	54	15,22,23	1.05	1 (6%)	16,32,35	1.74	1 (6%)
54	PSU	1y	55	54	17,21,22	1.50	3 (17%)	20,30,33	3.17	5 (25%)
32	5MC	1a	967	32	15,22,23	1.24	1 (6%)	19,32,35	1.29	2 (10%)
55	5MC	1x	32	55	15,22,23	1.25	1 (6%)	19,32,35	1.53	4 (21%)
1	4OC	1A	1942	1	15,22,24	0.76	0	17,31,35	1.65	2 (11%)
1	PSU	2A	2605	1	17,21,22	1.54	3 (17%)	20,30,33	3.11	6 (30%)
1	PSU	1A	2617	1,56	17,21,22	1.76	5 (29%)	20,30,33	3.04	6 (30%)
55	5MU	2x	54	55	15,22,23	1.07	1 (6%)	16,32,35	1.72	2 (12%)
1	2MU	1A	2564	1,56	14,22,24	0.99	1 (7%)	14,31,36	0.85	1 (7%)
1	OMG	1A	2263	1,55,56	18,26,27	1.21	2 (11%)	20,38,41	2.18	6 (30%)
43	0TD	2l	92	43	4,9,10	3.16	1 (25%)	3,11,13	5.17	1 (33%)
32	5MC	2a	1404	32	15,22,23	1.36	1 (6%)	19,32,35	1.38	3 (15%)
54	PSU	2w	32	54	17,21,22	1.48	2 (11%)	20,30,33	3.20	5 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	2y	55	54	-	6/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	4/5/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	1/3/25/26	0/3/3/3
32	4OC	2a	1402	32	-	3/9/29/30	0/2/2/2
1	5MC	1A	1964	1	-	0/5/25/26	0/2/2/2
1	5MC	1A	1984	1	-	2/5/25/26	0/2/2/2
32	5MC	2a	1407	32,56	-	0/5/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/5/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	3/7/37/38	0/3/3/3
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/5/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	0/5/25/26	0/2/2/2
1	2MU	2A	2552	1,56	-	1/7/27/28	0/2/2/2
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/5/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/5/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/5/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/11/33/34	0/3/3/3
1	2MA	1A	2515	1,56	-	1/3/25/26	0/3/3/3
32	7MG	1a	527	32	-	3/7/37/38	0/3/3/3
54	MIA	2y	37	54	-	2/3/25/34	0/3/3/3
54	4SU	2y	8	54	-	0/5/25/26	0/2/2/2
55	PSU	1x	55	55,56	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/7/27/30	0/2/2/2
32	2MG	2a	1207	32,56	-	0/5/27/28	0/3/3/3
54	7MG	2y	46	54	-	3/7/37/38	0/3/3/3
43	0TD	1l	92	43	-	2/3/12/14	-
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
32	5MC	2a	967	32	-	0/5/25/26	0/2/2/2
54	7MG	1y	46	54	-	4/7/37/38	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/5/25/26	0/2/2/2
1	5MU	1A	1937	1	-	2/5/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/5/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	2A	1962	1,56	-	2/5/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1961	1,56	-	0/5/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	3/7/29/30	0/3/3/3
54	MIA	2w	37	54	-	1/7/29/34	0/3/3/3
54	4SU	1w	8	54	-	0/5/25/26	0/2/2/2
54	5MU	1y	54	54	-	4/5/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	1/7/29/30	0/3/3/3
54	7MG	1w	46	54	-	2/7/37/38	0/3/3/3
55	4SU	2x	8	55,56	-	0/5/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55,56	-	0/5/27/28	0/3/3/3
55	5MU	1x	54	55	-	0/5/25/26	0/2/2/2
54	7MG	2w	46	54	-	4/7/37/38	0/3/3/3
54	5MU	2y	54	54	-	2/5/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	2/5/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/5/25/26	0/2/2/2
1	4OC	1A	1942	1	-	0/7/27/30	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2617	1,56	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/5/25/26	0/2/2/2
1	2MU	1A	2564	1,56	-	0/7/27/28	0/2/2/2
1	OMG	1A	2263	1,55,56	-	0/5/27/28	0/3/3/3
43	0TD	2l	92	43	-	1/3/12/14	-
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
54	PSU	2w	32	54	-	1/7/25/26	0/2/2/2

All (149) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	37	MIA	C13-C14	7.28	1.53	1.32
54	1w	37	MIA	C2-S10	-6.91	1.69	1.75
54	2w	37	MIA	C2-S10	-6.61	1.70	1.75
43	1l	92	0TD	CB-SB	-6.16	1.69	1.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-6.06	1.69	1.84
1	2A	1911	PSU	C5-C1'	-5.34	1.47	1.52
1	1A	2617	PSU	C5-C1'	-5.21	1.47	1.52
32	2a	527	7MG	C6-C5	5.19	1.48	1.41
54	2w	46	7MG	C6-C5	5.07	1.48	1.41
54	1y	46	7MG	C5-C4	5.01	1.49	1.39
54	1y	46	7MG	C6-C5	4.97	1.48	1.41
32	2a	967	5MC	C5-C4	4.95	1.49	1.41
32	1a	527	7MG	C6-C5	4.91	1.48	1.41
32	2a	1404	5MC	C5-C4	4.91	1.49	1.41
54	2y	46	7MG	C6-C5	4.86	1.48	1.41
1	2A	1942	5MC	C5-C4	4.83	1.48	1.41
54	2y	46	7MG	C5-C4	4.80	1.48	1.39
32	1a	1404	5MC	C5-C4	4.75	1.48	1.41
54	1w	46	7MG	C6-C5	4.71	1.47	1.41
32	2a	1400	5MC	C5-C4	4.57	1.48	1.41
32	2a	1407	5MC	C5-C4	4.54	1.48	1.41
54	1w	46	7MG	C5-C4	4.53	1.48	1.39
55	2x	55	PSU	C5-C1'	-4.52	1.48	1.52
1	2A	1962	5MC	C5-C4	4.52	1.48	1.41
54	2w	46	7MG	C5-C4	4.49	1.48	1.39
32	1a	527	7MG	C5-C4	4.47	1.47	1.39
55	2x	32	5MC	C5-C4	4.47	1.48	1.41
1	1A	1984	5MC	C5-C4	4.43	1.48	1.41
32	1a	1207	2MG	C6-C5	4.39	1.48	1.41
32	1a	967	5MC	C5-C4	4.37	1.48	1.41
32	1a	1400	5MC	C5-C4	4.35	1.48	1.41
1	1A	1964	5MC	C5-C4	4.33	1.48	1.41
55	1x	32	5MC	C5-C4	4.26	1.48	1.41
32	1a	516	PSU	C5-C1'	-4.25	1.48	1.52
32	2a	966	M2G	C6-C5	4.25	1.48	1.41
32	1a	966	M2G	C6-C5	4.22	1.48	1.41
54	1w	39	PSU	C5-C1'	-4.22	1.48	1.52
54	2y	8	4SU	C4-S4	-4.22	1.59	1.67
32	2a	527	7MG	C5-C4	4.22	1.47	1.39
54	1w	8	4SU	C4-S4	-4.21	1.59	1.67
32	2a	1207	2MG	C6-C5	4.19	1.48	1.41
32	1a	1407	5MC	C5-C4	4.18	1.47	1.41
55	2x	8	4SU	C4-S4	-4.16	1.59	1.67
54	2y	39	PSU	C5-C1'	-4.12	1.48	1.52
54	2y	55	PSU	C5-C1'	-4.11	1.48	1.52
1	1A	2263	OMG	C6-C5	4.06	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2515	2MA	C6-C5	4.05	1.47	1.41
1	2A	2605	PSU	C5-C1'	-4.05	1.48	1.52
1	2A	2251	OMG	C6-C5	4.02	1.48	1.41
55	1x	55	PSU	C5-C1'	-3.99	1.48	1.52
54	2w	32	PSU	C4-C5	3.95	1.49	1.41
1	2A	2503	2MA	C6-C5	3.93	1.47	1.41
1	2A	1917	PSU	C5-C1'	-3.92	1.48	1.52
54	2w	8	4SU	C4-S4	-3.88	1.60	1.67
54	1y	54	5MU	C4-C5	3.86	1.49	1.41
32	2a	516	PSU	C5-C1'	-3.86	1.49	1.52
54	1w	32	PSU	C5-C1'	-3.82	1.49	1.52
54	1w	55	PSU	C4-C5	3.81	1.49	1.41
54	1y	32	PSU	C5-C1'	-3.76	1.49	1.52
55	1x	8	4SU	C4-S4	-3.74	1.60	1.67
55	1x	8	4SU	C2-N3	-3.62	1.31	1.38
32	1a	966	M2G	C2-N2	3.61	1.40	1.34
54	1y	55	PSU	C5-C1'	-3.61	1.49	1.52
54	1y	32	PSU	C4-C5	3.58	1.49	1.41
54	2w	55	PSU	C4-C5	3.58	1.49	1.41
32	1a	516	PSU	C4-C5	3.57	1.49	1.41
54	1y	55	PSU	C4-C5	3.56	1.49	1.41
1	1A	1933	PSU	C4-C5	3.55	1.49	1.41
54	2y	55	PSU	C4-C5	3.55	1.49	1.41
54	1y	39	PSU	C4-C5	3.54	1.49	1.41
54	1y	8	4SU	C4-S4	-3.54	1.61	1.67
54	2y	32	PSU	C4-C5	3.53	1.49	1.41
54	1y	46	7MG	C5-N7	-3.53	1.33	1.39
54	2w	54	5MU	C4-C5	3.52	1.49	1.41
54	2y	46	7MG	C5-N7	-3.50	1.33	1.39
54	2y	54	5MU	C4-C5	3.46	1.48	1.41
1	2A	1917	PSU	C4-C5	3.46	1.48	1.41
1	1A	1937	5MU	C4-C5	3.45	1.48	1.41
54	2y	32	PSU	C5-C1'	-3.45	1.49	1.52
54	1w	32	PSU	C4-C5	3.44	1.48	1.41
54	1w	46	7MG	C5-N7	-3.42	1.34	1.39
55	2x	55	PSU	C4-C5	3.42	1.48	1.41
54	1y	39	PSU	C5-C1'	-3.41	1.49	1.52
55	1x	54	5MU	C4-C5	3.41	1.48	1.41
32	1a	527	7MG	C5-N7	-3.41	1.34	1.39
55	2x	54	5MU	C4-C5	3.38	1.48	1.41
54	1w	54	5MU	C4-C5	3.33	1.48	1.41
54	2y	39	PSU	C4-C5	3.31	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	55	PSU	C5-C1'	-3.30	1.49	1.52
32	2a	516	PSU	C4-C5	3.29	1.48	1.41
32	2a	527	7MG	C5-N7	-3.27	1.34	1.39
1	1A	1939	PSU	C4-C5	3.26	1.48	1.41
54	2w	46	7MG	C5-N7	-3.24	1.34	1.39
1	2A	1939	5MU	C4-C5	3.24	1.48	1.41
54	2w	39	PSU	C4-C5	3.23	1.48	1.41
54	2w	32	PSU	C5-C1'	-3.23	1.49	1.52
54	1w	39	PSU	C4-C5	3.22	1.48	1.41
54	2w	55	PSU	C5-C1'	-3.20	1.49	1.52
55	1x	55	PSU	C4-C5	3.19	1.48	1.41
1	1A	1939	PSU	C5-C1'	-3.15	1.49	1.52
1	2A	1915	5MU	C4-C5	3.14	1.48	1.41
1	2A	2605	PSU	C4-C5	3.11	1.48	1.41
1	2A	1911	PSU	C4-C5	3.06	1.48	1.41
32	2a	966	M2G	C2-N2	3.06	1.39	1.34
54	2w	39	PSU	C5-C1'	-3.03	1.49	1.52
1	1A	1961	5MU	C4-C5	3.01	1.47	1.41
1	1A	2617	PSU	C4-C5	2.89	1.47	1.41
55	2x	8	4SU	C2-N3	-2.85	1.32	1.38
1	1A	1933	PSU	C5-C1'	-2.83	1.49	1.52
54	2y	37	MIA	C5-C4	2.79	1.48	1.40
32	2a	1518	MA6	C5-C4	2.72	1.48	1.40
54	2y	37	MIA	C2-N3	2.71	1.36	1.32
54	1y	37	MIA	C5-C4	2.69	1.48	1.40
54	1y	37	MIA	C2-N3	2.67	1.36	1.32
32	2a	966	M2G	C5-C4	2.58	1.47	1.40
54	2w	37	MIA	C5-C4	2.58	1.47	1.40
32	2a	1519	MA6	C5-C4	2.57	1.47	1.40
32	1a	1518	MA6	C5-C4	2.55	1.47	1.40
54	1w	37	MIA	C5-C4	2.54	1.47	1.40
1	2A	2251	OMG	C5-C4	2.52	1.47	1.40
32	1a	1519	MA6	C5-C4	2.50	1.47	1.40
32	1a	527	7MG	C4-N9	-2.49	1.33	1.38
32	1a	966	M2G	C5-C4	2.47	1.47	1.40
32	2a	1207	2MG	C5-C4	2.42	1.47	1.40
54	2w	46	7MG	C4-N9	-2.35	1.33	1.38
32	1a	516	PSU	O4'-C1'	-2.35	1.41	1.44
32	2a	1498	UR3	C4-N3	2.34	1.41	1.38
54	1w	46	7MG	C4-N9	-2.34	1.34	1.38
1	1A	2263	OMG	C5-C4	2.33	1.47	1.40
1	1A	2564	2MU	C2-N3	-2.31	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1207	2MG	C5-C4	2.30	1.47	1.40
1	1A	2617	PSU	C2-N3	-2.28	1.33	1.38
1	2A	2605	PSU	C2-N3	-2.26	1.33	1.38
32	2a	527	7MG	C4-N9	-2.25	1.34	1.38
32	1a	1498	UR3	C4-N3	2.21	1.41	1.38
1	1A	2617	PSU	O4'-C1'	-2.21	1.41	1.44
54	1y	55	PSU	O4'-C1'	-2.17	1.41	1.44
1	2A	2503	2MA	C5-C4	2.12	1.46	1.40
54	1w	39	PSU	O4'-C1'	-2.11	1.41	1.44
54	1w	8	4SU	C2-N3	-2.10	1.34	1.38
1	1A	2617	PSU	C2-N1	-2.09	1.34	1.38
54	1y	46	7MG	C4-N3	2.09	1.36	1.34
54	1y	54	5MU	C2-N3	-2.09	1.34	1.38
1	1A	2515	2MA	C5-C4	2.07	1.46	1.40
32	1a	516	PSU	C2-N3	-2.06	1.34	1.38
32	1a	516	PSU	C2-N1	-2.05	1.34	1.38
54	1y	39	PSU	O4'-C1'	-2.02	1.41	1.44
54	2w	37	MIA	C6-N1	2.01	1.35	1.32
32	2a	516	PSU	O4'-C1'	-2.01	1.41	1.44

All (351) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	46	7MG	N3-C4-N9	10.01	139.76	126.91
54	2y	46	7MG	N3-C4-N9	9.89	139.61	126.91
54	2w	39	PSU	N1-C2-N3	-9.71	120.71	128.43
54	2y	39	PSU	N1-C2-N3	-9.28	121.05	128.43
55	1x	8	4SU	C2-N3-C4	9.22	128.52	115.15
54	1y	39	PSU	N1-C2-N3	-9.10	121.19	128.43
54	2w	32	PSU	N1-C2-N3	-9.06	121.23	128.43
55	1x	55	PSU	N1-C2-N3	-9.05	121.23	128.43
1	1A	1933	PSU	N1-C2-N3	-9.01	121.27	128.43
54	2w	46	7MG	N3-C4-N9	8.95	138.40	126.91
32	2a	527	7MG	N3-C4-N9	8.92	138.37	126.91
54	1w	32	PSU	N1-C2-N3	-8.90	121.35	128.43
54	1w	46	7MG	N3-C4-N9	8.90	138.34	126.91
54	1y	32	PSU	N1-C2-N3	-8.89	121.37	128.43
43	2l	92	0TD	CSB-SB-CB	-8.86	84.42	101.85
54	2y	32	PSU	N1-C2-N3	-8.82	121.42	128.43
32	2a	516	PSU	N1-C2-N3	-8.73	121.49	128.43
32	1a	527	7MG	N3-C4-N9	8.69	138.07	126.91
54	1y	55	PSU	N1-C2-N3	-8.67	121.54	128.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	55	PSU	N1-C2-N3	-8.61	121.59	128.43
54	1w	55	PSU	N1-C2-N3	-8.59	121.61	128.43
54	2w	39	PSU	C4-N3-C2	8.34	122.18	115.14
55	2x	55	PSU	N1-C2-N3	-8.31	121.82	128.43
54	2w	55	PSU	N1-C2-N3	-8.29	121.84	128.43
1	2A	1917	PSU	N1-C2-N3	-8.29	121.84	128.43
1	1A	1939	PSU	N1-C2-N3	-8.26	121.86	128.43
54	1w	37	MIA	C12-C13-C14	-8.22	111.14	127.14
1	2A	1911	PSU	N1-C2-N3	-8.18	121.92	128.43
32	1a	516	PSU	N1-C2-N3	-8.06	122.03	128.43
1	1A	2617	PSU	N1-C2-N3	-8.03	122.05	128.43
1	2A	2605	PSU	N1-C2-N3	-7.90	122.15	128.43
54	1y	54	5MU	C4-N3-C2	7.90	121.81	115.14
54	1w	39	PSU	N1-C2-N3	-7.88	122.17	128.43
54	2y	39	PSU	C4-N3-C2	7.76	121.70	115.14
54	1y	39	PSU	C4-N3-C2	7.50	121.48	115.14
54	1w	32	PSU	C4-N3-C2	7.40	121.39	115.14
54	1y	55	PSU	C4-N3-C2	7.39	121.38	115.14
55	2x	8	4SU	C2-N3-C4	7.39	125.86	115.15
55	1x	54	5MU	C4-N3-C2	7.38	121.38	115.14
54	1w	54	5MU	C4-N3-C2	7.32	121.33	115.14
54	2w	32	PSU	C4-N3-C2	7.32	121.32	115.14
54	2y	32	PSU	C4-N3-C2	7.30	121.31	115.14
54	1w	55	PSU	C4-N3-C2	7.30	121.30	115.14
54	1y	32	PSU	C4-N3-C2	7.20	121.22	115.14
55	1x	55	PSU	C4-N3-C2	7.13	121.16	115.14
54	2w	54	5MU	C4-N3-C2	7.01	121.06	115.14
1	2A	1915	5MU	C4-N3-C2	6.81	120.89	115.14
1	1A	1933	PSU	C4-N3-C2	6.79	120.88	115.14
32	2a	516	PSU	C4-N3-C2	6.76	120.85	115.14
1	2A	1911	PSU	C4-N3-C2	6.75	120.84	115.14
54	2w	55	PSU	C4-N3-C2	6.74	120.83	115.14
54	2y	55	PSU	C4-N3-C2	6.73	120.83	115.14
1	2A	2605	PSU	C4-N3-C2	6.71	120.81	115.14
55	2x	55	PSU	C4-N3-C2	6.54	120.66	115.14
1	1A	2515	2MA	C2-N3-C4	6.50	120.80	115.52
1	2A	1917	PSU	C4-N3-C2	6.49	120.62	115.14
1	1A	1939	PSU	C4-N3-C2	6.44	120.58	115.14
1	2A	2503	2MA	C2-N3-C4	6.36	120.69	115.52
1	1A	1961	5MU	C4-N3-C2	6.35	120.51	115.14
32	1a	516	PSU	C4-N3-C2	6.32	120.48	115.14
54	2y	54	5MU	C4-N3-C2	6.27	120.44	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1937	5MU	C4-N3-C2	6.24	120.41	115.14
1	2A	1939	5MU	C4-N3-C2	6.21	120.38	115.14
1	1A	2617	PSU	C4-N3-C2	6.06	120.26	115.14
55	2x	54	5MU	C4-N3-C2	5.94	120.16	115.14
54	1w	39	PSU	C4-N3-C2	5.89	120.11	115.14
54	2y	46	7MG	C5-C4-N3	-5.79	117.04	126.49
54	1y	55	PSU	C5-C4-N3	-5.76	117.93	125.36
54	2y	39	PSU	C5-C4-N3	-5.64	118.10	125.36
54	1y	46	7MG	C6-N1-C2	5.62	124.85	115.93
54	1y	46	7MG	C5-C4-N3	-5.56	117.41	126.49
1	2A	1911	PSU	C5-C4-N3	-5.56	118.20	125.36
54	2w	46	7MG	N7-C8-N9	-5.54	95.45	103.38
54	1w	55	PSU	C5-C4-N3	-5.54	118.22	125.36
54	1y	32	PSU	C5-C4-N3	-5.54	118.22	125.36
32	2a	527	7MG	N7-C8-N9	-5.50	95.51	103.38
54	1w	32	PSU	C5-C4-N3	-5.46	118.32	125.36
54	2y	46	7MG	C6-N1-C2	5.46	124.60	115.93
54	1y	39	PSU	C5-C4-N3	-5.45	118.33	125.36
55	2x	55	PSU	C5-C4-N3	-5.45	118.34	125.36
54	2y	55	PSU	C5-C4-N3	-5.45	118.34	125.36
54	2y	32	PSU	C5-C4-N3	-5.44	118.35	125.36
55	1x	55	PSU	C5-C4-N3	-5.42	118.37	125.36
54	2w	39	PSU	C5-C4-N3	-5.41	118.39	125.36
32	1a	516	PSU	C5-C4-N3	-5.33	118.49	125.36
54	2w	32	PSU	C5-C4-N3	-5.30	118.53	125.36
32	1a	966	M2G	C2-N3-C4	5.29	121.29	115.28
54	2y	39	PSU	C5-C1'-C2'	-5.28	105.89	115.32
54	1w	46	7MG	N7-C8-N9	-5.27	95.85	103.38
1	2A	1917	PSU	C5-C4-N3	-5.25	118.60	125.36
32	1a	966	M2G	C6-N1-C2	5.23	122.41	116.18
1	1A	2263	OMG	C2-N3-C4	5.22	121.32	115.36
54	2w	55	PSU	C5-C4-N3	-5.21	118.65	125.36
32	1a	527	7MG	N7-C8-N9	-5.18	95.96	103.38
1	2A	2605	PSU	C5-C4-N3	-5.16	118.72	125.36
32	2a	527	7MG	C5-C4-N3	-5.11	118.14	126.49
32	2a	516	PSU	C5-C4-N3	-5.08	118.82	125.36
54	1w	39	PSU	C5-C4-N3	-5.05	118.85	125.36
32	1a	527	7MG	C5-C4-N3	-5.03	118.28	126.49
54	2w	46	7MG	C5-C4-N3	-4.96	118.40	126.49
1	1A	2617	PSU	C5-C4-N3	-4.95	118.98	125.36
54	1w	46	7MG	C6-N1-C2	4.94	123.78	115.93
1	1A	1942	4OC	C2-N3-C4	4.92	121.33	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1939	PSU	C5-C4-N3	-4.92	119.02	125.36
1	1A	2515	2MA	C5-C6-N1	-4.90	117.92	123.06
54	1y	8	4SU	C2-N3-C4	4.90	122.26	115.15
1	1A	1933	PSU	C5-C4-N3	-4.86	119.09	125.36
54	1w	46	7MG	C5-C4-N3	-4.86	118.56	126.49
32	2a	966	M2G	C2-N3-C4	4.86	120.79	115.28
32	1a	1207	2MG	C2-N3-C4	4.83	120.77	115.28
54	1w	55	PSU	C5-C1'-C2'	-4.81	106.74	115.32
54	1w	37	MIA	C5-C6-N1	-4.80	116.82	120.81
54	2y	46	7MG	C6-C5-C4	4.78	120.33	115.20
1	2A	2251	OMG	C2-N3-C4	4.73	120.76	115.36
32	2a	966	M2G	C6-N1-C2	4.71	121.79	116.18
55	1x	8	4SU	C5-C4-N3	-4.69	117.56	123.83
54	1y	46	7MG	C6-C5-C4	4.63	120.17	115.20
54	2y	46	7MG	N7-C8-N9	-4.60	96.81	103.38
54	2w	55	PSU	C5-C1'-C2'	-4.59	107.13	115.32
54	1y	46	7MG	N7-C8-N9	-4.58	96.83	103.38
1	2A	1920	4OC	C2-N3-C4	4.52	120.93	116.34
1	1A	2617	PSU	C5-C6-N1	-4.50	118.92	124.44
55	2x	55	PSU	C5-C6-N1	-4.48	118.93	124.44
32	2a	1207	2MG	C2-N3-C4	4.47	120.36	115.28
1	2A	1911	PSU	C5-C1'-C2'	-4.46	107.36	115.32
32	1a	1207	2MG	C6-N1-C2	4.46	123.16	115.18
54	1w	8	4SU	C2-N3-C4	4.44	121.59	115.15
32	2a	1402	4OC	CM4-N4-C4	-4.42	119.17	122.97
32	1a	527	7MG	C6-N1-C2	4.41	122.94	115.93
32	1a	1207	2MG	C5-C6-N1	-4.39	117.43	123.43
54	2w	46	7MG	C6-N1-C2	4.36	122.86	115.93
43	1l	92	0TD	CSB-SB-CB	4.35	110.41	101.85
32	2a	1207	2MG	C5-C6-N1	-4.34	117.50	123.43
32	2a	527	7MG	C6-N1-C2	4.33	122.81	115.93
32	1a	1207	2MG	C6-C5-C4	-4.33	116.67	120.80
1	2A	1911	PSU	C5-C6-N1	-4.32	119.14	124.44
54	2y	55	PSU	C6-N1-C2	4.31	122.47	115.36
54	1w	46	7MG	C6-C5-C4	4.30	119.82	115.20
54	1w	39	PSU	C5-C6-N1	-4.29	119.17	124.44
32	1a	516	PSU	C5-C6-N1	-4.27	119.19	124.44
1	1A	1933	PSU	C6-N1-C2	4.24	122.36	115.36
54	2w	37	MIA	C2-N3-C4	4.22	121.14	115.32
32	1a	516	PSU	C6-N1-C2	4.22	122.32	115.36
32	1a	527	7MG	C6-C5-C4	4.22	119.73	115.20
1	2A	1917	PSU	C5-C6-N1	-4.22	119.26	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2617	PSU	C6-N1-C2	4.17	122.24	115.36
55	2x	55	PSU	C6-N1-C2	4.16	122.23	115.36
55	1x	55	PSU	C6-N1-C2	4.16	122.23	115.36
32	2a	516	PSU	C5-C6-N1	-4.15	119.34	124.44
1	2A	2503	2MA	C5-C6-N1	-4.15	118.71	123.06
1	2A	1917	PSU	C6-N1-C2	4.14	122.19	115.36
1	2A	1917	PSU	C5-C1'-C2'	-4.14	107.94	115.32
32	2a	516	PSU	C6-N1-C2	4.13	122.17	115.36
54	1y	39	PSU	C6-N1-C2	4.13	122.17	115.36
54	2y	55	PSU	C5-C6-N1	-4.12	119.37	124.44
54	2w	32	PSU	C6-N1-C2	4.10	122.13	115.36
1	2A	2605	PSU	C5-C1'-C2'	-4.08	108.05	115.32
32	2a	1207	2MG	C6-C5-C4	-4.07	116.91	120.80
55	1x	32	5MC	C2-N3-C4	4.06	120.92	116.02
54	1w	39	PSU	C6-N1-C2	4.06	122.06	115.36
1	2A	2605	PSU	C5-C6-N1	-4.06	119.45	124.44
54	1w	37	MIA	C15-C14-C13	-4.05	110.93	122.65
54	1y	46	7MG	C5-C6-N1	-4.05	114.81	123.14
1	1A	1939	PSU	C6-N1-C2	4.05	122.04	115.36
54	1y	32	PSU	C6-N1-C2	4.05	122.04	115.36
54	2w	55	PSU	C6-N1-C2	4.05	122.03	115.36
54	2y	39	PSU	C6-N1-C2	4.02	122.00	115.36
55	1x	55	PSU	C5-C6-N1	-4.02	119.50	124.44
54	1w	46	7MG	C5-C6-N1	-4.02	114.89	123.14
54	1w	32	PSU	C6-N1-C2	4.01	121.98	115.36
55	2x	32	5MC	C2-N3-C4	4.01	120.86	116.02
32	2a	1207	2MG	C6-N1-C2	3.99	122.32	115.18
1	2A	1911	PSU	C6-N1-C2	3.99	121.94	115.36
54	2y	46	7MG	C5-C6-N1	-3.98	114.96	123.14
54	2w	39	PSU	C6-N1-C2	3.96	121.90	115.36
1	1A	2263	OMG	C6-N1-C2	3.96	122.22	115.93
32	1a	966	M2G	C6-C5-C4	-3.95	117.03	120.80
54	2y	32	PSU	C6-N1-C2	3.94	121.86	115.36
54	2w	46	7MG	C6-C5-C4	3.94	119.43	115.20
32	1a	1207	2MG	CM2-N2-C2	-3.93	118.85	123.59
1	1A	2263	OMG	C5-C6-N1	-3.91	118.08	123.43
32	2a	527	7MG	C6-C5-C4	3.91	119.40	115.20
32	2a	966	M2G	C5-C6-N1	-3.91	118.09	123.43
54	2w	55	PSU	C5-C6-N1	-3.90	119.65	124.44
54	1w	55	PSU	C6-N1-C2	3.90	121.79	115.36
32	1a	1404	5MC	C2-N3-C4	3.88	120.70	116.02
32	1a	966	M2G	C5-C6-N1	-3.87	118.14	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	39	PSU	C5-C6-N1	-3.86	119.69	124.44
55	2x	8	4SU	C5-C4-N3	-3.86	118.67	123.83
1	1A	1939	PSU	C5-C6-N1	-3.83	119.73	124.44
54	1y	39	PSU	C5-C6-N1	-3.83	119.74	124.44
1	2A	2605	PSU	C6-N1-C2	3.82	121.67	115.36
54	1y	55	PSU	C6-N1-C2	3.82	121.66	115.36
32	1a	527	7MG	C5-C6-N1	-3.77	115.40	123.14
54	2y	8	4SU	C2-N3-C4	3.74	120.58	115.15
1	2A	1942	5MC	C2-N3-C4	3.74	120.53	116.02
32	1a	1402	4OC	CM4-N4-C4	-3.73	119.76	122.97
32	2a	1207	2MG	CM2-N2-C2	-3.73	119.09	123.59
54	1w	32	PSU	C5-C6-N1	-3.73	119.86	124.44
1	2A	1962	5MC	C2-N3-C4	3.72	120.51	116.02
54	2y	32	PSU	C5-C6-N1	-3.72	119.87	124.44
54	1y	8	4SU	C5-C4-N3	-3.72	118.86	123.83
54	1y	32	PSU	C5-C6-N1	-3.71	119.88	124.44
54	2y	37	MIA	N3-C2-N1	-3.69	122.91	128.68
1	1A	2263	OMG	C6-C5-C4	-3.68	117.29	120.80
54	2w	37	MIA	C5-C6-N1	-3.68	117.76	120.81
1	2A	2251	OMG	C6-N1-C2	3.65	121.73	115.93
32	2a	1518	MA6	C4-C5-N7	-3.64	105.60	109.40
54	1w	37	MIA	C2-N3-C4	3.62	120.31	115.32
54	2w	46	7MG	C5-C6-N1	-3.60	115.74	123.14
54	1y	37	MIA	N3-C2-N1	-3.60	123.05	128.68
1	2A	2251	OMG	C5-C6-N1	-3.59	118.52	123.43
1	1A	1984	5MC	C2-N3-C4	3.59	120.35	116.02
54	2w	39	PSU	C5-C6-N1	-3.58	120.04	124.44
1	1A	2617	PSU	C5-C1'-C2'	-3.57	108.96	115.32
54	1w	37	MIA	C16-C14-C13	-3.57	112.34	122.65
32	1a	1400	5MC	C2-N3-C4	3.55	120.31	116.02
32	2a	527	7MG	C5-C6-N1	-3.55	115.85	123.14
32	2a	1407	5MC	C2-N3-C4	3.54	120.29	116.02
32	1a	1207	2MG	C4-C5-N7	-3.54	105.71	109.40
32	2a	1404	5MC	C2-N3-C4	3.53	120.28	116.02
32	2a	1207	2MG	N2-C2-N1	3.53	120.35	116.96
32	2a	1518	MA6	C9-N6-C6	-3.51	108.88	119.51
32	1a	967	5MC	C2-N3-C4	3.51	120.26	116.02
1	1A	1933	PSU	C5-C6-N1	-3.50	120.14	124.44
32	2a	967	5MC	C2-N3-C4	3.49	120.23	116.02
32	2a	1400	5MC	C2-N3-C4	3.48	120.22	116.02
32	2a	1207	2MG	C4-C5-N7	-3.48	105.77	109.40
1	2A	2251	OMG	C6-C5-C4	-3.47	117.48	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1518	MA6	N3-C2-N1	-3.44	123.30	128.68
32	1a	1518	MA6	C4-C5-N7	-3.44	105.81	109.40
32	2a	966	M2G	C6-C5-C4	-3.44	117.51	120.80
54	2w	32	PSU	C5-C6-N1	-3.43	120.22	124.44
32	1a	1400	5MC	N4-C4-N3	3.41	121.85	117.03
32	1a	1519	MA6	N3-C2-N1	-3.37	123.41	128.68
1	1A	1964	5MC	C2-N3-C4	3.37	120.09	116.02
54	1w	55	PSU	C5-C6-N1	-3.36	120.31	124.44
54	1y	55	PSU	C5-C6-N1	-3.33	120.34	124.44
1	1A	2263	OMG	N3-C2-N1	-3.33	122.78	127.22
32	1a	1407	5MC	C2-N3-C4	3.30	120.00	116.02
32	2a	1518	MA6	N3-C2-N1	-3.28	123.56	128.68
32	2a	1519	MA6	C9-N6-C6	-3.27	109.62	119.51
32	2a	1400	5MC	N4-C4-N3	3.24	121.62	117.03
1	2A	1939	5MU	C5-C6-N1	-3.23	118.71	122.19
32	2a	1519	MA6	C4-C5-N7	-3.22	106.04	109.40
54	2w	8	4SU	C2-N3-C4	3.20	119.78	115.15
32	1a	1519	MA6	N1-C6-N6	3.15	120.37	117.06
32	1a	1519	MA6	C9-N6-C6	-3.14	109.99	119.51
55	1x	55	PSU	C5-C1'-C2'	-3.12	109.75	115.32
32	2a	516	PSU	C5-C1'-C2'	-3.11	109.78	115.32
1	1A	1961	5MU	C5-C6-N1	-3.10	118.86	122.19
32	2a	1404	5MC	N4-C4-N3	3.06	121.36	117.03
1	2A	1962	5MC	N4-C4-N3	3.05	121.34	117.03
32	1a	1518	MA6	C9-N6-C6	-3.05	110.28	119.51
54	1w	37	MIA	C2-N1-C6	3.05	122.65	117.19
54	2w	37	MIA	C12-N6-C6	-3.03	120.26	122.87
32	2a	1519	MA6	N3-C2-N1	-2.99	124.00	128.68
32	1a	1207	2MG	N2-C2-N1	2.98	119.82	116.96
1	2A	2251	OMG	N3-C2-N1	-2.95	123.29	127.22
54	2w	37	MIA	C4-C5-N7	-2.94	106.33	109.40
1	1A	1964	5MC	C5-C6-N1	-2.93	119.04	122.19
1	1A	1942	4OC	N4-C4-N3	2.87	121.03	116.49
32	2a	527	7MG	C8-N7-C5	2.86	116.37	108.94
32	2a	1407	5MC	N4-C4-N3	2.81	121.01	117.03
32	1a	967	5MC	N4-C4-N3	2.81	121.00	117.03
54	2w	46	7MG	C8-N7-C5	2.80	116.22	108.94
32	1a	1519	MA6	C4-C5-N7	-2.78	106.50	109.40
55	2x	32	5MC	N4-C4-N3	2.77	120.95	117.03
54	2w	37	MIA	C2-N1-C6	2.76	122.13	117.19
54	1y	37	MIA	C4-C5-N7	-2.73	106.55	109.40
55	1x	32	5MC	N4-C4-N3	2.72	120.88	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	32	PSU	C5-C1'-C2'	-2.70	110.50	115.32
32	1a	527	7MG	C8-N7-C5	2.70	115.96	108.94
54	2y	37	MIA	C4-C5-N7	-2.70	106.59	109.40
1	2A	1942	5MC	N4-C4-N3	2.69	120.83	117.03
54	2w	8	4SU	C5-C4-N3	-2.68	120.24	123.83
54	1w	8	4SU	C5-C4-N3	-2.65	120.28	123.83
54	1w	46	7MG	C8-N7-C5	2.64	115.80	108.94
1	1A	2263	OMG	C4-C5-N7	-2.62	106.67	109.40
1	1A	1964	5MC	N4-C4-N3	2.61	120.73	117.03
55	2x	55	PSU	C5-C1'-C2'	-2.61	110.66	115.32
54	1y	46	7MG	C5-C4-N9	-2.58	102.82	106.44
32	1a	1407	5MC	N4-C4-N3	2.58	120.68	117.03
54	2y	8	4SU	C5-C4-N3	-2.56	120.40	123.83
54	2y	46	7MG	C8-N7-C5	2.56	115.60	108.94
55	2x	54	5MU	C5-C6-N1	-2.55	119.44	122.19
32	2a	967	5MC	N4-C4-N3	2.53	120.61	117.03
54	1y	46	7MG	C8-N7-C5	2.52	115.49	108.94
1	1A	2515	2MA	C4-C5-N7	-2.51	106.78	109.40
32	1a	966	M2G	C4-C5-N7	-2.51	106.78	109.40
1	1A	1984	5MC	N4-C4-N3	2.50	120.57	117.03
54	2y	46	7MG	C2-N3-C4	2.49	120.77	113.89
1	2A	2251	OMG	C4-C5-N7	-2.44	106.85	109.40
54	1w	37	MIA	C4-C5-N7	-2.44	106.86	109.40
1	1A	1939	PSU	C5-C1'-C2'	-2.44	110.97	115.32
54	2w	37	MIA	C11-S10-C2	-2.43	100.45	102.27
32	2a	1404	5MC	C5-C6-N1	-2.43	119.57	122.19
32	1a	1407	5MC	C5-C6-N1	-2.43	119.57	122.19
32	2a	1407	5MC	C5-C6-N1	-2.41	119.59	122.19
55	1x	32	5MC	CM5-C5-C4	-2.41	119.28	121.72
32	2a	966	M2G	C4-C5-N7	-2.40	106.90	109.40
32	2a	967	5MC	C5-C6-N1	-2.40	119.61	122.19
54	1w	46	7MG	C5-C4-N9	-2.38	103.11	106.44
32	1a	1207	2MG	C1'-N9-C4	-2.38	122.46	126.64
32	1a	1404	5MC	C5-C6-N1	-2.34	119.68	122.19
54	2w	46	7MG	C5-C4-N9	-2.33	103.18	106.44
54	2w	37	MIA	N3-C2-N1	-2.31	122.73	126.98
32	2a	1519	MA6	N1-C6-N6	2.31	119.49	117.06
54	1w	32	PSU	C5-C1'-C2'	-2.31	111.20	115.32
54	1y	46	7MG	C2-N3-C4	2.30	120.24	113.89
32	1a	1207	2MG	N3-C2-N1	-2.28	122.62	126.23
32	2a	1518	MA6	C10-N6-C9	-2.28	108.79	116.12
1	2A	1920	4OC	N4-C4-N3	2.27	120.07	116.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1962	5MC	C5-C6-N1	-2.25	119.77	122.19
32	1a	1400	5MC	CM5-C5-C4	-2.24	119.45	121.72
32	2a	527	7MG	C2-N3-C4	2.23	120.05	113.89
1	1A	1984	5MC	C5-C6-N1	-2.22	119.80	122.19
54	2y	46	7MG	C5-C4-N9	-2.22	103.33	106.44
1	2A	2503	2MA	C4-C5-N7	-2.22	107.09	109.40
55	1x	32	5MC	C5-C6-N1	-2.21	119.81	122.19
1	2A	1915	5MU	C5-C6-N1	-2.20	119.82	122.19
32	1a	516	PSU	O4'-C1'-C2'	2.18	108.20	104.66
1	1A	1964	5MC	CM5-C5-C4	-2.18	119.52	121.72
32	2a	1207	2MG	C1'-N9-C4	-2.16	122.84	126.64
54	1w	37	MIA	N3-C2-N1	-2.15	123.03	126.98
54	2w	46	7MG	C2-N3-C4	2.12	119.76	113.89
54	1y	54	5MU	C5-C6-N1	-2.12	119.91	122.19
32	2a	1400	5MC	C5-C6-N1	-2.12	119.91	122.19
32	2a	527	7MG	C5-C4-N9	-2.12	103.48	106.44
32	1a	1518	MA6	C10-N6-C9	-2.11	109.32	116.12
32	2a	1498	UR3	C3U-N3-C4	2.10	120.90	118.12
32	2a	516	PSU	O4'-C1'-C2'	2.08	108.03	104.66
1	2A	2552	2MU	C5-C4-N3	-2.08	118.74	123.31
1	1A	2564	2MU	C5-C4-N3	-2.07	118.74	123.31
54	2y	55	PSU	O4'-C1'-C2'	2.07	108.01	104.66
32	1a	527	7MG	C2-N3-C4	2.06	119.59	113.89
54	2w	54	5MU	C5-C6-N1	-2.05	119.98	122.19
1	2A	2552	2MU	O5'-C5'-C4'	-2.05	102.02	108.99
32	1a	1400	5MC	C5-C6-N1	-2.04	119.99	122.19
54	1y	46	7MG	N2-C2-N3	2.04	120.43	117.25
1	1A	1937	5MU	C5-C6-N1	-2.04	120.00	122.19
54	1y	46	7MG	C4-N9-C1'	2.04	131.44	126.60
54	1w	37	MIA	C12-N6-C6	-2.04	119.53	122.55
32	2a	966	M2G	CM1-N2-C2	-2.03	119.35	121.29
54	2w	39	PSU	O4'-C1'-C2'	2.02	107.93	104.66
32	1a	1518	MA6	N1-C6-N6	2.02	119.18	117.06
54	2y	37	MIA	C2-N1-C6	2.01	122.19	118.75
55	2x	32	5MC	C5-C6-N1	-2.01	120.03	122.19
32	1a	527	7MG	C5-C4-N9	-2.00	103.64	106.44
32	1a	527	7MG	CM7-N7-C5	2.00	131.71	124.01
54	2y	32	PSU	O4'-C1'-C2'	2.00	107.90	104.66

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	2y	55	PSU	C2'-C1'-C5-C4
54	2y	55	PSU	C2'-C1'-C5-C6
54	2y	55	PSU	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C1'-N1-C6
1	1A	1984	5MC	O4'-C1'-N1-C6
1	1A	1984	5MC	C2'-C1'-N1-C6
32	2a	1400	5MC	O4'-C1'-N1-C6
32	2a	1400	5MC	C2'-C1'-N1-C6
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10
54	1w	37	MIA	C12-C13-C14-C16
54	1y	8	4SU	C2'-C1'-N1-C6
54	1y	8	4SU	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
54	1y	46	7MG	C4'-C5'-O5'-P
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1518	MA6	C5-C6-N6-C10
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
54	1y	54	5MU	C2'-C1'-N1-C6
54	1y	54	5MU	O4'-C1'-N1-C6
54	1y	54	5MU	C3'-C4'-C5'-O5'
54	1y	54	5MU	O4'-C4'-C5'-O5'
54	2w	37	MIA	N1-C6-N6-C12
54	2y	37	MIA	C3'-C4'-C5'-O5'
54	2y	54	5MU	C2'-C1'-N1-C6
32	1a	967	5MC	O4'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
54	2y	55	PSU	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	967	5MC	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	527	7MG	C3'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
54	2w	46	7MG	O4'-C4'-C5'-O5'
32	2a	1518	MA6	N1-C6-N6-C9
54	2y	37	MIA	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
54	2w	46	7MG	C3'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C10

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Mol	Chain	Res	Type	Atoms
32	2a	527	7MG	C3'-C4'-C5'-O5'
1	1A	1937	5MU	O4'-C4'-C5'-O5'
54	2y	46	7MG	C2'-C1'-N9-C8
32	2a	1519	MA6	C4'-C5'-O5'-P
54	2y	46	7MG	O4'-C1'-N9-C4
32	1a	1519	MA6	C5-C6-N6-C10
54	1y	46	7MG	C2'-C1'-N9-C8
32	2a	527	7MG	C4'-C5'-O5'-P
54	1y	8	4SU	C4'-C5'-O5'-P
32	2a	527	7MG	O4'-C4'-C5'-O5'
32	1a	527	7MG	C4'-C5'-O5'-P
54	1w	46	7MG	C4'-C5'-O5'-P
54	1w	46	7MG	C2'-C1'-N9-C8
54	2y	55	PSU	O4'-C1'-C5-C6
54	2y	55	PSU	O4'-C1'-C5-C4
43	1l	92	0TD	CA-CB-SB-CSB
1	2A	2552	2MU	O4'-C4'-C5'-O5'
1	1A	2515	2MA	O4'-C4'-C5'-O5'
54	2y	46	7MG	O4'-C1'-N9-C8
54	2w	46	7MG	C2'-C1'-N9-C8
54	2w	32	PSU	C2'-C1'-C5-C6
54	2y	54	5MU	C3'-C4'-C5'-O5'
54	1y	46	7MG	O4'-C1'-N9-C8
1	2A	2503	2MA	O4'-C4'-C5'-O5'
54	1y	46	7MG	C3'-C4'-C5'-O5'
1	1A	1937	5MU	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1402	4OC	C5-C4-N4-CM4
54	2w	46	7MG	C4'-C5'-O5'-P

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1939	PSU	1	0
1	2A	2503	2MA	3	0
1	2A	1917	PSU	1	0
1	2A	1939	5MU	1	0
1	2A	1920	4OC	2	0
1	1A	1961	5MU	1	0
1	1A	2564	2MU	1	0
1	1A	2263	OMG	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3095 ligands modelled in this entry, 3085 are monoatomic - leaving 10 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	$\# Z > 2$
57	CPT	2A	3903	1	0,3,4	0.00	-	-		
57	CPT	2a	3235	32	0,3,4	0.00	-	-		
57	CPT	1A	4210	1	0,3,4	0.00	-	-		
57	CPT	1A	4209	1	0,3,4	0.00	-	-		
57	CPT	2I	201	8	0,3,4	0.00	-	-		
60	SF4	2d	501	35	0,12,12	0.00	-	-		
60	SF4	1d	501	35	0,12,12	0.00	-	-		
57	CPT	1I	3002	8	0,3,4	0.00	-	-		
57	CPT	2A	3904	1	0,3,4	0.00	-	-		
57	CPT	1a	1930	32	0,3,4	0.00	-	-		

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

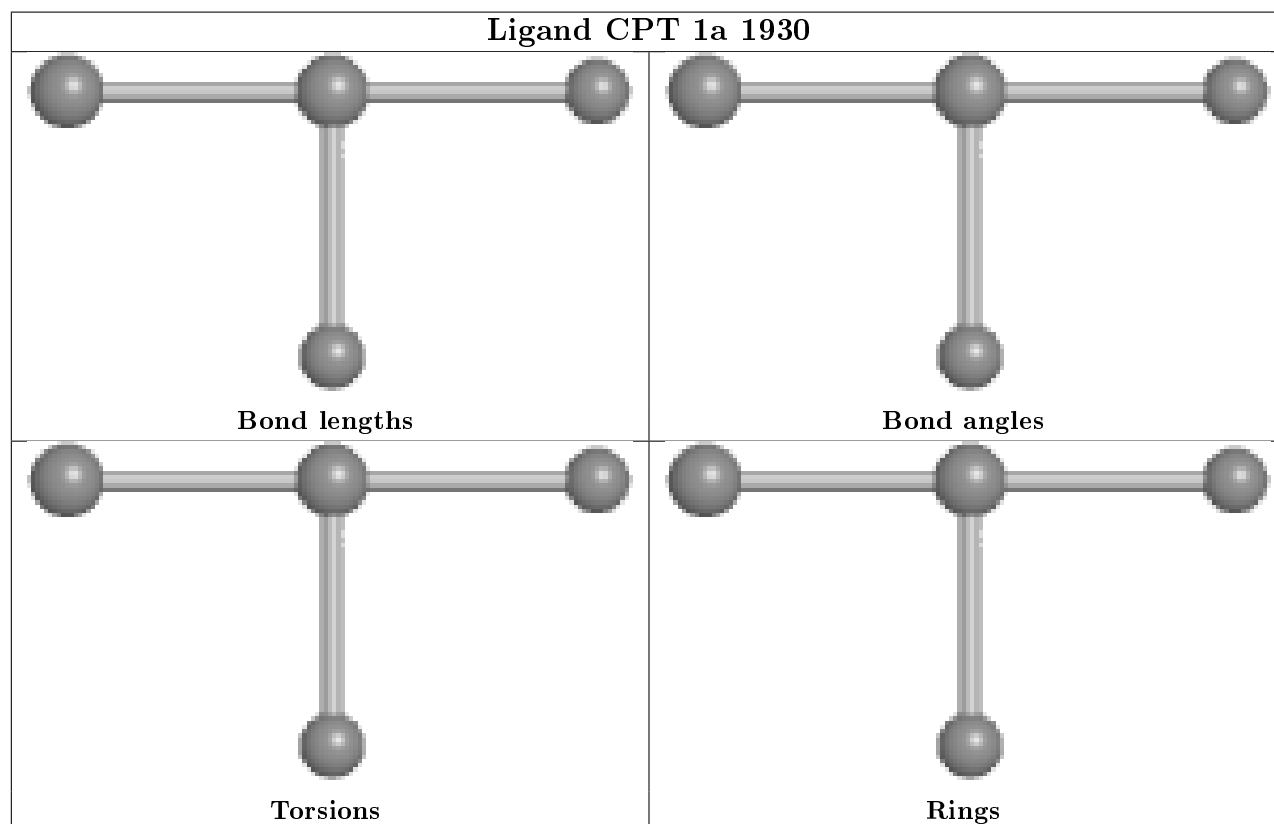
There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	2A	3903	CPT	1	0
57	1A	4209	CPT	1	0
57	2I	201	CPT	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	0.29	49 (1%) 70 63	24, 45, 94, 107	0
1	2A	2789/2915 (95%)	-0.12	33 (1%) 79 73	27, 48, 92, 107	0
2	1B	120/121 (99%)	-0.05	0 100 100	40, 60, 72, 93	0
2	2B	120/121 (99%)	-0.23	1 (0%) 86 81	46, 65, 75, 93	0
3	1D	275/276 (99%)	0.21	2 (0%) 87 84	23, 43, 59, 79	0
3	2D	275/276 (99%)	0.01	0 100 100	24, 44, 61, 79	0
4	1E	204/206 (99%)	0.20	0 100 100	25, 50, 66, 82	0
4	2E	204/206 (99%)	0.29	4 (1%) 65 56	27, 52, 68, 85	0
5	1F	203/210 (96%)	0.24	2 (0%) 82 77	26, 54, 77, 90	0
5	2F	203/210 (96%)	0.34	9 (4%) 34 24	28, 57, 79, 89	0
6	1G	181/182 (99%)	0.32	5 (2%) 53 43	49, 69, 80, 95	0
6	2G	181/182 (99%)	0.90	33 (18%) 1 1	52, 72, 83, 98	0
7	1H	173/180 (96%)	0.04	1 (0%) 89 86	54, 68, 77, 85	0
7	2H	173/180 (96%)	1.91	76 (43%) 0 0	57, 72, 81, 86	0
8	1I	146/148 (98%)	0.33	3 (2%) 63 54	51, 75, 85, 90	0
8	2I	146/148 (98%)	0.26	10 (6%) 17 10	53, 74, 86, 92	0
9	1N	140/140 (100%)	0.16	0 100 100	34, 51, 73, 78	0
9	2N	140/140 (100%)	0.24	1 (0%) 87 84	37, 55, 75, 81	0
10	1O	122/122 (100%)	-0.12	0 100 100	25, 41, 58, 68	0
10	2O	122/122 (100%)	0.48	4 (3%) 46 36	45, 62, 74, 80	0
11	1P	149/150 (99%)	0.22	1 (0%) 87 84	27, 57, 78, 87	0
11	2P	149/150 (99%)	0.87	23 (15%) 2 1	29, 60, 79, 88	0
12	1Q	141/141 (100%)	0.37	2 (1%) 75 70	36, 53, 69, 84	0
12	2Q	141/141 (100%)	0.50	11 (7%) 13 7	38, 57, 73, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	0.05	0 100 100	32, 42, 57, 67	0
13	2R	118/118 (100%)	0.19	2 (1%) 70 63	35, 45, 58, 69	0
14	1S	110/112 (98%)	0.12	0 100 100	45, 60, 73, 77	0
14	2S	110/112 (98%)	0.58	7 (6%) 19 12	49, 64, 76, 79	0
15	1T	131/146 (89%)	0.15	0 100 100	42, 54, 76, 86	0
15	2T	131/146 (89%)	0.55	5 (3%) 40 30	46, 57, 76, 86	0
16	1U	116/118 (98%)	0.29	1 (0%) 84 80	28, 45, 61, 75	0
16	2U	116/118 (98%)	0.09	2 (1%) 70 63	34, 49, 65, 77	0
17	1V	101/101 (100%)	0.13	0 100 100	31, 54, 70, 82	0
17	2V	101/101 (100%)	0.57	6 (5%) 22 14	34, 58, 73, 81	0
18	1W	112/113 (99%)	0.17	2 (1%) 68 61	30, 40, 64, 88	0
18	2W	112/113 (99%)	-0.05	1 (0%) 84 80	33, 42, 65, 90	0
19	1X	95/96 (98%)	-0.21	0 100 100	24, 38, 64, 78	0
19	2X	95/96 (98%)	0.63	5 (5%) 26 17	43, 61, 75, 87	0
20	1Y	107/110 (97%)	0.12	1 (0%) 84 80	47, 61, 74, 84	0
20	2Y	107/110 (97%)	0.37	3 (2%) 53 43	51, 64, 76, 86	0
21	1Z	154/206 (74%)	0.49	6 (3%) 39 29	55, 73, 89, 97	0
21	2Z	160/206 (77%)	1.09	25 (15%) 2 1	58, 76, 91, 98	0
22	10	83/85 (97%)	0.27	1 (1%) 79 73	23, 40, 62, 71	0
22	20	83/85 (97%)	0.41	1 (1%) 79 73	46, 65, 76, 84	0
23	11	97/98 (98%)	0.19	3 (3%) 49 39	27, 45, 72, 79	0
23	21	97/98 (98%)	0.45	4 (4%) 37 27	41, 56, 79, 88	0
24	12	70/72 (97%)	0.05	0 100 100	43, 58, 71, 82	0
24	22	70/72 (97%)	0.64	3 (4%) 35 25	46, 61, 75, 82	0
25	13	59/60 (98%)	0.29	1 (1%) 70 63	36, 50, 70, 83	0
25	23	59/60 (98%)	0.62	5 (8%) 10 5	41, 53, 74, 84	0
26	14	69/71 (97%)	0.79	13 (18%) 1 1	68, 82, 92, 97	0
26	24	69/71 (97%)	1.13	15 (21%) 0 0	72, 83, 92, 95	0
27	15	59/60 (98%)	0.05	1 (1%) 70 63	27, 41, 66, 71	0
27	25	59/60 (98%)	-0.08	0 100 100	29, 45, 67, 71	0
28	16	53/54 (98%)	0.18	0 100 100	41, 50, 65, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.34	4 (7%) 14 8	42, 53, 67, 73	0
29	17	48/49 (97%)	0.21	1 (2%) 63 54	26, 32, 62, 71	0
29	27	48/49 (97%)	0.08	3 (6%) 20 12	28, 35, 62, 70	0
30	18	64/65 (98%)	0.20	0 100 100	35, 44, 55, 68	0
30	28	64/65 (98%)	0.46	2 (3%) 49 39	38, 47, 58, 67	0
31	19	37/37 (100%)	0.11	0 100 100	31, 40, 58, 65	0
31	29	37/37 (100%)	0.97	5 (13%) 3 1	52, 71, 80, 81	0
32	1a	1488/1521 (97%)	0.03	22 (1%) 73 68	35, 63, 92, 109	0
32	2a	1491/1521 (98%)	0.11	31 (2%) 63 54	47, 77, 96, 107	0
33	1b	231/256 (90%)	0.29	11 (4%) 30 21	65, 82, 89, 96	0
33	2b	231/256 (90%)	0.88	31 (13%) 3 1	68, 83, 90, 98	0
34	1c	206/239 (86%)	0.32	7 (3%) 45 35	63, 76, 84, 91	0
34	2c	206/239 (86%)	1.63	73 (35%) 0 0	67, 78, 86, 91	0
35	1d	208/209 (99%)	0.14	1 (0%) 91 88	59, 71, 82, 87	0
35	2d	208/209 (99%)	0.61	11 (5%) 26 17	60, 72, 83, 88	0
36	1e	148/162 (91%)	0.17	0 100 100	57, 70, 79, 87	0
36	2e	148/162 (91%)	0.37	2 (1%) 75 70	60, 72, 81, 88	0
37	1f	100/101 (99%)	0.00	1 (1%) 82 77	48, 65, 77, 82	0
37	2f	100/101 (99%)	-0.05	1 (1%) 82 77	53, 70, 79, 86	0
38	1g	155/156 (99%)	0.60	15 (9%) 7 4	63, 72, 83, 95	0
38	2g	155/156 (99%)	1.09	29 (18%) 1 1	64, 74, 84, 95	0
39	1h	137/138 (99%)	0.19	2 (1%) 73 68	59, 72, 79, 88	0
39	2h	137/138 (99%)	0.70	5 (3%) 42 32	63, 74, 81, 88	0
40	1i	127/128 (99%)	0.66	12 (9%) 8 4	49, 73, 85, 91	0
40	2i	127/128 (99%)	2.02	60 (47%) 0 0	69, 83, 91, 93	0
41	1j	97/105 (92%)	0.65	11 (11%) 5 3	60, 80, 90, 93	0
41	2j	96/105 (91%)	2.08	40 (41%) 0 0	63, 81, 91, 97	0
42	1k	114/129 (88%)	0.66	7 (6%) 21 13	53, 68, 78, 85	0
42	2k	114/129 (88%)	0.24	3 (2%) 56 46	53, 69, 79, 85	0
43	1l	121/132 (91%)	0.04	1 (0%) 86 81	45, 58, 70, 84	0
43	2l	121/132 (91%)	0.02	0 100 100	46, 61, 72, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.30	5 (4%) 37 27	50, 67, 80, 88	0
44	2m	122/126 (96%)	1.28	34 (27%) 0 0	67, 83, 89, 93	0
45	1n	60/61 (98%)	0.44	2 (3%) 46 36	62, 71, 76, 81	0
45	2n	60/61 (98%)	2.76	44 (73%) 0 0	67, 74, 80, 85	0
46	1o	88/89 (98%)	0.49	5 (5%) 23 15	55, 68, 79, 83	0
46	2o	88/89 (98%)	0.20	0 100 100	58, 70, 80, 83	0
47	1p	82/88 (93%)	0.69	5 (6%) 21 13	57, 68, 79, 81	0
47	2p	82/88 (93%)	0.38	0 100 100	60, 68, 78, 84	0
48	1q	99/105 (94%)	0.56	2 (2%) 65 56	57, 70, 79, 83	0
48	2q	99/105 (94%)	0.97	10 (10%) 7 4	58, 71, 81, 84	0
49	1r	68/88 (77%)	0.68	4 (5%) 22 14	58, 68, 80, 83	0
49	2r	68/88 (77%)	0.01	2 (2%) 51 41	59, 69, 80, 85	0
50	1s	83/93 (89%)	0.52	3 (3%) 42 32	67, 76, 85, 92	0
50	2s	83/93 (89%)	1.20	19 (22%) 0 0	71, 79, 86, 93	0
51	1t	96/106 (90%)	1.40	25 (26%) 0 0	59, 70, 82, 89	0
51	2t	96/106 (90%)	1.32	21 (21%) 0 0	59, 70, 82, 89	0
52	1u	23/27 (85%)	0.63	0 100 100	64, 71, 77, 82	0
52	2u	23/27 (85%)	2.00	12 (52%) 0 0	67, 73, 79, 83	0
53	1v	13/24 (54%)	0.39	1 (7%) 13 7	43, 51, 74, 97	0
53	2v	13/24 (54%)	0.48	1 (7%) 13 7	63, 82, 98, 100	0
54	1w	67/76 (88%)	0.38	6 (8%) 9 5	49, 84, 99, 106	0
54	1y	67/76 (88%)	0.46	3 (4%) 33 23	39, 91, 99, 103	0
54	2w	65/76 (85%)	0.41	6 (9%) 9 5	62, 95, 102, 105	0
54	2y	66/76 (86%)	0.61	1 (1%) 73 68	49, 97, 101, 102	0
55	1x	72/77 (93%)	0.07	1 (1%) 75 70	33, 66, 82, 91	0
55	2x	72/77 (93%)	-0.01	0 100 100	50, 79, 88, 95	0
All	All	20873/21748 (95%)	0.31	986 (4%) 31 22	23, 63, 89, 109	0

All (986) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	10.0
41	2j	47	PHE	8.1

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Mol	Chain	Res	Type	RSRZ
38	1g	82	GLY	7.8
38	2g	82	GLY	7.6
21	2Z	144	LEU	7.3
33	2b	165	VAL	7.2
45	2n	39	LEU	7.1
1	2A	883	G	6.7
44	2m	123	ALA	6.6
32	2a	1030(B)	C	6.6
1	1A	931	C	6.5
45	2n	2	ALA	6.3
45	2n	25	VAL	6.3
34	2c	198	VAL	6.1
38	2g	80	VAL	6.1
51	2t	24	LEU	6.0
38	1g	79	ARG	5.9
54	1w	70	G	5.8
38	1g	83	ALA	5.8
34	2c	13	GLY	5.6
45	2n	34	TYR	5.6
41	2j	40	LEU	5.5
11	2P	1	MET	5.5
38	1g	80	VAL	5.5
7	2H	45	VAL	5.4
34	2c	182	ILE	5.4
41	2j	10	GLY	5.4
26	14	54	GLY	5.3
1	1A	942	A	5.2
32	1a	1030(B)	C	5.1
34	2c	33	LEU	5.1
40	2i	19	LEU	5.0
38	2g	156	TRP	5.0
1	1A	932	C	5.0
38	2g	16	LEU	4.9
7	2H	2	SER	4.9
45	2n	10	ALA	4.9
33	2b	215	LEU	4.8
6	2G	137	GLU	4.8
40	2i	7	THR	4.8
34	2c	204	LEU	4.8
26	24	51	ASP	4.7
6	2G	146	TYR	4.7
40	2i	109	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
26	24	49	PHE	4.6
38	2g	85	TYR	4.6
51	1t	95	ALA	4.6
44	2m	102	ARG	4.6
44	2m	6	GLY	4.6
32	2a	1034	G	4.5
1	2A	2146	C	4.5
33	2b	121	LEU	4.5
48	2q	80	GLY	4.5
41	2j	64	GLU	4.5
32	1a	1036	G	4.5
6	2G	140	ILE	4.5
21	1Z	149	SER	4.5
12	2Q	104	PHE	4.4
41	2j	55	LYS	4.4
21	2Z	155	LEU	4.4
34	2c	189	ALA	4.4
41	2j	63	PHE	4.4
5	2F	21	ALA	4.4
54	2w	71	G	4.4
50	2s	71	LEU	4.4
41	2j	44	VAL	4.4
1	2A	885	C	4.4
1	2A	884	C	4.3
44	2m	90	LEU	4.3
1	2A	2131	G	4.3
7	2H	115	VAL	4.3
1	1A	1555	C	4.3
1	2A	896	A	4.3
44	2m	15	VAL	4.3
44	2m	3	ARG	4.3
34	2c	14	ILE	4.3
45	2n	37	PHE	4.3
6	2G	139	LEU	4.3
54	1w	71	G	4.3
7	2H	98	LEU	4.2
51	2t	26	ASN	4.2
17	2V	101	GLY	4.2
7	2H	123	PHE	4.2
34	2c	155	GLY	4.1
7	2H	159	GLU	4.1
34	2c	158	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
40	2i	115	GLY	4.1
41	2j	62	HIS	4.1
7	2H	93	GLY	4.1
34	2c	188	LEU	4.1
40	2i	17	VAL	4.1
26	24	50	VAL	4.1
23	11	2	SER	4.1
51	1t	55	ILE	4.0
32	1a	1030(A)	G	4.0
41	2j	72	VAL	4.0
1	2A	1509	C	4.0
40	2i	26	VAL	4.0
6	1G	146	TYR	4.0
7	2H	166	GLY	4.0
38	1g	156	TRP	4.0
33	2b	122	PHE	4.0
41	2j	48	THR	4.0
45	2n	23	ARG	4.0
32	2a	1030(C)	G	4.0
7	2H	37	VAL	4.0
26	14	57	GLU	4.0
35	2d	47	ARG	4.0
51	2t	21	LYS	4.0
23	21	2	SER	4.0
1	1A	2167	C	3.9
32	1a	1030(C)	G	3.9
33	2b	48	MET	3.9
32	1a	204	U	3.9
7	2H	148	ILE	3.9
34	2c	21	ARG	3.9
34	2c	60	ALA	3.9
11	2P	123	LEU	3.9
38	2g	79	ARG	3.9
45	2n	35	ARG	3.9
34	2c	186	PHE	3.9
7	2H	145	ALA	3.9
26	14	4	GLY	3.9
40	2i	9	ARG	3.9
41	2j	46	ARG	3.9
16	1U	117	GLN	3.9
41	2j	66	ARG	3.8
21	2Z	156	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
34	2c	41	GLY	3.8
1	2A	882	G	3.8
34	2c	185	GLY	3.8
33	2b	118	LEU	3.8
45	2n	53	LEU	3.8
7	2H	24	VAL	3.8
34	2c	206	GLU	3.8
21	2Z	149	SER	3.8
34	2c	201	TYR	3.8
34	1c	13	GLY	3.8
45	2n	22	THR	3.8
6	2G	142	PRO	3.8
6	2G	152	LEU	3.7
45	2n	50	LYS	3.7
33	2b	135	GLN	3.7
17	2V	14	VAL	3.7
32	2a	1257	U	3.7
44	2m	73	GLU	3.7
50	2s	80	TYR	3.7
6	2G	133	LEU	3.7
7	2H	72	ILE	3.7
40	2i	125	TYR	3.7
38	2g	83	ALA	3.7
26	24	56	VAL	3.7
33	1b	215	LEU	3.7
35	2d	176	LEU	3.7
25	23	60	GLU	3.7
7	2H	43	VAL	3.7
52	2u	14	TRP	3.7
7	2H	46	GLU	3.7
34	2c	65	ALA	3.7
41	2j	11	PHE	3.7
41	1j	98	ILE	3.7
31	29	12	ASP	3.6
41	2j	87	THR	3.7
41	1j	95	GLU	3.6
25	23	26	LEU	3.6
51	2t	23	ARG	3.6
20	2Y	91	GLU	3.6
40	2i	110	GLU	3.6
40	2i	15	ALA	3.6
44	2m	66	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
35	2d	160	GLN	3.6
40	2i	81	ILE	3.6
34	2c	184	TYR	3.6
34	2c	132	ARG	3.6
52	2u	17	THR	3.6
26	24	54	GLY	3.6
40	2i	90	PRO	3.6
51	2t	80	ARG	3.6
7	2H	76	VAL	3.6
52	2u	10	ARG	3.6
32	2a	1030(A)	G	3.6
7	2H	34	GLU	3.6
26	14	66	SER	3.6
50	2s	79	THR	3.6
40	2i	65	VAL	3.5
45	2n	11	LYS	3.5
50	2s	30	LEU	3.5
51	1t	80	ARG	3.5
45	2n	61	TRP	3.5
34	2c	6	HIS	3.5
45	2n	24	CYS	3.5
19	2X	92	LEU	3.5
45	2n	6	LEU	3.5
11	2P	94	GLU	3.5
32	2a	1026	G	3.5
33	2b	92	TYR	3.5
41	2j	20	ALA	3.5
1	1A	1127	U	3.5
1	1A	930	G	3.5
1	1A	1105	G	3.5
34	2c	157	ILE	3.5
50	1s	40	ILE	3.5
39	2h	83	ILE	3.5
34	2c	8	ILE	3.5
44	2m	60	VAL	3.5
40	2i	30	GLY	3.4
41	2j	59	SER	3.4
45	2n	38	GLY	3.4
26	24	45	GLY	3.4
38	2g	7	ALA	3.4
7	2H	144	VAL	3.4
7	2H	47	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
42	1k	92	GLU	3.4
21	2Z	50	GLN	3.4
40	2i	52	ALA	3.4
41	2j	96	ILE	3.4
50	2s	12	ASP	3.4
40	2i	114	TYR	3.4
32	2a	80	G	3.4
7	2H	113	VAL	3.4
20	2Y	106	LEU	3.4
32	1a	1030	C	3.4
1	2A	2158	A	3.4
39	2h	2	LEU	3.4
40	2i	4	TYR	3.4
7	2H	48	GLY	3.3
15	2T	1	MET	3.3
40	2i	61	ALA	3.3
1	2A	2896	C	3.3
33	2b	187	LEU	3.3
48	2q	11	VAL	3.3
32	2a	1035	A	3.3
44	1m	124	PRO	3.3
29	27	47	ARG	3.3
35	2d	168	ARG	3.3
5	2F	7	TYR	3.3
28	26	20	ASN	3.3
51	2t	9	ASN	3.3
7	2H	105	LEU	3.3
40	2i	27	THR	3.3
7	2H	52	VAL	3.3
33	2b	133	LYS	3.3
7	2H	44	VAL	3.3
38	2g	140	ASP	3.3
1	1A	1104	G	3.3
14	2S	57	LYS	3.3
34	2c	50	ALA	3.3
40	2i	18	PHE	3.3
1	1A	2163	G	3.3
32	2a	1036	G	3.3
40	2i	75	ASP	3.3
7	1H	2	SER	3.3
34	2c	196	LEU	3.3
1	2A	2132	U	3.3

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Mol	Chain	Res	Type	RSRZ
7	2H	13	LYS	3.3
45	2n	12	ARG	3.3
11	2P	125	VAL	3.2
31	29	13	LYS	3.2
50	2s	83	HIS	3.2
54	2w	45	U	3.2
1	1A	1103	A	3.2
1	2A	229	A	3.2
34	2c	190	ARG	3.2
6	2G	155	MET	3.2
6	2G	136	ARG	3.2
21	2Z	137	ILE	3.2
54	1y	20	U	3.2
21	2Z	170	THR	3.2
1	2A	2145	C	3.2
5	2F	23	ASP	3.2
40	2i	119	ALA	3.2
42	1k	14	VAL	3.2
52	2u	23	PRO	3.2
13	2R	69	ASP	3.2
34	2c	124	ILE	3.2
1	2A	888	C	3.2
41	2j	65	LEU	3.2
6	2G	157	ILE	3.2
32	1a	1446	U	3.2
44	2m	13	LYS	3.2
6	2G	49	ASP	3.2
41	1j	20	ALA	3.2
52	2u	6	ARG	3.2
51	2t	20	LEU	3.2
45	2n	4	LYS	3.1
26	24	32	TYR	3.1
45	2n	29	ARG	3.1
45	2n	57	ARG	3.1
7	2H	165	ALA	3.1
11	2P	140	ALA	3.1
34	2c	37	GLN	3.1
7	2H	94	TYR	3.1
7	2H	41	MET	3.1
40	2i	54	ASP	3.1
11	2P	124	LYS	3.1
1	1A	936	C	3.1

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Mol	Chain	Res	Type	RSRZ
21	2Z	121	HIS	3.1
34	2c	87	LEU	3.1
32	1a	1447	A	3.1
31	29	37	GLY	3.1
40	2i	108	VAL	3.1
11	2P	126	VAL	3.1
29	27	48	LYS	3.1
41	2j	56	HIS	3.1
41	2j	50	ILE	3.1
40	2i	14	VAL	3.1
19	2X	1	MET	3.1
45	2n	31	ARG	3.1
1	1A	1141	A	3.1
20	1Y	1	MET	3.1
40	2i	5	TYR	3.1
7	2H	89	ILE	3.1
45	2n	42	ILE	3.1
44	2m	120	LYS	3.1
12	2Q	61	GLY	3.1
21	1Z	100	VAL	3.0
34	2c	180	ALA	3.0
1	1A	935	C	3.0
35	2d	98	GLU	3.0
38	1g	85	TYR	3.0
33	2b	136	VAL	3.0
45	1n	2	ALA	3.0
1	1A	934	A	3.0
1	1A	2168	C	3.0
3	1D	275	LYS	3.0
33	2b	127	ILE	3.0
40	2i	70	LYS	3.0
7	2H	122	THR	3.0
11	2P	109	GLY	3.0
41	1j	10	GLY	3.0
50	2s	68	GLY	3.0
6	2G	39	ILE	3.0
10	2O	10	VAL	3.0
32	2a	1033	G	3.0
32	2a	1202	G	3.0
39	2h	13	ILE	3.0
7	2H	49	VAL	3.0
7	2H	133	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
26	24	63	TYR	3.0
21	2Z	96	VAL	3.0
41	2j	49	VAL	3.0
1	1A	1144	A	3.0
7	2H	71	LEU	3.0
24	22	1	MET	3.0
1	1A	929	G	3.0
6	2G	59	GLU	3.0
32	1a	1257	U	3.0
41	2j	88	LEU	3.0
32	1a	1030(D)	A	3.0
32	2a	1030(D)	A	3.0
26	14	55	ARG	3.0
45	2n	54	PRO	3.0
1	1A	1139	G	3.0
7	2H	6	ARG	3.0
51	1t	47	GLY	3.0
46	1o	87	ILE	3.0
21	2Z	70	LEU	2.9
40	2i	92	TYR	2.9
44	2m	65	LYS	2.9
33	2b	152	PHE	2.9
34	2c	71	ALA	2.9
45	2n	55	GLY	2.9
11	2P	149	GLU	2.9
32	2a	1030	C	2.9
45	2n	26	ARG	2.9
51	2t	22	ARG	2.9
34	2c	187	ALA	2.9
6	2G	41	GLN	2.9
34	2c	4	LYS	2.9
51	2t	63	ILE	2.9
12	2Q	109	VAL	2.9
34	2c	200	ALA	2.9
48	2q	22	LEU	2.9
54	1w	44	G	2.9
54	1y	47	U	2.9
7	2H	74	ASN	2.9
38	1g	78	ARG	2.9
45	2n	41	ARG	2.9
41	1j	96	ILE	2.9
51	1t	69	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	1A	2153	G	2.9
32	2a	1031	G	2.9
7	2H	162	ILE	2.9
6	2G	159	VAL	2.9
29	17	48	LYS	2.9
40	2i	64	THR	2.9
41	2j	71	LEU	2.9
1	1A	2154	U	2.9
32	1a	1024	G	2.9
40	2i	36	TYR	2.9
11	2P	144	GLU	2.9
21	2Z	145	GLU	2.9
5	2F	208	GLY	2.9
33	1b	163	PHE	2.9
1	2A	2127	G	2.9
7	2H	51	ARG	2.9
37	1f	46	ARG	2.9
38	1g	81	GLY	2.9
24	22	61	LEU	2.9
38	1g	153	HIS	2.8
11	2P	118	GLY	2.8
51	2t	83	ARG	2.8
41	2j	85	LEU	2.8
51	2t	29	LYS	2.8
50	2s	69	HIS	2.8
33	2b	220	ASP	2.8
44	2m	71	ARG	2.8
40	2i	101	PHE	2.8
47	1p	21	VAL	2.8
6	1G	182	LYS	2.8
33	2b	132	LYS	2.8
1	2A	2173	A	2.8
6	2G	161	THR	2.8
41	2j	70	ARG	2.8
40	2i	38	GLN	2.8
1	1A	1140	U	2.8
34	2c	79	ARG	2.8
51	1t	86	ARG	2.8
45	2n	7	ILE	2.8
32	2a	1001(A)	G	2.8
42	1k	81	ASP	2.8
51	1t	74	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
50	2s	52	TYR	2.8
11	1P	105	LEU	2.8
7	2H	36	PRO	2.8
11	2P	97	PRO	2.8
18	1W	111	HIS	2.8
34	2c	57	ILE	2.8
41	2j	98	ILE	2.8
6	2G	34	LEU	2.8
40	2i	28	VAL	2.8
21	2Z	122	ARG	2.8
1	1A	1128	U	2.8
44	2m	4	ILE	2.8
8	1I	117	GLU	2.8
19	2X	93	GLU	2.8
34	2c	32	LEU	2.8
31	29	15	LYS	2.8
40	2i	87	GLN	2.8
17	2V	42	GLY	2.8
33	2b	216	SER	2.8
26	14	58	ARG	2.8
38	1g	16	LEU	2.8
1	1A	933	C	2.8
1	1A	2176	G	2.8
32	2a	1021	G	2.8
54	2w	70	G	2.8
7	2H	126	PRO	2.8
35	2d	49	ARG	2.8
38	2g	78	ARG	2.8
6	2G	182	LYS	2.8
6	1G	145	THR	2.8
33	2b	37	ASN	2.7
28	26	54	ILE	2.7
40	2i	63	ILE	2.7
11	2P	105	LEU	2.7
17	2V	94	LEU	2.7
45	2n	47	LEU	2.7
38	2g	147	ALA	2.7
54	1w	3	C	2.7
7	2H	7	LEU	2.7
26	14	50	VAL	2.7
54	2w	44	G	2.7
40	1i	106	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
34	2c	145	GLY	2.7
51	1t	83	ARG	2.7
41	2j	38	ILE	2.7
34	2c	138	VAL	2.7
40	2i	56	LEU	2.7
1	1A	943	C	2.7
7	2H	19	VAL	2.7
7	2H	128	PRO	2.7
26	14	56	VAL	2.7
33	2b	188	ALA	2.7
36	2e	94	ALA	2.7
38	2g	40	ALA	2.7
40	2i	62	TYR	2.7
12	2Q	66	ILE	2.7
33	2b	70	PHE	2.7
6	2G	92	VAL	2.7
5	2F	131	GLY	2.7
35	2d	165	MET	2.7
38	1g	154	TYR	2.7
21	2Z	69	THR	2.7
35	1d	110	PHE	2.7
1	1A	1133	G	2.7
6	2G	17	PRO	2.7
6	2G	28	VAL	2.7
51	2t	13	LEU	2.7
21	2Z	138	GLU	2.7
49	2r	46	GLU	2.7
12	1Q	33	GLY	2.7
1	1A	2134	G	2.7
40	1i	15	ALA	2.7
40	1i	76	ALA	2.7
51	2t	30	LYS	2.7
44	2m	87	TYR	2.7
54	1w	20	U	2.7
38	2g	84	ASN	2.7
6	2G	2	PRO	2.7
34	2c	199	LYS	2.7
34	2c	149	ALA	2.7
7	2H	56	SER	2.6
32	1a	1531	A	2.6
26	24	53	GLU	2.6
34	2c	175	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
40	2i	102	LEU	2.6
4	2E	115	GLY	2.6
45	2n	28	GLY	2.6
1	2A	886	C	2.6
1	2A	2128	C	2.6
32	2a	1117	G	2.6
34	2c	39	ILE	2.6
40	2i	88	TYR	2.6
11	2P	122	PRO	2.6
40	2i	10	ARG	2.6
40	2i	107	ARG	2.6
52	2u	13	ILE	2.6
8	2l	12	LEU	2.6
32	1a	1003	G	2.6
32	1a	1034	G	2.6
44	1m	87	TYR	2.6
1	1A	1142	A	2.6
40	2i	53	VAL	2.6
10	2O	41	ALA	2.6
38	2g	8	GLU	2.6
6	2G	62	LEU	2.6
11	2P	88	LEU	2.6
38	2g	77	SER	2.6
34	2c	173	VAL	2.6
40	2i	6	GLY	2.6
1	1A	1114	G	2.6
1	2A	2155	G	2.6
33	2b	211	ILE	2.6
7	2H	80	SER	2.6
12	2Q	28	ALA	2.6
40	2i	106	ALA	2.6
41	2j	41	PRO	2.6
38	2g	33	ASP	2.6
7	2H	18	GLU	2.6
44	2m	5	ALA	2.6
7	2H	101	ARG	2.6
1	2A	652(B)	A	2.6
11	2P	106	LEU	2.6
8	2l	3	VAL	2.6
48	2q	42	TYR	2.6
51	1t	71	THR	2.6
1	1A	2174	G	2.6

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Mol	Chain	Res	Type	RSRZ
7	2H	124	GLU	2.6
32	2a	204	U	2.6
41	2j	68	HIS	2.6
51	1t	24	LEU	2.6
32	2a	1024	G	2.6
11	2P	95	VAL	2.6
31	29	16	VAL	2.6
7	2H	3	ARG	2.6
38	2g	62	PHE	2.6
45	2n	30	ALA	2.6
49	1r	25	THR	2.5
51	1t	84	LEU	2.5
52	2u	8	THR	2.5
1	1A	2165	C	2.5
12	2Q	60	ARG	2.5
14	2S	20	ARG	2.5
25	23	6	VAL	2.5
40	2i	95	LYS	2.5
51	2t	34	LYS	2.5
54	1y	56	C	2.5
52	2u	18	TYR	2.5
34	2c	203	PHE	2.5
34	2c	51	GLY	2.5
19	2X	68	ARG	2.5
46	1o	68	ARG	2.5
44	1m	2	ALA	2.5
40	2i	124	GLN	2.5
44	2m	122	LYS	2.5
32	1a	1035	A	2.5
7	2H	119	GLU	2.5
34	2c	202	ILE	2.5
51	2t	25	ARG	2.5
34	2c	91	LEU	2.5
21	2Z	173	ALA	2.5
25	13	60	GLU	2.5
6	2G	181	ARG	2.5
26	24	68	ARG	2.5
51	1t	70	SER	2.5
38	1g	42	ILE	2.5
40	2i	41	VAL	2.5
34	2c	146	ALA	2.5
1	2A	2174	C	2.5

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Mol	Chain	Res	Type	RSRZ
32	2a	1116	C	2.5
14	2S	35	ILE	2.5
40	1i	81	ILE	2.5
33	2b	69	LEU	2.5
45	2n	58	LYS	2.5
7	2H	81	GLU	2.5
33	2b	140	HIS	2.5
45	2n	8	GLU	2.5
50	2s	14	HIS	2.5
8	2I	19	VAL	2.5
34	2c	64	VAL	2.5
42	1k	91	ARG	2.5
41	1j	92	THR	2.5
54	2y	34	G	2.5
40	2i	127	LYS	2.5
40	2i	79	LEU	2.5
50	2s	35	SER	2.5
41	1j	97	GLU	2.5
44	2m	8	GLU	2.5
33	2b	163	PHE	2.5
7	2H	77	LYS	2.5
38	2g	51	GLN	2.5
52	2u	16	GLY	2.5
7	2H	106	THR	2.5
11	2P	110	TYR	2.5
33	1b	61	LEU	2.5
41	2j	34	VAL	2.4
21	2Z	51	ALA	2.4
33	2b	47	THR	2.4
34	2c	193	TYR	2.4
1	1A	2151	C	2.4
45	2n	36	PHE	2.4
50	2s	32	LYS	2.4
50	2s	82	GLY	2.4
53	1v	12	A	2.4
21	1Z	168	GLU	2.4
51	1t	53	LEU	2.4
34	2c	80	GLY	2.4
6	2G	151	ALA	2.4
46	1o	65	ARG	2.4
21	1Z	169	GLU	2.4
7	2H	64	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
16	2U	88	ILE	2.4
48	2q	74	LEU	2.4
41	2j	15	THR	2.4
44	1m	23	TYR	2.4
7	2H	57	ASP	2.4
18	2W	112	GLY	2.4
33	2b	101	MET	2.4
33	1b	78	GLN	2.4
40	2i	42	ARG	2.4
51	1t	18	GLN	2.4
24	22	24	LEU	2.4
38	2g	154	TYR	2.4
7	2H	31	GLY	2.4
38	1g	77	SER	2.4
5	2F	24	LEU	2.4
7	2H	107	VAL	2.4
21	2Z	147	GLY	2.4
27	15	60	VAL	2.4
40	2i	93	ARG	2.4
44	2m	23	TYR	2.4
7	2H	138	LYS	2.4
45	2n	51	GLY	2.4
26	24	57	GLU	2.4
52	2u	5	ASP	2.4
26	24	13	ARG	2.4
44	2m	94	ARG	2.4
44	2m	121	LYS	2.4
38	2g	129	GLU	2.4
21	2Z	148	ASP	2.4
32	2a	1004	A	2.4
32	2a	1005	A	2.4
34	1c	62	ASP	2.4
34	2c	154	SER	2.4
44	2m	42	ALA	2.4
49	1r	87	ARG	2.4
12	2Q	33	GLY	2.4
51	2t	98	PRO	2.4
1	1A	2137	G	2.4
34	2c	15	THR	2.4
39	2h	120	THR	2.4
9	2N	23	LEU	2.4
51	1t	100	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
26	14	68	ARG	2.3
32	2a	1220	G	2.3
33	2b	120	ALA	2.3
50	2s	81	ARG	2.3
52	2u	22	ARG	2.3
8	2I	34	GLY	2.3
1	1A	1106	U	2.3
48	2q	40	LYS	2.3
34	2c	131	ARG	2.3
50	1s	39	THR	2.3
33	2b	44	LEU	2.3
33	2b	200	ILE	2.3
35	2d	19	LEU	2.3
51	2t	36	LEU	2.3
11	2P	91	PHE	2.3
34	2c	197	GLY	2.3
1	1A	1110	C	2.3
1	2A	652(T)	C	2.3
4	2E	175	VAL	2.3
21	2Z	139	VAL	2.3
32	1a	1029	C	2.3
41	1j	72	VAL	2.3
54	2w	4	C	2.3
6	2G	115	ARG	2.3
33	2b	94	ASN	2.3
26	14	59	PHE	2.3
44	2m	64	TRP	2.3
1	1A	1130	A	2.3
26	24	46	GLN	2.3
44	2m	17	VAL	2.3
45	2n	56	VAL	2.3
1	1A	1138	C	2.3
34	2c	183	ASP	2.3
50	2s	13	ASP	2.3
51	1t	32	ALA	2.3
41	2j	8	LEU	2.3
6	2G	29	TRP	2.3
40	1i	31	GLN	2.3
7	2H	65	HIS	2.3
32	1a	1532	U	2.3
32	2a	89	C	2.3
41	2j	58	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
50	2s	50	ALA	2.3
51	2t	55	ILE	2.3
6	2G	93	THR	2.3
42	2k	46	GLY	2.3
38	1g	17	VAL	2.3
1	1A	2183	C	2.3
42	2k	35	PRO	2.3
45	2n	15	LYS	2.3
11	2P	147	LEU	2.3
34	2c	61	ALA	2.3
11	2P	79	ARG	2.3
40	2i	72	GLY	2.3
47	1p	42	ARG	2.3
45	2n	52	GLN	2.3
7	2H	17	VAL	2.3
8	1I	142	VAL	2.3
1	2A	2111	C	2.3
15	2T	99	LEU	2.3
22	10	7	LEU	2.3
7	2H	14	GLY	2.3
32	2a	983	A	2.3
38	2g	19	GLY	2.3
22	20	69	PHE	2.3
4	2E	184	VAL	2.3
7	2H	129	THR	2.3
33	1b	133	LYS	2.3
48	2q	9	VAL	2.3
1	1A	1143	U	2.3
41	2j	9	ARG	2.3
51	1t	64	ASP	2.3
5	2F	12	LEU	2.3
33	1b	77	ALA	2.3
8	2I	4	ILE	2.3
40	2i	37	PHE	2.3
54	2w	73	A	2.3
7	2H	33	LEU	2.2
8	2I	111	PRO	2.2
26	14	69	LYS	2.2
40	2i	43	ALA	2.2
44	2m	18	ALA	2.2
51	2t	91	LEU	2.2
32	2a	1039	C	2.2

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Mol	Chain	Res	Type	RSRZ
54	1w	72	C	2.2
34	2c	3	ASN	2.2
44	2m	91	ARG	2.2
8	2I	108	THR	2.2
34	1c	87	LEU	2.2
33	2b	214	ILE	2.2
7	2H	116	GLU	2.2
1	1A	1126	C	2.2
21	2Z	126	VAL	2.2
46	1o	72	ARG	2.2
48	2q	18	THR	2.2
6	2G	90	LEU	2.2
17	2V	62	LEU	2.2
34	1c	12	LEU	2.2
50	1s	47	HIS	2.2
48	1q	27	PHE	2.2
42	1k	25	TYR	2.2
51	2t	17	ARG	2.2
1	1A	1146	C	2.2
45	1n	17	LYS	2.2
21	1Z	170	THR	2.2
21	2Z	76	LEU	2.2
23	1l	98	LEU	2.2
35	2d	188	LEU	2.2
48	2q	76	LEU	2.2
33	1b	222	ILE	2.2
1	2A	652(U)	G	2.2
1	2A	2802	G	2.2
6	2G	138	GLN	2.2
32	1a	1026	G	2.2
34	2c	30	ARG	2.2
34	2c	59	ARG	2.2
42	2k	25	TYR	2.2
34	1c	64	VAL	2.2
41	1j	8	LEU	2.2
23	2l	76	ARG	2.2
12	2Q	1	MET	2.2
1	2A	2133	G	2.2
47	1p	39	TYR	2.2
17	2V	5	VAL	2.2
44	2m	119	GLY	2.2
52	2u	11	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
7	2H	103	LEU	2.2
8	1I	52	ARG	2.2
11	2P	85	LEU	2.2
41	2j	89	ASP	2.2
40	2i	55	ALA	2.2
41	2j	42	THR	2.2
45	2n	49	HIS	2.2
23	2I	81	LYS	2.2
26	14	62	ARG	2.2
38	2g	76	ARG	2.2
46	1o	89	GLY	2.2
32	1a	1027	C	2.2
38	2g	99	LEU	2.2
41	1j	16	LEU	2.2
45	2n	44	LEU	2.2
7	2H	96	ALA	2.2
34	2c	49	SER	2.2
44	2m	92	HIS	2.2
3	1D	276	LYS	2.2
6	2G	149	VAL	2.2
7	2H	86	GLU	2.2
8	2I	107	VAL	2.2
37	2f	59	TYR	2.2
42	1k	75	TYR	2.2
10	2O	122	LEU	2.2
1	1A	1111	U	2.2
1	2A	894	C	2.2
40	1i	19	LEU	2.2
41	1j	40	LEU	2.2
49	1r	40	LEU	2.2
51	1t	62	LEU	2.2
34	2c	100	ALA	2.2
50	2s	49	ILE	2.2
7	2H	112	PRO	2.2
33	2b	111	ARG	2.2
51	1t	68	LYS	2.2
1	2A	1508	A	2.2
19	2X	69	TYR	2.2
44	2m	74	VAL	2.2
40	1i	8	GLY	2.1
14	2S	58	LEU	2.1
7	2H	4	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
51	1t	59	ALA	2.1
6	2G	112	PRO	2.1
32	1a	1002	G	2.1
32	1a	1023	G	2.1
44	2m	67	GLU	2.1
40	2i	103	THR	2.1
45	2n	27	CYS	2.1
32	2a	1447	A	2.1
40	1i	18	PHE	2.1
45	2n	16	PHE	2.1
30	28	16	ILE	2.1
34	2c	167	TRP	2.1
11	2P	92	GLU	2.1
39	2h	136	GLU	2.1
41	2j	61	GLU	2.1
45	2n	46	GLU	2.1
1	2A	2154	G	2.1
40	2i	8	GLY	2.1
48	1q	33	GLY	2.1
34	2c	10	PHE	2.1
49	2r	85	LEU	2.1
51	1t	29	LYS	2.1
51	1t	39	LYS	2.1
44	2m	50	GLU	2.1
36	2e	10	MET	2.1
55	1x	67	C	2.1
40	1i	53	VAL	2.1
42	1k	80	VAL	2.1
48	2q	85	VAL	2.1
1	1A	2173	G	2.1
26	24	52	THR	2.1
8	2I	72	LEU	2.1
26	14	32	TYR	2.1
35	2d	68	TYR	2.1
7	2H	132	ARG	2.1
14	2S	41	ASP	2.1
1	1A	944	C	2.1
30	28	34	TRP	2.1
21	2Z	129	SER	2.1
34	2c	207	VAL	2.1
12	2Q	37	LEU	2.1
38	2g	4	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
34	2c	35	GLU	2.1
34	2c	47	LEU	2.1
39	1h	133	LEU	2.1
10	2O	81	ASP	2.1
50	2s	43	GLU	2.1
16	2U	104	GLN	2.1
23	21	58	ILE	2.1
40	1i	82	ALA	2.1
38	1g	84	ASN	2.1
5	2F	172	TRP	2.1
21	1Z	141	VAL	2.1
34	2c	22	TRP	2.1
51	1t	89	ARG	2.1
41	2j	16	LEU	2.1
51	2t	71	THR	2.1
32	2a	78	G	2.1
43	1l	14	GLY	2.1
6	1G	181	ARG	2.1
29	27	46	VAL	2.1
38	2g	32	ARG	2.1
40	2i	20	ARG	2.1
7	2H	25	LYS	2.1
7	2H	137	ASP	2.1
38	2g	13	GLN	2.1
45	2n	13	THR	2.1
1	1A	1112	U	2.1
50	2s	40	ILE	2.1
18	1W	112	GLY	2.1
15	2T	111	ARG	2.1
7	2H	29	PRO	2.1
7	2H	114	VAL	2.1
32	2a	1003	G	2.1
38	2g	155	ARG	2.1
34	2c	153	VAL	2.1
13	2R	65	LEU	2.1
15	2T	48	ILE	2.1
34	2c	56	ASP	2.1
1	2A	2144	U	2.1
15	2T	131	ALA	2.1
34	1c	65	ALA	2.1
44	1m	18	ALA	2.1
47	1p	4	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
32	1a	841	U	2.1
12	2Q	59	ARG	2.1
7	2H	141	VAL	2.1
8	2I	74	ASN	2.1
14	2S	33	LYS	2.1
33	1b	165	VAL	2.1
44	2m	12	ASN	2.1
6	1G	139	LEU	2.0
40	2i	99	LEU	2.0
1	1A	2150	C	2.0
34	1c	20	SER	2.0
7	2H	92	ILE	2.0
7	2H	121	ILE	2.0
41	2j	6	ILE	2.0
44	2m	78	ILE	2.0
49	1r	73	ALA	2.0
5	1F	89	VAL	2.0
47	1p	2	VAL	2.0
14	2S	32	LEU	2.0
28	26	11	LEU	2.0
38	2g	22	LEU	2.0
32	2a	79	G	2.0
32	2a	1131	G	2.0
53	2v	24	A	2.0
1	2A	1026	U	2.0
39	1h	3	THR	2.0
20	2Y	3	VAL	2.0
26	24	42	PHE	2.0
33	1b	94	ASN	2.0
33	1b	98	LEU	2.0
51	1t	20	LEU	2.0
12	1Q	59	ARG	2.0
4	2E	18	ASP	2.0
41	2j	93	GLY	2.0
1	2A	887	A	2.0
2	2B	119	G	2.0
21	2Z	42	VAL	2.0
28	26	5	VAL	2.0
34	2c	151	VAL	2.0
38	2g	9	VAL	2.0
40	1i	86	VAL	2.0
21	2Z	5	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
35	2d	161	ASN	2.0
12	2Q	22	LYS	2.0
25	23	27	GLY	2.0
51	1t	31	SER	2.0
1	2A	277	C	2.0
34	2c	23	TYR	2.0
45	2n	21	TYR	2.0
1	1A	1109	G	2.0
1	1A	1221	G	2.0
5	2F	6	VAL	2.0
25	23	54	VAL	2.0
40	2i	83	ARG	2.0
5	1F	41	LEU	2.0
6	2G	135	LEU	2.0
21	2Z	68	PRO	2.0
23	11	82	LEU	2.0
33	1b	76	GLN	2.0
40	1i	47	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
54	PSU	2y	55	20/21	0.73	0.29	92,98,114,119	0
54	5MU	1y	54	21/22	0.78	0.22	73,89,102,120	0
54	7MG	2w	46	24/25	0.79	0.23	86,100,114,145	0
54	PSU	1y	55	20/21	0.79	0.26	86,98,106,123	0
54	4SU	1y	8	20/21	0.81	0.18	87,98,107,113	0
54	7MG	2y	46	24/25	0.82	0.18	93,98,105,125	0
54	5MU	2y	54	21/22	0.83	0.25	82,92,106,130	0
54	4SU	2w	8	20/21	0.84	0.17	84,95,110,123	0
54	4SU	2y	8	20/21	0.84	0.13	89,98,109,120	0
54	PSU	2y	32	20/21	0.85	0.20	74,90,101,111	0
54	MIA	2y	37	22/30	0.85	0.20	71,86,96,112	0
54	7MG	1y	46	24/25	0.87	0.21	83,94,107,126	0
54	4SU	1w	8	20/21	0.87	0.15	75,82,99,108	0
54	7MG	1w	46	24/25	0.87	0.15	74,87,111,126	0
54	PSU	2w	55	20/21	0.88	0.18	66,88,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
54	PSU	2y	39	20/21	0.90	0.20	74,86,97,100	0
54	PSU	1y	39	20/21	0.90	0.19	69,80,87,89	0
54	MIA	1y	37	22/30	0.91	0.12	65,81,88,93	0
55	4SU	2x	8	20/21	0.91	0.19	66,79,93,93	0
55	PSU	1x	55	20/21	0.91	0.17	62,72,91,96	0
54	PSU	1w	55	20/21	0.91	0.15	67,77,89,95	0
54	PSU	1y	32	20/21	0.92	0.18	68,86,94,94	0
54	PSU	2w	39	20/21	0.92	0.18	61,81,86,87	0
55	PSU	2x	55	20/21	0.92	0.15	73,79,92,97	0
55	5MU	2x	54	21/22	0.93	0.17	74,83,90,105	0
54	PSU	2w	32	20/21	0.93	0.19	67,83,98,106	0
54	5MU	2w	54	21/22	0.93	0.14	62,80,88,92	0
32	2MG	2a	1207	24/25	0.94	0.13	70,80,89,102	0
32	M2G	2a	966	25/26	0.94	0.21	53,67,78,82	0
32	5MC	2a	967	21/22	0.94	0.17	57,71,78,79	0
55	5MU	1x	54	21/22	0.94	0.15	56,73,78,85	0
43	0TD	2l	92	10/11	0.94	0.19	53,60,64,85	0
32	4OC	2a	1402	22/23	0.94	0.17	52,64,71,74	0
32	PSU	2a	516	20/21	0.95	0.16	54,68,81,87	0
1	PSU	1A	1939	20/21	0.95	0.20	50,57,64,65	0
1	PSU	2A	1911	20/21	0.95	0.17	42,57,65,65	0
1	5MC	2A	1962	21/22	0.95	0.22	37,42,53,60	0
55	5MC	2x	32	21/22	0.95	0.21	65,72,77,83	0
1	PSU	2A	1917	20/21	0.95	0.15	52,62,66,70	0
1	5MU	2A	1915	21/22	0.95	0.14	52,64,68,68	0
43	0TD	1l	92	10/11	0.95	0.22	47,57,60,73	0
54	MIA	2w	37	25/30	0.95	0.16	66,79,88,95	0
55	4SU	1x	8	20/21	0.95	0.18	50,61,71,83	0
32	7MG	2a	527	24/25	0.95	0.16	52,64,75,87	0
32	MA6	2a	1518	24/25	0.96	0.18	50,65,75,80	0
32	5MC	2a	1407	21/22	0.96	0.20	40,55,59,68	0
1	5MU	1A	1937	21/22	0.96	0.19	49,62,65,68	0
1	5MC	2A	1942	21/22	0.96	0.19	42,53,59,66	0
54	PSU	1w	32	20/21	0.96	0.13	58,66,79,81	0
32	7MG	1a	527	24/25	0.96	0.16	37,48,54,61	0
32	5MC	2a	1400	21/22	0.96	0.20	50,68,78,89	0
32	MA6	2a	1519	24/25	0.96	0.20	44,61,71,73	0
32	2MG	1a	1207	24/25	0.96	0.14	56,65,69,76	0
32	5MC	2a	1404	21/22	0.96	0.17	47,56,60,67	0
1	4OC	2A	1920	21/23	0.97	0.15	43,52,58,61	0
32	5MC	1a	1407	21/22	0.97	0.19	31,42,48,51	0
32	UR3	2a	1498	21/22	0.97	0.17	49,56,60,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	PSU	1a	516	20/21	0.97	0.15	39,51,60,64	0
1	PSU	1A	1933	20/21	0.97	0.19	38,55,63,65	0
1	5MC	1A	1984	21/22	0.97	0.22	33,39,46,58	0
55	5MC	1x	32	21/22	0.97	0.18	42,47,58,59	0
1	PSU	2A	2605	20/21	0.97	0.18	25,32,38,38	0
54	5MU	1w	54	21/22	0.97	0.17	48,62,67,73	0
1	2MU	1A	2564	21/23	0.97	0.22	29,36,42,46	0
32	5MC	1a	1400	21/22	0.97	0.17	31,45,56,63	0
54	MIA	1w	37	29/30	0.97	0.17	31,47,60,67	0
54	PSU	1w	39	20/21	0.97	0.15	35,56,64,66	0
32	5MC	1a	1404	21/22	0.97	0.19	30,36,44,47	0
32	MA6	1a	1519	24/25	0.98	0.20	35,39,47,51	0
1	2MU	2A	2552	21/23	0.98	0.15	29,38,45,51	0
1	2MA	2A	2503	23/24	0.98	0.18	22,28,37,40	0
32	5MC	1a	967	21/22	0.98	0.16	45,53,65,65	0
1	OMG	1A	2263	24/25	0.98	0.19	24,33,37,37	0
1	4OC	1A	1942	21/23	0.98	0.21	37,48,53,57	0
32	M2G	1a	966	25/26	0.98	0.18	46,54,60,69	0
1	PSU	1A	2617	20/21	0.98	0.20	25,30,34,35	0
32	MA6	1a	1518	24/25	0.98	0.19	30,41,47,50	0
1	5MU	1A	1961	21/22	0.98	0.21	25,31,36,41	0
1	5MC	1A	1964	21/22	0.98	0.20	39,51,57,64	0
32	4OC	1a	1402	22/23	0.98	0.18	34,43,56,68	0
1	OMG	2A	2251	24/25	0.98	0.17	29,36,40,41	0
1	5MU	2A	1939	21/22	0.98	0.19	28,34,38,40	0
32	UR3	1a	1498	21/22	0.99	0.19	29,37,45,49	0
1	2MA	1A	2515	23/24	0.99	0.19	20,27,33,37	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
56	MG	2B	3011	1/1	0.01	0.58	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4085	1/1	0.16	0.27	99,99,99,99	0
56	MG	1a	1871	1/1	0.26	0.18	79,79,79,79	0
56	MG	2a	3146	1/1	0.27	0.13	114,114,114,114	0
56	MG	2l	3001	1/1	0.28	0.69	62,62,62,62	0
56	MG	2a	3031	1/1	0.28	0.55	76,76,76,76	0
56	MG	2A	3792	1/1	0.32	0.44	61,61,61,61	0
56	MG	1A	4054	1/1	0.33	0.26	73,73,73,73	0
56	MG	2a	3109	1/1	0.35	0.38	89,89,89,89	0
56	MG	2a	3173	1/1	0.37	0.29	104,104,104,104	0
56	MG	2y	3006	1/1	0.41	0.10	106,106,106,106	0
56	MG	1A	4048	1/1	0.41	0.11	68,68,68,68	0
56	MG	2v	102	1/1	0.41	0.49	93,93,93,93	0
56	MG	1B	227	1/1	0.42	0.63	106,106,106,106	0
56	MG	1w	103	1/1	0.42	0.57	80,80,80,80	0
56	MG	2a	3064	1/1	0.44	0.48	83,83,83,83	0
56	MG	2A	3360	1/1	0.44	0.14	70,70,70,70	0
56	MG	2a	3131	1/1	0.44	0.18	90,90,90,90	0
56	MG	2a	3056	1/1	0.45	0.21	71,71,71,71	0
56	MG	2a	3162	1/1	0.45	0.24	100,100,100,100	0
56	MG	1A	3351	1/1	0.45	0.55	72,72,72,72	0
56	MG	1l	203	1/1	0.46	0.11	75,75,75,75	0
56	MG	1A	4068	1/1	0.47	0.28	83,83,83,83	0
56	MG	2a	3029	1/1	0.48	1.16	90,90,90,90	0
56	MG	1x	110	1/1	0.49	0.20	75,75,75,75	0
56	MG	1A	4083	1/1	0.50	0.15	63,63,63,63	0
56	MG	1A	4141	1/1	0.50	0.11	63,63,63,63	0
56	MG	2A	3816	1/1	0.50	0.32	75,75,75,75	0
56	MG	2A	3665	1/1	0.50	0.25	53,53,53,53	0
56	MG	1A	3357	1/1	0.51	0.30	69,69,69,69	0
56	MG	1A	3366	1/1	0.53	0.78	60,60,60,60	0
56	MG	2A	3411	1/1	0.53	0.75	52,52,52,52	0
56	MG	1a	1615	1/1	0.53	0.53	87,87,87,87	0
56	MG	2a	3003	1/1	0.54	0.20	75,75,75,75	0
56	MG	1a	1710	1/1	0.55	0.22	79,79,79,79	0
56	MG	2A	3382	1/1	0.55	0.43	55,55,55,55	0
56	MG	2a	3026	1/1	0.56	1.04	88,88,88,88	0
56	MG	1A	4116	1/1	0.56	0.35	85,85,85,85	0
56	MG	2a	3140	1/1	0.56	0.21	95,95,95,95	0
56	MG	2A	3872	1/1	0.57	0.33	63,63,63,63	0
56	MG	10	102	1/1	0.57	0.59	77,77,77,77	0
56	MG	2A	3798	1/1	0.57	0.21	75,75,75,75	0
56	MG	1A	3417	1/1	0.57	0.76	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4166	1/1	0.58	0.18	70,70,70,70	0
56	MG	1A	4180	1/1	0.58	0.39	62,62,62,62	0
56	MG	1A	3369	1/1	0.58	1.00	66,66,66,66	0
56	MG	2a	3182	1/1	0.58	0.16	74,74,74,74	0
56	MG	1A	3260	1/1	0.59	0.33	57,57,57,57	0
56	MG	1A	4014	1/1	0.59	0.08	81,81,81,81	0
56	MG	2a	3222	1/1	0.60	0.43	94,94,94,94	0
56	MG	2A	3059	1/1	0.61	0.24	57,57,57,57	0
56	MG	1x	102	1/1	0.61	0.55	74,74,74,74	0
56	MG	2A	3831	1/1	0.61	0.10	57,57,57,57	0
56	MG	1A	4099	1/1	0.61	0.10	82,82,82,82	0
56	MG	2A	3284	1/1	0.62	0.23	56,56,56,56	0
56	MG	1A	3646	1/1	0.63	0.29	49,49,49,49	0
56	MG	1A	3540	1/1	0.63	0.34	60,60,60,60	0
56	MG	1A	3222	1/1	0.63	0.60	71,71,71,71	0
56	MG	2A	3864	1/1	0.63	0.12	73,73,73,73	0
56	MG	1B	228	1/1	0.63	0.32	80,80,80,80	0
56	MG	2A	3343	1/1	0.63	1.04	63,63,63,63	0
56	MG	1a	1725	1/1	0.63	0.12	62,62,62,62	0
56	MG	1A	4009	1/1	0.64	0.14	81,81,81,81	0
56	MG	1A	3756	1/1	0.64	0.15	67,67,67,67	0
56	MG	2A	3332	1/1	0.64	0.38	53,53,53,53	0
56	MG	1a	1914	1/1	0.64	0.13	84,84,84,84	0
56	MG	2A	3410	1/1	0.64	0.36	71,71,71,71	0
56	MG	2A	3683	1/1	0.64	0.18	49,49,49,49	0
56	MG	1G	3002	1/1	0.64	0.17	63,63,63,63	0
56	MG	2a	3204	1/1	0.64	0.18	90,90,90,90	0
56	MG	1A	3915	1/1	0.65	0.20	51,51,51,51	0
56	MG	1A	4050	1/1	0.65	0.08	57,57,57,57	0
56	MG	1x	113	1/1	0.65	0.24	48,48,48,48	0
56	MG	2A	3894	1/1	0.65	0.24	60,60,60,60	0
56	MG	2A	3832	1/1	0.65	0.20	69,69,69,69	0
56	MG	2A	3837	1/1	0.65	0.17	48,48,48,48	0
56	MG	2a	3116	1/1	0.66	0.17	73,73,73,73	0
56	MG	1a	1658	1/1	0.66	0.25	84,84,84,84	0
56	MG	1A	4162	1/1	0.66	0.16	68,68,68,68	0
56	MG	2A	3823	1/1	0.66	0.49	79,79,79,79	0
56	MG	1A	3386	1/1	0.66	0.20	63,63,63,63	0
56	MG	2A	3527	1/1	0.67	0.13	38,38,38,38	0
56	MG	2A	3868	1/1	0.67	0.23	71,71,71,71	0
56	MG	2A	3874	1/1	0.67	0.12	74,74,74,74	0
56	MG	1a	1915	1/1	0.67	0.07	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3169	1/1	0.67	0.14	80,80,80,80	0
56	MG	2A	3617	1/1	0.67	0.20	47,47,47,47	0
56	MG	2a	3054	1/1	0.67	0.20	61,61,61,61	0
56	MG	1a	1881	1/1	0.67	0.09	73,73,73,73	0
56	MG	1A	3600	1/1	0.67	0.14	64,64,64,64	0
56	MG	1A	3007	1/1	0.68	0.35	52,52,52,52	0
56	MG	1A	4087	1/1	0.68	0.36	79,79,79,79	0
56	MG	1a	1874	1/1	0.68	0.11	82,82,82,82	0
56	MG	1A	4146	1/1	0.68	0.88	80,80,80,80	0
56	MG	2A	3734	1/1	0.68	0.27	67,67,67,67	0
56	MG	2A	3090	1/1	0.68	0.10	71,71,71,71	0
56	MG	1a	1607	1/1	0.68	0.14	71,71,71,71	0
56	MG	1w	108	1/1	0.68	0.20	63,63,63,63	0
56	MG	1l	102	1/1	0.68	0.35	58,58,58,58	0
56	MG	2A	3388	1/1	0.68	0.18	65,65,65,65	0
56	MG	2a	3066	1/1	0.68	0.30	77,77,77,77	0
56	MG	1A	3383	1/1	0.68	0.53	72,72,72,72	0
56	MG	1A	3890	1/1	0.68	0.12	65,65,65,65	0
56	MG	2A	3362	1/1	0.68	0.29	61,61,61,61	0
56	MG	1a	1751	1/1	0.68	0.12	78,78,78,78	0
56	MG	2a	3034	1/1	0.68	0.40	64,64,64,64	0
56	MG	2A	3068	1/1	0.69	0.19	56,56,56,56	0
56	MG	1A	3987	1/1	0.69	0.09	71,71,71,71	0
56	MG	1a	1861	1/1	0.69	0.31	102,102,102,102	0
56	MG	2a	3007	1/1	0.69	0.16	70,70,70,70	0
56	MG	1a	1693	1/1	0.69	0.16	66,66,66,66	0
56	MG	1A	4123	1/1	0.69	0.17	78,78,78,78	0
56	MG	1A	3358	1/1	0.69	0.35	64,64,64,64	0
56	MG	2A	3713	1/1	0.69	0.12	63,63,63,63	0
56	MG	2A	3495	1/1	0.69	0.58	66,66,66,66	0
56	MG	1A	4063	1/1	0.70	0.38	63,63,63,63	0
56	MG	1A	4111	1/1	0.70	0.21	92,92,92,92	0
56	MG	2a	3086	1/1	0.70	0.60	81,81,81,81	0
56	MG	1A	4151	1/1	0.70	0.28	59,59,59,59	0
56	MG	1a	1887	1/1	0.70	0.16	57,57,57,57	0
56	MG	1A	3464	1/1	0.70	0.19	50,50,50,50	0
56	MG	1A	4015	1/1	0.70	0.22	73,73,73,73	0
56	MG	2a	3044	1/1	0.70	0.17	70,70,70,70	0
56	MG	1A	4038	1/1	0.70	0.15	71,71,71,71	0
56	MG	2a	3170	1/1	0.70	0.13	79,79,79,79	0
56	MG	1A	3981	1/1	0.70	0.17	41,41,41,41	0
56	MG	1A	3265	1/1	0.70	0.19	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3265	1/1	0.70	0.34	61,61,61,61	0
56	MG	1A	3091	1/1	0.70	0.57	72,72,72,72	0
56	MG	1A	3112	1/1	0.70	0.48	54,54,54,54	0
56	MG	1A	3634	1/1	0.70	0.21	68,68,68,68	0
56	MG	1A	3370	1/1	0.70	0.84	55,55,55,55	0
56	MG	1I	3001	1/1	0.70	0.34	76,76,76,76	0
56	MG	1A	4207	1/1	0.70	0.28	60,60,60,60	0
56	MG	1A	4135	1/1	0.71	0.11	67,67,67,67	0
56	MG	2A	3888	1/1	0.71	0.13	42,42,42,42	0
56	MG	2A	3380	1/1	0.71	0.14	67,67,67,67	0
56	MG	2A	3271	1/1	0.71	0.21	59,59,59,59	0
56	MG	2A	3113	1/1	0.71	0.23	71,71,71,71	0
56	MG	1A	3255	1/1	0.71	0.24	60,60,60,60	0
56	MG	1a	1750	1/1	0.71	0.11	75,75,75,75	0
56	MG	1A	3312	1/1	0.71	0.41	67,67,67,67	0
56	MG	1a	1814	1/1	0.71	0.15	71,71,71,71	0
56	MG	1A	3730	1/1	0.71	0.18	44,44,44,44	0
56	MG	2a	3174	1/1	0.71	0.12	88,88,88,88	0
56	MG	2A	3058	1/1	0.71	0.37	68,68,68,68	0
56	MG	2A	3326	1/1	0.71	0.27	57,57,57,57	0
56	MG	2A	3057	1/1	0.72	0.40	68,68,68,68	0
56	MG	2A	3757	1/1	0.72	0.19	54,54,54,54	0
56	MG	2A	3476	1/1	0.72	0.22	63,63,63,63	0
56	MG	1A	4024	1/1	0.72	0.10	48,48,48,48	0
57	CPT	1a	1930	4/5	0.72	0.45	60,62,73,353	0
56	MG	1a	1649	1/1	0.72	0.09	62,62,62,62	0
56	MG	2A	3672	1/1	0.72	0.12	68,68,68,68	0
56	MG	1A	3227	1/1	0.72	0.29	65,65,65,65	0
56	MG	2a	3060	1/1	0.72	0.51	82,82,82,82	0
56	MG	1A	3934	1/1	0.72	0.12	64,64,64,64	0
56	MG	2B	3009	1/1	0.72	0.14	61,61,61,61	0
56	MG	1a	1723	1/1	0.72	0.71	69,69,69,69	0
56	MG	2a	3047	1/1	0.72	0.15	72,72,72,72	0
56	MG	1A	3397	1/1	0.72	0.36	44,44,44,44	0
56	MG	2A	3593	1/1	0.72	0.30	71,71,71,71	0
56	MG	1a	1867	1/1	0.73	0.11	83,83,83,83	0
56	MG	1t	3001	1/1	0.73	0.35	65,65,65,65	0
56	MG	2A	3797	1/1	0.73	0.26	50,50,50,50	0
56	MG	2A	3835	1/1	0.73	0.13	32,32,32,32	0
56	MG	1A	3274	1/1	0.73	0.38	71,71,71,71	0
56	MG	1A	4179	1/1	0.73	0.22	51,51,51,51	0
56	MG	2A	3688	1/1	0.73	0.24	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3377	1/1	0.73	0.75	64,64,64,64	0
56	MG	2a	3143	1/1	0.73	0.16	82,82,82,82	0
56	MG	2x	103	1/1	0.73	0.33	83,83,83,83	0
56	MG	1A	4121	1/1	0.73	0.14	91,91,91,91	0
56	MG	1A	3246	1/1	0.73	0.19	54,54,54,54	0
56	MG	2A	3329	1/1	0.73	0.21	58,58,58,58	0
56	MG	2a	3020	1/1	0.73	0.27	61,61,61,61	0
56	MG	1A	4066	1/1	0.73	0.44	82,82,82,82	0
56	MG	2a	3234	1/1	0.73	0.15	76,76,76,76	0
56	MG	1A	4138	1/1	0.73	0.20	76,76,76,76	0
56	MG	1a	1754	1/1	0.73	0.18	63,63,63,63	0
56	MG	1A	3406	1/1	0.73	0.25	54,54,54,54	0
56	MG	1A	4008	1/1	0.73	0.07	84,84,84,84	0
56	MG	2A	3479	1/1	0.73	0.57	58,58,58,58	0
56	MG	1A	3352	1/1	0.73	0.27	66,66,66,66	0
56	MG	1a	1899	1/1	0.74	0.20	86,86,86,86	0
56	MG	1A	4153	1/1	0.74	0.15	90,90,90,90	0
56	MG	1A	3251	1/1	0.74	0.66	57,57,57,57	0
56	MG	2a	3148	1/1	0.74	0.10	75,75,75,75	0
56	MG	1A	3960	1/1	0.74	0.13	50,50,50,50	0
56	MG	2A	3725	1/1	0.74	0.12	52,52,52,52	0
56	MG	2A	3261	1/1	0.74	0.31	65,65,65,65	0
56	MG	2a	3191	1/1	0.74	0.19	65,65,65,65	0
56	MG	2A	3769	1/1	0.74	0.14	54,54,54,54	0
56	MG	1a	1679	1/1	0.74	0.14	75,75,75,75	0
56	MG	1A	3215	1/1	0.74	0.20	56,56,56,56	0
56	MG	1A	3151	1/1	0.74	0.86	54,54,54,54	0
56	MG	2a	3152	1/1	0.74	0.20	69,69,69,69	0
56	MG	2a	3057	1/1	0.74	0.79	97,97,97,97	0
56	MG	2A	3387	1/1	0.74	0.58	64,64,64,64	0
56	MG	20	101	1/1	0.74	0.21	60,60,60,60	0
56	MG	1A	4053	1/1	0.74	0.17	41,41,41,41	0
56	MG	1A	3560	1/1	0.74	0.44	55,55,55,55	0
56	MG	2A	3810	1/1	0.74	0.10	59,59,59,59	0
56	MG	1A	3575	1/1	0.74	0.43	54,54,54,54	0
56	MG	1A	4124	1/1	0.74	0.07	67,67,67,67	0
56	MG	1a	1602	1/1	0.74	0.44	83,83,83,83	0
56	MG	2A	3756	1/1	0.74	0.18	40,40,40,40	0
56	MG	1A	3403	1/1	0.74	0.39	53,53,53,53	0
56	MG	1A	3375	1/1	0.75	0.94	60,60,60,60	0
56	MG	1A	4037	1/1	0.75	0.11	64,64,64,64	0
56	MG	1A	3059	1/1	0.75	0.24	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3165	1/1	0.75	0.19	72,72,72,72	0
56	MG	1a	1878	1/1	0.75	0.07	70,70,70,70	0
56	MG	2a	3055	1/1	0.75	0.30	67,67,67,67	0
56	MG	2A	3303	1/1	0.75	0.24	45,45,45,45	0
56	MG	1A	3392	1/1	0.75	0.59	55,55,55,55	0
56	MG	2A	3334	1/1	0.75	0.34	54,54,54,54	0
56	MG	2A	3373	1/1	0.75	0.17	72,72,72,72	0
56	MG	2w	103	1/1	0.75	0.52	83,83,83,83	0
56	MG	1G	3003	1/1	0.75	0.28	67,67,67,67	0
56	MG	2A	3394	1/1	0.75	0.59	61,61,61,61	0
56	MG	1A	3297	1/1	0.75	0.26	67,67,67,67	0
56	MG	1A	3384	1/1	0.75	0.24	51,51,51,51	0
56	MG	1A	4125	1/1	0.75	0.09	77,77,77,77	0
56	MG	1a	1781	1/1	0.75	0.22	58,58,58,58	0
56	MG	1Z	302	1/1	0.75	0.23	64,64,64,64	0
56	MG	1A	3460	1/1	0.75	0.24	62,62,62,62	0
56	MG	2A	3297	1/1	0.75	0.18	54,54,54,54	0
56	MG	1A	3331	1/1	0.75	0.17	67,67,67,67	0
56	MG	2A	3719	1/1	0.75	0.25	55,55,55,55	0
56	MG	2a	3100	1/1	0.75	0.12	67,67,67,67	0
56	MG	1A	4186	1/1	0.75	0.47	66,66,66,66	0
56	MG	2a	3025	1/1	0.75	0.17	68,68,68,68	0
56	MG	2a	3192	1/1	0.75	0.10	74,74,74,74	0
56	MG	2A	3092	1/1	0.75	0.58	34,34,34,34	0
56	MG	1A	3296	1/1	0.76	0.17	53,53,53,53	0
56	MG	1A	3372	1/1	0.76	0.37	74,74,74,74	0
56	MG	2A	3214	1/1	0.76	0.64	64,64,64,64	0
56	MG	1A	4114	1/1	0.76	0.50	87,87,87,87	0
56	MG	2A	3408	1/1	0.76	0.24	60,60,60,60	0
56	MG	1Q	204	1/1	0.76	0.10	33,33,33,33	0
56	MG	10	105	1/1	0.76	0.16	66,66,66,66	0
56	MG	1A	3367	1/1	0.76	0.51	56,56,56,56	0
56	MG	15	102	1/1	0.76	0.51	42,42,42,42	0
56	MG	1A	3256	1/1	0.76	0.15	73,73,73,73	0
56	MG	1A	4002	1/1	0.76	0.26	45,45,45,45	0
56	MG	1A	3496	1/1	0.76	0.33	57,57,57,57	0
56	MG	1A	4113	1/1	0.76	0.11	60,60,60,60	0
56	MG	1A	3192	1/1	0.76	0.18	57,57,57,57	0
56	MG	1A	4072	1/1	0.76	0.37	95,95,95,95	0
56	MG	1a	1690	1/1	0.76	0.26	71,71,71,71	0
56	MG	1A	3639	1/1	0.76	0.22	56,56,56,56	0
56	MG	1a	1673	1/1	0.76	0.29	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1726	1/1	0.76	0.15	85,85,85,85	0
56	MG	1A	3212	1/1	0.76	0.26	53,53,53,53	0
56	MG	2A	3288	1/1	0.76	0.20	56,56,56,56	0
56	MG	2A	3671	1/1	0.76	0.34	57,57,57,57	0
56	MG	2A	3188	1/1	0.76	0.13	57,57,57,57	0
56	MG	2A	3296	1/1	0.76	0.34	55,55,55,55	0
56	MG	1a	1659	1/1	0.76	0.09	68,68,68,68	0
56	MG	1A	4154	1/1	0.76	0.23	88,88,88,88	0
56	MG	2A	3274	1/1	0.76	0.25	52,52,52,52	0
56	MG	1A	3633	1/1	0.76	0.29	55,55,55,55	0
56	MG	2A	3029	1/1	0.76	0.12	51,51,51,51	0
56	MG	1A	3270	1/1	0.76	0.14	64,64,64,64	0
56	MG	1A	3468	1/1	0.76	0.25	68,68,68,68	0
56	MG	23	3001	1/1	0.76	0.69	56,56,56,56	0
56	MG	1a	1742	1/1	0.76	0.16	73,73,73,73	0
56	MG	1A	3978	1/1	0.76	0.21	35,35,35,35	0
56	MG	2A	3548	1/1	0.76	0.13	49,49,49,49	0
56	MG	1a	1732	1/1	0.76	0.18	57,57,57,57	0
56	MG	2v	103	1/1	0.76	0.41	67,67,67,67	0
56	MG	2A	3301	1/1	0.76	0.43	64,64,64,64	0
56	MG	2A	3460	1/1	0.76	0.27	66,66,66,66	0
56	MG	1A	3002	1/1	0.76	0.31	59,59,59,59	0
56	MG	2A	3875	1/1	0.77	0.25	48,48,48,48	0
56	MG	2A	3550	1/1	0.77	0.15	41,41,41,41	0
56	MG	2A	3152	1/1	0.77	0.16	53,53,53,53	0
56	MG	2A	3089	1/1	0.77	0.17	60,60,60,60	0
56	MG	1A	3467	1/1	0.77	0.26	65,65,65,65	0
56	MG	1A	3363	1/1	0.77	0.34	58,58,58,58	0
56	MG	2A	3073	1/1	0.77	0.24	43,43,43,43	0
56	MG	2A	3521	1/1	0.77	0.09	53,53,53,53	0
56	MG	2A	3858	1/1	0.77	0.24	52,52,52,52	0
56	MG	2A	3200	1/1	0.77	0.38	73,73,73,73	0
56	MG	2A	3255	1/1	0.77	0.24	60,60,60,60	0
56	MG	1A	3601	1/1	0.77	0.12	70,70,70,70	0
56	MG	2A	3879	1/1	0.77	0.08	91,91,91,91	0
56	MG	1A	4119	1/1	0.77	0.29	73,73,73,73	0
56	MG	2E	303	1/1	0.77	0.14	51,51,51,51	0
56	MG	1A	3862	1/1	0.77	0.24	31,31,31,31	0
56	MG	1A	3745	1/1	0.77	0.28	49,49,49,49	0
56	MG	1A	3817	1/1	0.77	0.15	67,67,67,67	0
56	MG	2A	3516	1/1	0.77	0.06	57,57,57,57	0
56	MG	1x	118	1/1	0.77	0.35	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1872	1/1	0.77	0.10	85,85,85,85	0
56	MG	1A	4199	1/1	0.77	0.22	36,36,36,36	0
56	MG	1a	1755	1/1	0.77	0.13	62,62,62,62	0
56	MG	2A	3312	1/1	0.77	0.24	60,60,60,60	0
56	MG	2A	3400	1/1	0.77	0.22	77,77,77,77	0
56	MG	2A	3251	1/1	0.77	0.44	68,68,68,68	0
56	MG	2A	3201	1/1	0.77	0.17	61,61,61,61	0
56	MG	2A	3064	1/1	0.77	0.09	64,64,64,64	0
56	MG	1A	3688	1/1	0.77	0.45	53,53,53,53	0
56	MG	2A	3173	1/1	0.77	0.08	61,61,61,61	0
56	MG	1A	3984	1/1	0.77	0.27	49,49,49,49	0
56	MG	1A	4208	1/1	0.77	0.30	79,79,79,79	0
56	MG	2A	3393	1/1	0.77	0.15	67,67,67,67	0
56	MG	1a	1917	1/1	0.77	0.17	55,55,55,55	0
56	MG	1A	3506	1/1	0.77	0.34	55,55,55,55	0
56	MG	2a	3073	1/1	0.78	0.13	58,58,58,58	0
56	MG	2A	3210	1/1	0.78	0.38	61,61,61,61	0
56	MG	1A	3519	1/1	0.78	0.11	71,71,71,71	0
56	MG	2A	3355	1/1	0.78	0.35	73,73,73,73	0
56	MG	2A	3195	1/1	0.78	0.45	53,53,53,53	0
56	MG	1a	1798	1/1	0.78	0.15	66,66,66,66	0
56	MG	2A	3687	1/1	0.78	0.16	53,53,53,53	0
56	MG	2p	3001	1/1	0.78	0.22	63,63,63,63	0
56	MG	1A	3720	1/1	0.78	0.15	37,37,37,37	0
56	MG	1B	204	1/1	0.78	0.27	61,61,61,61	0
56	MG	2A	3803	1/1	0.78	0.15	64,64,64,64	0
56	MG	1A	3457	1/1	0.78	0.25	63,63,63,63	0
56	MG	1A	3024	1/1	0.78	0.18	53,53,53,53	0
56	MG	1A	3409	1/1	0.78	0.21	64,64,64,64	0
56	MG	2A	3177	1/1	0.78	0.31	46,46,46,46	0
56	MG	2A	3582	1/1	0.78	0.10	76,76,76,76	0
56	MG	2A	3270	1/1	0.78	0.46	65,65,65,65	0
56	MG	1a	1612	1/1	0.78	0.18	62,62,62,62	0
56	MG	1a	1851	1/1	0.78	0.16	76,76,76,76	0
56	MG	1a	1805	1/1	0.78	0.17	63,63,63,63	0
56	MG	1a	1880	1/1	0.78	0.17	51,51,51,51	0
56	MG	1A	4065	1/1	0.78	0.09	64,64,64,64	0
56	MG	2A	3243	1/1	0.78	0.40	60,60,60,60	0
56	MG	2A	3456	1/1	0.78	0.56	52,52,52,52	0
56	MG	2A	3589	1/1	0.78	0.20	65,65,65,65	0
56	MG	2A	3358	1/1	0.78	0.18	78,78,78,78	0
56	MG	2B	3020	1/1	0.78	0.14	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3888	1/1	0.78	0.19	54,54,54,54	0
56	MG	1A	3695	1/1	0.79	0.16	37,37,37,37	0
56	MG	2A	3222	1/1	0.79	0.27	72,72,72,72	0
56	MG	16	102	1/1	0.79	0.62	68,68,68,68	0
56	MG	2A	3800	1/1	0.79	0.15	67,67,67,67	0
56	MG	1a	1902	1/1	0.79	0.10	77,77,77,77	0
56	MG	2a	3142	1/1	0.79	0.14	86,86,86,86	0
56	MG	2B	3002	1/1	0.79	0.30	60,60,60,60	0
56	MG	1A	4201	1/1	0.79	0.19	51,51,51,51	0
56	MG	2A	3342	1/1	0.79	0.37	53,53,53,53	0
56	MG	2B	3015	1/1	0.79	0.19	62,62,62,62	0
56	MG	1A	3327	1/1	0.79	0.33	56,56,56,56	0
56	MG	2a	3059	1/1	0.79	0.17	61,61,61,61	0
56	MG	2A	3551	1/1	0.79	0.14	44,44,44,44	0
56	MG	1a	1677	1/1	0.79	0.27	70,70,70,70	0
56	MG	1A	3649	1/1	0.79	0.39	79,79,79,79	0
56	MG	2a	3167	1/1	0.79	0.08	75,75,75,75	0
56	MG	2F	303	1/1	0.79	0.31	52,52,52,52	0
56	MG	1A	4147	1/1	0.79	0.13	79,79,79,79	0
56	MG	1B	234	1/1	0.79	0.27	78,78,78,78	0
56	MG	1A	4013	1/1	0.79	0.09	50,50,50,50	0
56	MG	2v	105	1/1	0.79	0.17	76,76,76,76	0
56	MG	1a	1919	1/1	0.79	0.10	54,54,54,54	0
56	MG	1A	3484	1/1	0.79	0.23	58,58,58,58	0
56	MG	2a	3023	1/1	0.79	0.28	72,72,72,72	0
56	MG	1a	1793	1/1	0.79	0.26	65,65,65,65	0
56	MG	1A	3321	1/1	0.79	0.21	57,57,57,57	0
56	MG	2a	3139	1/1	0.79	0.19	85,85,85,85	0
56	MG	1x	117	1/1	0.79	0.17	78,78,78,78	0
56	MG	1A	3359	1/1	0.79	0.22	53,53,53,53	0
56	MG	1A	4255	1/1	0.79	0.19	48,48,48,48	0
56	MG	2a	3004	1/1	0.79	0.12	68,68,68,68	0
56	MG	2A	3604	1/1	0.79	0.22	34,34,34,34	0
56	MG	1A	3425	1/1	0.79	0.20	54,54,54,54	0
56	MG	2a	3137	1/1	0.79	0.06	87,87,87,87	0
56	MG	2y	3002	1/1	0.79	0.20	58,58,58,58	0
56	MG	1A	3517	1/1	0.80	0.38	53,53,53,53	0
56	MG	1a	1776	1/1	0.80	0.42	69,69,69,69	0
56	MG	2a	3048	1/1	0.80	0.11	58,58,58,58	0
56	MG	2A	3726	1/1	0.80	0.09	64,64,64,64	0
56	MG	2A	3352	1/1	0.80	0.25	47,47,47,47	0
56	MG	1A	3684	1/1	0.80	0.24	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3078	1/1	0.80	0.15	50,50,50,50	0
56	MG	1a	1728	1/1	0.80	0.09	62,62,62,62	0
56	MG	2A	3422	1/1	0.80	0.20	56,56,56,56	0
56	MG	1A	3797	1/1	0.80	0.20	49,49,49,49	0
56	MG	1A	3374	1/1	0.80	0.29	53,53,53,53	0
56	MG	1A	3472	1/1	0.80	0.20	59,59,59,59	0
56	MG	2a	3134	1/1	0.80	0.15	74,74,74,74	0
56	MG	1A	3595	1/1	0.80	0.26	49,49,49,49	0
56	MG	1a	1620	1/1	0.80	0.13	54,54,54,54	0
56	MG	1A	4168	1/1	0.80	0.11	66,66,66,66	0
56	MG	1A	3308	1/1	0.80	0.79	62,62,62,62	0
56	MG	1a	1864	1/1	0.80	0.10	94,94,94,94	0
56	MG	2A	3247	1/1	0.80	0.47	56,56,56,56	0
56	MG	2a	3216	1/1	0.80	0.18	66,66,66,66	0
56	MG	1A	3512	1/1	0.80	0.43	59,59,59,59	0
56	MG	2a	3107	1/1	0.80	0.30	75,75,75,75	0
56	MG	1A	3049	1/1	0.80	0.29	45,45,45,45	0
56	MG	1A	4011	1/1	0.80	0.20	73,73,73,73	0
56	MG	2l	3002	1/1	0.80	0.17	62,62,62,62	0
56	MG	2a	3157	1/1	0.80	0.09	79,79,79,79	0
56	MG	1A	3995	1/1	0.80	0.20	51,51,51,51	0
56	MG	1E	309	1/1	0.80	0.14	54,54,54,54	0
56	MG	2A	3727	1/1	0.80	0.15	53,53,53,53	0
56	MG	2A	3248	1/1	0.80	0.41	66,66,66,66	0
56	MG	2A	3824	1/1	0.80	0.21	80,80,80,80	0
56	MG	1A	3615	1/1	0.80	0.18	33,33,33,33	0
56	MG	1F	308	1/1	0.80	0.11	45,45,45,45	0
56	MG	2A	3290	1/1	0.80	0.28	62,62,62,62	0
56	MG	2a	3006	1/1	0.80	0.17	65,65,65,65	0
56	MG	1a	1709	1/1	0.80	0.07	73,73,73,73	0
56	MG	2A	3339	1/1	0.80	0.24	56,56,56,56	0
56	MG	2A	3431	1/1	0.80	0.24	58,58,58,58	0
56	MG	1A	3941	1/1	0.80	0.23	29,29,29,29	0
56	MG	1a	1891	1/1	0.80	0.13	91,91,91,91	0
56	MG	1A	4205	1/1	0.80	0.18	46,46,46,46	0
56	MG	2a	3188	1/1	0.80	0.19	78,78,78,78	0
56	MG	1A	4193	1/1	0.80	0.15	49,49,49,49	0
56	MG	1w	111	1/1	0.80	0.29	84,84,84,84	0
56	MG	2a	3133	1/1	0.80	0.15	94,94,94,94	0
56	MG	2a	3214	1/1	0.80	0.14	63,63,63,63	0
56	MG	1A	4240	1/1	0.80	0.25	51,51,51,51	0
56	MG	2A	3809	1/1	0.80	0.23	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3146	1/1	0.80	0.21	56,56,56,56	0
56	MG	2v	106	1/1	0.80	0.22	68,68,68,68	0
56	MG	1a	1694	1/1	0.80	0.40	62,62,62,62	0
56	MG	2A	3853	1/1	0.80	0.13	63,63,63,63	0
56	MG	1A	4118	1/1	0.81	0.09	66,66,66,66	0
56	MG	1A	3599	1/1	0.81	0.25	64,64,64,64	0
56	MG	2A	3414	1/1	0.81	0.32	52,52,52,52	0
56	MG	1A	4007	1/1	0.81	0.13	51,51,51,51	0
56	MG	2A	3761	1/1	0.81	0.51	47,47,47,47	0
56	MG	1A	3801	1/1	0.81	0.15	60,60,60,60	0
56	MG	1a	1641	1/1	0.81	0.17	73,73,73,73	0
56	MG	1A	3800	1/1	0.81	0.13	57,57,57,57	0
56	MG	2N	8001	1/1	0.81	0.14	53,53,53,53	0
56	MG	1G	3005	1/1	0.81	0.11	65,65,65,65	0
56	MG	2a	3024	1/1	0.81	0.17	65,65,65,65	0
56	MG	1X	106	1/1	0.81	0.24	56,56,56,56	0
56	MG	1E	302	1/1	0.81	0.19	51,51,51,51	0
56	MG	1A	4046	1/1	0.81	0.17	69,69,69,69	0
56	MG	1A	4051	1/1	0.81	0.15	55,55,55,55	0
56	MG	1A	3315	1/1	0.81	0.23	51,51,51,51	0
56	MG	1a	1705	1/1	0.81	0.15	65,65,65,65	0
56	MG	2A	3645	1/1	0.81	0.19	40,40,40,40	0
56	MG	2a	3018	1/1	0.81	0.17	62,62,62,62	0
56	MG	1A	3757	1/1	0.81	0.14	51,51,51,51	0
56	MG	2A	3005	1/1	0.81	0.15	56,56,56,56	0
56	MG	2a	3221	1/1	0.81	0.10	81,81,81,81	0
56	MG	2A	3489	1/1	0.81	0.51	82,82,82,82	0
56	MG	2A	3783	1/1	0.81	0.15	42,42,42,42	0
56	MG	1y	3005	1/1	0.81	0.44	83,83,83,83	0
56	MG	2A	3885	1/1	0.81	0.26	50,50,50,50	0
56	MG	2A	3340	1/1	0.81	0.47	75,75,75,75	0
56	MG	1A	4078	1/1	0.81	0.19	24,24,24,24	0
56	MG	1W	3002	1/1	0.81	0.21	51,51,51,51	0
56	MG	1A	3904	1/1	0.81	0.11	57,57,57,57	0
56	MG	1A	4100	1/1	0.81	0.08	95,95,95,95	0
56	MG	1a	1832	1/1	0.81	0.15	59,59,59,59	0
56	MG	2f	3002	1/1	0.81	0.22	63,63,63,63	0
56	MG	1A	4034	1/1	0.81	0.16	24,24,24,24	0
56	MG	2a	3058	1/1	0.81	0.54	76,76,76,76	0
56	MG	1A	3480	1/1	0.81	0.24	53,53,53,53	0
56	MG	1A	4165	1/1	0.81	0.09	45,45,45,45	0
56	MG	1B	215	1/1	0.81	0.09	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4115	1/1	0.81	0.13	86,86,86,86	0
56	MG	2A	3313	1/1	0.81	0.42	71,71,71,71	0
56	MG	1B	210	1/1	0.81	0.92	62,62,62,62	0
56	MG	1A	3431	1/1	0.81	0.46	47,47,47,47	0
56	MG	1A	3152	1/1	0.81	0.24	51,51,51,51	0
56	MG	2a	3196	1/1	0.81	0.24	71,71,71,71	0
56	MG	2A	3540	1/1	0.81	0.10	54,54,54,54	0
56	MG	1A	3626	1/1	0.81	0.11	64,64,64,64	0
56	MG	1A	3643	1/1	0.81	0.14	51,51,51,51	0
56	MG	2A	3229	1/1	0.81	0.27	55,55,55,55	0
56	MG	2A	3287	1/1	0.81	0.25	60,60,60,60	0
56	MG	1a	1713	1/1	0.81	0.61	79,79,79,79	0
56	MG	1A	3662	1/1	0.81	0.27	59,59,59,59	0
56	MG	1A	3354	1/1	0.81	0.24	55,55,55,55	0
56	MG	1A	4091	1/1	0.81	0.14	75,75,75,75	0
56	MG	1a	1809	1/1	0.82	0.13	64,64,64,64	0
56	MG	1D	312	1/1	0.82	0.21	63,63,63,63	0
56	MG	2A	3050	1/1	0.82	0.46	47,47,47,47	0
56	MG	2a	3156	1/1	0.82	0.10	77,77,77,77	0
56	MG	2a	3187	1/1	0.82	0.22	78,78,78,78	0
56	MG	1A	3538	1/1	0.82	0.20	50,50,50,50	0
56	MG	2A	3420	1/1	0.82	0.16	61,61,61,61	0
56	MG	1A	3677	1/1	0.82	0.22	57,57,57,57	0
56	MG	2A	3359	1/1	0.82	0.15	73,73,73,73	0
56	MG	2a	3075	1/1	0.82	0.20	70,70,70,70	0
56	MG	1A	3611	1/1	0.82	0.20	59,59,59,59	0
56	MG	2A	3309	1/1	0.82	0.15	66,66,66,66	0
56	MG	2A	3262	1/1	0.82	0.36	55,55,55,55	0
56	MG	1A	3364	1/1	0.82	0.21	52,52,52,52	0
56	MG	1A	3879	1/1	0.82	0.10	57,57,57,57	0
56	MG	1A	3330	1/1	0.82	0.15	67,67,67,67	0
56	MG	2a	3113	1/1	0.82	0.55	73,73,73,73	0
56	MG	1a	1665	1/1	0.82	0.12	67,67,67,67	0
56	MG	2A	3258	1/1	0.82	0.20	55,55,55,55	0
56	MG	1A	3804	1/1	0.82	0.14	66,66,66,66	0
56	MG	1A	3149	1/1	0.82	0.55	42,42,42,42	0
56	MG	2a	3027	1/1	0.82	0.20	69,69,69,69	0
56	MG	1A	3690	1/1	0.82	0.14	52,52,52,52	0
56	MG	1A	3648	1/1	0.82	0.23	53,53,53,53	0
56	MG	1A	3430	1/1	0.82	0.15	50,50,50,50	0
56	MG	1a	1875	1/1	0.82	0.13	55,55,55,55	0
56	MG	1A	3518	1/1	0.82	0.11	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4171	1/1	0.82	0.17	74,74,74,74	0
56	MG	1A	3269	1/1	0.82	0.28	57,57,57,57	0
56	MG	1a	1759	1/1	0.82	0.19	53,53,53,53	0
56	MG	2A	3354	1/1	0.82	0.10	69,69,69,69	0
56	MG	2A	3202	1/1	0.82	0.16	53,53,53,53	0
56	MG	1a	1618	1/1	0.82	0.16	51,51,51,51	0
56	MG	1A	3692	1/1	0.82	0.27	73,73,73,73	0
56	MG	2A	3066	1/1	0.82	0.17	55,55,55,55	0
56	MG	1A	3947	1/1	0.82	0.11	47,47,47,47	0
56	MG	1A	3225	1/1	0.82	0.41	53,53,53,53	0
56	MG	1a	1876	1/1	0.82	0.12	65,65,65,65	0
56	MG	1A	3081	1/1	0.82	0.31	44,44,44,44	0
56	MG	2A	3618	1/1	0.82	0.12	46,46,46,46	0
56	MG	1A	4145	1/1	0.82	0.23	35,35,35,35	0
56	MG	2a	3052	1/1	0.82	0.31	65,65,65,65	0
56	MG	2A	3298	1/1	0.82	0.16	67,67,67,67	0
56	MG	1A	3469	1/1	0.82	0.19	60,60,60,60	0
56	MG	1A	4084	1/1	0.82	0.21	78,78,78,78	0
56	MG	2A	3001	1/1	0.82	0.35	49,49,49,49	0
56	MG	1A	3226	1/1	0.82	0.40	51,51,51,51	0
56	MG	2U	203	1/1	0.82	0.63	57,57,57,57	0
56	MG	2a	3068	1/1	0.82	0.13	71,71,71,71	0
56	MG	1a	1784	1/1	0.82	0.11	59,59,59,59	0
56	MG	1A	3244	1/1	0.83	0.19	55,55,55,55	0
56	MG	2x	102	1/1	0.83	0.55	71,71,71,71	0
56	MG	2A	3198	1/1	0.83	0.26	48,48,48,48	0
56	MG	1a	1691	1/1	0.83	0.29	79,79,79,79	0
56	MG	2E	304	1/1	0.83	0.18	55,55,55,55	0
56	MG	2A	3363	1/1	0.83	0.27	65,65,65,65	0
56	MG	2A	3820	1/1	0.83	0.23	75,75,75,75	0
56	MG	1A	3793	1/1	0.83	0.17	36,36,36,36	0
56	MG	1A	3373	1/1	0.83	0.15	61,61,61,61	0
56	MG	1A	3029	1/1	0.83	0.20	41,41,41,41	0
56	MG	1A	3336	1/1	0.83	0.29	59,59,59,59	0
56	MG	2A	3676	1/1	0.83	0.22	55,55,55,55	0
56	MG	2a	3036	1/1	0.83	0.30	60,60,60,60	0
56	MG	1A	3791	1/1	0.83	0.34	61,61,61,61	0
56	MG	1A	3952	1/1	0.83	0.22	52,52,52,52	0
56	MG	1A	3683	1/1	0.83	0.15	76,76,76,76	0
56	MG	1A	3867	1/1	0.83	0.10	62,62,62,62	0
56	MG	1A	4184	1/1	0.83	0.21	33,33,33,33	0
56	MG	1a	1792	1/1	0.83	0.21	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3376	1/1	0.83	0.20	59,59,59,59	0
56	MG	2g	8001	1/1	0.83	0.08	61,61,61,61	0
56	MG	1A	3577	1/1	0.83	0.17	69,69,69,69	0
56	MG	1a	1868	1/1	0.83	0.17	75,75,75,75	0
56	MG	1B	208	1/1	0.83	0.13	71,71,71,71	0
56	MG	1A	3678	1/1	0.83	0.30	50,50,50,50	0
56	MG	1A	3053	1/1	0.83	0.12	62,62,62,62	0
56	MG	2A	3900	1/1	0.83	0.29	53,53,53,53	0
56	MG	1A	3189	1/1	0.83	0.20	43,43,43,43	0
56	MG	1A	4157	1/1	0.83	0.11	61,61,61,61	0
56	MG	2Q	3003	1/1	0.83	0.15	41,41,41,41	0
56	MG	2a	3200	1/1	0.83	0.14	71,71,71,71	0
56	MG	2A	3026	1/1	0.83	0.92	56,56,56,56	0
56	MG	2a	3127	1/1	0.83	0.25	67,67,67,67	0
56	MG	1B	209	1/1	0.83	0.46	73,73,73,73	0
56	MG	1a	1782	1/1	0.83	0.12	58,58,58,58	0
56	MG	1a	1707	1/1	0.83	0.24	59,59,59,59	0
56	MG	2A	3321	1/1	0.83	0.32	62,62,62,62	0
56	MG	1A	3515	1/1	0.83	0.50	55,55,55,55	0
56	MG	1A	4137	1/1	0.83	0.20	72,72,72,72	0
56	MG	1A	3299	1/1	0.83	0.22	54,54,54,54	0
56	MG	1A	3343	1/1	0.83	0.39	60,60,60,60	0
56	MG	2B	3001	1/1	0.83	0.15	66,66,66,66	0
56	MG	2A	3158	1/1	0.83	0.32	58,58,58,58	0
56	MG	1A	3631	1/1	0.83	0.20	57,57,57,57	0
56	MG	2A	3644	1/1	0.83	0.17	46,46,46,46	0
56	MG	2A	3920	1/1	0.83	0.72	60,60,60,60	0
56	MG	1A	3713	1/1	0.83	0.14	50,50,50,50	0
56	MG	2A	3765	1/1	0.83	0.18	62,62,62,62	0
56	MG	1A	3997	1/1	0.83	0.18	68,68,68,68	0
56	MG	1l	202	1/1	0.83	0.23	63,63,63,63	0
56	MG	1a	1909	1/1	0.83	0.07	64,64,64,64	0
56	MG	1A	4159	1/1	0.83	0.16	60,60,60,60	0
56	MG	2a	3013	1/1	0.83	0.20	66,66,66,66	0
56	MG	1A	3026	1/1	0.83	0.23	56,56,56,56	0
56	MG	2A	3815	1/1	0.83	0.13	69,69,69,69	0
56	MG	2A	3722	1/1	0.83	0.17	48,48,48,48	0
56	MG	2A	3266	1/1	0.83	0.20	62,62,62,62	0
56	MG	1A	3185	1/1	0.83	0.18	41,41,41,41	0
56	MG	1A	4017	1/1	0.83	0.20	29,29,29,29	0
56	MG	1A	3805	1/1	0.83	0.23	62,62,62,62	0
56	MG	2a	3155	1/1	0.83	0.11	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3085	1/1	0.83	0.25	55,55,55,55	0
56	MG	1A	4139	1/1	0.83	0.13	34,34,34,34	0
56	MG	2A	3204	1/1	0.83	0.14	58,58,58,58	0
56	MG	2A	3454	1/1	0.83	0.19	48,48,48,48	0
56	MG	2A	3865	1/1	0.83	0.16	57,57,57,57	0
56	MG	2A	3771	1/1	0.83	0.14	47,47,47,47	0
56	MG	1w	104	1/1	0.83	0.13	54,54,54,54	0
56	MG	1a	1811	1/1	0.83	0.33	68,68,68,68	0
56	MG	1a	1859	1/1	0.83	0.21	77,77,77,77	0
56	MG	1A	3605	1/1	0.83	0.16	48,48,48,48	0
56	MG	2a	3194	1/1	0.84	0.12	77,77,77,77	0
56	MG	2a	3132	1/1	0.84	0.10	59,59,59,59	0
56	MG	2A	3241	1/1	0.84	0.76	44,44,44,44	0
56	MG	1F	302	1/1	0.84	0.58	66,66,66,66	0
56	MG	1A	3489	1/1	0.84	0.42	52,52,52,52	0
56	MG	1A	4140	1/1	0.84	0.31	74,74,74,74	0
56	MG	1A	4128	1/1	0.84	0.17	57,57,57,57	0
56	MG	2A	3514	1/1	0.84	0.16	48,48,48,48	0
56	MG	1a	1749	1/1	0.84	0.19	62,62,62,62	0
56	MG	1A	4074	1/1	0.84	0.12	58,58,58,58	0
56	MG	2A	3866	1/1	0.84	0.11	63,63,63,63	0
56	MG	2a	3080	1/1	0.84	0.42	62,62,62,62	0
56	MG	2A	3206	1/1	0.84	0.18	59,59,59,59	0
56	MG	1a	1688	1/1	0.84	0.29	71,71,71,71	0
56	MG	2A	3375	1/1	0.84	0.44	59,59,59,59	0
56	MG	10	104	1/1	0.84	0.74	53,53,53,53	0
56	MG	1A	3598	1/1	0.84	0.22	54,54,54,54	0
56	MG	1A	3455	1/1	0.84	0.41	41,41,41,41	0
56	MG	2A	3109	1/1	0.84	0.09	58,58,58,58	0
56	MG	2a	3168	1/1	0.84	0.09	68,68,68,68	0
56	MG	2A	3086	1/1	0.84	0.13	51,51,51,51	0
56	MG	2a	3225	1/1	0.84	0.17	68,68,68,68	0
56	MG	2A	3753	1/1	0.84	0.13	66,66,66,66	0
56	MG	1A	3318	1/1	0.84	0.31	57,57,57,57	0
56	MG	2A	3179	1/1	0.84	0.26	55,55,55,55	0
56	MG	2A	3870	1/1	0.84	0.11	45,45,45,45	0
56	MG	1A	3082	1/1	0.84	0.61	50,50,50,50	0
56	MG	1A	3580	1/1	0.84	0.14	57,57,57,57	0
56	MG	1A	4088	1/1	0.84	0.14	62,62,62,62	0
56	MG	1a	1663	1/1	0.84	0.10	73,73,73,73	0
56	MG	2A	3854	1/1	0.84	0.28	42,42,42,42	0
56	MG	2A	3311	1/1	0.84	0.58	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2y	3003	1/1	0.84	0.30	71,71,71,71	0
56	MG	2A	3227	1/1	0.84	0.20	62,62,62,62	0
56	MG	1x	107	1/1	0.84	0.14	66,66,66,66	0
56	MG	1O	3001	1/1	0.84	0.48	82,82,82,82	0
56	MG	28	103	1/1	0.84	0.24	63,63,63,63	0
56	MG	1a	1714	1/1	0.84	0.34	75,75,75,75	0
56	MG	1A	3247	1/1	0.84	1.13	71,71,71,71	0
56	MG	2A	3169	1/1	0.84	0.15	49,49,49,49	0
56	MG	2A	3447	1/1	0.84	0.34	51,51,51,51	0
56	MG	1a	1711	1/1	0.84	0.11	54,54,54,54	0
56	MG	2A	3423	1/1	0.84	0.13	61,61,61,61	0
56	MG	1a	1639	1/1	0.84	0.07	56,56,56,56	0
56	MG	2A	3682	1/1	0.84	0.18	56,56,56,56	0
56	MG	2A	3383	1/1	0.84	0.37	59,59,59,59	0
56	MG	1A	3865	1/1	0.84	0.20	29,29,29,29	0
56	MG	1A	3113	1/1	0.84	0.15	61,61,61,61	0
56	MG	1A	3475	1/1	0.84	0.33	48,48,48,48	0
56	MG	1A	3220	1/1	0.84	0.18	47,47,47,47	0
56	MG	2A	3172	1/1	0.84	0.40	55,55,55,55	0
56	MG	2a	3177	1/1	0.84	0.13	69,69,69,69	0
56	MG	1a	1683	1/1	0.84	0.14	80,80,80,80	0
56	MG	1A	4098	1/1	0.84	0.09	81,81,81,81	0
56	MG	2a	3083	1/1	0.84	0.13	62,62,62,62	0
56	MG	2a	3121	1/1	0.84	0.07	78,78,78,78	0
56	MG	1x	116	1/1	0.84	0.13	65,65,65,65	0
56	MG	1a	1644	1/1	0.84	0.23	79,79,79,79	0
56	MG	1A	3102	1/1	0.84	0.20	42,42,42,42	0
56	MG	1A	4059	1/1	0.84	0.15	65,65,65,65	0
56	MG	2A	3892	1/1	0.84	0.45	52,52,52,52	0
56	MG	1A	3557	1/1	0.84	0.20	59,59,59,59	0
56	MG	1a	1763	1/1	0.84	0.37	65,65,65,65	0
56	MG	1a	1605	1/1	0.84	0.49	72,72,72,72	0
56	MG	1a	1834	1/1	0.84	0.25	60,60,60,60	0
56	MG	1B	230	1/1	0.84	0.10	82,82,82,82	0
56	MG	1A	3052	1/1	0.84	0.39	59,59,59,59	0
56	MG	1A	3132	1/1	0.84	0.36	58,58,58,58	0
56	MG	1a	1604	1/1	0.84	0.37	63,63,63,63	0
56	MG	1A	3320	1/1	0.84	0.12	55,55,55,55	0
56	MG	1A	3338	1/1	0.84	0.21	50,50,50,50	0
56	MG	1a	1854	1/1	0.84	0.25	68,68,68,68	0
56	MG	2A	3112	1/1	0.84	0.11	60,60,60,60	0
56	MG	1A	3644	1/1	0.84	0.19	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3452	1/1	0.84	0.20	60,60,60,60	0
56	MG	1A	3316	1/1	0.85	0.17	51,51,51,51	0
56	MG	1a	1900	1/1	0.85	0.08	62,62,62,62	0
56	MG	1A	4195	1/1	0.85	0.73	59,59,59,59	0
56	MG	2A	3714	1/1	0.85	0.16	58,58,58,58	0
56	MG	2A	3855	1/1	0.85	0.17	47,47,47,47	0
56	MG	1A	3647	1/1	0.85	0.20	40,40,40,40	0
56	MG	1a	1715	1/1	0.85	0.25	62,62,62,62	0
56	MG	1a	1802	1/1	0.85	0.10	63,63,63,63	0
56	MG	1A	3881	1/1	0.85	0.09	78,78,78,78	0
56	MG	1a	1734	1/1	0.85	0.16	67,67,67,67	0
56	MG	2A	3470	1/1	0.85	0.50	60,60,60,60	0
56	MG	1B	207	1/1	0.85	0.11	65,65,65,65	0
56	MG	1A	3034	1/1	0.85	0.78	51,51,51,51	0
56	MG	1A	3273	1/1	0.85	0.41	45,45,45,45	0
56	MG	1A	3988	1/1	0.85	0.14	58,58,58,58	0
56	MG	1A	3292	1/1	0.85	0.23	62,62,62,62	0
56	MG	1A	3333	1/1	0.85	0.13	55,55,55,55	0
56	MG	1A	3441	1/1	0.85	0.26	48,48,48,48	0
56	MG	2A	3395	1/1	0.85	0.08	61,61,61,61	0
56	MG	1A	3079	1/1	0.85	0.17	46,46,46,46	0
56	MG	2A	3503	1/1	0.85	0.10	45,45,45,45	0
56	MG	1A	4232	1/1	0.85	1.31	62,62,62,62	0
56	MG	2A	3230	1/1	0.85	0.33	58,58,58,58	0
56	MG	2A	3549	1/1	0.85	0.14	52,52,52,52	0
56	MG	1A	3231	1/1	0.85	0.16	54,54,54,54	0
56	MG	2A	3384	1/1	0.85	0.30	70,70,70,70	0
56	MG	10	106	1/1	0.85	0.13	70,70,70,70	0
56	MG	2A	3002	1/1	0.85	0.41	61,61,61,61	0
56	MG	2A	3361	1/1	0.85	0.12	57,57,57,57	0
56	MG	2A	3091	1/1	0.85	0.26	55,55,55,55	0
56	MG	1A	3930	1/1	0.85	0.14	44,44,44,44	0
56	MG	1a	1818	1/1	0.85	0.42	45,45,45,45	0
56	MG	2A	3344	1/1	0.85	1.10	71,71,71,71	0
56	MG	2A	3244	1/1	0.85	0.25	46,46,46,46	0
56	MG	1A	3826	1/1	0.85	0.21	61,61,61,61	0
56	MG	2A	3409	1/1	0.85	0.37	51,51,51,51	0
56	MG	1B	205	1/1	0.85	0.19	48,48,48,48	0
56	MG	1a	1700	1/1	0.85	0.16	55,55,55,55	0
56	MG	1A	4133	1/1	0.85	0.14	57,57,57,57	0
56	MG	1A	3974	1/1	0.85	0.20	35,35,35,35	0
56	MG	2a	3237	1/1	0.85	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4010	1/1	0.85	0.45	85,85,85,85	0
56	MG	1x	111	1/1	0.85	0.10	61,61,61,61	0
56	MG	2w	104	1/1	0.85	0.17	81,81,81,81	0
56	MG	1A	3483	1/1	0.85	0.15	43,43,43,43	0
56	MG	1A	3492	1/1	0.85	0.29	47,47,47,47	0
56	MG	1A	3208	1/1	0.85	0.28	52,52,52,52	0
56	MG	2A	3902	1/1	0.85	0.30	61,61,61,61	0
56	MG	1A	3783	1/1	0.85	0.22	37,37,37,37	0
56	MG	2a	3120	1/1	0.85	0.11	77,77,77,77	0
56	MG	2A	3793	1/1	0.85	0.19	56,56,56,56	0
56	MG	1A	4220	1/1	0.85	0.28	48,48,48,48	0
56	MG	2A	3746	1/1	0.85	0.11	76,76,76,76	0
56	MG	1A	4117	1/1	0.85	0.09	83,83,83,83	0
56	MG	25	101	1/1	0.85	0.34	57,57,57,57	0
56	MG	1A	3371	1/1	0.85	0.34	56,56,56,56	0
56	MG	1S	3002	1/1	0.85	0.58	63,63,63,63	0
56	MG	1a	1804	1/1	0.85	0.16	67,67,67,67	0
56	MG	1a	1611	1/1	0.85	0.17	63,63,63,63	0
56	MG	1A	3776	1/1	0.85	0.20	43,43,43,43	0
56	MG	2a	3123	1/1	0.85	0.09	61,61,61,61	0
56	MG	2A	3328	1/1	0.85	0.48	58,58,58,58	0
56	MG	1A	3340	1/1	0.85	0.16	65,65,65,65	0
56	MG	2A	3077	1/1	0.85	0.16	46,46,46,46	0
56	MG	1y	3003	1/1	0.85	0.18	85,85,85,85	0
56	MG	2A	3685	1/1	0.85	0.11	44,44,44,44	0
56	MG	1A	3958	1/1	0.85	0.18	48,48,48,48	0
56	MG	2A	3246	1/1	0.85	0.28	59,59,59,59	0
56	MG	2A	3335	1/1	0.85	0.10	52,52,52,52	0
56	MG	2a	3219	1/1	0.85	0.19	81,81,81,81	0
56	MG	1A	3899	1/1	0.85	0.17	35,35,35,35	0
56	MG	2A	3404	1/1	0.85	0.25	55,55,55,55	0
56	MG	1A	3337	1/1	0.85	0.26	48,48,48,48	0
56	MG	1A	3573	1/1	0.85	0.27	51,51,51,51	0
56	MG	1A	3587	1/1	0.85	0.16	54,54,54,54	0
56	MG	1A	3399	1/1	0.85	0.36	72,72,72,72	0
56	MG	2A	3154	1/1	0.85	0.17	50,50,50,50	0
56	MG	1A	3501	1/1	0.85	0.35	62,62,62,62	0
56	MG	1A	4222	1/1	0.85	0.31	45,45,45,45	0
56	MG	1a	1704	1/1	0.85	0.41	67,67,67,67	0
56	MG	2A	3207	1/1	0.85	0.12	38,38,38,38	0
56	MG	2A	3203	1/1	0.85	0.21	48,48,48,48	0
56	MG	1A	3413	1/1	0.85	0.20	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1B	202	1/1	0.85	0.26	56,56,56,56	0
56	MG	1A	3640	1/1	0.86	0.20	40,40,40,40	0
56	MG	1A	3555	1/1	0.86	0.21	72,72,72,72	0
56	MG	1a	1682	1/1	0.86	0.14	69,69,69,69	0
56	MG	2A	3429	1/1	0.86	0.19	55,55,55,55	0
56	MG	1A	3860	1/1	0.86	0.21	36,36,36,36	0
56	MG	2A	3159	1/1	0.86	0.38	44,44,44,44	0
56	MG	2A	3424	1/1	0.86	0.12	65,65,65,65	0
56	MG	1A	3726	1/1	0.86	0.19	30,30,30,30	0
56	MG	1A	4149	1/1	0.86	0.10	61,61,61,61	0
56	MG	2A	3132	1/1	0.86	0.08	53,53,53,53	0
56	MG	1A	3680	1/1	0.86	0.14	64,64,64,64	0
56	MG	2A	3642	1/1	0.86	0.27	44,44,44,44	0
56	MG	1a	1762	1/1	0.86	0.23	60,60,60,60	0
56	MG	1A	3169	1/1	0.86	0.18	59,59,59,59	0
56	MG	1D	305	1/1	0.86	0.24	48,48,48,48	0
56	MG	1A	3660	1/1	0.86	0.29	61,61,61,61	0
56	MG	1A	3931	1/1	0.86	0.31	59,59,59,59	0
56	MG	1a	1916	1/1	0.86	0.12	79,79,79,79	0
56	MG	2A	3240	1/1	0.86	0.38	41,41,41,41	0
56	MG	1A	3849	1/1	0.86	0.16	55,55,55,55	0
56	MG	1A	3237	1/1	0.86	0.60	39,39,39,39	0
56	MG	1A	3544	1/1	0.86	0.17	65,65,65,65	0
56	MG	2W	204	1/1	0.86	0.43	51,51,51,51	0
56	MG	2a	3032	1/1	0.86	0.42	65,65,65,65	0
56	MG	1a	1654	1/1	0.86	0.23	52,52,52,52	0
56	MG	1a	1743	1/1	0.86	0.23	66,66,66,66	0
56	MG	1a	1858	1/1	0.86	0.15	74,74,74,74	0
56	MG	1A	3243	1/1	0.86	0.58	47,47,47,47	0
56	MG	2A	3385	1/1	0.86	0.23	55,55,55,55	0
56	MG	2A	3127	1/1	0.86	0.10	48,48,48,48	0
56	MG	1A	3140	1/1	0.86	0.33	37,37,37,37	0
56	MG	1a	1866	1/1	0.86	0.09	62,62,62,62	0
56	MG	2A	3324	1/1	0.86	0.35	57,57,57,57	0
56	MG	1A	4197	1/1	0.86	0.33	59,59,59,59	0
56	MG	1B	229	1/1	0.86	0.20	66,66,66,66	0
56	MG	2W	203	1/1	0.86	0.11	49,49,49,49	0
56	MG	2B	3017	1/1	0.86	0.10	68,68,68,68	0
56	MG	2T	3001	1/1	0.86	0.70	74,74,74,74	0
56	MG	1A	4093	1/1	0.86	0.21	39,39,39,39	0
56	MG	2A	3294	1/1	0.86	0.70	59,59,59,59	0
56	MG	1a	1729	1/1	0.86	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
56	MG	1A	3463	1/1	0.86	0.31	59,59,59,59	0
56	MG	2A	3785	1/1	0.86	0.37	57,57,57,57	0
56	MG	2a	3090	1/1	0.86	0.13	64,64,64,64	0
56	MG	1A	3288	1/1	0.86	0.23	54,54,54,54	0
56	MG	2A	3755	1/1	0.86	0.21	47,47,47,47	0
56	MG	1a	1667	1/1	0.86	0.12	59,59,59,59	0
56	MG	1A	3604	1/1	0.86	0.13	42,42,42,42	0
56	MG	2a	3112	1/1	0.86	0.18	70,70,70,70	0
56	MG	1a	1842	1/1	0.86	0.19	61,61,61,61	0
56	MG	1a	1813	1/1	0.86	0.13	76,76,76,76	0
56	MG	2W	202	1/1	0.86	0.39	66,66,66,66	0
56	MG	2A	3104	1/1	0.86	0.17	60,60,60,60	0
56	MG	2a	3105	1/1	0.86	0.09	57,57,57,57	0
56	MG	2A	3106	1/1	0.86	0.09	52,52,52,52	0
56	MG	2A	3126	1/1	0.86	0.09	50,50,50,50	0
56	MG	1A	4090	1/1	0.86	0.18	54,54,54,54	0
56	MG	1A	3728	1/1	0.86	0.10	60,60,60,60	0
56	MG	2a	3038	1/1	0.86	0.28	58,58,58,58	0
56	MG	1A	3971	1/1	0.86	0.16	31,31,31,31	0
56	MG	1a	1897	1/1	0.86	0.31	95,95,95,95	0
56	MG	1A	3624	1/1	0.86	0.25	60,60,60,60	0
56	MG	1A	3618	1/1	0.86	0.33	53,53,53,53	0
56	MG	2A	3100	1/1	0.86	0.10	72,72,72,72	0
56	MG	1A	3565	1/1	0.86	0.16	67,67,67,67	0
56	MG	2A	3819	1/1	0.86	0.07	64,64,64,64	0
56	MG	2A	3913	1/1	0.86	0.76	46,46,46,46	0
56	MG	2A	3677	1/1	0.86	0.13	44,44,44,44	0
56	MG	2A	3427	1/1	0.86	0.36	58,58,58,58	0
56	MG	2A	3056	1/1	0.86	0.41	46,46,46,46	0
56	MG	2A	3055	1/1	0.86	0.18	55,55,55,55	0
56	MG	1a	1817	1/1	0.86	0.31	56,56,56,56	0
56	MG	1A	4081	1/1	0.86	0.18	99,99,99,99	0
56	MG	1A	3632	1/1	0.86	0.35	60,60,60,60	0
56	MG	1m	201	1/1	0.86	0.14	59,59,59,59	0
56	MG	1A	4150	1/1	0.86	0.13	36,36,36,36	0
56	MG	1A	3248	1/1	0.86	0.13	67,67,67,67	0
56	MG	1A	3442	1/1	0.86	0.55	40,40,40,40	0
56	MG	1A	3721	1/1	0.86	0.12	37,37,37,37	0
56	MG	2a	3069	1/1	0.86	0.23	65,65,65,65	0
56	MG	1a	1901	1/1	0.86	0.10	70,70,70,70	0
56	MG	1A	3535	1/1	0.86	0.28	56,56,56,56	0
56	MG	1a	1907	1/1	0.87	0.14	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3149	1/1	0.87	0.11	86,86,86,86	0
56	MG	1w	107	1/1	0.87	0.27	70,70,70,70	0
56	MG	1F	309	1/1	0.87	0.16	62,62,62,62	0
56	MG	1A	4132	1/1	0.87	0.14	54,54,54,54	0
56	MG	2A	3218	1/1	0.87	0.12	63,63,63,63	0
56	MG	2A	3213	1/1	0.87	0.27	54,54,54,54	0
56	MG	2A	3245	1/1	0.87	0.29	51,51,51,51	0
56	MG	2A	3223	1/1	0.87	0.21	50,50,50,50	0
56	MG	2A	3692	1/1	0.87	0.36	65,65,65,65	0
56	MG	1A	3448	1/1	0.87	0.24	59,59,59,59	0
56	MG	1A	3636	1/1	0.87	0.18	66,66,66,66	0
56	MG	2A	3374	1/1	0.87	0.15	76,76,76,76	0
56	MG	2A	3087	1/1	0.87	0.39	57,57,57,57	0
56	MG	1N	3005	1/1	0.87	0.19	69,69,69,69	0
56	MG	1A	3205	1/1	0.87	0.24	27,27,27,27	0
56	MG	2A	3825	1/1	0.87	0.18	58,58,58,58	0
56	MG	1A	3759	1/1	0.87	0.24	34,34,34,34	0
56	MG	2A	3621	1/1	0.87	0.19	32,32,32,32	0
56	MG	2A	3863	1/1	0.87	0.26	68,68,68,68	0
56	MG	1A	3671	1/1	0.87	0.22	49,49,49,49	0
56	MG	1A	3967	1/1	0.87	0.40	61,61,61,61	0
56	MG	1A	3084	1/1	0.87	0.23	42,42,42,42	0
56	MG	28	101	1/1	0.87	0.15	75,75,75,75	0
56	MG	1A	3491	1/1	0.87	0.51	58,58,58,58	0
56	MG	1E	313	1/1	0.87	0.29	47,47,47,47	0
56	MG	1A	3629	1/1	0.87	0.26	62,62,62,62	0
56	MG	1a	1927	1/1	0.87	0.07	71,71,71,71	0
56	MG	1A	3405	1/1	0.87	0.27	51,51,51,51	0
56	MG	2A	3346	1/1	0.87	0.34	55,55,55,55	0
56	MG	1a	1722	1/1	0.87	0.28	58,58,58,58	0
56	MG	2A	3861	1/1	0.87	0.09	67,67,67,67	0
56	MG	2j	8001	1/1	0.87	0.12	80,80,80,80	0
56	MG	1A	3586	1/1	0.87	0.19	44,44,44,44	0
56	MG	1A	3504	1/1	0.87	0.31	51,51,51,51	0
56	MG	1Z	301	1/1	0.87	0.19	50,50,50,50	0
56	MG	1A	3252	1/1	0.87	0.17	66,66,66,66	0
56	MG	1A	3342	1/1	0.87	0.20	54,54,54,54	0
56	MG	1a	1671	1/1	0.87	0.23	53,53,53,53	0
56	MG	1A	3040	1/1	0.87	0.20	43,43,43,43	0
56	MG	2A	3181	1/1	0.87	0.17	49,49,49,49	0
56	MG	2A	3024	1/1	0.87	0.12	42,42,42,42	0
56	MG	1A	3616	1/1	0.87	0.41	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3449	1/1	0.87	0.39	57,57,57,57	0
56	MG	1A	3812	1/1	0.87	0.15	39,39,39,39	0
56	MG	1a	1921	1/1	0.87	0.33	55,55,55,55	0
56	MG	1A	3582	1/1	0.87	0.21	37,37,37,37	0
56	MG	2a	3128	1/1	0.87	0.15	60,60,60,60	0
56	MG	2A	3848	1/1	0.87	0.12	79,79,79,79	0
56	MG	1a	1840	1/1	0.87	0.17	50,50,50,50	0
56	MG	2A	3253	1/1	0.87	0.23	57,57,57,57	0
56	MG	1a	1633	1/1	0.87	0.23	62,62,62,62	0
56	MG	1A	3802	1/1	0.87	0.15	58,58,58,58	0
56	MG	1a	1800	1/1	0.87	0.19	56,56,56,56	0
56	MG	1A	3576	1/1	0.87	0.23	54,54,54,54	0
56	MG	2A	3176	1/1	0.87	0.09	62,62,62,62	0
56	MG	1B	226	1/1	0.87	0.10	54,54,54,54	0
56	MG	1A	3365	1/1	0.87	0.60	53,53,53,53	0
56	MG	1A	3889	1/1	0.87	0.17	49,49,49,49	0
56	MG	1E	307	1/1	0.87	0.16	67,67,67,67	0
56	MG	1a	1774	1/1	0.87	0.13	51,51,51,51	0
56	MG	2A	3033	1/1	0.87	0.13	53,53,53,53	0
56	MG	2j	8002	1/1	0.87	0.43	79,79,79,79	0
56	MG	1A	3837	1/1	0.87	0.18	29,29,29,29	0
56	MG	2A	3189	1/1	0.87	0.19	51,51,51,51	0
56	MG	1a	1906	1/1	0.87	0.13	50,50,50,50	0
56	MG	2A	3773	1/1	0.87	0.20	67,67,67,67	0
56	MG	2A	3317	1/1	0.87	0.17	53,53,53,53	0
56	MG	1A	3539	1/1	0.87	0.12	57,57,57,57	0
56	MG	1A	3858	1/1	0.87	0.22	34,34,34,34	0
56	MG	1A	3172	1/1	0.87	0.18	60,60,60,60	0
56	MG	1A	3380	1/1	0.87	0.22	50,50,50,50	0
56	MG	1A	3686	1/1	0.87	0.25	52,52,52,52	0
56	MG	2a	3039	1/1	0.87	0.17	45,45,45,45	0
56	MG	1x	103	1/1	0.87	0.24	59,59,59,59	0
56	MG	1A	3533	1/1	0.87	0.42	53,53,53,53	0
56	MG	1A	4058	1/1	0.87	0.57	65,65,65,65	0
56	MG	2A	3724	1/1	0.87	0.10	48,48,48,48	0
56	MG	1a	1812	1/1	0.87	0.14	58,58,58,58	0
56	MG	1x	104	1/1	0.87	0.26	68,68,68,68	0
56	MG	1A	3253	1/1	0.87	0.26	48,48,48,48	0
56	MG	1A	3975	1/1	0.87	0.27	48,48,48,48	0
56	MG	2A	3442	1/1	0.87	0.35	48,48,48,48	0
56	MG	1A	3486	1/1	0.87	0.17	52,52,52,52	0
56	MG	1a	1724	1/1	0.87	0.24	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3061	1/1	0.87	0.10	69,69,69,69	0
56	MG	2A	3466	1/1	0.87	0.26	50,50,50,50	0
56	MG	1A	3707	1/1	0.87	0.20	43,43,43,43	0
56	MG	1a	1778	1/1	0.87	0.45	65,65,65,65	0
56	MG	1A	3295	1/1	0.87	0.18	55,55,55,55	0
56	MG	2A	3293	1/1	0.87	1.25	64,64,64,64	0
56	MG	2A	3040	1/1	0.87	0.35	42,42,42,42	0
56	MG	1A	3487	1/1	0.87	0.36	62,62,62,62	0
56	MG	2A	3499	1/1	0.87	0.32	41,41,41,41	0
56	MG	2A	3080	1/1	0.87	0.22	57,57,57,57	0
56	MG	2A	3263	1/1	0.87	0.20	58,58,58,58	0
56	MG	2A	3153	1/1	0.87	0.07	63,63,63,63	0
56	MG	2A	3366	1/1	0.87	0.46	52,52,52,52	0
56	MG	1A	3069	1/1	0.87	0.14	45,45,45,45	0
56	MG	2A	3232	1/1	0.87	0.20	52,52,52,52	0
56	MG	2A	3350	1/1	0.87	0.11	44,44,44,44	0
56	MG	2A	3194	1/1	0.87	0.20	63,63,63,63	0
56	MG	1a	1849	1/1	0.87	0.09	54,54,54,54	0
56	MG	1A	3520	1/1	0.87	0.21	52,52,52,52	0
56	MG	2A	3813	1/1	0.87	0.25	39,39,39,39	0
56	MG	25	103	1/1	0.87	0.31	61,61,61,61	0
56	MG	2A	3457	1/1	0.87	0.41	66,66,66,66	0
56	MG	2a	3144	1/1	0.87	0.08	88,88,88,88	0
56	MG	1A	3402	1/1	0.87	0.30	53,53,53,53	0
56	MG	1A	3553	1/1	0.87	0.26	76,76,76,76	0
56	MG	2a	3129	1/1	0.87	0.30	65,65,65,65	0
56	MG	2A	3817	1/1	0.87	0.18	63,63,63,63	0
56	MG	1a	1795	1/1	0.87	0.18	67,67,67,67	0
56	MG	2A	3446	1/1	0.87	0.19	49,49,49,49	0
56	MG	2A	3357	1/1	0.87	0.39	66,66,66,66	0
56	MG	2A	3733	1/1	0.88	0.15	38,38,38,38	0
56	MG	2A	3276	1/1	0.88	0.29	49,49,49,49	0
56	MG	2A	3657	1/1	0.88	0.12	65,65,65,65	0
56	MG	1A	4156	1/1	0.88	0.08	54,54,54,54	0
56	MG	1A	3681	1/1	0.88	0.21	73,73,73,73	0
56	MG	1a	1753	1/1	0.88	0.15	74,74,74,74	0
56	MG	1A	3909	1/1	0.88	0.10	50,50,50,50	0
56	MG	2A	3696	1/1	0.88	0.16	50,50,50,50	0
56	MG	1A	3725	1/1	0.88	0.09	53,53,53,53	0
56	MG	1A	3437	1/1	0.88	0.47	59,59,59,59	0
56	MG	1a	1810	1/1	0.88	0.10	64,64,64,64	0
56	MG	1a	1664	1/1	0.88	0.09	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3545	1/1	0.88	0.19	30,30,30,30	0
56	MG	2A	3292	1/1	0.88	0.16	55,55,55,55	0
56	MG	1A	4104	1/1	0.88	0.07	32,32,32,32	0
56	MG	2a	3145	1/1	0.88	0.13	71,71,71,71	0
56	MG	2A	3367	1/1	0.88	0.09	59,59,59,59	0
56	MG	1A	3548	1/1	0.88	0.31	37,37,37,37	0
56	MG	2a	3082	1/1	0.88	0.12	64,64,64,64	0
56	MG	1A	3188	1/1	0.88	0.18	61,61,61,61	0
56	MG	2A	3841	1/1	0.88	0.14	66,66,66,66	0
56	MG	1A	3196	1/1	0.88	0.57	44,44,44,44	0
56	MG	2A	3628	1/1	0.88	0.15	53,53,53,53	0
56	MG	2A	3807	1/1	0.88	0.09	50,50,50,50	0
56	MG	1a	1609	1/1	0.88	0.09	64,64,64,64	0
56	MG	2D	303	1/1	0.88	1.02	51,51,51,51	0
56	MG	1A	4248	1/1	0.88	0.29	53,53,53,53	0
56	MG	2A	3128	1/1	0.88	0.18	56,56,56,56	0
56	MG	1A	3874	1/1	0.88	0.20	29,29,29,29	0
56	MG	2A	3748	1/1	0.88	0.08	61,61,61,61	0
56	MG	1A	3267	1/1	0.88	0.23	57,57,57,57	0
56	MG	1A	3085	1/1	0.88	0.30	48,48,48,48	0
56	MG	1A	3204	1/1	0.88	0.18	48,48,48,48	0
56	MG	1B	223	1/1	0.88	0.12	75,75,75,75	0
56	MG	1a	1672	1/1	0.88	0.19	61,61,61,61	0
56	MG	1A	3957	1/1	0.88	0.10	57,57,57,57	0
56	MG	1A	3574	1/1	0.88	0.26	49,49,49,49	0
56	MG	2A	3403	1/1	0.88	0.20	54,54,54,54	0
56	MG	2A	3706	1/1	0.88	0.19	60,60,60,60	0
56	MG	1A	3532	1/1	0.88	0.21	51,51,51,51	0
56	MG	2a	3195	1/1	0.88	0.28	85,85,85,85	0
56	MG	1a	1787	1/1	0.88	0.10	61,61,61,61	0
56	MG	1I	101	1/1	0.88	0.16	44,44,44,44	0
56	MG	1A	3583	1/1	0.88	0.24	51,51,51,51	0
56	MG	2A	3097	1/1	0.88	0.12	64,64,64,64	0
56	MG	2x	105	1/1	0.88	0.38	59,59,59,59	0
56	MG	2A	3775	1/1	0.88	0.18	40,40,40,40	0
56	MG	1A	3875	1/1	0.88	0.06	69,69,69,69	0
56	MG	1A	3735	1/1	0.88	0.16	61,61,61,61	0
56	MG	2A	3537	1/1	0.88	0.09	50,50,50,50	0
56	MG	1A	3378	1/1	0.88	0.17	63,63,63,63	0
56	MG	1A	3663	1/1	0.88	0.17	39,39,39,39	0
56	MG	2A	3228	1/1	0.88	0.64	53,53,53,53	0
56	MG	2A	3264	1/1	0.88	0.16	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3379	1/1	0.88	0.31	58,58,58,58	0
56	MG	1A	3317	1/1	0.88	0.16	53,53,53,53	0
56	MG	2a	3037	1/1	0.88	0.55	92,92,92,92	0
56	MG	1A	3314	1/1	0.88	0.26	53,53,53,53	0
56	MG	2A	3139	1/1	0.88	0.26	45,45,45,45	0
56	MG	2A	3076	1/1	0.88	0.33	39,39,39,39	0
56	MG	2A	3318	1/1	0.88	0.35	61,61,61,61	0
56	MG	2A	3014	1/1	0.88	0.35	40,40,40,40	0
56	MG	2a	3124	1/1	0.88	0.11	81,81,81,81	0
56	MG	2A	3883	1/1	0.88	0.41	44,44,44,44	0
56	MG	2A	3160	1/1	0.88	0.26	42,42,42,42	0
56	MG	2A	3721	1/1	0.88	0.19	45,45,45,45	0
56	MG	2A	3897	1/1	0.88	0.31	71,71,71,71	0
56	MG	1a	1716	1/1	0.88	0.39	53,53,53,53	0
56	MG	2a	3008	1/1	0.88	0.13	67,67,67,67	0
56	MG	2A	3426	1/1	0.88	0.07	47,47,47,47	0
56	MG	1a	1757	1/1	0.88	0.17	71,71,71,71	0
56	MG	1A	3356	1/1	0.88	0.34	76,76,76,76	0
56	MG	1A	3458	1/1	0.88	0.33	55,55,55,55	0
56	MG	1a	1780	1/1	0.88	0.22	70,70,70,70	0
56	MG	1A	3067	1/1	0.88	0.15	44,44,44,44	0
56	MG	2A	3138	1/1	0.88	0.38	40,40,40,40	0
59	ZN	29	501	1/1	0.88	0.06	79,79,79,79	0
56	MG	2A	3814	1/1	0.88	0.28	56,56,56,56	0
56	MG	2a	3166	1/1	0.88	0.06	81,81,81,81	0
56	MG	2A	3208	1/1	0.88	0.29	50,50,50,50	0
56	MG	2A	3370	1/1	0.88	0.52	62,62,62,62	0
56	MG	1A	3500	1/1	0.88	0.62	50,50,50,50	0
56	MG	2A	3042	1/1	0.88	0.20	59,59,59,59	0
56	MG	1N	3007	1/1	0.88	0.57	56,56,56,56	0
56	MG	12	3001	1/1	0.88	0.24	56,56,56,56	0
56	MG	2a	3085	1/1	0.88	0.31	57,57,57,57	0
56	MG	1A	3513	1/1	0.88	0.60	36,36,36,36	0
56	MG	1a	1624	1/1	0.88	0.08	60,60,60,60	0
56	MG	1a	1806	1/1	0.88	0.20	53,53,53,53	0
56	MG	1A	3073	1/1	0.88	0.31	52,52,52,52	0
56	MG	2A	3796	1/1	0.88	0.14	64,64,64,64	0
56	MG	1A	3121	1/1	0.88	0.47	54,54,54,54	0
56	MG	2A	3226	1/1	0.88	0.39	51,51,51,51	0
56	MG	1A	3554	1/1	0.88	0.16	53,53,53,53	0
56	MG	1A	3768	1/1	0.88	0.21	28,28,28,28	0
56	MG	1a	1839	1/1	0.88	0.15	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4057	1/1	0.88	0.23	47,47,47,47	0
56	MG	2A	3211	1/1	0.88	0.37	56,56,56,56	0
56	MG	1A	3853	1/1	0.88	0.20	24,24,24,24	0
56	MG	1a	1646	1/1	0.88	0.09	59,59,59,59	0
56	MG	1B	221	1/1	0.88	0.16	65,65,65,65	0
56	MG	1A	3263	1/1	0.88	0.21	61,61,61,61	0
56	MG	1A	3920	1/1	0.88	0.17	60,60,60,60	0
56	MG	2A	3878	1/1	0.88	0.17	64,64,64,64	0
56	MG	1E	303	1/1	0.88	0.45	46,46,46,46	0
56	MG	2a	3224	1/1	0.88	0.17	67,67,67,67	0
56	MG	1A	3778	1/1	0.88	0.09	66,66,66,66	0
56	MG	2a	3099	1/1	0.88	0.10	60,60,60,60	0
56	MG	2A	3065	1/1	0.88	0.10	59,59,59,59	0
56	MG	2A	3279	1/1	0.88	0.14	60,60,60,60	0
56	MG	1A	3679	1/1	0.88	0.15	44,44,44,44	0
56	MG	2a	3043	1/1	0.88	0.23	61,61,61,61	0
56	MG	1A	3545	1/1	0.88	0.14	62,62,62,62	0
56	MG	2w	107	1/1	0.88	0.11	63,63,63,63	0
56	MG	1A	3106	1/1	0.88	0.52	47,47,47,47	0
56	MG	2A	3101	1/1	0.88	0.14	51,51,51,51	0
56	MG	2A	3405	1/1	0.88	0.10	72,72,72,72	0
56	MG	1O	3003	1/1	0.88	0.21	50,50,50,50	0
56	MG	1U	206	1/1	0.88	0.45	41,41,41,41	0
56	MG	2A	3205	1/1	0.88	0.18	45,45,45,45	0
56	MG	2A	3304	1/1	0.88	0.12	52,52,52,52	0
56	MG	2A	3416	1/1	0.88	0.27	52,52,52,52	0
56	MG	1A	3921	1/1	0.88	0.12	53,53,53,53	0
56	MG	1A	3423	1/1	0.88	0.47	61,61,61,61	0
56	MG	2A	3560	1/1	0.88	0.21	41,41,41,41	0
56	MG	1A	4045	1/1	0.88	0.06	57,57,57,57	0
56	MG	2a	3164	1/1	0.88	0.06	88,88,88,88	0
56	MG	1a	1873	1/1	0.89	0.05	90,90,90,90	0
56	MG	1A	3788	1/1	0.89	0.15	27,27,27,27	0
56	MG	1Q	203	1/1	0.89	0.16	53,53,53,53	0
56	MG	2a	3103	1/1	0.89	0.08	65,65,65,65	0
56	MG	1A	3456	1/1	0.89	0.23	57,57,57,57	0
56	MG	1A	3147	1/1	0.89	0.21	45,45,45,45	0
56	MG	1a	1708	1/1	0.89	0.18	48,48,48,48	0
56	MG	1A	3928	1/1	0.89	0.14	47,47,47,47	0
56	MG	2a	3077	1/1	0.89	0.15	59,59,59,59	0
56	MG	1A	4108	1/1	0.89	0.07	44,44,44,44	0
56	MG	1A	3219	1/1	0.89	0.10	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3650	1/1	0.89	0.25	45,45,45,45	0
56	MG	1A	3011	1/1	0.89	0.19	42,42,42,42	0
56	MG	2A	3436	1/1	0.89	0.19	54,54,54,54	0
56	MG	2A	3475	1/1	0.89	0.24	49,49,49,49	0
56	MG	1a	1740	1/1	0.89	0.09	53,53,53,53	0
56	MG	2A	3768	1/1	0.89	0.25	66,66,66,66	0
56	MG	1A	3348	1/1	0.89	0.26	53,53,53,53	0
56	MG	2A	3717	1/1	0.89	0.46	55,55,55,55	0
56	MG	1x	115	1/1	0.89	0.28	49,49,49,49	0
56	MG	1A	3645	1/1	0.89	0.25	59,59,59,59	0
56	MG	2A	3281	1/1	0.89	0.22	34,34,34,34	0
56	MG	1s	3001	1/1	0.89	0.09	61,61,61,61	0
56	MG	1A	3635	1/1	0.89	0.25	59,59,59,59	0
56	MG	1A	3526	1/1	0.89	0.25	46,46,46,46	0
56	MG	1A	3828	1/1	0.89	0.08	47,47,47,47	0
56	MG	1a	1892	1/1	0.89	0.09	66,66,66,66	0
56	MG	1A	3774	1/1	0.89	0.19	75,75,75,75	0
56	MG	2A	3579	1/1	0.89	0.14	39,39,39,39	0
56	MG	1c	301	1/1	0.89	0.19	66,66,66,66	0
56	MG	2A	3030	1/1	0.89	0.12	35,35,35,35	0
56	MG	1A	4136	1/1	0.89	0.10	59,59,59,59	0
56	MG	1A	3180	1/1	0.89	0.33	52,52,52,52	0
56	MG	2A	3701	1/1	0.89	0.17	66,66,66,66	0
56	MG	1A	3926	1/1	0.89	0.20	62,62,62,62	0
56	MG	1F	304	1/1	0.89	0.12	44,44,44,44	0
56	MG	2A	3592	1/1	0.89	0.14	52,52,52,52	0
56	MG	2a	3022	1/1	0.89	0.32	67,67,67,67	0
56	MG	2a	3011	1/1	0.89	0.06	69,69,69,69	0
56	MG	1A	3422	1/1	0.89	0.25	56,56,56,56	0
56	MG	1a	1797	1/1	0.89	0.24	66,66,66,66	0
56	MG	2A	3779	1/1	0.89	0.14	73,73,73,73	0
56	MG	1A	3514	1/1	0.89	0.18	51,51,51,51	0
56	MG	2A	3555	1/1	0.89	0.14	36,36,36,36	0
56	MG	2A	3061	1/1	0.89	0.15	51,51,51,51	0
56	MG	2A	3842	1/1	0.89	0.18	35,35,35,35	0
56	MG	1A	3353	1/1	0.89	0.12	69,69,69,69	0
56	MG	2A	3882	1/1	0.89	0.27	51,51,51,51	0
56	MG	1a	1852	1/1	0.89	0.13	66,66,66,66	0
56	MG	2A	3300	1/1	0.89	0.30	63,63,63,63	0
56	MG	1A	4006	1/1	0.89	0.22	57,57,57,57	0
56	MG	2A	3471	1/1	0.89	0.33	59,59,59,59	0
56	MG	1A	3325	1/1	0.89	0.33	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3209	1/1	0.89	0.18	57,57,57,57	0
56	MG	2A	3458	1/1	0.89	0.44	57,57,57,57	0
56	MG	1A	3433	1/1	0.89	0.26	57,57,57,57	0
56	MG	1A	3672	1/1	0.89	0.17	40,40,40,40	0
56	MG	1a	1745	1/1	0.89	0.36	58,58,58,58	0
56	MG	2A	3557	1/1	0.89	0.08	51,51,51,51	0
56	MG	1a	1879	1/1	0.89	0.17	49,49,49,49	0
56	MG	1A	3239	1/1	0.89	0.15	55,55,55,55	0
56	MG	17	102	1/1	0.89	0.33	62,62,62,62	0
56	MG	2a	3229	1/1	0.89	0.23	81,81,81,81	0
56	MG	2A	3918	1/1	0.89	0.95	52,52,52,52	0
56	MG	1a	1636	1/1	0.89	0.12	66,66,66,66	0
56	MG	2A	3506	1/1	0.89	0.11	38,38,38,38	0
56	MG	2a	3141	1/1	0.89	0.14	57,57,57,57	0
56	MG	1A	3394	1/1	0.89	0.24	63,63,63,63	0
56	MG	2A	3805	1/1	0.89	0.12	64,64,64,64	0
56	MG	2A	3668	1/1	0.89	0.12	41,41,41,41	0
56	MG	1a	1766	1/1	0.89	0.37	62,62,62,62	0
56	MG	20	102	1/1	0.89	0.19	56,56,56,56	0
56	MG	2A	3345	1/1	0.89	0.36	58,58,58,58	0
56	MG	1A	3444	1/1	0.89	0.24	45,45,45,45	0
56	MG	2A	3583	1/1	0.89	0.07	56,56,56,56	0
56	MG	2A	3529	1/1	0.89	0.16	35,35,35,35	0
56	MG	2A	3585	1/1	0.89	0.13	49,49,49,49	0
56	MG	1A	3361	1/1	0.89	0.27	63,63,63,63	0
56	MG	1A	3412	1/1	0.89	0.27	56,56,56,56	0
56	MG	2a	3115	1/1	0.89	0.22	61,61,61,61	0
56	MG	1a	1662	1/1	0.89	0.14	47,47,47,47	0
56	MG	2A	3487	1/1	0.89	0.19	45,45,45,45	0
56	MG	2A	3553	1/1	0.89	0.11	42,42,42,42	0
56	MG	1a	1718	1/1	0.89	0.11	57,57,57,57	0
56	MG	1A	3360	1/1	0.89	0.31	54,54,54,54	0
56	MG	1A	3642	1/1	0.89	0.28	53,53,53,53	0
56	MG	1A	3285	1/1	0.89	0.93	43,43,43,43	0
56	MG	2A	3744	1/1	0.89	0.13	71,71,71,71	0
56	MG	2a	3181	1/1	0.89	0.19	62,62,62,62	0
56	MG	1A	3382	1/1	0.89	0.32	53,53,53,53	0
56	MG	2A	3772	1/1	0.89	0.10	59,59,59,59	0
56	MG	1A	3436	1/1	0.89	0.37	47,47,47,47	0
56	MG	1a	1894	1/1	0.89	0.05	71,71,71,71	0
56	MG	1A	3401	1/1	0.89	0.20	46,46,46,46	0
56	MG	1A	3980	1/1	0.89	0.21	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3495	1/1	0.89	0.44	48,48,48,48	0
56	MG	1A	3741	1/1	0.89	0.07	58,58,58,58	0
56	MG	1A	3830	1/1	0.89	0.15	53,53,53,53	0
56	MG	1A	3474	1/1	0.89	0.17	51,51,51,51	0
56	MG	2A	3280	1/1	0.89	0.48	59,59,59,59	0
56	MG	2A	3415	1/1	0.89	0.24	59,59,59,59	0
56	MG	1a	1756	1/1	0.89	0.17	66,66,66,66	0
56	MG	1A	3592	1/1	0.89	0.15	41,41,41,41	0
56	MG	2A	3381	1/1	0.89	0.12	53,53,53,53	0
56	MG	1A	4004	1/1	0.89	0.21	56,56,56,56	0
56	MG	1A	3302	1/1	0.89	0.32	33,33,33,33	0
56	MG	2A	3093	1/1	0.89	0.70	48,48,48,48	0
56	MG	2A	3739	1/1	0.89	0.13	52,52,52,52	0
56	MG	1a	1670	1/1	0.89	0.34	56,56,56,56	0
56	MG	1A	3065	1/1	0.89	0.20	61,61,61,61	0
56	MG	1A	4082	1/1	0.89	0.14	90,90,90,90	0
56	MG	1A	3498	1/1	0.89	0.22	64,64,64,64	0
56	MG	2A	3482	1/1	0.89	0.67	48,48,48,48	0
56	MG	1O	3005	1/1	0.89	0.35	68,68,68,68	0
56	MG	1A	3850	1/1	0.89	0.23	25,25,25,25	0
56	MG	2a	3159	1/1	0.89	0.13	62,62,62,62	0
56	MG	2A	3860	1/1	0.89	0.08	70,70,70,70	0
56	MG	2A	3552	1/1	0.89	0.20	34,34,34,34	0
56	MG	2A	3759	1/1	0.89	0.17	37,37,37,37	0
56	MG	2a	3017	1/1	0.89	0.07	71,71,71,71	0
56	MG	1A	3956	1/1	0.89	0.20	55,55,55,55	0
56	MG	1A	3445	1/1	0.89	0.37	59,59,59,59	0
56	MG	2A	3192	1/1	0.89	0.46	52,52,52,52	0
56	MG	18	101	1/1	0.89	0.37	77,77,77,77	0
56	MG	1N	3002	1/1	0.89	0.13	46,46,46,46	0
56	MG	1A	3485	1/1	0.89	0.11	51,51,51,51	0
56	MG	2A	3512	1/1	0.89	0.14	53,53,53,53	0
56	MG	2A	3498	1/1	0.89	0.16	62,62,62,62	0
56	MG	1A	3322	1/1	0.89	0.36	50,50,50,50	0
56	MG	1A	3446	1/1	0.89	0.12	55,55,55,55	0
56	MG	2A	3571	1/1	0.89	0.16	36,36,36,36	0
56	MG	1A	3459	1/1	0.89	0.35	53,53,53,53	0
56	MG	1A	3945	1/1	0.89	0.20	35,35,35,35	0
56	MG	1B	236	1/1	0.89	0.12	33,33,33,33	0
56	MG	2A	3185	1/1	0.89	0.27	60,60,60,60	0
56	MG	2A	3330	1/1	0.89	0.21	69,69,69,69	0
56	MG	2A	3580	1/1	0.89	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
56	MG	1A	3393	1/1	0.89	0.31	67,67,67,67	0
56	MG	1F	303	1/1	0.89	0.15	57,57,57,57	0
56	MG	2W	201	1/1	0.89	0.11	61,61,61,61	0
56	MG	2A	3098	1/1	0.89	0.15	51,51,51,51	0
56	MG	2A	3417	1/1	0.89	0.16	60,60,60,60	0
56	MG	1a	1748	1/1	0.89	0.05	53,53,53,53	0
56	MG	2a	3089	1/1	0.89	0.20	70,70,70,70	0
56	MG	1A	3913	1/1	0.89	0.24	45,45,45,45	0
56	MG	1a	1632	1/1	0.89	0.22	62,62,62,62	0
56	MG	1A	3542	1/1	0.89	0.28	50,50,50,50	0
56	MG	1A	3451	1/1	0.89	0.26	63,63,63,63	0
56	MG	1A	3224	1/1	0.89	0.22	50,50,50,50	0
56	MG	1F	307	1/1	0.89	0.12	35,35,35,35	0
56	MG	1A	3704	1/1	0.89	0.19	38,38,38,38	0
56	MG	2A	3212	1/1	0.89	0.19	58,58,58,58	0
56	MG	2A	3217	1/1	0.89	0.16	59,59,59,59	0
56	MG	1A	3979	1/1	0.89	0.18	46,46,46,46	0
56	MG	1A	4043	1/1	0.89	0.13	38,38,38,38	0
56	MG	2A	3131	1/1	0.89	0.20	56,56,56,56	0
56	MG	1x	109	1/1	0.90	0.30	74,74,74,74	0
56	MG	1A	3164	1/1	0.90	0.30	66,66,66,66	0
56	MG	1A	3018	1/1	0.90	0.30	50,50,50,50	0
56	MG	1A	4204	1/1	0.90	0.23	50,50,50,50	0
56	MG	2A	3191	1/1	0.90	0.27	52,52,52,52	0
56	MG	2A	3268	1/1	0.90	0.13	59,59,59,59	0
56	MG	2A	3450	1/1	0.90	0.18	56,56,56,56	0
56	MG	2a	3209	1/1	0.90	0.12	61,61,61,61	0
56	MG	1A	3094	1/1	0.90	0.09	52,52,52,52	0
56	MG	2A	3622	1/1	0.90	0.15	47,47,47,47	0
56	MG	2A	3908	1/1	0.90	0.23	43,43,43,43	0
56	MG	1f	3002	1/1	0.90	0.27	61,61,61,61	0
56	MG	2A	3603	1/1	0.90	0.06	44,44,44,44	0
56	MG	2a	3189	1/1	0.90	0.12	54,54,54,54	0
56	MG	1A	3814	1/1	0.90	0.16	64,64,64,64	0
56	MG	1A	4172	1/1	0.90	0.18	46,46,46,46	0
56	MG	1a	1844	1/1	0.90	0.14	52,52,52,52	0
56	MG	1A	3502	1/1	0.90	0.19	55,55,55,55	0
56	MG	2A	3216	1/1	0.90	0.24	54,54,54,54	0
56	MG	2A	3365	1/1	0.90	0.18	58,58,58,58	0
56	MG	1A	3567	1/1	0.90	0.18	38,38,38,38	0
56	MG	1A	3465	1/1	0.90	0.46	53,53,53,53	0
56	MG	1A	4071	1/1	0.90	0.20	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3603	1/1	0.90	0.14	51,51,51,51	0
56	MG	1A	4218	1/1	0.90	0.17	36,36,36,36	0
56	MG	1A	3466	1/1	0.90	0.25	58,58,58,58	0
56	MG	2A	3469	1/1	0.90	0.41	61,61,61,61	0
56	MG	1A	4221	1/1	0.90	0.23	35,35,35,35	0
56	MG	1A	3588	1/1	0.90	0.13	50,50,50,50	0
56	MG	1a	1856	1/1	0.90	0.13	38,38,38,38	0
56	MG	1A	3233	1/1	0.90	0.27	65,65,65,65	0
56	MG	2A	3215	1/1	0.90	0.20	61,61,61,61	0
56	MG	2A	3474	1/1	0.90	0.36	53,53,53,53	0
56	MG	1A	3345	1/1	0.90	0.28	57,57,57,57	0
56	MG	2a	3201	1/1	0.90	0.06	70,70,70,70	0
56	MG	2q	204	1/1	0.90	0.10	68,68,68,68	0
56	MG	1A	3471	1/1	0.90	0.50	65,65,65,65	0
56	MG	2A	3877	1/1	0.90	0.07	71,71,71,71	0
56	MG	1A	3324	1/1	0.90	0.18	62,62,62,62	0
56	MG	1A	3737	1/1	0.90	0.13	35,35,35,35	0
56	MG	2A	3766	1/1	0.90	0.16	51,51,51,51	0
56	MG	1A	3016	1/1	0.90	0.15	50,50,50,50	0
56	MG	1A	3613	1/1	0.90	0.16	55,55,55,55	0
56	MG	1A	4211	1/1	0.90	0.23	61,61,61,61	0
56	MG	1a	1822	1/1	0.90	0.17	45,45,45,45	0
56	MG	2A	3121	1/1	0.90	0.25	53,53,53,53	0
56	MG	2A	3371	1/1	0.90	0.15	53,53,53,53	0
56	MG	25	104	1/1	0.90	0.17	51,51,51,51	0
56	MG	1A	4021	1/1	0.90	0.14	36,36,36,36	0
56	MG	2A	3219	1/1	0.90	0.26	56,56,56,56	0
56	MG	1A	3278	1/1	0.90	0.22	55,55,55,55	0
56	MG	2A	3536	1/1	0.90	0.12	60,60,60,60	0
56	MG	2A	3282	1/1	0.90	0.34	64,64,64,64	0
56	MG	1A	3884	1/1	0.90	0.23	63,63,63,63	0
56	MG	2F	302	1/1	0.90	0.21	63,63,63,63	0
56	MG	1A	4019	1/1	0.90	0.11	47,47,47,47	0
56	MG	1A	4105	1/1	0.90	0.15	33,33,33,33	0
56	MG	1A	3499	1/1	0.90	0.20	62,62,62,62	0
56	MG	2A	3062	1/1	0.90	0.09	54,54,54,54	0
56	MG	2A	3703	1/1	0.90	0.08	64,64,64,64	0
56	MG	1A	3562	1/1	0.90	0.15	45,45,45,45	0
56	MG	2A	3069	1/1	0.90	0.13	38,38,38,38	0
56	MG	1A	3693	1/1	0.90	0.22	57,57,57,57	0
56	MG	1a	1767	1/1	0.90	0.16	51,51,51,51	0
56	MG	1a	1747	1/1	0.90	0.07	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1845	1/1	0.90	0.13	75,75,75,75	0
56	MG	1a	1826	1/1	0.90	0.14	68,68,68,68	0
56	MG	1A	4174	1/1	0.90	0.12	83,83,83,83	0
56	MG	2a	3104	1/1	0.90	0.18	81,81,81,81	0
56	MG	1A	4086	1/1	0.90	0.33	57,57,57,57	0
56	MG	2A	3627	1/1	0.90	0.23	43,43,43,43	0
56	MG	2A	3822	1/1	0.90	0.06	78,78,78,78	0
56	MG	2A	3072	1/1	0.90	0.15	47,47,47,47	0
56	MG	1f	3001	1/1	0.90	0.15	44,44,44,44	0
56	MG	1a	1603	1/1	0.90	0.18	87,87,87,87	0
56	MG	1A	4076	1/1	0.90	0.19	30,30,30,30	0
56	MG	1A	3706	1/1	0.90	0.16	23,23,23,23	0
56	MG	2A	3273	1/1	0.90	0.17	58,58,58,58	0
56	MG	1A	3493	1/1	0.90	0.31	33,33,33,33	0
56	MG	1A	4219	1/1	0.90	0.20	41,41,41,41	0
56	MG	1A	3703	1/1	0.90	0.26	47,47,47,47	0
56	MG	2A	3801	1/1	0.90	0.14	59,59,59,59	0
56	MG	2A	3433	1/1	0.90	0.19	46,46,46,46	0
56	MG	1A	3685	1/1	0.90	0.20	69,69,69,69	0
56	MG	2A	3019	1/1	0.90	0.14	40,40,40,40	0
56	MG	2A	3675	1/1	0.90	0.22	42,42,42,42	0
56	MG	2a	3053	1/1	0.90	0.27	82,82,82,82	0
56	MG	1A	3429	1/1	0.90	0.35	48,48,48,48	0
56	MG	2A	3652	1/1	0.90	0.55	45,45,45,45	0
56	MG	2A	3448	1/1	0.90	0.33	61,61,61,61	0
56	MG	1a	1853	1/1	0.90	0.09	48,48,48,48	0
56	MG	1A	3056	1/1	0.90	0.21	50,50,50,50	0
56	MG	1a	1619	1/1	0.90	0.08	55,55,55,55	0
56	MG	2E	307	1/1	0.90	0.07	61,61,61,61	0
56	MG	2A	3740	1/1	0.90	0.18	73,73,73,73	0
56	MG	2A	3610	1/1	0.90	0.10	62,62,62,62	0
56	MG	2a	3117	1/1	0.90	0.15	63,63,63,63	0
56	MG	1T	202	1/1	0.90	0.50	59,59,59,59	0
56	MG	1A	4169	1/1	0.90	0.13	77,77,77,77	0
56	MG	2A	3310	1/1	0.90	0.20	49,49,49,49	0
56	MG	1A	3803	1/1	0.90	0.27	48,48,48,48	0
56	MG	2A	3308	1/1	0.90	0.11	56,56,56,56	0
56	MG	1A	3996	1/1	0.90	0.14	48,48,48,48	0
56	MG	2A	3425	1/1	0.90	0.41	73,73,73,73	0
56	MG	1a	1684	1/1	0.90	0.22	55,55,55,55	0
56	MG	2A	3840	1/1	0.90	0.10	49,49,49,49	0
56	MG	2w	106	1/1	0.90	0.10	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3811	1/1	0.90	0.11	34,34,34,34	0
56	MG	1a	1650	1/1	0.90	0.22	54,54,54,54	0
56	MG	2A	3561	1/1	0.90	0.07	37,37,37,37	0
56	MG	2A	3283	1/1	0.90	0.09	53,53,53,53	0
56	MG	1A	3396	1/1	0.90	0.42	43,43,43,43	0
56	MG	2A	3004	1/1	0.90	0.38	44,44,44,44	0
56	MG	2A	3237	1/1	0.90	0.22	48,48,48,48	0
56	MG	2A	3609	1/1	0.90	0.20	60,60,60,60	0
56	MG	2r	3001	1/1	0.90	0.27	75,75,75,75	0
59	ZN	2Y	501	1/1	0.90	0.07	101,101,101,101	0
56	MG	1A	4257	1/1	0.90	0.16	41,41,41,41	0
56	MG	1A	4244	1/1	0.90	0.15	39,39,39,39	0
56	MG	1a	1824	1/1	0.90	0.13	67,67,67,67	0
56	MG	1A	3421	1/1	0.90	0.25	46,46,46,46	0
56	MG	1A	3339	1/1	0.90	0.15	53,53,53,53	0
56	MG	1A	3115	1/1	0.90	0.25	44,44,44,44	0
56	MG	1a	1825	1/1	0.90	0.21	57,57,57,57	0
56	MG	2A	3530	1/1	0.90	0.11	45,45,45,45	0
56	MG	1a	1627	1/1	0.90	0.09	46,46,46,46	0
56	MG	1A	3427	1/1	0.90	0.19	44,44,44,44	0
56	MG	1a	1629	1/1	0.90	0.10	43,43,43,43	0
56	MG	2A	3762	1/1	0.90	0.16	54,54,54,54	0
56	MG	2a	3208	1/1	0.90	0.17	70,70,70,70	0
56	MG	1A	3617	1/1	0.90	0.18	48,48,48,48	0
56	MG	2A	3102	1/1	0.90	0.11	55,55,55,55	0
56	MG	1A	3766	1/1	0.90	0.26	26,26,26,26	0
56	MG	1A	3846	1/1	0.90	0.12	47,47,47,47	0
56	MG	1A	3961	1/1	0.90	0.52	60,60,60,60	0
56	MG	2a	3093	1/1	0.90	0.14	55,55,55,55	0
56	MG	1a	1816	1/1	0.90	0.54	59,59,59,59	0
56	MG	1A	3202	1/1	0.90	0.15	46,46,46,46	0
56	MG	2A	3455	1/1	0.90	0.29	44,44,44,44	0
56	MG	2A	3220	1/1	0.90	0.21	46,46,46,46	0
56	MG	1A	3497	1/1	0.90	0.14	59,59,59,59	0
56	MG	1Q	205	1/1	0.90	0.16	41,41,41,41	0
56	MG	1A	3620	1/1	0.90	0.60	59,59,59,59	0
56	MG	2a	3212	1/1	0.90	0.12	71,71,71,71	0
56	MG	2x	101	1/1	0.90	0.10	48,48,48,48	0
56	MG	1A	3387	1/1	0.90	0.41	63,63,63,63	0
56	MG	1A	4129	1/1	0.90	0.07	56,56,56,56	0
56	MG	2A	3899	1/1	0.90	0.38	61,61,61,61	0
56	MG	1A	3893	1/1	0.90	0.15	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1630	1/1	0.90	0.16	57,57,57,57	0
56	MG	2a	3050	1/1	0.90	0.09	69,69,69,69	0
56	MG	2a	3110	1/1	0.90	0.36	53,53,53,53	0
56	MG	1A	3257	1/1	0.90	0.26	49,49,49,49	0
56	MG	2A	3186	1/1	0.90	0.29	54,54,54,54	0
56	MG	1A	4040	1/1	0.90	0.12	74,74,74,74	0
56	MG	1A	3841	1/1	0.90	0.19	42,42,42,42	0
56	MG	1N	3003	1/1	0.90	0.17	53,53,53,53	0
56	MG	2A	3481	1/1	0.90	0.16	55,55,55,55	0
56	MG	1A	3782	1/1	0.90	0.24	26,26,26,26	0
56	MG	1a	1877	1/1	0.90	0.07	72,72,72,72	0
56	MG	12	3002	1/1	0.90	0.42	48,48,48,48	0
56	MG	2B	3004	1/1	0.90	0.08	79,79,79,79	0
56	MG	2A	3782	1/1	0.90	0.10	44,44,44,44	0
56	MG	1E	312	1/1	0.90	0.11	62,62,62,62	0
56	MG	1A	3723	1/1	0.90	0.16	37,37,37,37	0
56	MG	2a	3074	1/1	0.90	0.12	63,63,63,63	0
56	MG	1A	3898	1/1	0.90	0.13	54,54,54,54	0
56	MG	1A	3585	1/1	0.90	0.28	49,49,49,49	0
56	MG	1A	3856	1/1	0.90	0.37	56,56,56,56	0
56	MG	1B	211	1/1	0.90	0.20	62,62,62,62	0
56	MG	1A	3857	1/1	0.90	0.21	29,29,29,29	0
56	MG	1A	3181	1/1	0.90	0.23	53,53,53,53	0
56	MG	1B	225	1/1	0.90	0.12	42,42,42,42	0
56	MG	1A	3408	1/1	0.90	0.30	48,48,48,48	0
56	MG	1a	1885	1/1	0.90	0.12	78,78,78,78	0
56	MG	1A	3385	1/1	0.90	0.18	63,63,63,63	0
56	MG	1A	4079	1/1	0.90	0.17	36,36,36,36	0
56	MG	2A	3921	1/1	0.90	0.28	65,65,65,65	0
56	MG	2w	102	1/1	0.90	0.28	60,60,60,60	0
56	MG	2A	3235	1/1	0.90	0.21	52,52,52,52	0
56	MG	1E	308	1/1	0.91	0.19	34,34,34,34	0
56	MG	2a	3096	1/1	0.91	0.06	70,70,70,70	0
56	MG	1a	1896	1/1	0.91	0.07	77,77,77,77	0
56	MG	19	101	1/1	0.91	0.11	49,49,49,49	0
56	MG	1A	3051	1/1	0.91	0.30	43,43,43,43	0
56	MG	2A	3118	1/1	0.91	0.17	52,52,52,52	0
56	MG	2a	3175	1/1	0.91	0.09	58,58,58,58	0
56	MG	1A	3148	1/1	0.91	0.39	40,40,40,40	0
56	MG	1A	3651	1/1	0.91	0.12	47,47,47,47	0
56	MG	2A	3025	1/1	0.91	1.40	55,55,55,55	0
56	MG	2A	3178	1/1	0.91	0.31	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3063	1/1	0.91	0.30	64,64,64,64	0
56	MG	2A	3821	1/1	0.91	0.09	76,76,76,76	0
56	MG	1a	1889	1/1	0.91	0.08	77,77,77,77	0
56	MG	2v	104	1/1	0.91	0.13	61,61,61,61	0
56	MG	1a	1614	1/1	0.91	0.19	63,63,63,63	0
56	MG	2A	3569	1/1	0.91	0.13	32,32,32,32	0
56	MG	1A	3870	1/1	0.91	0.23	35,35,35,35	0
56	MG	1A	3440	1/1	0.91	0.38	38,38,38,38	0
56	MG	1A	3807	1/1	0.91	0.14	44,44,44,44	0
56	MG	1x	114	1/1	0.91	0.20	59,59,59,59	0
56	MG	1A	3109	1/1	0.91	0.16	50,50,50,50	0
56	MG	1A	3184	1/1	0.91	0.10	61,61,61,61	0
56	MG	1A	3276	1/1	0.91	0.19	55,55,55,55	0
56	MG	1A	3117	1/1	0.91	0.36	46,46,46,46	0
56	MG	2A	3764	1/1	0.91	0.11	51,51,51,51	0
56	MG	1A	3105	1/1	0.91	0.12	31,31,31,31	0
56	MG	1A	4075	1/1	0.91	0.19	21,21,21,21	0
56	MG	2A	3502	1/1	0.91	0.10	54,54,54,54	0
56	MG	2D	301	1/1	0.91	0.27	51,51,51,51	0
56	MG	2A	3036	1/1	0.91	0.14	50,50,50,50	0
56	MG	2a	3183	1/1	0.91	0.21	39,39,39,39	0
56	MG	1X	102	1/1	0.91	0.23	45,45,45,45	0
56	MG	2a	3227	1/1	0.91	0.15	68,68,68,68	0
56	MG	2a	3206	1/1	0.91	0.10	58,58,58,58	0
56	MG	2A	3047	1/1	0.91	0.10	44,44,44,44	0
56	MG	1a	1883	1/1	0.91	0.15	47,47,47,47	0
56	MG	2A	3286	1/1	0.91	0.28	52,52,52,52	0
56	MG	1A	3481	1/1	0.91	0.35	52,52,52,52	0
56	MG	1A	3609	1/1	0.91	0.16	50,50,50,50	0
56	MG	1a	1791	1/1	0.91	0.29	71,71,71,71	0
56	MG	2A	3567	1/1	0.91	0.16	33,33,33,33	0
56	MG	2A	3486	1/1	0.91	0.47	46,46,46,46	0
56	MG	1a	1642	1/1	0.91	0.18	51,51,51,51	0
56	MG	1A	3503	1/1	0.91	0.36	56,56,56,56	0
56	MG	1A	3627	1/1	0.91	0.26	55,55,55,55	0
56	MG	1A	3159	1/1	0.91	0.36	35,35,35,35	0
56	MG	2A	3053	1/1	0.91	0.10	55,55,55,55	0
56	MG	1a	1913	1/1	0.91	0.09	80,80,80,80	0
56	MG	2A	3910	1/1	0.91	0.65	58,58,58,58	0
56	MG	2q	202	1/1	0.91	0.28	74,74,74,74	0
56	MG	1A	3282	1/1	0.91	0.61	51,51,51,51	0
56	MG	1A	3344	1/1	0.91	0.12	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3573	1/1	0.91	0.17	49,49,49,49	0
56	MG	1A	3998	1/1	0.91	0.42	48,48,48,48	0
56	MG	1a	1621	1/1	0.91	0.25	59,59,59,59	0
56	MG	1a	1706	1/1	0.91	0.12	54,54,54,54	0
56	MG	1A	3190	1/1	0.91	0.30	40,40,40,40	0
56	MG	1A	4164	1/1	0.91	0.11	55,55,55,55	0
56	MG	2a	3193	1/1	0.91	0.22	63,63,63,63	0
56	MG	1a	1739	1/1	0.91	0.11	49,49,49,49	0
56	MG	2a	3213	1/1	0.91	0.20	60,60,60,60	0
56	MG	1A	3198	1/1	0.91	0.15	67,67,67,67	0
56	MG	2A	3134	1/1	0.91	0.10	39,39,39,39	0
56	MG	1a	1720	1/1	0.91	0.20	62,62,62,62	0
56	MG	1A	3610	1/1	0.91	0.29	61,61,61,61	0
56	MG	1A	3155	1/1	0.91	0.32	47,47,47,47	0
56	MG	1a	1821	1/1	0.91	0.15	66,66,66,66	0
56	MG	1R	201	1/1	0.91	0.18	54,54,54,54	0
57	CPT	1A	4210	4/5	0.91	0.10	77,103,121,207	0
56	MG	2a	3016	1/1	0.91	0.16	55,55,55,55	0
56	MG	1A	3722	1/1	0.91	0.16	21,21,21,21	0
56	MG	1A	3966	1/1	0.91	0.81	45,45,45,45	0
56	MG	1A	3400	1/1	0.91	0.17	56,56,56,56	0
56	MG	1a	1730	1/1	0.91	0.11	57,57,57,57	0
56	MG	1A	3473	1/1	0.91	0.15	59,59,59,59	0
56	MG	1a	1869	1/1	0.91	0.34	101,101,101,101	0
56	MG	2A	3291	1/1	0.91	0.12	61,61,61,61	0
56	MG	2A	3670	1/1	0.91	0.18	42,42,42,42	0
56	MG	1a	1912	1/1	0.91	0.15	69,69,69,69	0
56	MG	2A	3463	1/1	0.91	0.18	59,59,59,59	0
56	MG	1A	4130	1/1	0.91	0.10	49,49,49,49	0
56	MG	1A	3390	1/1	0.91	0.41	55,55,55,55	0
56	MG	1A	3570	1/1	0.91	0.23	54,54,54,54	0
56	MG	2A	3774	1/1	0.91	0.07	57,57,57,57	0
56	MG	1A	3004	1/1	0.91	0.26	35,35,35,35	0
56	MG	1A	3479	1/1	0.91	0.32	57,57,57,57	0
56	MG	2A	3162	1/1	0.91	0.15	56,56,56,56	0
56	MG	1A	3232	1/1	0.91	0.40	55,55,55,55	0
56	MG	2A	3743	1/1	0.91	0.10	79,79,79,79	0
56	MG	2A	3389	1/1	0.91	0.22	52,52,52,52	0
56	MG	1A	4243	1/1	0.91	0.59	40,40,40,40	0
56	MG	1A	3559	1/1	0.91	0.50	35,35,35,35	0
56	MG	1a	1865	1/1	0.91	0.11	51,51,51,51	0
56	MG	1A	3170	1/1	0.91	0.22	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4234	1/1	0.91	0.69	46,46,46,46	0
56	MG	2A	3319	1/1	0.91	0.39	57,57,57,57	0
56	MG	2A	3697	1/1	0.91	0.05	42,42,42,42	0
56	MG	2A	3325	1/1	0.91	0.58	47,47,47,47	0
56	MG	2A	3323	1/1	0.91	0.10	48,48,48,48	0
56	MG	2A	3348	1/1	0.91	0.14	55,55,55,55	0
56	MG	2A	3802	1/1	0.91	0.18	43,43,43,43	0
56	MG	1A	3777	1/1	0.91	0.17	33,33,33,33	0
56	MG	2a	3076	1/1	0.91	0.10	64,64,64,64	0
56	MG	2A	3869	1/1	0.91	0.07	54,54,54,54	0
56	MG	1A	3218	1/1	0.91	0.44	55,55,55,55	0
56	MG	1A	3878	1/1	0.91	0.05	63,63,63,63	0
56	MG	2a	3065	1/1	0.91	0.45	47,47,47,47	0
56	MG	1A	3739	1/1	0.91	0.16	30,30,30,30	0
56	MG	1a	1771	1/1	0.91	0.26	51,51,51,51	0
56	MG	2A	3507	1/1	0.91	0.12	49,49,49,49	0
56	MG	1a	1815	1/1	0.91	0.17	57,57,57,57	0
56	MG	1a	1789	1/1	0.91	0.20	69,69,69,69	0
56	MG	2A	3174	1/1	0.91	0.11	66,66,66,66	0
56	MG	2x	104	1/1	0.91	0.26	58,58,58,58	0
56	MG	2A	3067	1/1	0.91	0.37	56,56,56,56	0
56	MG	2y	3004	1/1	0.91	0.18	69,69,69,69	0
56	MG	2A	3081	1/1	0.91	0.29	51,51,51,51	0
56	MG	2A	3599	1/1	0.91	0.22	55,55,55,55	0
56	MG	2y	3005	1/1	0.91	0.13	79,79,79,79	0
56	MG	2A	3616	1/1	0.91	0.26	31,31,31,31	0
56	MG	1A	3751	1/1	0.91	0.14	40,40,40,40	0
56	MG	1a	1777	1/1	0.91	0.38	51,51,51,51	0
56	MG	2a	3005	1/1	0.91	0.18	54,54,54,54	0
56	MG	2A	3378	1/1	0.91	0.18	58,58,58,58	0
56	MG	1a	1928	1/1	0.91	0.12	57,57,57,57	0
56	MG	2U	201	1/1	0.91	0.28	56,56,56,56	0
56	MG	2A	3209	1/1	0.91	0.12	61,61,61,61	0
56	MG	2A	3760	1/1	0.91	0.18	64,64,64,64	0
56	MG	2A	3901	1/1	0.91	0.20	77,77,77,77	0
56	MG	1A	3795	1/1	0.91	0.14	43,43,43,43	0
56	MG	2A	3322	1/1	0.91	0.11	58,58,58,58	0
56	MG	1A	3258	1/1	0.91	0.11	53,53,53,53	0
56	MG	1H	201	1/1	0.91	0.10	46,46,46,46	0
56	MG	1A	3859	1/1	0.91	0.18	37,37,37,37	0
56	MG	1A	3834	1/1	0.91	0.25	28,28,28,28	0
56	MG	2a	3176	1/1	0.91	0.09	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3285	1/1	0.91	0.32	55,55,55,55	0
56	MG	2A	3018	1/1	0.91	0.17	56,56,56,56	0
56	MG	2A	3754	1/1	0.91	0.12	71,71,71,71	0
56	MG	1A	3937	1/1	0.91	0.33	56,56,56,56	0
56	MG	2a	3021	1/1	0.91	0.12	72,72,72,72	0
56	MG	1U	201	1/1	0.91	0.45	53,53,53,53	0
56	MG	2a	3019	1/1	0.91	0.16	48,48,48,48	0
56	MG	1A	3404	1/1	0.91	0.56	69,69,69,69	0
56	MG	1A	3300	1/1	0.91	0.28	52,52,52,52	0
56	MG	1y	3004	1/1	0.91	0.26	78,78,78,78	0
56	MG	1A	4064	1/1	0.91	0.16	39,39,39,39	0
56	MG	2A	3522	1/1	0.91	0.07	63,63,63,63	0
56	MG	1A	3259	1/1	0.91	0.23	61,61,61,61	0
56	MG	1a	1687	1/1	0.91	0.20	73,73,73,73	0
56	MG	2a	3072	1/1	0.91	0.17	49,49,49,49	0
56	MG	1A	3854	1/1	0.91	0.15	49,49,49,49	0
56	MG	1a	1783	1/1	0.91	0.06	88,88,88,88	0
56	MG	1A	3906	1/1	0.91	0.11	55,55,55,55	0
56	MG	1A	3831	1/1	0.91	0.11	46,46,46,46	0
56	MG	2w	105	1/1	0.91	0.32	71,71,71,71	0
56	MG	2A	3123	1/1	0.91	0.21	50,50,50,50	0
56	MG	1A	3536	1/1	0.91	0.26	56,56,56,56	0
56	MG	1A	3279	1/1	0.91	0.21	40,40,40,40	0
56	MG	1A	3088	1/1	0.91	0.30	54,54,54,54	0
56	MG	2A	3032	1/1	0.91	0.20	57,57,57,57	0
56	MG	2A	3108	1/1	0.91	0.20	39,39,39,39	0
56	MG	2x	106	1/1	0.91	0.23	57,57,57,57	0
56	MG	2A	3168	1/1	0.91	0.19	50,50,50,50	0
56	MG	1a	1746	1/1	0.91	0.07	66,66,66,66	0
56	MG	1A	3391	1/1	0.91	0.50	71,71,71,71	0
56	MG	2a	3071	1/1	0.91	0.09	71,71,71,71	0
56	MG	1A	3291	1/1	0.91	0.14	49,49,49,49	0
56	MG	1A	3329	1/1	0.91	0.19	54,54,54,54	0
59	ZN	24	501	1/1	0.91	0.04	114,114,114,114	0
56	MG	2A	3461	1/1	0.91	0.33	47,47,47,47	0
56	MG	2A	3401	1/1	0.91	0.17	50,50,50,50	0
56	MG	1A	4215	1/1	0.91	0.48	73,73,73,73	0
56	MG	1A	4206	1/1	0.91	0.42	45,45,45,45	0
56	MG	1A	4163	1/1	0.91	0.13	70,70,70,70	0
56	MG	2a	3030	1/1	0.91	0.14	52,52,52,52	0
56	MG	2a	3185	1/1	0.91	0.13	87,87,87,87	0
56	MG	1A	4067	1/1	0.91	0.06	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3516	1/1	0.91	0.14	48,48,48,48	0
56	MG	2A	3862	1/1	0.91	0.08	62,62,62,62	0
56	MG	2A	3135	1/1	0.91	0.54	51,51,51,51	0
56	MG	2a	3231	1/1	0.91	0.07	77,77,77,77	0
56	MG	1A	3275	1/1	0.91	0.59	45,45,45,45	0
56	MG	2A	3911	1/1	0.91	0.19	43,43,43,43	0
56	MG	1a	1648	1/1	0.91	0.08	53,53,53,53	0
56	MG	18	103	1/1	0.91	0.45	57,57,57,57	0
56	MG	1A	3044	1/1	0.91	0.45	48,48,48,48	0
56	MG	2A	3795	1/1	0.91	0.23	63,63,63,63	0
56	MG	1a	1846	1/1	0.91	0.26	56,56,56,56	0
56	MG	1A	4106	1/1	0.91	0.15	28,28,28,28	0
56	MG	1A	3505	1/1	0.91	0.40	44,44,44,44	0
56	MG	1A	3418	1/1	0.91	0.25	49,49,49,49	0
56	MG	1A	3779	1/1	0.91	0.22	31,31,31,31	0
56	MG	2A	3574	1/1	0.91	0.13	32,32,32,32	0
56	MG	1A	4194	1/1	0.91	0.20	55,55,55,55	0
56	MG	2A	3659	1/1	0.91	0.08	45,45,45,45	0
56	MG	1A	3490	1/1	0.91	0.16	50,50,50,50	0
56	MG	1A	3411	1/1	0.91	0.22	58,58,58,58	0
56	MG	1a	1773	1/1	0.91	0.15	53,53,53,53	0
56	MG	1a	1827	1/1	0.92	0.10	66,66,66,66	0
56	MG	1a	1870	1/1	0.92	0.35	81,81,81,81	0
56	MG	1A	3395	1/1	0.92	0.89	46,46,46,46	0
56	MG	1A	3428	1/1	0.92	0.21	46,46,46,46	0
56	MG	1A	3699	1/1	0.92	0.18	24,24,24,24	0
56	MG	1a	1920	1/1	0.92	0.25	59,59,59,59	0
56	MG	2A	3008	1/1	0.92	0.15	41,41,41,41	0
56	MG	2A	3681	1/1	0.92	0.20	66,66,66,66	0
56	MG	2A	3881	1/1	0.92	0.14	71,71,71,71	0
56	MG	2A	3689	1/1	0.92	0.17	53,53,53,53	0
56	MG	1A	3482	1/1	0.92	0.10	53,53,53,53	0
56	MG	2A	3520	1/1	0.92	0.18	55,55,55,55	0
56	MG	2A	3338	1/1	0.92	1.03	64,64,64,64	0
56	MG	1A	3135	1/1	0.92	0.29	39,39,39,39	0
56	MG	1A	4188	1/1	0.92	0.18	37,37,37,37	0
56	MG	1A	4052	1/1	0.92	0.10	67,67,67,67	0
56	MG	2A	3031	1/1	0.92	0.15	46,46,46,46	0
56	MG	2A	3392	1/1	0.92	0.18	72,72,72,72	0
56	MG	2a	3009	1/1	0.92	0.13	72,72,72,72	0
56	MG	2A	3439	1/1	0.92	0.26	38,38,38,38	0
56	MG	2A	3843	1/1	0.92	0.13	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3465	1/1	0.92	0.22	52,52,52,52	0
56	MG	2A	3347	1/1	0.92	0.15	51,51,51,51	0
56	MG	1A	3134	1/1	0.92	0.16	45,45,45,45	0
56	MG	1A	3829	1/1	0.92	0.08	54,54,54,54	0
56	MG	1a	1882	1/1	0.92	0.15	52,52,52,52	0
56	MG	2A	3239	1/1	0.92	0.82	54,54,54,54	0
56	MG	1A	3199	1/1	0.92	0.74	56,56,56,56	0
56	MG	2a	3091	1/1	0.92	0.12	62,62,62,62	0
56	MG	1w	106	1/1	0.92	0.10	63,63,63,63	0
56	MG	2A	3133	1/1	0.92	0.16	63,63,63,63	0
56	MG	2A	3851	1/1	0.92	0.09	51,51,51,51	0
56	MG	1A	4035	1/1	0.92	0.16	39,39,39,39	0
56	MG	1A	3851	1/1	0.92	0.19	45,45,45,45	0
56	MG	1A	4213	1/1	0.92	0.11	52,52,52,52	0
56	MG	2A	3145	1/1	0.92	0.29	49,49,49,49	0
56	MG	1A	3074	1/1	0.92	0.11	35,35,35,35	0
56	MG	1A	3543	1/1	0.92	0.20	71,71,71,71	0
56	MG	2A	3484	1/1	0.92	0.13	57,57,57,57	0
56	MG	1A	3811	1/1	0.92	0.14	45,45,45,45	0
56	MG	1A	3673	1/1	0.92	0.11	50,50,50,50	0
56	MG	17	103	1/1	0.92	0.18	48,48,48,48	0
56	MG	2Q	3001	1/1	0.92	0.08	59,59,59,59	0
56	MG	13	101	1/1	0.92	0.32	50,50,50,50	0
56	MG	1a	1926	1/1	0.92	0.16	55,55,55,55	0
56	MG	1A	4003	1/1	0.92	0.17	57,57,57,57	0
56	MG	2A	3640	1/1	0.92	0.25	45,45,45,45	0
56	MG	1A	3083	1/1	0.92	0.14	41,41,41,41	0
56	MG	1A	3341	1/1	0.92	0.21	46,46,46,46	0
56	MG	2A	3519	1/1	0.92	0.24	57,57,57,57	0
56	MG	1a	1758	1/1	0.92	0.18	49,49,49,49	0
56	MG	1A	3160	1/1	0.92	0.64	49,49,49,49	0
56	MG	2A	3023	1/1	0.92	0.14	57,57,57,57	0
56	MG	2A	3626	1/1	0.92	0.29	48,48,48,48	0
56	MG	1A	3063	1/1	0.92	0.29	51,51,51,51	0
56	MG	1A	3355	1/1	0.92	0.22	60,60,60,60	0
56	MG	1A	3838	1/1	0.92	0.15	54,54,54,54	0
56	MG	1A	3912	1/1	0.92	0.14	44,44,44,44	0
56	MG	1A	3955	1/1	0.92	0.26	37,37,37,37	0
56	MG	1a	1847	1/1	0.92	0.13	51,51,51,51	0
56	MG	2D	302	1/1	0.92	0.13	27,27,27,27	0
56	MG	1A	3993	1/1	0.92	0.28	55,55,55,55	0
56	MG	1A	3416	1/1	0.92	0.24	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3447	1/1	0.92	0.42	58,58,58,58	0
56	MG	1A	3420	1/1	0.92	0.31	50,50,50,50	0
56	MG	2a	3150	1/1	0.92	0.09	61,61,61,61	0
56	MG	2A	3122	1/1	0.92	0.19	47,47,47,47	0
56	MG	2A	3459	1/1	0.92	0.30	46,46,46,46	0
56	MG	1a	1931	1/1	0.92	0.10	49,49,49,49	0
56	MG	2A	3509	1/1	0.92	0.16	55,55,55,55	0
56	MG	1A	3158	1/1	0.92	0.14	47,47,47,47	0
56	MG	1A	3376	1/1	0.92	0.15	48,48,48,48	0
56	MG	1A	4103	1/1	0.92	0.15	26,26,26,26	0
56	MG	1a	1765	1/1	0.92	0.34	53,53,53,53	0
56	MG	1a	1692	1/1	0.92	0.10	55,55,55,55	0
56	MG	1A	3449	1/1	0.92	0.15	52,52,52,52	0
56	MG	1A	4077	1/1	0.92	0.24	26,26,26,26	0
56	MG	1A	3579	1/1	0.92	0.13	45,45,45,45	0
56	MG	1A	3844	1/1	0.92	0.15	40,40,40,40	0
56	MG	2A	3587	1/1	0.92	0.16	46,46,46,46	0
56	MG	2A	3827	1/1	0.92	0.20	64,64,64,64	0
56	MG	2a	3002	1/1	0.92	0.42	72,72,72,72	0
56	MG	1A	3596	1/1	0.92	0.22	44,44,44,44	0
56	MG	2A	3224	1/1	0.92	0.21	55,55,55,55	0
56	MG	1A	4227	1/1	0.92	0.37	38,38,38,38	0
56	MG	1A	3200	1/1	0.92	0.21	49,49,49,49	0
56	MG	2A	3784	1/1	0.92	0.23	48,48,48,48	0
56	MG	1A	3767	1/1	0.92	0.15	24,24,24,24	0
56	MG	1A	3558	1/1	0.92	0.18	48,48,48,48	0
56	MG	2A	3559	1/1	0.92	0.20	38,38,38,38	0
56	MG	1A	3240	1/1	0.92	0.29	39,39,39,39	0
56	MG	2B	3016	1/1	0.92	0.15	63,63,63,63	0
56	MG	2A	3413	1/1	0.92	0.28	61,61,61,61	0
56	MG	2a	3035	1/1	0.92	0.13	81,81,81,81	0
56	MG	1A	3946	1/1	0.92	0.16	34,34,34,34	0
56	MG	1A	3214	1/1	0.92	0.24	58,58,58,58	0
56	MG	1a	1929	1/1	0.92	0.08	57,57,57,57	0
56	MG	2A	3730	1/1	0.92	0.14	40,40,40,40	0
56	MG	1A	3217	1/1	0.92	0.34	59,59,59,59	0
56	MG	2A	3257	1/1	0.92	0.28	70,70,70,70	0
56	MG	23	3002	1/1	0.92	0.19	53,53,53,53	0
56	MG	1A	3792	1/1	0.92	0.18	30,30,30,30	0
56	MG	2a	3062	1/1	0.92	0.20	85,85,85,85	0
56	MG	2A	3063	1/1	0.92	0.14	46,46,46,46	0
56	MG	2A	3445	1/1	0.92	0.15	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3586	1/1	0.92	0.17	60,60,60,60	0
56	MG	1A	3900	1/1	0.92	0.08	64,64,64,64	0
56	MG	1a	1622	1/1	0.92	0.18	55,55,55,55	0
56	MG	2a	3158	1/1	0.92	0.09	47,47,47,47	0
56	MG	1A	3731	1/1	0.92	0.19	57,57,57,57	0
56	MG	1A	3943	1/1	0.92	0.10	68,68,68,68	0
56	MG	2A	3651	1/1	0.92	0.07	61,61,61,61	0
56	MG	1a	1695	1/1	0.92	0.20	65,65,65,65	0
56	MG	1A	3625	1/1	0.92	0.27	66,66,66,66	0
56	MG	2A	3751	1/1	0.92	0.15	46,46,46,46	0
56	MG	2a	3202	1/1	0.92	0.12	65,65,65,65	0
56	MG	1A	3847	1/1	0.92	0.11	60,60,60,60	0
56	MG	1A	4018	1/1	0.92	0.13	45,45,45,45	0
56	MG	1A	3785	1/1	0.92	0.23	33,33,33,33	0
56	MG	2A	3543	1/1	0.92	0.14	56,56,56,56	0
56	MG	2A	3896	1/1	0.92	0.39	53,53,53,53	0
56	MG	1A	3334	1/1	0.92	0.32	54,54,54,54	0
56	MG	1T	201	1/1	0.92	0.14	57,57,57,57	0
56	MG	1w	110	1/1	0.92	0.16	78,78,78,78	0
56	MG	2A	3912	1/1	0.92	0.09	41,41,41,41	0
56	MG	1A	3319	1/1	0.92	0.33	58,58,58,58	0
56	MG	1A	3568	1/1	0.92	0.14	46,46,46,46	0
56	MG	2A	3715	1/1	0.92	0.15	57,57,57,57	0
56	MG	1A	3036	1/1	0.92	0.32	43,43,43,43	0
56	MG	2A	3873	1/1	0.92	0.23	57,57,57,57	0
56	MG	1A	3326	1/1	0.92	0.14	53,53,53,53	0
56	MG	13	102	1/1	0.92	0.17	46,46,46,46	0
56	MG	2A	3735	1/1	0.92	0.09	49,49,49,49	0
56	MG	1a	1675	1/1	0.92	0.17	53,53,53,53	0
56	MG	2a	3151	1/1	0.92	0.09	74,74,74,74	0
56	MG	1A	3983	1/1	0.92	0.20	73,73,73,73	0
56	MG	1A	4177	1/1	0.92	0.12	36,36,36,36	0
56	MG	1B	222	1/1	0.92	0.14	59,59,59,59	0
56	MG	2a	3014	1/1	0.92	0.21	70,70,70,70	0
56	MG	2A	3421	1/1	0.92	0.23	60,60,60,60	0
56	MG	2A	3758	1/1	0.92	0.17	53,53,53,53	0
56	MG	2A	3781	1/1	0.92	0.10	47,47,47,47	0
56	MG	2A	3045	1/1	0.92	0.09	48,48,48,48	0
58	K	1A	4256	1/1	0.92	0.18	65,65,65,65	0
56	MG	1a	1785	1/1	0.92	0.07	71,71,71,71	0
56	MG	1a	1808	1/1	0.92	0.28	61,61,61,61	0
56	MG	1A	3143	1/1	0.92	0.13	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	23	3003	1/1	0.92	0.21	48,48,48,48	0
56	MG	1A	3968	1/1	0.92	0.08	63,63,63,63	0
56	MG	1a	1635	1/1	0.92	0.33	62,62,62,62	0
56	MG	1A	3156	1/1	0.92	0.97	47,47,47,47	0
56	MG	2A	3602	1/1	0.92	0.12	52,52,52,52	0
56	MG	1A	3732	1/1	0.92	0.16	35,35,35,35	0
56	MG	1A	4062	1/1	0.92	0.08	76,76,76,76	0
56	MG	1A	3746	1/1	0.92	0.10	51,51,51,51	0
56	MG	1A	3424	1/1	0.92	0.21	75,75,75,75	0
56	MG	2A	3705	1/1	0.92	0.22	58,58,58,58	0
56	MG	1x	101	1/1	0.92	0.25	45,45,45,45	0
56	MG	1A	3589	1/1	0.92	0.26	53,53,53,53	0
56	MG	1A	3944	1/1	0.92	0.09	69,69,69,69	0
56	MG	2a	3108	1/1	0.92	0.05	57,57,57,57	0
56	MG	2A	3505	1/1	0.92	0.20	58,58,58,58	0
56	MG	2A	3533	1/1	0.92	0.09	44,44,44,44	0
56	MG	1A	3552	1/1	0.92	0.21	34,34,34,34	0
56	MG	2A	3558	1/1	0.92	0.14	38,38,38,38	0
56	MG	1A	3652	1/1	0.92	0.16	52,52,52,52	0
56	MG	2a	3236	1/1	0.92	0.10	65,65,65,65	0
56	MG	1A	3717	1/1	0.92	0.17	49,49,49,49	0
56	MG	1A	4120	1/1	0.92	0.12	76,76,76,76	0
56	MG	2A	3674	1/1	0.92	0.16	49,49,49,49	0
56	MG	2G	3001	1/1	0.92	0.21	46,46,46,46	0
56	MG	2A	3799	1/1	0.92	0.06	58,58,58,58	0
56	MG	1A	3929	1/1	0.92	0.16	62,62,62,62	0
56	MG	2A	3595	1/1	0.92	0.23	56,56,56,56	0
56	MG	2A	3828	1/1	0.92	0.09	64,64,64,64	0
56	MG	2A	3419	1/1	0.92	0.10	46,46,46,46	0
56	MG	2A	3182	1/1	0.92	0.14	62,62,62,62	0
56	MG	1A	3950	1/1	0.92	0.15	68,68,68,68	0
56	MG	2A	3022	1/1	0.92	0.17	37,37,37,37	0
56	MG	2A	3906	1/1	0.92	0.18	64,64,64,64	0
56	MG	2A	3249	1/1	0.92	0.34	64,64,64,64	0
56	MG	1A	3019	1/1	0.92	0.20	45,45,45,45	0
56	MG	1A	4126	1/1	0.92	0.16	67,67,67,67	0
56	MG	1A	3245	1/1	0.92	0.16	60,60,60,60	0
56	MG	1A	3903	1/1	0.92	0.09	51,51,51,51	0
56	MG	1A	3593	1/1	0.92	0.13	50,50,50,50	0
56	MG	1A	3781	1/1	0.92	0.20	26,26,26,26	0
56	MG	1A	3933	1/1	0.92	0.14	81,81,81,81	0
56	MG	2A	3790	1/1	0.92	0.19	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3544	1/1	0.92	0.10	41,41,41,41	0
56	MG	1A	4202	1/1	0.92	0.20	39,39,39,39	0
56	MG	1a	1848	1/1	0.92	0.29	44,44,44,44	0
56	MG	2a	3226	1/1	0.93	0.16	79,79,79,79	0
56	MG	1A	3691	1/1	0.93	0.22	55,55,55,55	0
56	MG	2A	3480	1/1	0.93	0.37	50,50,50,50	0
56	MG	1A	3836	1/1	0.93	0.20	42,42,42,42	0
56	MG	2a	3136	1/1	0.93	0.24	83,83,83,83	0
56	MG	1A	3949	1/1	0.93	0.50	41,41,41,41	0
56	MG	2A	3488	1/1	0.93	0.31	53,53,53,53	0
56	MG	2A	3196	1/1	0.93	0.16	57,57,57,57	0
56	MG	1A	4189	1/1	0.93	0.14	33,33,33,33	0
56	MG	1A	3676	1/1	0.93	0.22	46,46,46,46	0
56	MG	2A	3546	1/1	0.93	0.11	34,34,34,34	0
56	MG	2A	3629	1/1	0.93	0.17	56,56,56,56	0
56	MG	1A	3228	1/1	0.93	0.17	37,37,37,37	0
56	MG	2A	3699	1/1	0.93	0.12	64,64,64,64	0
56	MG	1A	3062	1/1	0.93	0.32	56,56,56,56	0
56	MG	2a	3102	1/1	0.93	0.25	63,63,63,63	0
56	MG	1A	4246	1/1	0.93	0.43	40,40,40,40	0
56	MG	2A	3812	1/1	0.93	0.19	48,48,48,48	0
56	MG	1A	4047	1/1	0.93	0.14	58,58,58,58	0
56	MG	2a	3211	1/1	0.93	0.10	71,71,71,71	0
56	MG	1A	3103	1/1	0.93	0.84	47,47,47,47	0
58	K	2A	3922	1/1	0.93	0.13	72,72,72,72	0
56	MG	1X	101	1/1	0.93	0.15	38,38,38,38	0
56	MG	2A	3594	1/1	0.93	0.07	45,45,45,45	0
56	MG	2A	3349	1/1	0.93	0.14	61,61,61,61	0
56	MG	1a	1769	1/1	0.93	0.14	44,44,44,44	0
56	MG	1a	1661	1/1	0.93	0.18	73,73,73,73	0
56	MG	1E	304	1/1	0.93	0.19	51,51,51,51	0
56	MG	2A	3631	1/1	0.93	0.08	47,47,47,47	0
56	MG	1A	4056	1/1	0.93	0.20	51,51,51,51	0
56	MG	1A	3076	1/1	0.93	0.51	43,43,43,43	0
56	MG	1A	3435	1/1	0.93	0.43	53,53,53,53	0
56	MG	1A	3138	1/1	0.93	0.87	49,49,49,49	0
56	MG	1a	1843	1/1	0.93	0.12	50,50,50,50	0
56	MG	1A	3939	1/1	0.93	0.14	51,51,51,51	0
56	MG	1A	4198	1/1	0.93	0.08	45,45,45,45	0
56	MG	1A	3549	1/1	0.93	0.83	50,50,50,50	0
56	MG	2A	3336	1/1	0.93	0.13	62,62,62,62	0
56	MG	1A	4028	1/1	0.93	0.08	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4032	1/1	0.93	0.12	57,57,57,57	0
56	MG	1A	3621	1/1	0.93	0.19	40,40,40,40	0
56	MG	2A	3163	1/1	0.93	0.34	55,55,55,55	0
56	MG	2E	305	1/1	0.93	0.19	53,53,53,53	0
56	MG	1a	1638	1/1	0.93	0.09	45,45,45,45	0
56	MG	2A	3320	1/1	0.93	0.21	55,55,55,55	0
56	MG	1a	1626	1/1	0.93	0.21	48,48,48,48	0
56	MG	2A	3260	1/1	0.93	0.10	73,73,73,73	0
56	MG	1a	1904	1/1	0.93	0.08	56,56,56,56	0
56	MG	2A	3107	1/1	0.93	0.40	50,50,50,50	0
56	MG	2Z	8001	1/1	0.93	0.06	65,65,65,65	0
59	ZN	2n	102	1/1	0.93	0.04	85,85,85,85	0
56	MG	1D	308	1/1	0.93	0.51	56,56,56,56	0
56	MG	1A	4102	1/1	0.93	0.12	32,32,32,32	0
56	MG	2a	3220	1/1	0.93	0.12	62,62,62,62	0
56	MG	2A	3137	1/1	0.93	0.19	52,52,52,52	0
56	MG	2A	3391	1/1	0.93	0.11	58,58,58,58	0
56	MG	2A	3635	1/1	0.93	0.17	53,53,53,53	0
56	MG	1A	3833	1/1	0.93	0.14	37,37,37,37	0
56	MG	2t	3001	1/1	0.93	0.07	63,63,63,63	0
56	MG	2A	3577	1/1	0.93	0.20	35,35,35,35	0
56	MG	1A	4101	1/1	0.93	0.07	61,61,61,61	0
56	MG	2A	3406	1/1	0.93	0.08	52,52,52,52	0
56	MG	1a	1717	1/1	0.93	0.10	63,63,63,63	0
56	MG	1A	4142	1/1	0.93	0.10	64,64,64,64	0
56	MG	2A	3233	1/1	0.93	0.20	61,61,61,61	0
56	MG	2A	3581	1/1	0.93	0.12	42,42,42,42	0
56	MG	1A	3982	1/1	0.93	0.13	32,32,32,32	0
56	MG	1A	4231	1/1	0.93	0.40	55,55,55,55	0
56	MG	25	105	1/1	0.93	0.10	55,55,55,55	0
56	MG	1a	1637	1/1	0.93	0.34	56,56,56,56	0
56	MG	1A	3187	1/1	0.93	0.61	51,51,51,51	0
56	MG	1a	1850	1/1	0.93	0.12	59,59,59,59	0
56	MG	1R	203	1/1	0.93	0.12	36,36,36,36	0
56	MG	2E	308	1/1	0.93	0.96	59,59,59,59	0
56	MG	1A	4230	1/1	0.93	0.60	45,45,45,45	0
56	MG	2A	3576	1/1	0.93	0.14	29,29,29,29	0
56	MG	1A	3578	1/1	0.93	0.23	61,61,61,61	0
56	MG	1A	3092	1/1	0.93	0.15	53,53,53,53	0
56	MG	1a	1652	1/1	0.93	0.24	41,41,41,41	0
56	MG	1a	1884	1/1	0.93	0.13	54,54,54,54	0
56	MG	1A	4005	1/1	0.93	0.13	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3491	1/1	0.93	0.34	37,37,37,37	0
56	MG	1A	3197	1/1	0.93	0.12	55,55,55,55	0
56	MG	2A	3611	1/1	0.93	0.05	60,60,60,60	0
56	MG	2A	3524	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3101	1/1	0.93	0.10	66,66,66,66	0
56	MG	2A	3095	1/1	0.93	0.19	48,48,48,48	0
56	MG	2B	3008	1/1	0.93	0.11	50,50,50,50	0
56	MG	2A	3275	1/1	0.93	0.14	67,67,67,67	0
56	MG	1A	3954	1/1	0.93	0.24	62,62,62,62	0
56	MG	1A	3098	1/1	0.93	0.22	57,57,57,57	0
56	MG	1U	203	1/1	0.93	0.62	46,46,46,46	0
56	MG	1A	3347	1/1	0.93	0.51	42,42,42,42	0
56	MG	2A	3661	1/1	0.93	0.08	39,39,39,39	0
56	MG	2A	3120	1/1	0.93	0.16	34,34,34,34	0
56	MG	1A	3638	1/1	0.93	0.18	54,54,54,54	0
56	MG	2a	3095	1/1	0.93	0.26	50,50,50,50	0
56	MG	2A	3052	1/1	0.93	0.14	61,61,61,61	0
56	MG	1A	3753	1/1	0.93	0.16	32,32,32,32	0
56	MG	1a	1863	1/1	0.93	0.12	76,76,76,76	0
56	MG	1A	3349	1/1	0.93	0.21	41,41,41,41	0
56	MG	2a	3138	1/1	0.93	0.12	83,83,83,83	0
56	MG	10	103	1/1	0.93	1.00	54,54,54,54	0
56	MG	1a	1601	1/1	0.93	0.23	50,50,50,50	0
56	MG	2A	3070	1/1	0.93	0.16	34,34,34,34	0
56	MG	2A	3256	1/1	0.93	0.15	58,58,58,58	0
56	MG	2A	3856	1/1	0.93	0.16	44,44,44,44	0
56	MG	1A	3594	1/1	0.93	0.24	40,40,40,40	0
56	MG	1A	4196	1/1	0.93	0.18	37,37,37,37	0
56	MG	1A	3163	1/1	0.93	0.26	49,49,49,49	0
56	MG	1a	1886	1/1	0.93	0.08	54,54,54,54	0
56	MG	2A	3694	1/1	0.93	0.07	60,60,60,60	0
56	MG	1N	3006	1/1	0.93	0.14	46,46,46,46	0
56	MG	1R	202	1/1	0.93	0.21	36,36,36,36	0
56	MG	1A	3005	1/1	0.93	0.22	53,53,53,53	0
56	MG	1F	301	1/1	0.93	0.27	68,68,68,68	0
56	MG	1F	305	1/1	0.93	0.55	39,39,39,39	0
56	MG	2A	3660	1/1	0.93	0.16	57,57,57,57	0
56	MG	1a	1608	1/1	0.93	0.10	47,47,47,47	0
56	MG	1A	4027	1/1	0.93	0.13	41,41,41,41	0
56	MG	1A	3210	1/1	0.93	0.08	67,67,67,67	0
56	MG	1a	1922	1/1	0.93	0.16	52,52,52,52	0
56	MG	2A	3167	1/1	0.93	0.31	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3335	1/1	0.93	0.32	56,56,56,56	0
56	MG	1a	1761	1/1	0.93	0.23	55,55,55,55	0
57	CPT	2A	3904	4/5	0.93	0.13	79,102,124,194	4
56	MG	1D	309	1/1	0.93	0.15	41,41,41,41	0
56	MG	1A	3507	1/1	0.93	0.29	72,72,72,72	0
56	MG	2A	3171	1/1	0.93	0.13	61,61,61,61	0
56	MG	1A	3133	1/1	0.93	0.35	36,36,36,36	0
56	MG	2a	3230	1/1	0.93	0.11	66,66,66,66	0
56	MG	1a	1779	1/1	0.93	0.16	56,56,56,56	0
56	MG	2A	3221	1/1	0.93	0.12	49,49,49,49	0
56	MG	1A	3141	1/1	0.93	0.28	43,43,43,43	0
56	MG	2A	3269	1/1	0.93	0.20	50,50,50,50	0
56	MG	1B	231	1/1	0.93	0.18	56,56,56,56	0
56	MG	1A	3765	1/1	0.93	0.21	28,28,28,28	0
56	MG	2A	3017	1/1	0.93	0.22	44,44,44,44	0
56	MG	1a	1772	1/1	0.93	0.12	56,56,56,56	0
56	MG	1A	3054	1/1	0.93	0.17	53,53,53,53	0
56	MG	1U	204	1/1	0.93	0.90	66,66,66,66	0
56	MG	1A	3277	1/1	0.93	0.46	47,47,47,47	0
56	MG	1A	3045	1/1	0.93	0.15	38,38,38,38	0
56	MG	1A	3799	1/1	0.93	0.14	47,47,47,47	0
56	MG	1A	3948	1/1	0.93	0.14	53,53,53,53	0
56	MG	1A	3659	1/1	0.93	0.31	41,41,41,41	0
56	MG	1A	3193	1/1	0.93	0.44	44,44,44,44	0
56	MG	1A	4229	1/1	0.93	0.44	45,45,45,45	0
56	MG	1A	3940	1/1	0.93	0.33	47,47,47,47	0
56	MG	1A	3716	1/1	0.93	0.11	44,44,44,44	0
56	MG	1a	1678	1/1	0.93	0.08	52,52,52,52	0
56	MG	1A	3494	1/1	0.93	0.09	45,45,45,45	0
56	MG	2y	3007	1/1	0.93	0.14	84,84,84,84	0
56	MG	2A	3142	1/1	0.93	0.12	51,51,51,51	0
56	MG	1A	3454	1/1	0.93	0.25	51,51,51,51	0
56	MG	1A	3414	1/1	0.93	0.37	62,62,62,62	0
56	MG	2A	3277	1/1	0.93	0.56	63,63,63,63	0
56	MG	1A	3241	1/1	0.93	0.22	37,37,37,37	0
56	MG	2A	3054	1/1	0.93	0.11	44,44,44,44	0
56	MG	2a	3070	1/1	0.93	0.10	76,76,76,76	0
56	MG	1A	3119	1/1	0.93	0.16	41,41,41,41	0
56	MG	1A	3932	1/1	0.93	0.08	40,40,40,40	0
56	MG	2A	3808	1/1	0.93	0.09	60,60,60,60	0
56	MG	1A	3328	1/1	0.93	0.34	53,53,53,53	0
56	MG	1a	1645	1/1	0.93	0.20	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3655	1/1	0.93	0.21	50,50,50,50	0
56	MG	2a	3232	1/1	0.93	0.09	43,43,43,43	0
56	MG	1A	3571	1/1	0.93	0.29	58,58,58,58	0
56	MG	1A	3478	1/1	0.93	0.20	47,47,47,47	0
56	MG	1A	4109	1/1	0.93	0.12	40,40,40,40	0
56	MG	2A	3048	1/1	0.93	0.18	53,53,53,53	0
56	MG	2Q	3002	1/1	0.93	0.38	47,47,47,47	0
56	MG	1A	3511	1/1	0.93	0.44	44,44,44,44	0
56	MG	2a	3203	1/1	0.93	0.25	50,50,50,50	0
56	MG	2A	3523	1/1	0.93	0.11	31,31,31,31	0
56	MG	1A	3798	1/1	0.93	0.13	54,54,54,54	0
56	MG	1A	3508	1/1	0.93	0.35	41,41,41,41	0
56	MG	2a	3033	1/1	0.93	0.10	55,55,55,55	0
56	MG	2a	3045	1/1	0.93	0.12	68,68,68,68	0
56	MG	1A	3658	1/1	0.93	0.18	65,65,65,65	0
56	MG	2A	3003	1/1	0.93	0.19	40,40,40,40	0
56	MG	2A	3496	1/1	0.93	0.21	51,51,51,51	0
56	MG	2A	3250	1/1	0.93	0.69	62,62,62,62	0
56	MG	1A	3379	1/1	0.93	0.13	64,64,64,64	0
56	MG	1A	3887	1/1	0.93	0.21	29,29,29,29	0
56	MG	1A	3527	1/1	0.93	0.17	55,55,55,55	0
56	MG	2A	3193	1/1	0.93	0.15	57,57,57,57	0
56	MG	1A	3075	1/1	0.93	0.15	32,32,32,32	0
56	MG	2A	3710	1/1	0.93	0.19	28,28,28,28	0
56	MG	1A	3790	1/1	0.93	0.18	46,46,46,46	0
56	MG	2A	3356	1/1	0.93	0.15	53,53,53,53	0
56	MG	2A	3238	1/1	0.93	0.29	43,43,43,43	0
56	MG	1a	1696	1/1	0.93	0.13	55,55,55,55	0
56	MG	1a	1703	1/1	0.93	0.27	51,51,51,51	0
56	MG	2A	3418	1/1	0.94	0.15	64,64,64,64	0
56	MG	1A	4239	1/1	0.94	0.64	33,33,33,33	0
56	MG	1A	3990	1/1	0.94	0.14	44,44,44,44	0
56	MG	2A	3236	1/1	0.94	0.26	61,61,61,61	0
56	MG	2A	3563	1/1	0.94	0.29	41,41,41,41	0
56	MG	1A	3021	1/1	0.94	0.16	43,43,43,43	0
56	MG	1S	3003	1/1	0.94	0.17	72,72,72,72	0
56	MG	1A	3666	1/1	0.94	0.22	43,43,43,43	0
56	MG	1A	3419	1/1	0.94	0.33	61,61,61,61	0
56	MG	2A	3650	1/1	0.94	0.08	50,50,50,50	0
56	MG	2A	3012	1/1	0.94	0.12	35,35,35,35	0
56	MG	2A	3157	1/1	0.94	0.24	45,45,45,45	0
56	MG	2a	3186	1/1	0.94	0.16	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1v	3001	1/1	0.94	0.20	64,64,64,64	0
56	MG	1E	310	1/1	0.94	0.69	49,49,49,49	0
56	MG	1a	1701	1/1	0.94	0.41	46,46,46,46	0
56	MG	1A	3368	1/1	0.94	0.51	62,62,62,62	0
56	MG	1a	1888	1/1	0.94	0.07	58,58,58,58	0
56	MG	1a	1712	1/1	0.94	0.10	37,37,37,37	0
56	MG	1A	3959	1/1	0.94	0.31	46,46,46,46	0
56	MG	1A	3426	1/1	0.94	0.20	52,52,52,52	0
56	MG	1A	3923	1/1	0.94	0.14	67,67,67,67	0
56	MG	1A	4112	1/1	0.94	0.16	43,43,43,43	0
56	MG	1A	3223	1/1	0.94	0.65	43,43,43,43	0
56	MG	2A	3295	1/1	0.94	0.40	43,43,43,43	0
56	MG	2A	3252	1/1	0.94	0.20	66,66,66,66	0
56	MG	2A	3836	1/1	0.94	0.12	46,46,46,46	0
56	MG	1A	3902	1/1	0.94	0.07	59,59,59,59	0
56	MG	1A	3839	1/1	0.94	0.08	50,50,50,50	0
56	MG	1a	1764	1/1	0.94	0.19	36,36,36,36	0
56	MG	2U	202	1/1	0.94	0.49	46,46,46,46	0
56	MG	1a	1760	1/1	0.94	0.20	48,48,48,48	0
56	MG	1A	4080	1/1	0.94	0.15	26,26,26,26	0
56	MG	1A	3911	1/1	0.94	0.09	36,36,36,36	0
56	MG	2A	3606	1/1	0.94	0.14	56,56,56,56	0
56	MG	2a	3163	1/1	0.94	0.13	46,46,46,46	0
56	MG	1a	1685	1/1	0.94	0.31	53,53,53,53	0
56	MG	2A	3225	1/1	0.94	0.23	54,54,54,54	0
56	MG	2B	3005	1/1	0.94	0.11	64,64,64,64	0
56	MG	1A	4158	1/1	0.94	0.15	49,49,49,49	0
56	MG	1A	3055	1/1	0.94	0.13	34,34,34,34	0
56	MG	2A	3368	1/1	0.94	0.36	65,65,65,65	0
56	MG	2A	3568	1/1	0.94	0.14	31,31,31,31	0
56	MG	1x	108	1/1	0.94	0.23	73,73,73,73	0
56	MG	2A	3151	1/1	0.94	0.14	53,53,53,53	0
56	MG	1A	3855	1/1	0.94	0.15	34,34,34,34	0
56	MG	2A	3886	1/1	0.94	0.15	53,53,53,53	0
56	MG	2A	3693	1/1	0.94	0.10	49,49,49,49	0
56	MG	2A	3623	1/1	0.94	0.10	57,57,57,57	0
56	MG	1a	1623	1/1	0.94	0.16	56,56,56,56	0
56	MG	2y	3001	1/1	0.94	0.10	58,58,58,58	0
56	MG	1a	1925	1/1	0.94	0.14	52,52,52,52	0
56	MG	2a	3233	1/1	0.94	0.19	60,60,60,60	0
56	MG	1A	3770	1/1	0.94	0.18	36,36,36,36	0
56	MG	1A	3010	1/1	0.94	0.15	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3415	1/1	0.94	0.14	57,57,57,57	0
56	MG	2A	3039	1/1	0.94	0.11	42,42,42,42	0
56	MG	1A	3816	1/1	0.94	0.20	58,58,58,58	0
56	MG	1A	3523	1/1	0.94	0.11	61,61,61,61	0
56	MG	1A	3438	1/1	0.94	0.40	41,41,41,41	0
56	MG	1a	1737	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	4127	1/1	0.94	0.07	38,38,38,38	0
56	MG	2a	3199	1/1	0.94	0.31	62,62,62,62	0
56	MG	1A	3630	1/1	0.94	0.30	39,39,39,39	0
56	MG	1a	1676	1/1	0.94	0.21	60,60,60,60	0
56	MG	2A	3051	1/1	0.94	0.30	54,54,54,54	0
56	MG	1V	201	1/1	0.94	0.22	41,41,41,41	0
59	ZN	14	501	1/1	0.94	0.08	104,104,104,104	0
56	MG	2A	3525	1/1	0.94	0.13	49,49,49,49	0
56	MG	1A	3020	1/1	0.94	0.24	38,38,38,38	0
56	MG	1A	3264	1/1	0.94	0.43	57,57,57,57	0
56	MG	1a	1631	1/1	0.94	0.07	51,51,51,51	0
56	MG	2A	3857	1/1	0.94	0.16	56,56,56,56	0
56	MG	2B	3012	1/1	0.94	0.12	58,58,58,58	0
56	MG	2a	3207	1/1	0.94	0.12	71,71,71,71	0
56	MG	2A	3718	1/1	0.94	0.14	30,30,30,30	0
56	MG	1a	1681	1/1	0.94	0.28	60,60,60,60	0
56	MG	1A	4251	1/1	0.94	0.52	49,49,49,49	0
56	MG	1A	3935	1/1	0.94	0.20	58,58,58,58	0
56	MG	1A	3668	1/1	0.94	0.17	48,48,48,48	0
56	MG	2A	3656	1/1	0.94	0.15	58,58,58,58	0
56	MG	1A	4012	1/1	0.94	0.08	68,68,68,68	0
56	MG	2A	3613	1/1	0.94	0.17	62,62,62,62	0
56	MG	1W	3001	1/1	0.94	0.20	45,45,45,45	0
56	MG	1A	3918	1/1	0.94	0.23	42,42,42,42	0
56	MG	1A	3090	1/1	0.94	0.40	62,62,62,62	0
56	MG	1A	3488	1/1	0.94	0.26	45,45,45,45	0
56	MG	1A	3877	1/1	0.94	0.09	40,40,40,40	0
56	MG	1A	3749	1/1	0.94	0.12	44,44,44,44	0
56	MG	2A	3893	1/1	0.94	0.10	42,42,42,42	0
56	MG	1A	3916	1/1	0.94	0.11	53,53,53,53	0
56	MG	1B	219	1/1	0.94	0.15	63,63,63,63	0
56	MG	2A	3372	1/1	0.94	0.14	54,54,54,54	0
56	MG	1A	3682	1/1	0.94	0.14	40,40,40,40	0
56	MG	2a	3125	1/1	0.94	0.22	48,48,48,48	0
56	MG	2A	3564	1/1	0.94	0.16	70,70,70,70	0
56	MG	1l	204	1/1	0.94	0.21	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3752	1/1	0.94	0.30	45,45,45,45	0
56	MG	1A	3122	1/1	0.94	0.23	53,53,53,53	0
56	MG	2E	302	1/1	0.94	0.14	48,48,48,48	0
56	MG	1A	3100	1/1	0.94	0.13	48,48,48,48	0
56	MG	1a	1674	1/1	0.94	0.16	66,66,66,66	0
56	MG	1A	3922	1/1	0.94	0.12	44,44,44,44	0
56	MG	2A	3542	1/1	0.94	0.11	49,49,49,49	0
56	MG	1A	4042	1/1	0.94	0.06	51,51,51,51	0
56	MG	1P	202	1/1	0.94	0.31	39,39,39,39	0
56	MG	2A	3620	1/1	0.94	0.21	40,40,40,40	0
56	MG	2A	3143	1/1	0.94	0.27	35,35,35,35	0
56	MG	2A	3510	1/1	0.94	0.22	26,26,26,26	0
56	MG	1a	1803	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	4070	1/1	0.94	0.18	51,51,51,51	0
56	MG	1A	3157	1/1	0.94	0.48	51,51,51,51	0
56	MG	1A	3541	1/1	0.94	0.19	48,48,48,48	0
56	MG	1a	1799	1/1	0.94	0.09	62,62,62,62	0
56	MG	1x	112	1/1	0.94	0.18	47,47,47,47	0
56	MG	2A	3638	1/1	0.94	0.34	44,44,44,44	0
56	MG	2a	3001	1/1	0.94	0.20	62,62,62,62	0
56	MG	1A	3528	1/1	0.94	0.20	35,35,35,35	0
56	MG	2A	3020	1/1	0.94	0.28	50,50,50,50	0
56	MG	2a	3126	1/1	0.94	0.13	49,49,49,49	0
56	MG	2F	304	1/1	0.94	0.62	52,52,52,52	0
56	MG	2A	3156	1/1	0.94	0.14	53,53,53,53	0
56	MG	1A	4190	1/1	0.94	0.14	58,58,58,58	0
56	MG	1a	1640	1/1	0.94	0.16	52,52,52,52	0
56	MG	2U	206	1/1	0.94	0.39	49,49,49,49	0
56	MG	1A	4250	1/1	0.94	0.14	38,38,38,38	0
56	MG	2a	3084	1/1	0.94	0.25	62,62,62,62	0
56	MG	1A	3118	1/1	0.94	0.20	49,49,49,49	0
56	MG	2A	3166	1/1	0.94	0.11	47,47,47,47	0
56	MG	2A	3845	1/1	0.94	0.09	53,53,53,53	0
56	MG	2B	3007	1/1	0.94	0.14	53,53,53,53	0
56	MG	1A	3006	1/1	0.94	0.13	49,49,49,49	0
56	MG	2A	3839	1/1	0.94	0.19	33,33,33,33	0
56	MG	1A	3674	1/1	0.94	0.08	33,33,33,33	0
56	MG	1A	3529	1/1	0.94	0.24	45,45,45,45	0
56	MG	2A	3909	1/1	0.94	0.21	51,51,51,51	0
56	MG	2A	3649	1/1	0.94	0.15	58,58,58,58	0
56	MG	2A	3515	1/1	0.94	0.18	25,25,25,25	0
56	MG	1A	3763	1/1	0.94	0.09	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3653	1/1	0.94	0.18	34,34,34,34	0
56	MG	2a	3049	1/1	0.94	0.22	50,50,50,50	0
56	MG	1A	4073	1/1	0.94	0.25	68,68,68,68	0
56	MG	2A	3402	1/1	0.94	0.26	47,47,47,47	0
56	MG	2A	3124	1/1	0.94	0.07	47,47,47,47	0
56	MG	1A	3718	1/1	0.94	0.17	35,35,35,35	0
56	MG	2A	3305	1/1	0.94	0.25	55,55,55,55	0
56	MG	2A	3190	1/1	0.94	0.24	64,64,64,64	0
56	MG	1A	3173	1/1	0.94	0.46	50,50,50,50	0
59	ZN	26	501	1/1	0.94	0.11	59,59,59,59	0
56	MG	2A	3331	1/1	0.94	0.20	64,64,64,64	0
56	MG	2A	3534	1/1	0.94	0.11	40,40,40,40	0
56	MG	1A	3670	1/1	0.94	0.12	45,45,45,45	0
56	MG	2A	3478	1/1	0.94	0.20	46,46,46,46	0
56	MG	2A	3826	1/1	0.94	0.10	81,81,81,81	0
56	MG	2A	3302	1/1	0.94	0.37	57,57,57,57	0
56	MG	1A	3410	1/1	0.94	0.28	40,40,40,40	0
56	MG	1A	3825	1/1	0.94	0.14	49,49,49,49	0
56	MG	1A	3510	1/1	0.94	0.45	50,50,50,50	0
56	MG	1A	3027	1/1	0.94	0.13	59,59,59,59	0
56	MG	2A	3412	1/1	0.94	0.31	53,53,53,53	0
56	MG	1a	1735	1/1	0.94	0.07	47,47,47,47	0
56	MG	2B	3013	1/1	0.94	0.15	72,72,72,72	0
56	MG	2a	3223	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	4181	1/1	0.94	0.34	47,47,47,47	0
56	MG	2A	3890	1/1	0.94	0.17	44,44,44,44	0
56	MG	2A	3591	1/1	0.94	0.08	46,46,46,46	0
56	MG	2A	3600	1/1	0.94	0.16	62,62,62,62	0
56	MG	1A	3293	1/1	0.94	0.17	57,57,57,57	0
56	MG	1A	3144	1/1	0.94	0.39	50,50,50,50	0
56	MG	1A	3124	1/1	0.94	0.43	39,39,39,39	0
56	MG	1A	3398	1/1	0.94	0.18	41,41,41,41	0
56	MG	2P	201	1/1	0.94	0.19	57,57,57,57	0
56	MG	1A	3938	1/1	0.94	0.11	60,60,60,60	0
56	MG	1A	3664	1/1	0.94	0.19	51,51,51,51	0
56	MG	1N	3004	1/1	0.94	1.17	60,60,60,60	0
56	MG	1A	3346	1/1	0.94	0.44	57,57,57,57	0
56	MG	1A	3590	1/1	0.94	0.21	44,44,44,44	0
56	MG	2a	3051	1/1	0.94	0.09	54,54,54,54	0
56	MG	2A	3646	1/1	0.94	0.18	50,50,50,50	0
56	MG	1A	4253	1/1	0.94	0.66	45,45,45,45	0
56	MG	1A	3114	1/1	0.94	0.23	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1D	311	1/1	0.94	0.14	51,51,51,51	0
56	MG	2A	3473	1/1	0.94	0.09	60,60,60,60	0
56	MG	1A	4185	1/1	0.94	0.13	43,43,43,43	0
56	MG	2A	3272	1/1	0.94	0.20	49,49,49,49	0
56	MG	2A	3554	1/1	0.94	0.22	33,33,33,33	0
56	MG	2A	3528	1/1	0.94	0.15	57,57,57,57	0
56	MG	2A	3333	1/1	0.94	0.16	53,53,53,53	0
56	MG	2A	3780	1/1	0.94	0.12	57,57,57,57	0
56	MG	1a	1666	1/1	0.94	0.38	49,49,49,49	0
56	MG	1A	4089	1/1	0.94	0.15	64,64,64,64	0
56	MG	1a	1731	1/1	0.94	0.18	55,55,55,55	0
56	MG	2A	3114	1/1	0.94	0.11	51,51,51,51	0
56	MG	2a	3165	1/1	0.94	0.10	68,68,68,68	0
56	MG	1A	3942	1/1	0.94	0.21	49,49,49,49	0
56	MG	1D	304	1/1	0.94	0.13	19,19,19,19	0
56	MG	1A	3452	1/1	0.94	0.12	55,55,55,55	0
56	MG	2A	3155	1/1	0.94	0.26	56,56,56,56	0
56	MG	1A	3787	1/1	0.94	0.07	35,35,35,35	0
56	MG	1A	3665	1/1	0.94	0.12	40,40,40,40	0
56	MG	2A	3905	1/1	0.94	0.22	33,33,33,33	0
56	MG	2A	3636	1/1	0.94	0.16	60,60,60,60	0
56	MG	2A	3655	1/1	0.94	0.18	58,58,58,58	0
56	MG	2A	3662	1/1	0.94	0.33	52,52,52,52	0
56	MG	1a	1794	1/1	0.94	0.34	52,52,52,52	0
56	MG	1A	3131	1/1	0.94	0.25	45,45,45,45	0
56	MG	2A	3578	1/1	0.94	0.12	29,29,29,29	0
56	MG	2a	3179	1/1	0.94	0.09	80,80,80,80	0
56	MG	1A	4216	1/1	0.94	0.15	28,28,28,28	0
56	MG	1A	3290	1/1	0.94	0.21	49,49,49,49	0
56	MG	2A	3490	1/1	0.94	0.09	49,49,49,49	0
56	MG	2E	301	1/1	0.94	0.19	53,53,53,53	0
56	MG	2A	3041	1/1	0.94	0.18	39,39,39,39	0
56	MG	1a	1836	1/1	0.94	0.12	44,44,44,44	0
56	MG	2A	3648	1/1	0.94	0.08	51,51,51,51	0
56	MG	2A	3231	1/1	0.94	0.43	49,49,49,49	0
56	MG	2a	3178	1/1	0.94	0.13	64,64,64,64	0
56	MG	1c	302	1/1	0.94	0.15	71,71,71,71	0
56	MG	1N	3001	1/1	0.94	0.44	56,56,56,56	0
56	MG	1A	3842	1/1	0.94	0.13	58,58,58,58	0
56	MG	2I	3004	1/1	0.94	0.14	61,61,61,61	0
56	MG	1A	3470	1/1	0.94	0.18	62,62,62,62	0
56	MG	1A	3747	1/1	0.94	0.16	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1G	3001	1/1	0.94	0.07	41,41,41,41	0
56	MG	2R	201	1/1	0.94	0.44	57,57,57,57	0
56	MG	1A	3780	1/1	0.94	0.16	55,55,55,55	0
56	MG	1A	3736	1/1	0.94	0.19	32,32,32,32	0
56	MG	1A	3272	1/1	0.94	0.33	55,55,55,55	0
56	MG	2A	3741	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	3530	1/1	0.94	0.27	43,43,43,43	0
56	MG	1A	3761	1/1	0.94	0.15	26,26,26,26	0
56	MG	1A	3657	1/1	0.94	0.17	49,49,49,49	0
56	MG	2A	3777	1/1	0.94	0.14	55,55,55,55	0
56	MG	2A	3508	1/1	0.94	0.05	35,35,35,35	0
56	MG	2A	3110	1/1	0.94	0.16	46,46,46,46	0
56	MG	1A	3313	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3201	1/1	0.94	0.17	28,28,28,28	0
56	MG	2A	3472	1/1	0.94	0.34	55,55,55,55	0
56	MG	2A	3736	1/1	0.94	0.10	36,36,36,36	0
56	MG	1A	3986	1/1	0.94	0.21	39,39,39,39	0
56	MG	1a	1770	1/1	0.94	0.14	48,48,48,48	0
56	MG	2A	3915	1/1	0.94	0.26	54,54,54,54	0
56	MG	1A	3962	1/1	0.94	0.82	58,58,58,58	0
56	MG	2A	3396	1/1	0.94	0.12	50,50,50,50	0
56	MG	1B	213	1/1	0.94	0.13	80,80,80,80	0
56	MG	2A	3667	1/1	0.94	0.17	36,36,36,36	0
56	MG	15	101	1/1	0.94	0.12	53,53,53,53	0
56	MG	1A	3719	1/1	0.95	0.15	53,53,53,53	0
56	MG	1A	3924	1/1	0.95	0.12	45,45,45,45	0
56	MG	1A	3992	1/1	0.95	0.10	73,73,73,73	0
56	MG	1A	3848	1/1	0.95	0.21	57,57,57,57	0
56	MG	2a	3046	1/1	0.95	0.09	50,50,50,50	0
56	MG	1a	1835	1/1	0.95	0.09	39,39,39,39	0
56	MG	1a	1788	1/1	0.95	0.09	38,38,38,38	0
56	MG	2A	3859	1/1	0.95	0.26	41,41,41,41	0
56	MG	1A	3281	1/1	0.95	0.34	53,53,53,53	0
56	MG	1A	3891	1/1	0.95	0.09	43,43,43,43	0
56	MG	2A	3742	1/1	0.95	0.13	43,43,43,43	0
56	MG	1A	3547	1/1	0.95	0.32	40,40,40,40	0
56	MG	1A	3017	1/1	0.95	0.32	44,44,44,44	0
56	MG	2A	3889	1/1	0.95	0.13	25,25,25,25	0
56	MG	1A	3116	1/1	0.95	0.29	33,33,33,33	0
56	MG	1A	3999	1/1	0.95	0.42	32,32,32,32	0
56	MG	1P	203	1/1	0.95	0.38	44,44,44,44	0
56	MG	1A	3669	1/1	0.95	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
56	MG	1A	3303	1/1	0.95	0.39	40,40,40,40	0
56	MG	2A	3919	1/1	0.95	0.12	39,39,39,39	0
56	MG	17	104	1/1	0.95	0.17	41,41,41,41	0
56	MG	2A	3084	1/1	0.95	0.18	54,54,54,54	0
56	MG	2A	3511	1/1	0.95	0.25	52,52,52,52	0
56	MG	2a	3154	1/1	0.95	0.14	48,48,48,48	0
56	MG	2e	3001	1/1	0.95	0.07	66,66,66,66	0
56	MG	2w	101	1/1	0.95	0.22	65,65,65,65	0
56	MG	1a	1733	1/1	0.95	0.23	41,41,41,41	0
56	MG	1x	106	1/1	0.95	0.35	50,50,50,50	0
56	MG	1a	1697	1/1	0.95	0.18	45,45,45,45	0
56	MG	1S	3001	1/1	0.95	0.36	52,52,52,52	0
56	MG	2A	3307	1/1	0.95	0.09	48,48,48,48	0
56	MG	2A	3829	1/1	0.95	0.09	34,34,34,34	0
56	MG	2A	3369	1/1	0.95	0.11	52,52,52,52	0
56	MG	1A	3661	1/1	0.95	0.47	61,61,61,61	0
56	MG	1A	3022	1/1	0.95	0.12	28,28,28,28	0
56	MG	1A	3591	1/1	0.95	0.26	48,48,48,48	0
56	MG	1A	3066	1/1	0.95	0.17	46,46,46,46	0
56	MG	2A	3398	1/1	0.95	0.18	48,48,48,48	0
56	MG	2A	3500	1/1	0.95	0.37	33,33,33,33	0
56	MG	1A	3917	1/1	0.95	0.18	36,36,36,36	0
56	MG	2A	3147	1/1	0.95	0.09	44,44,44,44	0
56	MG	2A	3846	1/1	0.95	0.12	31,31,31,31	0
56	MG	1a	1719	1/1	0.95	0.06	60,60,60,60	0
56	MG	1A	3820	1/1	0.95	0.13	38,38,38,38	0
56	MG	1A	3972	1/1	0.95	0.15	34,34,34,34	0
56	MG	2A	3170	1/1	0.95	0.13	38,38,38,38	0
56	MG	1a	1689	1/1	0.95	0.13	65,65,65,65	0
56	MG	1A	4203	1/1	0.95	0.71	50,50,50,50	0
56	MG	1A	3332	1/1	0.95	0.14	49,49,49,49	0
56	MG	1A	3033	1/1	0.95	0.62	39,39,39,39	0
56	MG	1A	3230	1/1	0.95	0.26	39,39,39,39	0
56	MG	1A	3970	1/1	0.95	0.09	43,43,43,43	0
56	MG	1A	3186	1/1	0.95	0.24	50,50,50,50	0
56	MG	1A	3183	1/1	0.95	0.18	54,54,54,54	0
56	MG	1W	3005	1/1	0.95	0.16	29,29,29,29	0
56	MG	2A	3289	1/1	0.95	0.39	52,52,52,52	0
56	MG	1A	3964	1/1	0.95	0.49	37,37,37,37	0
56	MG	2a	3088	1/1	0.95	0.13	63,63,63,63	0
56	MG	1A	3250	1/1	0.95	0.08	58,58,58,58	0
56	MG	2A	3103	1/1	0.95	0.20	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3105	1/1	0.95	0.08	44,44,44,44	0
56	MG	1a	1617	1/1	0.95	0.11	59,59,59,59	0
56	MG	2A	3440	1/1	0.95	0.18	42,42,42,42	0
56	MG	1A	3111	1/1	0.95	0.30	38,38,38,38	0
56	MG	1A	4092	1/1	0.95	0.15	57,57,57,57	0
56	MG	2A	3254	1/1	0.95	0.11	56,56,56,56	0
56	MG	1A	3057	1/1	0.95	0.11	38,38,38,38	0
56	MG	1a	1807	1/1	0.95	0.09	51,51,51,51	0
56	MG	1A	3130	1/1	0.95	0.14	57,57,57,57	0
56	MG	1A	3919	1/1	0.95	0.23	47,47,47,47	0
56	MG	2A	3129	1/1	0.95	0.23	56,56,56,56	0
56	MG	2A	3111	1/1	0.95	0.13	34,34,34,34	0
56	MG	2A	3663	1/1	0.95	0.14	43,43,43,43	0
56	MG	2A	3390	1/1	0.95	0.23	43,43,43,43	0
56	MG	2A	3849	1/1	0.95	0.07	60,60,60,60	0
56	MG	1A	3041	1/1	0.95	0.14	33,33,33,33	0
56	MG	1A	3301	1/1	0.95	0.31	58,58,58,58	0
56	MG	2a	3010	1/1	0.95	0.17	76,76,76,76	0
56	MG	1A	4023	1/1	0.95	0.15	19,19,19,19	0
56	MG	1A	3755	1/1	0.95	0.20	26,26,26,26	0
56	MG	2U	205	1/1	0.95	0.24	49,49,49,49	0
56	MG	1A	3014	1/1	0.95	0.20	32,32,32,32	0
56	MG	2A	3399	1/1	0.95	0.13	49,49,49,49	0
56	MG	1A	3985	1/1	0.95	0.14	59,59,59,59	0
56	MG	1A	3071	1/1	0.95	0.31	38,38,38,38	0
56	MG	1A	3089	1/1	0.95	0.20	48,48,48,48	0
56	MG	2B	3006	1/1	0.95	0.17	54,54,54,54	0
56	MG	2A	3314	1/1	0.95	0.12	48,48,48,48	0
56	MG	2a	3198	1/1	0.95	0.18	68,68,68,68	0
56	MG	2A	3654	1/1	0.95	0.27	54,54,54,54	0
56	MG	1A	3407	1/1	0.95	0.21	61,61,61,61	0
56	MG	1A	4000	1/1	0.95	0.18	29,29,29,29	0
56	MG	2A	3485	1/1	0.95	0.14	52,52,52,52	0
56	MG	1A	4029	1/1	0.95	0.09	59,59,59,59	0
56	MG	2A	3009	1/1	0.95	0.16	33,33,33,33	0
56	MG	2A	3917	1/1	0.95	0.19	52,52,52,52	0
56	MG	2a	3180	1/1	0.95	0.11	70,70,70,70	0
56	MG	1X	105	1/1	0.95	0.31	62,62,62,62	0
56	MG	1A	3058	1/1	0.95	0.15	60,60,60,60	0
56	MG	1A	3167	1/1	0.95	0.10	41,41,41,41	0
56	MG	2A	3364	1/1	0.95	0.16	56,56,56,56	0
56	MG	1A	3794	1/1	0.95	0.14	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1905	1/1	0.95	0.08	56,56,56,56	0
56	MG	1w	109	1/1	0.95	0.05	61,61,61,61	0
56	MG	1A	3242	1/1	0.95	0.84	40,40,40,40	0
56	MG	1A	3936	1/1	0.95	0.13	64,64,64,64	0
56	MG	1a	1830	1/1	0.95	0.19	36,36,36,36	0
56	MG	15	105	1/1	0.95	0.17	62,62,62,62	0
56	MG	11	103	1/1	0.95	0.14	55,55,55,55	0
56	MG	1A	3976	1/1	0.95	0.16	42,42,42,42	0
56	MG	1A	3030	1/1	0.95	0.25	40,40,40,40	0
56	MG	1O	3002	1/1	0.95	0.46	59,59,59,59	0
56	MG	1G	3004	1/1	0.95	0.09	54,54,54,54	0
56	MG	1A	3377	1/1	0.95	0.45	50,50,50,50	0
56	MG	2A	3088	1/1	0.95	0.13	55,55,55,55	0
56	MG	2E	306	1/1	0.95	0.21	42,42,42,42	0
56	MG	2A	3712	1/1	0.95	0.12	55,55,55,55	0
56	MG	2n	101	1/1	0.95	0.18	70,70,70,70	0
56	MG	2A	3669	1/1	0.95	0.09	37,37,37,37	0
56	MG	1A	3602	1/1	0.95	0.27	56,56,56,56	0
56	MG	1A	4173	1/1	0.95	0.15	41,41,41,41	0
56	MG	1A	3607	1/1	0.95	0.10	62,62,62,62	0
56	MG	1A	3569	1/1	0.95	0.49	43,43,43,43	0
56	MG	2A	3184	1/1	0.95	0.14	58,58,58,58	0
56	MG	1A	3597	1/1	0.95	0.50	49,49,49,49	0
56	MG	1A	3306	1/1	0.95	0.22	40,40,40,40	0
56	MG	1l	201	1/1	0.95	0.22	49,49,49,49	0
56	MG	1a	1890	1/1	0.95	0.10	37,37,37,37	0
56	MG	1A	3477	1/1	0.95	0.14	44,44,44,44	0
56	MG	1A	3694	1/1	0.95	0.21	36,36,36,36	0
56	MG	1A	3687	1/1	0.95	0.49	39,39,39,39	0
56	MG	2A	3637	1/1	0.95	0.15	35,35,35,35	0
56	MG	1A	3521	1/1	0.95	0.30	71,71,71,71	0
56	MG	1w	101	1/1	0.95	0.16	87,87,87,87	0
56	MG	1a	1643	1/1	0.95	0.15	57,57,57,57	0
56	MG	2A	3492	1/1	0.95	0.16	58,58,58,58	0
56	MG	1A	3216	1/1	0.95	0.16	52,52,52,52	0
56	MG	1A	3871	1/1	0.95	0.27	37,37,37,37	0
56	MG	2a	3028	1/1	0.95	0.25	47,47,47,47	0
56	MG	1A	4228	1/1	0.95	0.08	42,42,42,42	0
56	MG	1A	3350	1/1	0.95	0.74	39,39,39,39	0
56	MG	2a	3210	1/1	0.95	0.08	58,58,58,58	0
56	MG	1A	3546	1/1	0.95	0.17	50,50,50,50	0
56	MG	1B	220	1/1	0.95	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
56	MG	2A	3767	1/1	0.95	0.25	52,52,52,52	0
56	MG	1A	3821	1/1	0.95	0.10	40,40,40,40	0
56	MG	2A	3572	1/1	0.95	0.12	40,40,40,40	0
56	MG	1A	4161	1/1	0.95	0.13	23,23,23,23	0
56	MG	2A	3539	1/1	0.95	0.12	56,56,56,56	0
56	MG	1A	3266	1/1	0.95	0.17	54,54,54,54	0
56	MG	1a	1680	1/1	0.95	0.51	48,48,48,48	0
56	MG	1A	3061	1/1	0.95	0.13	56,56,56,56	0
56	MG	1A	3236	1/1	0.95	0.11	64,64,64,64	0
56	MG	2A	3612	1/1	0.95	0.19	41,41,41,41	0
56	MG	2B	3018	1/1	0.95	0.17	42,42,42,42	0
56	MG	2B	3019	1/1	0.95	0.20	66,66,66,66	0
56	MG	2A	3493	1/1	0.95	0.39	45,45,45,45	0
56	MG	2A	3451	1/1	0.95	0.19	54,54,54,54	0
56	MG	1a	1628	1/1	0.95	0.25	51,51,51,51	0
56	MG	1A	3710	1/1	0.95	0.22	44,44,44,44	0
56	MG	2A	3532	1/1	0.95	0.15	49,49,49,49	0
56	MG	2A	3441	1/1	0.95	0.28	36,36,36,36	0
56	MG	1A	4022	1/1	0.95	0.07	60,60,60,60	0
56	MG	2A	3011	1/1	0.95	0.08	47,47,47,47	0
56	MG	1A	4237	1/1	0.95	0.66	48,48,48,48	0
56	MG	1A	3551	1/1	0.95	0.28	33,33,33,33	0
56	MG	2A	3643	1/1	0.95	0.15	51,51,51,51	0
56	MG	2A	3830	1/1	0.95	0.17	56,56,56,56	0
56	MG	1A	4254	1/1	0.95	0.60	49,49,49,49	0
56	MG	1a	1911	1/1	0.95	0.06	57,57,57,57	0
56	MG	2A	3038	1/1	0.95	0.22	36,36,36,36	0
56	MG	2a	3092	1/1	0.95	0.18	77,77,77,77	0
56	MG	2A	3501	1/1	0.95	0.07	72,72,72,72	0
56	MG	2A	3679	1/1	0.95	0.10	51,51,51,51	0
56	MG	1a	1752	1/1	0.95	0.04	63,63,63,63	0
56	MG	1A	3969	1/1	0.95	0.12	44,44,44,44	0
56	MG	1a	1647	1/1	0.95	0.11	49,49,49,49	0
56	MG	1A	3362	1/1	0.95	0.12	54,54,54,54	0
56	MG	2a	3160	1/1	0.95	0.07	77,77,77,77	0
56	MG	1A	4226	1/1	0.95	0.43	38,38,38,38	0
56	MG	2A	3634	1/1	0.95	0.16	39,39,39,39	0
56	MG	1A	4192	1/1	0.95	0.47	52,52,52,52	0
56	MG	1A	3139	1/1	0.95	0.20	42,42,42,42	0
56	MG	1E	306	1/1	0.95	0.18	50,50,50,50	0
56	MG	2A	3150	1/1	0.95	0.21	38,38,38,38	0
56	MG	1A	3843	1/1	0.95	0.09	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3094	1/1	0.95	0.20	61,61,61,61	0
56	MG	1A	4183	1/1	0.95	0.36	33,33,33,33	0
56	MG	1A	3104	1/1	0.95	0.50	54,54,54,54	0
56	MG	1A	4217	1/1	0.95	0.14	57,57,57,57	0
56	MG	1A	3925	1/1	0.95	0.13	32,32,32,32	0
56	MG	1A	3729	1/1	0.95	0.10	48,48,48,48	0
56	MG	1A	3443	1/1	0.95	0.12	42,42,42,42	0
56	MG	1D	303	1/1	0.95	0.50	45,45,45,45	0
56	MG	1A	4061	1/1	0.95	0.08	72,72,72,72	0
56	MG	1A	3653	1/1	0.95	0.13	50,50,50,50	0
56	MG	2A	3770	1/1	0.95	0.10	52,52,52,52	0
56	MG	2A	3895	1/1	0.95	0.36	41,41,41,41	0
56	MG	2A	3078	1/1	0.95	0.28	41,41,41,41	0
56	MG	2a	3147	1/1	0.95	0.07	78,78,78,78	0
56	MG	1A	3434	1/1	0.95	0.18	51,51,51,51	0
56	MG	2A	3633	1/1	0.95	0.15	59,59,59,59	0
56	MG	1A	3612	1/1	0.95	0.22	41,41,41,41	0
56	MG	2B	3014	1/1	0.95	0.13	81,81,81,81	0
56	MG	2A	3116	1/1	0.95	0.36	40,40,40,40	0
56	MG	1D	310	1/1	0.95	0.34	27,27,27,27	0
56	MG	2A	3723	1/1	0.95	0.17	50,50,50,50	0
56	MG	1A	3108	1/1	0.95	0.52	42,42,42,42	0
56	MG	1a	1910	1/1	0.95	0.07	61,61,61,61	0
56	MG	2A	3789	1/1	0.95	0.07	50,50,50,50	0
56	MG	1A	3910	1/1	0.95	0.10	35,35,35,35	0
56	MG	2A	3680	1/1	0.95	0.10	51,51,51,51	0
56	MG	1x	105	1/1	0.95	0.19	62,62,62,62	0
56	MG	1a	1855	1/1	0.95	0.12	49,49,49,49	0
56	MG	2a	3184	1/1	0.95	0.10	58,58,58,58	0
56	MG	1A	3304	1/1	0.95	0.18	55,55,55,55	0
56	MG	2A	3916	1/1	0.95	0.50	41,41,41,41	0
56	MG	2A	3566	1/1	0.95	0.12	51,51,51,51	0
56	MG	2A	3598	1/1	0.95	0.12	46,46,46,46	0
56	MG	2A	3788	1/1	0.95	0.06	47,47,47,47	0
56	MG	2A	3852	1/1	0.95	0.07	72,72,72,72	0
56	MG	1A	4175	1/1	0.95	0.10	46,46,46,46	0
56	MG	2A	3242	1/1	0.95	0.16	46,46,46,46	0
56	MG	2B	3021	1/1	0.95	0.79	74,74,74,74	0
56	MG	2A	3483	1/1	0.95	0.20	52,52,52,52	0
56	MG	1A	3705	1/1	0.95	0.21	42,42,42,42	0
56	MG	2A	3007	1/1	0.95	0.13	54,54,54,54	0
56	MG	1A	3153	1/1	0.95	0.25	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3136	1/1	0.95	0.10	48,48,48,48	0
56	MG	2A	3720	1/1	0.95	0.21	57,57,57,57	0
56	MG	2a	3111	1/1	0.95	0.23	67,67,67,67	0
56	MG	2A	3467	1/1	0.95	0.26	56,56,56,56	0
56	MG	1a	1837	1/1	0.95	0.16	32,32,32,32	0
56	MG	1A	3566	1/1	0.95	0.07	46,46,46,46	0
56	MG	2A	3711	1/1	0.95	0.23	73,73,73,73	0
56	MG	1A	3120	1/1	0.95	0.61	41,41,41,41	0
56	MG	1A	3709	1/1	0.95	0.10	33,33,33,33	0
56	MG	1A	3175	1/1	0.96	0.46	43,43,43,43	0
56	MG	1A	3087	1/1	0.96	0.43	38,38,38,38	0
56	MG	2A	3695	1/1	0.96	0.09	43,43,43,43	0
56	MG	2q	201	1/1	0.96	0.07	55,55,55,55	0
56	MG	1A	3818	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3714	1/1	0.96	0.12	32,32,32,32	0
56	MG	1A	3294	1/1	0.96	0.26	32,32,32,32	0
56	MG	1A	3046	1/1	0.96	0.17	33,33,33,33	0
56	MG	1A	3137	1/1	0.96	0.44	38,38,38,38	0
56	MG	1A	4182	1/1	0.96	0.27	57,57,57,57	0
56	MG	2A	3513	1/1	0.96	0.16	28,28,28,28	0
56	MG	2A	3316	1/1	0.96	0.38	52,52,52,52	0
56	MG	1a	1744	1/1	0.96	0.14	45,45,45,45	0
56	MG	1A	3809	1/1	0.96	0.09	56,56,56,56	0
56	MG	1a	1860	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3667	1/1	0.96	0.16	44,44,44,44	0
56	MG	1B	233	1/1	0.96	0.16	82,82,82,82	0
56	MG	1a	1796	1/1	0.96	0.16	51,51,51,51	0
56	MG	1A	3696	1/1	0.96	0.13	49,49,49,49	0
56	MG	1a	1820	1/1	0.96	0.29	46,46,46,46	0
56	MG	2A	3615	1/1	0.96	0.13	47,47,47,47	0
56	MG	1A	3207	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	4131	1/1	0.96	0.12	24,24,24,24	0
56	MG	2A	3684	1/1	0.96	0.13	63,63,63,63	0
56	MG	2A	3074	1/1	0.96	0.08	38,38,38,38	0
56	MG	1A	3254	1/1	0.96	0.24	56,56,56,56	0
56	MG	1A	3206	1/1	0.96	0.32	39,39,39,39	0
56	MG	1A	3827	1/1	0.96	0.13	56,56,56,56	0
56	MG	1a	1741	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3550	1/1	0.96	0.28	34,34,34,34	0
56	MG	1A	3733	1/1	0.96	0.18	21,21,21,21	0
56	MG	1a	1841	1/1	0.96	0.07	52,52,52,52	0
56	MG	2A	3140	1/1	0.96	0.06	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3238	1/1	0.96	0.47	39,39,39,39	0
56	MG	1F	306	1/1	0.96	0.69	47,47,47,47	0
56	MG	1A	3128	1/1	0.96	0.25	49,49,49,49	0
56	MG	1A	4212	1/1	0.96	0.16	32,32,32,32	0
56	MG	2A	3891	1/1	0.96	0.12	40,40,40,40	0
56	MG	1A	3211	1/1	0.96	0.16	48,48,48,48	0
56	MG	1A	3476	1/1	0.96	0.52	53,53,53,53	0
56	MG	2A	3547	1/1	0.96	0.12	28,28,28,28	0
56	MG	1a	1895	1/1	0.96	0.06	58,58,58,58	0
56	MG	1a	1721	1/1	0.96	0.10	41,41,41,41	0
56	MG	2A	3747	1/1	0.96	0.34	47,47,47,47	0
56	MG	2A	3898	1/1	0.96	0.20	55,55,55,55	0
56	MG	1A	3656	1/1	0.96	0.28	53,53,53,53	0
56	MG	1A	3622	1/1	0.96	0.12	54,54,54,54	0
56	MG	2A	3035	1/1	0.96	0.34	30,30,30,30	0
56	MG	2a	3205	1/1	0.96	0.18	59,59,59,59	0
56	MG	1A	3738	1/1	0.96	0.12	34,34,34,34	0
56	MG	1A	3873	1/1	0.96	0.18	57,57,57,57	0
56	MG	1A	3129	1/1	0.96	0.11	41,41,41,41	0
56	MG	1a	1625	1/1	0.96	0.16	50,50,50,50	0
56	MG	1A	3896	1/1	0.96	0.18	38,38,38,38	0
56	MG	2a	3098	1/1	0.96	0.23	61,61,61,61	0
56	MG	1a	1829	1/1	0.96	0.18	27,27,27,27	0
56	MG	1A	3840	1/1	0.96	0.14	44,44,44,44	0
56	MG	2A	3117	1/1	0.96	0.10	54,54,54,54	0
56	MG	1a	1924	1/1	0.96	0.18	43,43,43,43	0
56	MG	1A	3563	1/1	0.96	0.57	44,44,44,44	0
56	MG	1A	3522	1/1	0.96	0.44	51,51,51,51	0
56	MG	1A	3861	1/1	0.96	0.17	31,31,31,31	0
56	MG	2a	3081	1/1	0.96	0.16	52,52,52,52	0
56	MG	1a	1768	1/1	0.96	0.18	47,47,47,47	0
56	MG	1A	3712	1/1	0.96	0.31	39,39,39,39	0
56	MG	1A	3235	1/1	0.96	0.23	52,52,52,52	0
56	MG	1A	3822	1/1	0.96	0.20	34,34,34,34	0
56	MG	2R	202	1/1	0.96	0.34	50,50,50,50	0
56	MG	1A	3032	1/1	0.96	0.86	47,47,47,47	0
56	MG	1A	3883	1/1	0.96	0.20	47,47,47,47	0
56	MG	1A	3742	1/1	0.96	0.14	43,43,43,43	0
56	MG	1A	4242	1/1	0.96	0.22	53,53,53,53	0
56	MG	1A	4016	1/1	0.96	0.16	58,58,58,58	0
56	MG	2A	3731	1/1	0.96	0.24	62,62,62,62	0
56	MG	2A	3584	1/1	0.96	0.27	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3885	1/1	0.96	0.20	36,36,36,36	0
56	MG	2A	3704	1/1	0.96	0.13	50,50,50,50	0
56	MG	27	101	1/1	0.96	0.18	45,45,45,45	0
56	MG	1A	3715	1/1	0.96	0.10	44,44,44,44	0
56	MG	2a	3106	1/1	0.96	0.19	66,66,66,66	0
56	MG	1X	103	1/1	0.96	0.14	34,34,34,34	0
56	MG	1A	3123	1/1	0.96	0.55	41,41,41,41	0
56	MG	1A	3864	1/1	0.96	0.18	24,24,24,24	0
56	MG	1A	4096	1/1	0.96	0.19	17,17,17,17	0
56	MG	1A	3832	1/1	0.96	0.05	48,48,48,48	0
56	MG	1a	1790	1/1	0.96	0.06	78,78,78,78	0
56	MG	1B	203	1/1	0.96	0.20	45,45,45,45	0
56	MG	2A	3834	1/1	0.96	0.13	65,65,65,65	0
56	MG	1A	3762	1/1	0.96	0.11	29,29,29,29	0
56	MG	1n	502	1/1	0.96	0.10	41,41,41,41	0
56	MG	1A	3078	1/1	0.96	0.08	46,46,46,46	0
56	MG	2A	3702	1/1	0.96	0.15	45,45,45,45	0
56	MG	2U	204	1/1	0.96	0.37	42,42,42,42	0
56	MG	1A	4033	1/1	0.96	0.17	49,49,49,49	0
56	MG	1a	1918	1/1	0.96	0.12	75,75,75,75	0
56	MG	2A	3658	1/1	0.96	0.31	36,36,36,36	0
56	MG	2A	3183	1/1	0.96	0.11	54,54,54,54	0
56	MG	1Q	201	1/1	0.96	0.16	37,37,37,37	0
56	MG	1A	3287	1/1	0.96	0.13	51,51,51,51	0
56	MG	2A	3161	1/1	0.96	0.08	54,54,54,54	0
56	MG	1A	3080	1/1	0.96	0.36	44,44,44,44	0
56	MG	1A	4095	1/1	0.96	0.29	51,51,51,51	0
56	MG	1A	3171	1/1	0.96	0.67	50,50,50,50	0
56	MG	1A	4152	1/1	0.96	0.15	24,24,24,24	0
56	MG	1a	1660	1/1	0.96	0.12	49,49,49,49	0
56	MG	1A	3608	1/1	0.96	0.12	37,37,37,37	0
56	MG	1A	3234	1/1	0.96	0.17	62,62,62,62	0
56	MG	1A	4236	1/1	0.96	0.20	37,37,37,37	0
56	MG	2A	3044	1/1	0.96	0.13	50,50,50,50	0
56	MG	1A	3744	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3012	1/1	0.96	0.12	32,32,32,32	0
56	MG	1D	301	1/1	0.96	0.18	46,46,46,46	0
56	MG	1A	3013	1/1	0.96	0.55	34,34,34,34	0
56	MG	1A	3953	1/1	0.96	0.10	54,54,54,54	0
56	MG	2A	3119	1/1	0.96	0.11	48,48,48,48	0
56	MG	2A	3565	1/1	0.96	0.13	53,53,53,53	0
56	MG	2A	3125	1/1	0.96	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3641	1/1	0.96	0.11	36,36,36,36	0
56	MG	1A	3001	1/1	0.96	0.08	47,47,47,47	0
56	MG	1A	3050	1/1	0.96	0.25	24,24,24,24	0
56	MG	1A	3808	1/1	0.96	0.12	50,50,50,50	0
56	MG	2A	3504	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	3537	1/1	0.96	0.18	33,33,33,33	0
56	MG	2A	3049	1/1	0.96	0.25	21,21,21,21	0
56	MG	1A	3097	1/1	0.96	0.20	31,31,31,31	0
56	MG	2A	3136	1/1	0.96	0.13	41,41,41,41	0
56	MG	1A	4235	1/1	0.96	0.55	37,37,37,37	0
56	MG	1a	1857	1/1	0.96	0.17	64,64,64,64	0
56	MG	1A	3754	1/1	0.96	0.18	21,21,21,21	0
56	MG	2A	3341	1/1	0.96	0.13	56,56,56,56	0
56	MG	2A	3844	1/1	0.96	0.06	60,60,60,60	0
56	MG	1A	3810	1/1	0.96	0.17	43,43,43,43	0
56	MG	1B	212	1/1	0.96	0.09	42,42,42,42	0
56	MG	2A	3006	1/1	0.96	0.19	51,51,51,51	0
56	MG	1A	3077	1/1	0.96	0.50	39,39,39,39	0
56	MG	2A	3327	1/1	0.96	0.20	54,54,54,54	0
56	MG	2A	3686	1/1	0.96	0.08	49,49,49,49	0
56	MG	2A	3518	1/1	0.96	0.14	32,32,32,32	0
56	MG	1A	3619	1/1	0.96	0.31	41,41,41,41	0
56	MG	1A	4148	1/1	0.96	0.11	43,43,43,43	0
56	MG	1A	3572	1/1	0.96	0.21	39,39,39,39	0
56	MG	1A	4069	1/1	0.96	0.13	89,89,89,89	0
56	MG	1A	3286	1/1	0.96	0.36	62,62,62,62	0
56	MG	2A	3750	1/1	0.96	0.30	44,44,44,44	0
56	MG	1A	3581	1/1	0.96	0.08	39,39,39,39	0
56	MG	2A	3013	1/1	0.96	0.16	42,42,42,42	0
56	MG	1A	3125	1/1	0.96	0.85	47,47,47,47	0
56	MG	2A	3698	1/1	0.96	0.18	32,32,32,32	0
56	MG	2A	3435	1/1	0.96	0.23	44,44,44,44	0
56	MG	2A	3082	1/1	0.96	0.06	49,49,49,49	0
56	MG	2a	3197	1/1	0.96	0.14	63,63,63,63	0
56	MG	1A	3628	1/1	0.96	0.16	49,49,49,49	0
56	MG	1A	4223	1/1	0.96	0.23	39,39,39,39	0
56	MG	2A	3306	1/1	0.96	0.14	44,44,44,44	0
56	MG	20	103	1/1	0.96	0.16	55,55,55,55	0
56	MG	1A	3110	1/1	0.96	0.28	40,40,40,40	0
56	MG	1a	1801	1/1	0.96	0.05	59,59,59,59	0
56	MG	1A	4191	1/1	0.96	0.16	25,25,25,25	0
56	MG	2A	3043	1/1	0.96	0.11	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3614	1/1	0.96	0.09	40,40,40,40	0
56	MG	1a	1775	1/1	0.96	0.29	60,60,60,60	0
56	MG	1A	3093	1/1	0.96	0.23	26,26,26,26	0
56	MG	1A	3194	1/1	0.96	0.22	49,49,49,49	0
56	MG	2A	3806	1/1	0.96	0.20	55,55,55,55	0
56	MG	1E	305	1/1	0.96	0.34	57,57,57,57	0
56	MG	1a	1833	1/1	0.96	0.38	70,70,70,70	0
56	MG	1a	1898	1/1	0.96	0.20	43,43,43,43	0
56	MG	2A	3871	1/1	0.96	0.28	67,67,67,67	0
56	MG	1A	3989	1/1	0.96	0.10	49,49,49,49	0
56	MG	2B	3003	1/1	0.96	0.11	58,58,58,58	0
56	MG	1a	1656	1/1	0.96	0.20	40,40,40,40	0
56	MG	1a	1634	1/1	0.96	0.21	14,14,14,14	0
56	MG	1A	4178	1/1	0.96	0.18	32,32,32,32	0
56	MG	1A	3025	1/1	0.96	0.35	45,45,45,45	0
56	MG	1A	3165	1/1	0.96	0.17	51,51,51,51	0
56	MG	1A	3606	1/1	0.96	0.15	54,54,54,54	0
56	MG	2A	3778	1/1	0.96	0.16	53,53,53,53	0
56	MG	2a	3041	1/1	0.96	0.34	43,43,43,43	0
56	MG	2A	3732	1/1	0.96	0.11	53,53,53,53	0
56	MG	1A	3305	1/1	0.96	0.24	35,35,35,35	0
56	MG	1A	3389	1/1	0.96	0.35	43,43,43,43	0
56	MG	1A	3637	1/1	0.96	0.11	51,51,51,51	0
56	MG	1A	3095	1/1	0.96	0.27	47,47,47,47	0
56	MG	1A	4160	1/1	0.96	0.16	72,72,72,72	0
59	ZN	1Y	501	1/1	0.96	0.11	79,79,79,79	0
56	MG	2a	3015	1/1	0.96	0.13	63,63,63,63	0
56	MG	1A	3750	1/1	0.96	0.15	45,45,45,45	0
56	MG	1a	1831	1/1	0.96	0.18	29,29,29,29	0
56	MG	1A	3743	1/1	0.96	0.25	43,43,43,43	0
56	MG	1A	3381	1/1	0.96	0.26	38,38,38,38	0
56	MG	1A	3009	1/1	0.96	0.20	33,33,33,33	0
56	MG	1a	1738	1/1	0.96	0.09	51,51,51,51	0
56	MG	2a	3067	1/1	0.96	0.05	62,62,62,62	0
56	MG	2A	3130	1/1	0.96	0.20	47,47,47,47	0
56	MG	2a	3172	1/1	0.96	0.07	62,62,62,62	0
56	MG	1A	3107	1/1	0.96	0.56	47,47,47,47	0
56	MG	2A	3096	1/1	0.96	0.09	42,42,42,42	0
56	MG	2A	3804	1/1	0.96	0.22	74,74,74,74	0
56	MG	1a	1655	1/1	0.96	0.17	42,42,42,42	0
56	MG	1A	3819	1/1	0.96	0.15	58,58,58,58	0
56	MG	2a	3040	1/1	0.96	0.25	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3003	1/1	0.96	0.20	30,30,30,30	0
56	MG	2X	102	1/1	0.96	0.23	66,66,66,66	0
56	MG	2A	3607	1/1	0.96	0.24	51,51,51,51	0
56	MG	1A	3698	1/1	0.96	0.21	48,48,48,48	0
56	MG	2A	3664	1/1	0.96	0.13	62,62,62,62	0
56	MG	1A	3043	1/1	0.96	0.28	34,34,34,34	0
56	MG	2A	3083	1/1	0.96	0.27	44,44,44,44	0
56	MG	1A	3015	1/1	0.96	0.14	30,30,30,30	0
56	MG	1Q	202	1/1	0.96	0.34	35,35,35,35	0
56	MG	1a	1606	1/1	0.96	0.09	68,68,68,68	0
56	MG	2A	3094	1/1	0.96	0.12	45,45,45,45	0
56	MG	2A	3907	1/1	0.96	0.12	38,38,38,38	0
56	MG	2a	3119	1/1	0.96	0.30	63,63,63,63	0
56	MG	2a	3130	1/1	0.96	0.14	67,67,67,67	0
56	MG	1A	3221	1/1	0.96	0.17	46,46,46,46	0
56	MG	18	102	1/1	0.96	0.27	45,45,45,45	0
56	MG	2A	3386	1/1	0.96	0.55	68,68,68,68	0
56	MG	2A	3666	1/1	0.96	0.10	47,47,47,47	0
56	MG	1A	3866	1/1	0.96	0.07	33,33,33,33	0
56	MG	1A	4247	1/1	0.96	0.15	34,34,34,34	0
56	MG	1A	3772	1/1	0.96	0.06	47,47,47,47	0
56	MG	1A	4020	1/1	0.96	0.10	65,65,65,65	0
56	MG	1A	3869	1/1	0.96	0.18	26,26,26,26	0
56	MG	1A	3623	1/1	0.96	0.07	36,36,36,36	0
56	MG	2A	3175	1/1	0.96	0.14	54,54,54,54	0
56	MG	1A	3461	1/1	0.96	0.38	45,45,45,45	0
56	MG	2a	3161	1/1	0.96	0.08	70,70,70,70	0
56	MG	1F	310	1/1	0.96	0.53	66,66,66,66	0
56	MG	2A	3428	1/1	0.96	0.16	46,46,46,46	0
56	MG	1A	3213	1/1	0.96	0.44	53,53,53,53	0
56	MG	1A	3775	1/1	0.96	0.28	30,30,30,30	0
56	MG	1A	3174	1/1	0.97	0.40	47,47,47,47	0
56	MG	2A	3353	1/1	0.97	0.42	73,73,73,73	0
56	MG	1A	4039	1/1	0.97	0.14	51,51,51,51	0
56	MG	2A	3673	1/1	0.97	0.17	33,33,33,33	0
56	MG	2A	3608	1/1	0.97	0.09	57,57,57,57	0
56	MG	1w	102	1/1	0.97	0.22	77,77,77,77	0
56	MG	1a	1727	1/1	0.97	0.11	38,38,38,38	0
56	MG	1A	3880	1/1	0.97	0.21	32,32,32,32	0
56	MG	2a	3228	1/1	0.97	0.29	66,66,66,66	0
56	MG	1Z	303	1/1	0.97	0.14	62,62,62,62	0
56	MG	2A	3575	1/1	0.97	0.06	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1U	205	1/1	0.97	0.34	42,42,42,42	0
56	MG	1a	1828	1/1	0.97	0.14	67,67,67,67	0
56	MG	1A	3179	1/1	0.97	0.11	39,39,39,39	0
56	MG	1A	3311	1/1	0.97	0.20	53,53,53,53	0
56	MG	1A	3689	1/1	0.97	0.34	30,30,30,30	0
56	MG	1A	4225	1/1	0.97	0.35	35,35,35,35	0
56	MG	1A	3991	1/1	0.97	0.45	53,53,53,53	0
56	MG	1A	3697	1/1	0.97	0.24	34,34,34,34	0
56	MG	1A	3048	1/1	0.97	0.15	34,34,34,34	0
56	MG	2A	3562	1/1	0.97	0.16	23,23,23,23	0
56	MG	1B	201	1/1	0.97	0.11	24,24,24,24	0
56	MG	16	103	1/1	0.97	0.10	53,53,53,53	0
56	MG	2A	3729	1/1	0.97	0.10	48,48,48,48	0
56	MG	1W	3003	1/1	0.97	0.53	45,45,45,45	0
56	MG	2A	3464	1/1	0.97	0.04	53,53,53,53	0
56	MG	1A	3150	1/1	0.97	0.19	43,43,43,43	0
56	MG	2A	3015	1/1	0.97	0.13	34,34,34,34	0
56	MG	2A	3700	1/1	0.97	0.09	56,56,56,56	0
56	MG	1A	3760	1/1	0.97	0.16	29,29,29,29	0
56	MG	1A	3298	1/1	0.97	0.24	49,49,49,49	0
56	MG	2A	3075	1/1	0.97	0.33	46,46,46,46	0
56	MG	1A	4044	1/1	0.97	0.11	50,50,50,50	0
56	MG	2A	3588	1/1	0.97	0.26	36,36,36,36	0
56	MG	1A	3178	1/1	0.97	0.16	18,18,18,18	0
56	MG	1A	3145	1/1	0.97	0.42	45,45,45,45	0
56	MG	1A	3654	1/1	0.97	0.28	52,52,52,52	0
56	MG	1A	4055	1/1	0.97	0.12	47,47,47,47	0
56	MG	2A	3497	1/1	0.97	0.45	58,58,58,58	0
56	MG	1A	3907	1/1	0.97	0.27	35,35,35,35	0
56	MG	1A	3161	1/1	0.97	0.21	46,46,46,46	0
56	MG	2a	3122	1/1	0.97	0.14	53,53,53,53	0
56	MG	1A	3914	1/1	0.97	0.15	41,41,41,41	0
56	MG	1A	3641	1/1	0.97	0.12	40,40,40,40	0
56	MG	1A	3764	1/1	0.97	0.10	40,40,40,40	0
56	MG	2B	3010	1/1	0.97	0.12	59,59,59,59	0
56	MG	2A	3786	1/1	0.97	0.05	42,42,42,42	0
56	MG	1a	1823	1/1	0.97	0.21	51,51,51,51	0
56	MG	1A	3784	1/1	0.97	0.12	65,65,65,65	0
56	MG	1A	3039	1/1	0.97	0.52	33,33,33,33	0
56	MG	2A	3624	1/1	0.97	0.12	45,45,45,45	0
56	MG	1A	3882	1/1	0.97	0.20	59,59,59,59	0
56	MG	1A	4214	1/1	0.97	0.21	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1a	1699	1/1	0.97	0.33	38,38,38,38	0
56	MG	1Y	502	1/1	0.97	0.08	50,50,50,50	0
56	MG	1P	201	1/1	0.97	0.56	34,34,34,34	0
56	MG	2A	3763	1/1	0.97	0.14	49,49,49,49	0
56	MG	1A	3284	1/1	0.97	0.34	40,40,40,40	0
56	MG	1A	4155	1/1	0.97	0.15	19,19,19,19	0
56	MG	1B	218	1/1	0.97	0.28	22,22,22,22	0
56	MG	1A	4224	1/1	0.97	0.41	49,49,49,49	0
56	MG	2A	3535	1/1	0.97	0.20	37,37,37,37	0
56	MG	1e	3001	1/1	0.97	0.14	61,61,61,61	0
56	MG	2A	3099	1/1	0.97	0.29	44,44,44,44	0
56	MG	2A	3267	1/1	0.97	0.12	56,56,56,56	0
56	MG	1A	4049	1/1	0.97	0.13	63,63,63,63	0
56	MG	1A	3727	1/1	0.97	0.12	26,26,26,26	0
56	MG	2A	3601	1/1	0.97	0.14	38,38,38,38	0
56	MG	1y	3001	1/1	0.97	0.60	42,42,42,42	0
56	MG	1d	502	1/1	0.97	0.34	55,55,55,55	0
56	MG	2F	301	1/1	0.97	0.21	44,44,44,44	0
56	MG	1B	235	1/1	0.97	0.12	52,52,52,52	0
56	MG	2A	3034	1/1	0.97	0.16	41,41,41,41	0
56	MG	1U	202	1/1	0.97	0.43	35,35,35,35	0
57	CPT	1A	4209	4/5	0.97	0.21	75,78,104,121	4
56	MG	1A	3166	1/1	0.97	0.64	42,42,42,42	0
56	MG	1E	311	1/1	0.97	0.08	34,34,34,34	0
56	MG	2A	3709	1/1	0.97	0.06	59,59,59,59	0
56	MG	1B	217	1/1	0.97	0.08	28,28,28,28	0
56	MG	2a	3218	1/1	0.97	0.09	49,49,49,49	0
56	MG	2A	3187	1/1	0.97	0.14	38,38,38,38	0
56	MG	2A	3462	1/1	0.97	0.25	42,42,42,42	0
56	MG	2V	201	1/1	0.97	0.13	50,50,50,50	0
56	MG	1A	3824	1/1	0.97	0.09	65,65,65,65	0
56	MG	1A	3509	1/1	0.97	0.25	38,38,38,38	0
56	MG	1A	3531	1/1	0.97	0.28	34,34,34,34	0
56	MG	1A	4249	1/1	0.97	0.29	46,46,46,46	0
56	MG	1B	206	1/1	0.97	0.37	51,51,51,51	0
56	MG	1a	1923	1/1	0.97	0.15	69,69,69,69	0
56	MG	2O	8001	1/1	0.97	0.12	50,50,50,50	0
56	MG	1A	3734	1/1	0.97	0.12	55,55,55,55	0
56	MG	1A	4134	1/1	0.97	0.05	36,36,36,36	0
56	MG	1A	3047	1/1	0.97	0.13	30,30,30,30	0
56	MG	2A	3787	1/1	0.97	0.04	51,51,51,51	0
56	MG	1A	3927	1/1	0.97	0.07	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3884	1/1	0.97	0.29	32,32,32,32	0
56	MG	2A	3477	1/1	0.97	0.36	44,44,44,44	0
56	MG	2I	3003	1/1	0.97	0.12	68,68,68,68	0
56	MG	1D	306	1/1	0.97	0.23	35,35,35,35	0
56	MG	2A	3199	1/1	0.97	0.44	55,55,55,55	0
56	MG	1A	3835	1/1	0.97	0.20	37,37,37,37	0
56	MG	2A	3716	1/1	0.97	0.14	29,29,29,29	0
56	MG	2A	3010	1/1	0.97	0.12	47,47,47,47	0
56	MG	1A	3584	1/1	0.97	0.26	57,57,57,57	0
56	MG	1B	224	1/1	0.97	0.16	76,76,76,76	0
56	MG	1A	3868	1/1	0.97	0.18	38,38,38,38	0
56	MG	1a	1686	1/1	0.97	0.17	42,42,42,42	0
56	MG	1A	3462	1/1	0.97	0.12	43,43,43,43	0
56	MG	1A	3786	1/1	0.97	0.21	48,48,48,48	0
56	MG	2A	3880	1/1	0.97	0.05	55,55,55,55	0
56	MG	1A	3806	1/1	0.97	0.14	33,33,33,33	0
56	MG	2A	3708	1/1	0.97	0.09	55,55,55,55	0
56	MG	2A	3259	1/1	0.97	0.20	59,59,59,59	0
56	MG	1A	4107	1/1	0.97	0.09	36,36,36,36	0
56	MG	2A	3468	1/1	0.97	0.35	62,62,62,62	0
56	MG	2A	3494	1/1	0.97	0.17	59,59,59,59	0
56	MG	1A	3064	1/1	0.97	0.11	37,37,37,37	0
56	MG	2A	3556	1/1	0.97	0.12	59,59,59,59	0
56	MG	1A	3702	1/1	0.97	0.15	56,56,56,56	0
56	MG	1a	1702	1/1	0.97	0.23	42,42,42,42	0
56	MG	2A	3745	1/1	0.97	0.15	51,51,51,51	0
56	MG	1A	3773	1/1	0.97	0.13	54,54,54,54	0
56	MG	2A	3351	1/1	0.97	0.29	48,48,48,48	0
56	MG	1a	1653	1/1	0.97	0.09	48,48,48,48	0
56	MG	1A	3453	1/1	0.97	0.25	42,42,42,42	0
56	MG	2A	3430	1/1	0.97	0.34	57,57,57,57	0
56	MG	2A	3630	1/1	0.97	0.19	35,35,35,35	0
56	MG	1A	3439	1/1	0.97	0.14	43,43,43,43	0
56	MG	1A	3740	1/1	0.97	0.09	42,42,42,42	0
56	MG	2A	3833	1/1	0.97	0.06	34,34,34,34	0
56	MG	1A	3796	1/1	0.97	0.09	32,32,32,32	0
56	MG	1A	3008	1/1	0.97	0.20	26,26,26,26	0
56	MG	2A	3776	1/1	0.97	0.20	33,33,33,33	0
56	MG	2A	3887	1/1	0.97	0.11	54,54,54,54	0
56	MG	1A	3675	1/1	0.97	0.15	53,53,53,53	0
56	MG	1A	3450	1/1	0.97	0.15	51,51,51,51	0
56	MG	1A	4167	1/1	0.97	0.13	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3647	1/1	0.97	0.25	39,39,39,39	0
56	MG	2A	3728	1/1	0.97	0.11	32,32,32,32	0
56	MG	2A	3164	1/1	0.97	0.50	43,43,43,43	0
56	MG	1A	4122	1/1	0.97	0.12	48,48,48,48	0
56	MG	1a	1698	1/1	0.97	0.17	36,36,36,36	0
56	MG	1a	1908	1/1	0.97	0.13	56,56,56,56	0
56	MG	2A	3149	1/1	0.97	0.26	35,35,35,35	0
56	MG	2A	3079	1/1	0.97	0.15	47,47,47,47	0
56	MG	1a	1903	1/1	0.97	0.16	49,49,49,49	0
56	MG	2A	3337	1/1	0.97	0.15	53,53,53,53	0
56	MG	2a	3118	1/1	0.97	0.15	70,70,70,70	0
56	MG	1A	3771	1/1	0.97	0.17	25,25,25,25	0
56	MG	2A	3570	1/1	0.97	0.10	41,41,41,41	0
56	MG	2a	3190	1/1	0.97	0.18	46,46,46,46	0
56	MG	1A	3758	1/1	0.97	0.10	36,36,36,36	0
56	MG	1y	3002	1/1	0.97	0.09	55,55,55,55	0
56	MG	2A	3605	1/1	0.97	0.13	44,44,44,44	0
56	MG	1A	3154	1/1	0.97	0.23	49,49,49,49	0
56	MG	1A	3963	1/1	0.97	0.41	38,38,38,38	0
56	MG	2X	101	1/1	0.97	0.10	45,45,45,45	0
56	MG	1A	4060	1/1	0.97	0.09	52,52,52,52	0
56	MG	2A	3678	1/1	0.97	0.11	29,29,29,29	0
56	MG	2A	3625	1/1	0.97	0.12	53,53,53,53	0
56	MG	2a	3215	1/1	0.97	0.18	69,69,69,69	0
56	MG	2a	3012	1/1	0.97	0.14	57,57,57,57	0
56	MG	1A	3556	1/1	0.97	0.53	45,45,45,45	0
56	MG	1A	4252	1/1	0.97	0.29	24,24,24,24	0
56	MG	1A	3564	1/1	0.97	0.35	40,40,40,40	0
56	MG	1A	3561	1/1	0.97	0.72	42,42,42,42	0
56	MG	1A	3168	1/1	0.97	0.27	36,36,36,36	0
56	MG	1A	3748	1/1	0.97	0.13	56,56,56,56	0
56	MG	1A	4238	1/1	0.97	0.45	39,39,39,39	0
56	MG	1A	3769	1/1	0.97	0.23	27,27,27,27	0
56	MG	1A	3323	1/1	0.97	0.23	43,43,43,43	0
56	MG	28	102	1/1	0.97	0.16	55,55,55,55	0
56	MG	1A	3534	1/1	0.97	0.25	19,19,19,19	0
56	MG	1a	1819	1/1	0.97	0.12	46,46,46,46	0
56	MG	2A	3614	1/1	0.97	0.17	54,54,54,54	0
56	MG	2A	3538	1/1	0.97	0.15	48,48,48,48	0
56	MG	2a	3171	1/1	0.97	0.10	71,71,71,71	0
57	CPT	2I	201	4/5	0.97	0.13	67,68,96,140	4
56	MG	1V	202	1/1	0.97	0.18	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2a	3101	1/1	0.97	0.23	40,40,40,40	0
56	MG	2A	3144	1/1	0.97	0.25	39,39,39,39	0
56	MG	1A	3162	1/1	0.97	0.79	40,40,40,40	0
56	MG	2A	3517	1/1	0.97	0.10	28,28,28,28	0
56	MG	1A	4176	1/1	0.97	0.17	55,55,55,55	0
56	MG	1A	3068	1/1	0.97	0.08	55,55,55,55	0
56	MG	2A	3407	1/1	0.97	0.14	62,62,62,62	0
56	MG	1D	302	1/1	0.97	0.42	44,44,44,44	0
56	MG	1A	3261	1/1	0.97	0.08	56,56,56,56	0
56	MG	10	107	1/1	0.97	0.15	55,55,55,55	0
56	MG	1A	3268	1/1	0.97	0.23	43,43,43,43	0
56	MG	1A	3525	1/1	0.97	0.48	47,47,47,47	0
56	MG	1A	3789	1/1	0.97	0.29	39,39,39,39	0
56	MG	1A	3177	1/1	0.97	0.12	42,42,42,42	0
56	MG	1a	1610	1/1	0.97	0.45	64,64,64,64	0
56	MG	1A	3195	1/1	0.97	0.61	39,39,39,39	0
56	MG	2a	3217	1/1	0.97	0.27	45,45,45,45	0
56	MG	1A	4026	1/1	0.97	0.12	30,30,30,30	0
56	MG	1A	3023	1/1	0.98	0.29	46,46,46,46	0
56	MG	1a	1651	1/1	0.98	0.23	39,39,39,39	0
56	MG	1a	1613	1/1	0.98	0.17	18,18,18,18	0
56	MG	1A	4025	1/1	0.98	0.05	53,53,53,53	0
56	MG	2A	3737	1/1	0.98	0.11	58,58,58,58	0
56	MG	1A	3035	1/1	0.98	0.08	54,54,54,54	0
56	MG	2A	3818	1/1	0.98	0.08	55,55,55,55	0
57	CPT	2A	3903	4/5	0.98	0.13	70,73,87,100	4
56	MG	2A	3071	1/1	0.98	0.28	31,31,31,31	0
56	MG	1a	1616	1/1	0.98	0.14	36,36,36,36	0
56	MG	1a	1862	1/1	0.98	0.10	49,49,49,49	0
56	MG	2v	101	1/1	0.98	0.27	55,55,55,55	0
56	MG	1A	3701	1/1	0.98	0.13	31,31,31,31	0
56	MG	1A	3994	1/1	0.98	0.13	44,44,44,44	0
56	MG	1A	3283	1/1	0.98	0.27	42,42,42,42	0
56	MG	1a	1736	1/1	0.98	0.23	44,44,44,44	0
56	MG	1A	3307	1/1	0.98	0.16	53,53,53,53	0
60	SF4	2d	501	8/8	0.98	0.12	58,66,75,87	0
56	MG	1B	216	1/1	0.98	0.14	37,37,37,37	0
56	MG	2a	3087	1/1	0.98	0.11	64,64,64,64	0
56	MG	1A	3249	1/1	0.98	0.20	44,44,44,44	0
56	MG	2P	202	1/1	0.98	0.06	41,41,41,41	0
56	MG	1A	3060	1/1	0.98	0.16	50,50,50,50	0
56	MG	1A	3070	1/1	0.98	0.20	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3749	1/1	0.98	0.11	49,49,49,49	0
56	MG	1b	3001	1/1	0.98	0.07	62,62,62,62	0
56	MG	2A	3914	1/1	0.98	0.49	38,38,38,38	0
56	MG	1A	3977	1/1	0.98	0.10	45,45,45,45	0
56	MG	2A	3180	1/1	0.98	0.18	22,22,22,22	0
56	MG	19	103	1/1	0.98	0.16	41,41,41,41	0
56	MG	1A	4200	1/1	0.98	0.06	55,55,55,55	0
56	MG	2A	3867	1/1	0.98	0.11	33,33,33,33	0
56	MG	1A	4030	1/1	0.98	0.07	29,29,29,29	0
56	MG	2A	3526	1/1	0.98	0.10	48,48,48,48	0
57	CPT	1I	3002	4/5	0.98	0.11	70,77,97,175	0
56	MG	1A	3271	1/1	0.98	0.31	47,47,47,47	0
56	MG	2A	3278	1/1	0.98	0.14	57,57,57,57	0
56	MG	1A	3289	1/1	0.98	0.41	59,59,59,59	0
56	MG	2A	3632	1/1	0.98	0.20	34,34,34,34	0
56	MG	1A	3524	1/1	0.98	0.39	43,43,43,43	0
56	MG	1A	3700	1/1	0.98	0.07	55,55,55,55	0
56	MG	2A	3791	1/1	0.98	0.10	46,46,46,46	0
56	MG	2A	3434	1/1	0.98	0.32	46,46,46,46	0
56	MG	1A	3072	1/1	0.98	0.18	15,15,15,15	0
56	MG	1A	3028	1/1	0.98	0.37	28,28,28,28	0
56	MG	1B	214	1/1	0.98	0.14	46,46,46,46	0
56	MG	1A	3711	1/1	0.98	0.19	51,51,51,51	0
56	MG	1A	3176	1/1	0.98	0.18	42,42,42,42	0
56	MG	1A	3965	1/1	0.98	0.16	45,45,45,45	0
56	MG	2a	3135	1/1	0.98	0.22	95,95,95,95	0
56	MG	1A	3191	1/1	0.98	0.54	48,48,48,48	0
56	MG	1B	232	1/1	0.98	0.13	44,44,44,44	0
56	MG	2A	3037	1/1	0.98	0.18	33,33,33,33	0
56	MG	1a	1893	1/1	0.98	0.12	36,36,36,36	0
56	MG	1A	3872	1/1	0.98	0.12	55,55,55,55	0
56	MG	1A	3897	1/1	0.98	0.41	44,44,44,44	0
56	MG	10	101	1/1	0.98	0.04	51,51,51,51	0
56	MG	2A	3850	1/1	0.98	0.13	68,68,68,68	0
57	CPT	2a	3235	4/5	0.98	0.12	85,87,90,125	0
56	MG	2d	502	1/1	0.98	0.09	58,58,58,58	0
56	MG	2A	3597	1/1	0.98	0.09	28,28,28,28	0
56	MG	1a	1668	1/1	0.98	0.10	48,48,48,48	0
56	MG	1A	3182	1/1	0.98	0.19	58,58,58,58	0
56	MG	2A	3438	1/1	0.98	0.35	44,44,44,44	0
56	MG	2A	3541	1/1	0.98	0.08	29,29,29,29	0
56	MG	1A	3127	1/1	0.98	0.38	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	3146	1/1	0.98	0.25	32,32,32,32	0
56	MG	17	101	1/1	0.98	0.16	38,38,38,38	0
56	MG	1A	4144	1/1	0.98	0.18	34,34,34,34	0
56	MG	2A	3838	1/1	0.98	0.17	31,31,31,31	0
56	MG	1e	3002	1/1	0.98	0.53	65,65,65,65	0
56	MG	1A	4031	1/1	0.98	0.05	34,34,34,34	0
56	MG	2A	3690	1/1	0.98	0.06	43,43,43,43	0
56	MG	1Y	503	1/1	0.98	0.68	54,54,54,54	0
56	MG	1A	4233	1/1	0.98	0.32	47,47,47,47	0
56	MG	1A	3388	1/1	0.98	0.41	45,45,45,45	0
56	MG	2A	3453	1/1	0.98	0.24	53,53,53,53	0
56	MG	1A	4041	1/1	0.98	0.07	71,71,71,71	0
56	MG	1A	3142	1/1	0.98	0.21	22,22,22,22	0
56	MG	2A	3707	1/1	0.98	0.10	50,50,50,50	0
56	MG	1W	3004	1/1	0.98	0.28	39,39,39,39	0
56	MG	1a	1786	1/1	0.98	0.04	53,53,53,53	0
56	MG	1A	3031	1/1	0.98	0.17	27,27,27,27	0
56	MG	1A	3895	1/1	0.98	0.07	48,48,48,48	0
56	MG	1A	3852	1/1	0.98	0.18	48,48,48,48	0
56	MG	2A	3531	1/1	0.98	0.20	21,21,21,21	0
56	MG	1A	3905	1/1	0.98	0.12	27,27,27,27	0
56	MG	2A	3596	1/1	0.98	0.14	29,29,29,29	0
56	MG	1A	3086	1/1	0.98	0.39	56,56,56,56	0
59	ZN	15	103	1/1	0.98	0.17	46,46,46,46	0
56	MG	1A	3038	1/1	0.98	0.42	46,46,46,46	0
56	MG	2a	3042	1/1	0.98	0.10	81,81,81,81	0
56	MG	2A	3046	1/1	0.98	0.04	37,37,37,37	0
56	MG	2q	203	1/1	0.98	0.24	72,72,72,72	0
56	MG	2A	3148	1/1	0.98	0.15	45,45,45,45	0
56	MG	1A	3752	1/1	0.98	0.10	34,34,34,34	0
56	MG	1b	3002	1/1	0.98	0.06	65,65,65,65	0
56	MG	1A	3096	1/1	0.98	0.15	46,46,46,46	0
56	MG	1A	3901	1/1	0.98	0.13	60,60,60,60	0
56	MG	2A	3639	1/1	0.98	0.30	49,49,49,49	0
56	MG	1a	1657	1/1	0.98	0.19	48,48,48,48	0
56	MG	1a	1838	1/1	0.98	0.14	39,39,39,39	0
56	MG	2a	3079	1/1	0.98	0.13	40,40,40,40	0
56	MG	2A	3794	1/1	0.98	0.08	74,74,74,74	0
56	MG	1A	3037	1/1	0.98	0.19	21,21,21,21	0
56	MG	2f	3001	1/1	0.98	0.20	41,41,41,41	0
56	MG	2A	3299	1/1	0.98	0.13	58,58,58,58	0
56	MG	1X	104	1/1	0.98	0.50	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	1A	4170	1/1	0.98	0.21	13,13,13,13	0
56	MG	1O	3004	1/1	0.98	0.21	54,54,54,54	0
56	MG	1A	3724	1/1	0.98	0.20	31,31,31,31	0
56	MG	2A	3590	1/1	0.98	0.17	30,30,30,30	0
56	MG	1A	3973	1/1	0.98	0.16	41,41,41,41	0
56	MG	2A	3315	1/1	0.98	0.33	62,62,62,62	0
56	MG	1A	4143	1/1	0.98	0.20	36,36,36,36	0
56	MG	1a	1669	1/1	0.98	0.05	47,47,47,47	0
56	MG	2A	3432	1/1	0.98	0.17	38,38,38,38	0
56	MG	1A	3042	1/1	0.98	0.10	33,33,33,33	0
56	MG	1A	4187	1/1	0.98	0.17	28,28,28,28	0
56	MG	1D	307	1/1	0.98	0.21	25,25,25,25	0
56	MG	1A	4110	1/1	0.98	0.12	36,36,36,36	0
56	MG	2A	3197	1/1	0.98	0.13	44,44,44,44	0
56	MG	2A	3021	1/1	0.98	0.21	34,34,34,34	0
56	MG	1A	3894	1/1	0.99	0.20	34,34,34,34	0
59	ZN	25	102	1/1	0.99	0.13	61,61,61,61	0
56	MG	1A	3951	1/1	0.99	0.08	43,43,43,43	0
56	MG	1A	4245	1/1	0.99	0.19	46,46,46,46	0
56	MG	2A	3397	1/1	0.99	0.06	36,36,36,36	0
56	MG	2a	3097	1/1	0.99	0.24	48,48,48,48	0
59	ZN	1n	501	1/1	0.99	0.15	59,59,59,59	0
56	MG	2A	3016	1/1	0.99	0.12	52,52,52,52	0
56	MG	1w	105	1/1	0.99	0.11	58,58,58,58	0
56	MG	1A	3886	1/1	0.99	0.21	26,26,26,26	0
56	MG	1E	301	1/1	0.99	0.18	14,14,14,14	0
56	MG	1A	3823	1/1	0.99	0.18	28,28,28,28	0
56	MG	2A	3028	1/1	0.99	0.45	47,47,47,47	0
56	MG	1A	3229	1/1	0.99	0.17	47,47,47,47	0
60	SF4	1d	501	8/8	0.99	0.18	55,59,67,69	0
56	MG	1A	3815	1/1	0.99	0.13	44,44,44,44	0
56	MG	1A	4036	1/1	0.99	0.06	71,71,71,71	0
56	MG	2a	3153	1/1	0.99	0.13	43,43,43,43	0
56	MG	2A	3060	1/1	0.99	0.26	50,50,50,50	0
56	MG	1A	3280	1/1	0.99	0.21	29,29,29,29	0
56	MG	1A	3908	1/1	0.99	0.08	47,47,47,47	0
56	MG	1A	3203	1/1	0.99	0.15	38,38,38,38	0
56	MG	1A	3126	1/1	0.99	0.19	40,40,40,40	0
56	MG	1A	3892	1/1	0.99	0.06	60,60,60,60	0
56	MG	1A	4001	1/1	0.99	0.16	32,32,32,32	0
56	MG	1A	3813	1/1	0.99	0.18	34,34,34,34	0
56	MG	1A	3432	1/1	0.99	0.36	40,40,40,40	0

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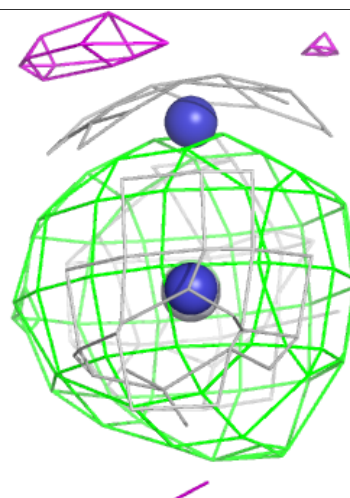
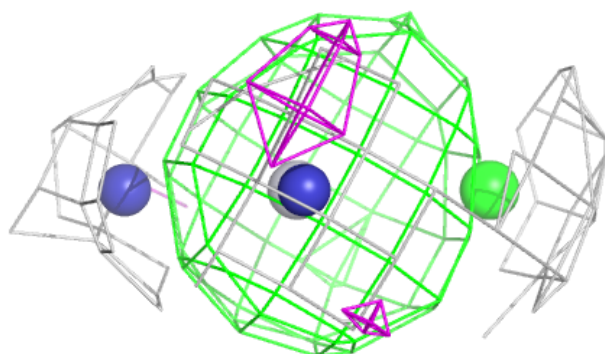
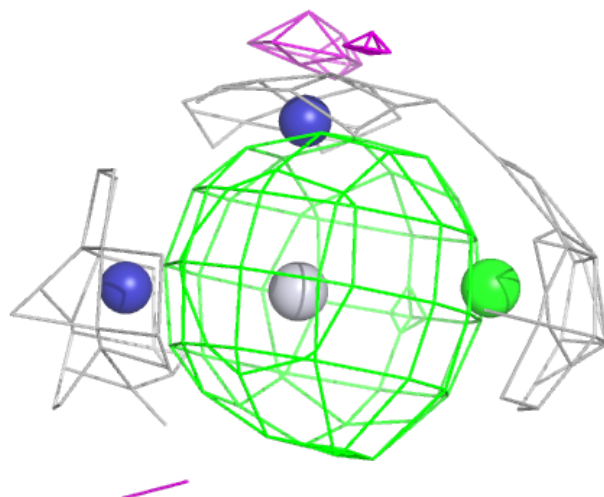
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
56	MG	2A	3027	1/1	0.99	0.10	27,27,27,27	0
56	MG	2A	3847	1/1	0.99	0.15	30,30,30,30	0
56	MG	1A	4094	1/1	0.99	0.09	22,22,22,22	0
56	MG	1A	3309	1/1	0.99	0.43	47,47,47,47	0
56	MG	2A	3443	1/1	0.99	0.19	43,43,43,43	0
56	MG	1W	3006	1/1	0.99	0.13	35,35,35,35	0
56	MG	1A	3708	1/1	0.99	0.27	16,16,16,16	0
56	MG	1A	3099	1/1	0.99	0.27	57,57,57,57	0
56	MG	1A	4241	1/1	0.99	0.15	23,23,23,23	0
56	MG	15	104	1/1	0.99	0.30	42,42,42,42	0
56	MG	1A	3863	1/1	0.99	0.12	59,59,59,59	0
56	MG	2A	3234	1/1	0.99	0.14	62,62,62,62	0
56	MG	1A	3310	1/1	0.99	0.18	42,42,42,42	0
56	MG	2A	3691	1/1	0.99	0.16	66,66,66,66	0
56	MG	1A	4097	1/1	0.99	0.08	23,23,23,23	0
56	MG	2A	3619	1/1	0.99	0.13	44,44,44,44	0
59	ZN	19	102	1/1	0.99	0.10	27,27,27,27	0
56	MG	2A	3444	1/1	0.99	0.31	32,32,32,32	0
56	MG	2a	3114	1/1	0.99	0.10	69,69,69,69	0
56	MG	1A	3262	1/1	0.99	0.10	58,58,58,58	0
56	MG	2A	3141	1/1	0.99	0.24	35,35,35,35	0
56	MG	2A	3115	1/1	0.99	0.21	46,46,46,46	0
56	MG	2A	3437	1/1	0.99	0.24	45,45,45,45	0
56	MG	2A	3876	1/1	0.99	0.10	62,62,62,62	0
56	MG	1A	3845	1/1	0.99	0.20	25,25,25,25	0
56	MG	2A	3738	1/1	0.99	0.08	63,63,63,63	0
56	MG	1A	3876	1/1	0.99	0.22	48,48,48,48	0
59	ZN	16	101	1/1	1.00	0.16	47,47,47,47	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CPT 1a 1930:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.